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Abstract Book

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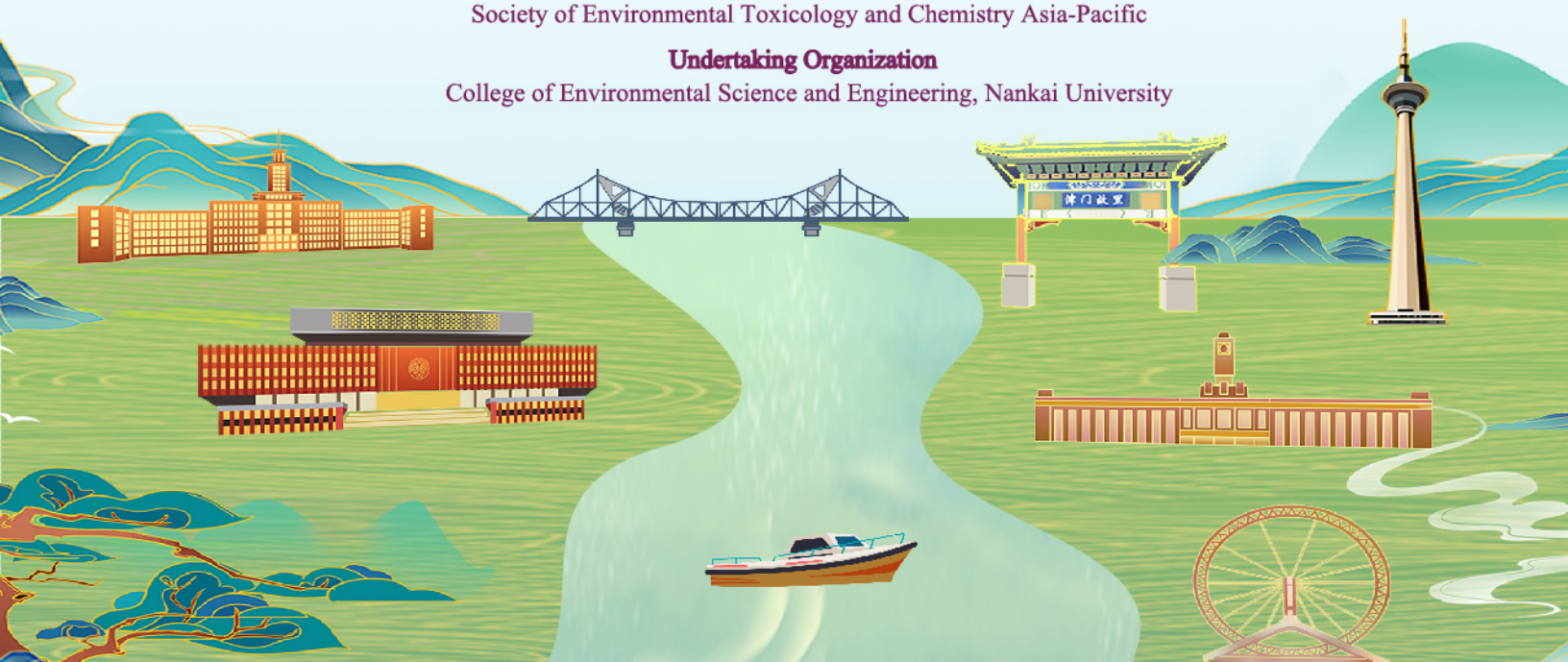

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Plastic-related Oligomers Migrated from Single and Multilayer Breast Milk Storage Bags

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Abstract

Breastmilk storage bags (BSB) simplify milk storage and save space, making them popular for infant feeding. To increase their durability, multilayer plastic materials are often used. However, made by using adhesives and layers of plastic films, multilayer plastic has raised concerns about exposure to various plastic-related chemicals, particularly plastic-related oligomers (PRO). In recent years, PRO has become a health concern for infants due to limited knowledge about their presence and toxicity. To date, no study has examined PRO migration from BSB. This study aims to assess PRO migration from single and multilayer BSB using simulant, cow's milk, and particularly, human breast milk.

Simulant, cow's milk, and human breast milk were stored in both single and multi-layer BSB at -20°C for two weeks and then reheated using 70°C water, following a typical household procedure. A modified QuEChERS method was used for cow's milk and human breast milk extraction, while the simulant was diluted with water. LC-QToF analysis was performed using a non-target approach for PRO identification, and pyrolysis-GC was employed to determine the material composition of the BSB layers.

The results showed similar PRO detection and concentration in the simulant and cow's milk samples, with multilayer bags exhibiting a higher number of PRO compared to single-layer bags. However, no PRO were detected in human breast milk samples after the storage and defrosting procedure. Our hypothesis is that the PRO were degraded by lipase presented in the milk, which could be either the bile salt–stimulated lipase unique to primate breastmilk, or a non-species specific lipase in milk but deactivated by the commercial pasteurization process.

This study concludes that PRO exposure is unlikely to occur when feeding infants with breast milk stored in BSB using typical and recommended storage and reheating procedures. Our results suggest that using alternative matrices (e.g., cow's milk) for PRO migration studies requires careful consideration due to compositional differences in human breast milk, such as the presence of lipase. Results from simulant and cow's milk migration studies indicate that multilayer plastic can introduce more PRO into foodstuff within. Although the exposure through breast milk feeding is limited, such materials are also used in other infant food packaging, notably food puree pouches, and the possibility of PRO exposure in these contexts needs to be assessed separately.

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Exploring the Use of Blood Microsampling Devices for Chemical Exposomics

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Abstract

Blood microsampling devices are a recent technology designed for accurate and high-frequency sampling of individuals outside the clinic. Because they are simple and minimally invasive, these devices can be deployed to a layperson and shipped back to the laboratory at room temperature, thereby facilitating sample collection in cohorts to comprehensively characterize the human chemical exposome. However, two challenges that may limit the application of blood microsamplers for trace analysis of environmental contaminants include: (i) the potential chemical background introduced by the devices, and (ii) the low sample volumes typically collected e.g., 10 – 50 µL. In this project, we aimed to characterize the chemical background of commercially available microsamplers, and implement new methods for low-volume analyses with application for parallel targeted and untargeted chemical exposomics by LC-HRMS. As a first step, we performed chemical background profiling in various commercially available blood microsampling devices, using high-purity water as a blood surrogate. We ranked the devices by the extent of background interferences, assessed in terms of total ion chromatogram intensities, total number of features detected, and the specific detection (Level 1) or annotation (Level 2) of environmental substances. For those samplers with the lowest chemical background, practicality criteria related to the use of the samplers (e.g., volume collected, and ease of use) were also considered during the assessment. In future work, the selected sampler(s) will be used for method development, focussing on high-throughput methods in 96-well plates. Overall, the goal is to support longitudinal studies of exposure in individuals, and larger cohort studies to explore the health effects of the chemical exposome.

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Enhanced Chemical Coverage and Toxicological Insight to the Airborne Exposome using Polydimethylsiloxane (PDMS) Foam Passive Samplers

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Abstract

The chemical exposome encompasses all environmental chemical exposures an individual encounters from conception to death. The air we breathe is a key pathway of exposure, and contributes to chronic disease and premature mortality around the world, yet its chemical composition is largely unexplored in most human environments. To advance airborne exposomics and broaden the chemical space examined, we developed and tested polydimethylsiloxane (PDMS) foam for passive air sampling in indoor and outdoor environments. This material captures both (semi-)volatile organic compounds and particulate matter and can be compatible with toxicity assays, facilitating molecular discovery, quantification, and toxicity assessment for a broad spectrum of airborne chemicals and their mixtures. We specifically optimized and validated GC-HRMS and LC-HRMS sample preparation methodologies for using over 200 prioritized substances from 20 different chemical classes, and demonstrate a method to assess the cytotoxicity of extracts in primary human lung fibroblasts. Together, these methods allow for comprehensive chemical analysis and toxicity assessment for the same passive air samples. In an indoor pilot study with samples collected over eight-weeks, 21 LC and 46 GC target analytes were detected with concentrations in the sampler ranging between 0.003 – 297.7 ng/cm^2, including the presence of 23 PCBs. LC- and GC- amenable chemicals such as DEET, tris(2-butoxyethyl) phosphate, or tributyl phosphate, were detected in both modes at similar concentrations, adding a confidence layer to the reported results. Additionally, suspect screening using MS-Dial software and public libraries (e.g. Mass Bank North America, or GNPS) allowed for the tentative identification of 39 (LC) and 62 (GC) chemicals at level 2. Finally, nontarget approaches such as feature-based molecular networking and network annotation propagation are being applied to further identify features of interest that can be linked with high cytotoxicity in human lung cells. PDMS foam disks have been deployed in over 200 homes across eight European countries as part of the Horizon Europe INQUIRE project. We will present novel results and preliminary data from this extensive sampling effort, highlighting the samplers' effectiveness in airborne exposure assessment, and toxicity evaluation to supports studies of the exposome and future chemical regulation.

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Evaluation of Mass Spectral Acquisition Strategies for Ecotoxicity-Based Feature Prioritization by MS2Tox in Non-Target Water Analysis

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Abstract

Identification of toxic chemicals in environmental waters by non-target liquid chromatography-high resolution mass spectrometry (LC-HMRS) workflows can be overwhelming due to the thousands of features detected in complex water samples. The machine-learning tool MS2Tox can be applied for toxicity-based prioritization of features without structural annotation, as it predicts acute fish lethality based only on MS^2 spectral information. Here, we compared two common MS^2 acquisition strategies in non-target LC-HRMS workflows for their molecular coverage, structural annotation accuracy (SIRIUS+CSI:FingerID), and accuracy of MS2Tox ecotoxicity predictions (i.e. acute fish lethality) for 191 reference chemicals spiked to LC-MS water, groundwater, surface water, and wastewater. Data-independent acquisition (DIA) showed higher MS^2 detection rates than data-dependent acquisition (DDA), leading to higher true positive rates for spectral library matching and formula prediction for the reference chemicals. However, DDA resulted in higher true positive rate in structural annotation of the spiked chemicals in three out of four water matrices. For MS2Tox accuracy, DDA showed higher accuracy than DIA, with root mean square errors of 0.62 and 0.71 log-mM, respectively. To evaluate relative confidence in MS2Tox predictions, we also introduced a *CombinedConfidence* score. These approaches were also applied to environmental water samples to prioritize potentially ecotoxic substances in both DDA and DIA datasets.

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Protein-guided identification of toxicity driving chemicals at the exposome-wide level

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Abstract

The exposure to a growing number of environmental contaminants has been associated with the increasing incidence of many human diseases. While over 350,000 compounds have been registered worldwide for production and use, the toxicity testing of each individual compound by traditional methods is infeasible. Over the past several years, my group propose a protein-guided ‘top-down’ strategy for identifying toxicity-driving contaminants from environmental mixtures—which consist of millions of unknown compounds—at the exposome-wide level. Case studies from our group will be presented to demonstrate the strengths of this strategy to identify previously unknown toxicity-driving chemicals including transformation products. The major discovery from our research is that a few chemicals often drive the bulky toxicity of environmental mixtures, which highlights an opportunity to channel our future research efforts towards these prioritized chemicals.

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Non-target Screening of Persistent Micropollutants and Their Ecotoxicological Evaluation in Wastewater Treatment and River

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Abstract

Tens of thousands of compounds are used in daily life, mostly discharged in wastewater and collected by domestic wastewater treatment plants (WWTPs). In addition to monitor well known hazardous compounds, it is necessary to understand the fate of the other pollutants, especially persistent compounds. Non-target screening analysis by high resolution mass spectrometry enables comprehensive detection of organic compounds. We screened the compounds persistently remained in the treated wastewater. We also studied the fate of such organic compounds in a river. We developed a method to obtain a list of features representing persistent compounds in the effluent of the WWTPs, which are significant for regular monitoring and survey. Primary effluent, secondary effluent, and final effluent were collected from 9 different WWTPs during three sampling events. River water samples were collected from upstream to downstream in a river for four times in a year. Non-target data processing was carried out for data obtained by liquid chromatograph quadrupole-Orbitrap hybrid mass spectrometer. A list of 436 features in positive and 298 in negative ionization mode were screened as persistent micropollutants in WWTPs. MS/MS analysis was applied for top 100 features in the peak intensity. The exact structure for five features were estimated, and confirmed by the authentic standard chemicals. Concentration of five compounds in the treated wastewater did not exceed the predicted no-effect concentration (PNEC), though the concentration of diphenhydramine was close to 1/10 PNEC. Further, tentative partial structures for 17 features were determined. PNEC was estimated by quantitative structure-activity relationship for all possible structures of the compounds. The PNEC values were low enough for the compounds to be possibly observed in the treated wastewater and in the environment. We also screened the persistent and frequently observed compounds in the river water. Three features were detected in all samples, whose formula were likely to be transformation products of alkylbenzene sulfonate or related surfactants. In addition, etodolac and 4-α-cumylphenol were tentatively determined among the frequently detected features by the database matching. This study provides the list of compounds that have priority for monitoring water environment to supplement the existing monitoring list of compounds.

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Association Between Personal Abiotic Airborne Exposures and Body Composition Changes Among Healthy Older Adults: A Combined Exposome-Wide and Lipidome Mediation Approach from the China BAPE Study

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Abstract

Background: Evidence suggested that the abiotic airborne exposures may be associated with changes in body composition. However, more evidence is needed to identify key pollutants linked to adverse health effects and their underlying biomolecular mechanisms, particularly in sensitive older adults.

Objectives: Our research aimed to systematically assess the relationship between the abiotic airborne exposures and changes in body composition among healthy older adults, as well as the potential mediating mechanism through the serum lipidome.

Methods: From September 2018 to January 2019, we conducted a monthly survey among 76 healthy adults (60-69 years old) in the China Biomarkers of Air Pollutant Exposure study, measuring their personal exposures to 632 abiotic airborne pollutions using MicroPEM and the Fresh Air Wristband, 18 body composition indicators from Inbody 770, and lipidomics from venous blood samples. We used an exposure-wide association study (ExWAS) and deletion/substitution/addition (DSA) model to unravel complex associations between exposure to contaminants mixtures and body composition, bayesian kernel machine regression (BKMR) model to assess the overall effect of key exposures on body composition, and mediation analysis to identify lipid intermediators.

Results: The ExWAS and DSA model identified that 2,4,5-T methyl ester (2,4,5-TME), 9,10-Anthracenedione (ATQ), 4b,8-dimethyl-2-isopropylphenanthrene, and 4b,5,6,7,8,8a,9,10-octahydro-(DMIP) were associated with increased body fat mass, fat mass indicators, percent body fat, and visceral fat area (VFA) in healthy older adults ($FDR_{B\text{-}H} < 0.05$). The BKMR model demonstrated a positive correlation between pollutants (anthracene, ATQ, copaene, di-epi-α-cedrene, and DMIP) with VFA. Mediation analysis revealed that phosphatidylcholine [PC, PC(16:1e/18:1), PC(16:2e/18:0)], and sphingolipid [SM, SM(d18:2/24:1)] mediated a significant portion, ranging from 12.27% to 26.03% (p value <0.05), of the observed increase in VFA.

Discussion: Based on the evidence from multiple model results, ATQ and DMIP were statistically significantly associated with the increased VFA levels of healthy older adults, potentially regulated through lipid intermediators. These findings may have important implications for identifying potentially harmful environmental chemicals and developing targeted strategies for the control and prevention of chronic diseases in the future, particularly as the global population is rapidly aging.

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A comprehensive screening of organophosphate esters and related substances in food contact materials

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Abstract

The occurrences of organophosphate esters in food contact materials are currently poorly studied. In this research, high-resolution mass spectrometry was used to establish a nontarget and suspect screening method to comprehensively screen organophosphate tri-esters (tri-OPEs), organophosphite antioxidants (OPAs), organophosphate di-esters (di-OPEs) and organothiophosphate esters (OTPEs) in food contact materials and foods in large supermarkets in Southern China. Twenty-eight tri-OPEs, six OPAs, 18 di-OPEs, and three OTPEs were identified in food contact materials, of which seven tri-OPEs, three OPAs, seven di-OPEs, and one OTPEs had not been reported in the previous environmental literature. Further quantitative results showed that AO168=O, AO168, di-ester of AO168=O, and AO168=S were the main compounds, with median concentrations of 7,260 ng/g (range: <8.50–103,879 ng/g), 31,920 ng/g (range: <9.80–657,399 ng/g), 1,079 ng/g (range: 23.4–158,414 ng/g), and 111 ng/g (range: <0.1–13,016 ng/g), respectively. Migration experiments have demonstrated that these compounds can migrate from food contact materials to food simulants. At the same time, the results of targeted quantitative analysis also showed that most of the compounds could be detected in food. Finally, the estimated daily intakes of detected substances were calculated. These results suggest that food contact materials are a major source of organophosphate esters in food.

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Profiling Metabolites and Exploring Metabolism of Parabens in Human Urine Using Non-Target Screening and Molecular Networking

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Abstract

Parabens are widely used as preservatives in food, pharmaceuticals, and cosmetics due to their excellent antimicrobial activities, cost effectiveness, and stability. Previous studies have demonstrated their harmful potential and their ubiquitousness in the environment and human tissues. This study revealed profiles of parabens and their metabolites in human urine of general population with different ages using non-target screening. Metabolism of parabens in human bodies was further explored through the filtered metabolites in combination of molecular networking analysis. A total of 34 paraben compounds were screened and filtered in the urine samples. Three compounds of confidence level 1 (CL1) were identified, which were methylparaben, ethylparaben, and propylparaben. Three compounds of CL2 were identified, namely 4-hydroxybenzoic acid, 3,4-dihydroxybenzoic acid and ethylparaben sulfate. In addition, 6 CL3 compounds

were tentatively identified, five of which were sulfonated metabolites of parabens. The remaining 22 were CL4 features without certain chemical structures. Distribution of the parabens and metabolites in the urines showed age dependent difference in terms of levels and compositions. This study provided insights into understanding metabolism and metabolic pathways of the parabens in human bodies.

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Unraveling Fluorotelomer Biotransformation: Insights from Analytical Chemistry and Microbiology

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Abstract

For decades, fluorotelomer compounds have been used to produce surfactants and fluorinated polymers in consumer and industrial products. Long-chain fluorotelomers were phased out and replaced with shorter-chained analogues since their biotransformation can result in long-chain perfluoroalkyl carboxylates (PFCAs). Early studies using ^{14}C-labeled fluorotelomer alcohols were conducted to clarify the relationship between fluorotelomer alcohols and PFCAs. Through the use of ^{14}C-labels and high-resolution mass spectrometry, pathways for FTOHs 8:2 and 6:2 were elucidated with high confidence, resulting in the discovery of new transformation intermediates. These studies showed that these compounds undergo a "one-carbon removal process" instead of the classical beta-oxidation. This process involves sequential -CF2- removal from fluorotelomers, leading to partial defluorination and n:3 acids (such as 5:3, 4:3 and 3:3 acids) formation under aerobic conditions.

Despite a relatively good understanding of these pathways, the microorganisms involved are understudied. Our study aims to enrich cultures capable of deep defluorination of fluorotelomer acids for future cost-effective biological treatments. We employed a dual-stage enrichment strategy: initially using diluted media for slow-growing microbes, followed by rich media to accelerate growth and degradation. After a year of enrichment with 5:3 acid, several degrading consortia were obtained. Further testing showed that one consortium degraded 5:3 acid into 4:3, 3:3, and 2:3 acids in 47 days. The consortium's defluorination potential for n:3 acids (n = 2-5) and 6:2 fluorotelomer unsaturated acids was evaluated, with defluorination rates of 24%, 85%, 33%, 55%, and 66%, respectively. Fluoride generation was quantified, which confirmed the extensive biotransformation.

Furthermore, based on the dilution plate technique, 23 bacteria were isolated and identified via 16S rRNA gene sequencing. However, none could perform defluorination alone. We also characterized the bacterial community structure in this enriched consortia using 16S rRNA gene amplicon analysis. This study is the first to identify and enrich microbes responsible for the one-carbon removal pathway in fluorotelomer

degradation. The unique culture we developed lays the groundwork for future engineered biological treatments to achieve extensive defluorination of fluorotelomers.

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Chemical Exposomics in Human Plasma by Lipid Removal and Large Volume Injection Gas Chromatography High-Resolution Mass Spectrometry

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Abstract

To achieve comprehensive and sensitive profiling of the chemical exposome in human blood, analytical workflows are evolving through advances in sample preparation and instrumental methods. We hypothesized that gas chromatography high-resolution mass spectrometry (GC-HRMS) workflows could be enhanced by minimizing lipid co-extractives during sample preparation, thereby enabling larger injection volumes and lower matrix interference for increased method sensitivity. A simple liquid-liquid extraction protocol with hexane (H) from acetonitrile-plasma (A-P) was validated for small human plasma sample volumes (100-200 µL) while optimizing for lipid removal, recovery and sensitivity of 103 representative target analytes (from 6 classes) in large volume injections (LVI) to an Orbitrap GC-HRMS. The HA-P method resulted in analyte recoveries that were quantitative for a wide range of analytes (i.e. K_{ow} >3), and relatively clean extracts that enabled LVI of 25 µL (25-50 µL of plasma equivalents on-column) with robustness over 60 consecutive injections. Without removal of plasma lipids, instrumental sensitivity dropped with increasing injection volume due to high background signal and the auto-gain control function of the Orbitrap. The method was sensitive for the broad range of target analytes, with a median method quantification limit of 0.08 ng/mL (range 0.005–4.83 ng/mL), and method accuracy was good for certified reference serum (SRM 1958). Applied to a small subset (n=32) of adult plasma samples (100 µL) from a Swedish cohort, half of the target analytes (i.e. 52 from 5 classes) were detected at least once; 8 of them displayed significant temporal trends. Nontarget analysis in the cohort also performed well, resulting in 112 structural annotations from spectral library matching, a 12.8% annotation rate overall. Follow-up confirmation with 8 authentic standards resulted in 7 Level 1 confirmations, including some anti-oxidants and UV stabilizers. The HA-P method with GC-HRMS is potentially scalable for higher throughput, and is complementary to liquid-chromatography based chemical exposomics protocols for application in future cohort studies.

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High-through analysis and Spatially resolved co-imaging of polyhalogenated compounds and their disrupted biological metabolites

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Abstract

A large group of polyhalogenated compounds has been added to the list of persistent organic pollutants in a global convention endorsed by over 100 nations. Once entering biotas, these pollutants are transported to focal sites of toxicological action and affected endogenous metabolites, which exhibited distinct tissue or organ distribution patterns. However, no study is available to achieve simultaneous mapping the spatial distributions of xenobiotics and endogenous metabolites for clarifying molecular mechanism of toxicities. Herein, we present a sensitive mass spectrometry imaging method—tetraphenyl phosphonium chloride-enhanced ionization coupled with air flow-assisted ionization-Orbitrap mass spectrometry—which simultaneously determined the spatial distributions of polyhalogenated xenobiotics and endogenous metabolites. The spatially resolved toxicokinetics and toxicodynamics of typical polyhalogenated compounds (chlorinated paraffins (CPs) and hexabromocyclododecane (HBCD)) were assessed in zebrafish. Co-imaging of polyhalogenated compounds and metabolites visualized the major accumulation organs and maternal transfer of HBCD and CPs, and clarified the reproductive toxicity of HBCD. CPs were accumulated in the liver, heart, and brain, and decreased the concentrations of polyamine-/inosine-related metabolites and lipid molecules in these organs. HBCD accumulated in the ovary and was effectively transferred to eggs, and it also disrupted the normal follicular development and impaired the production of mature eggs from the ovary by inhibiting expressions of the luteinizing hormone/choriogonadotropin receptor gene. The toxic effects of metabolic disruptions were validated by organ-specific histopathological examinations. These results highlight the necessary to assess the distributions and bioeffects of pollutants in a spatial perspective.

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Suppressing Effects of Perfluoro/polyfluoroalkyl Substances on Forskolin-Induced Syncytialization in BeWo Cells

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Abstract

Perfluoro/polyfluoroalkyl substances (PFAS) were widely detected in human samples, including placenta, but limited study evaluated the toxicity effects of PFAS on placental development. Here, BeWo cell with forskolin was used to investigate the toxic effects of PFAS on placental trophoblast syncytialization. After inducing 50 μM forskolin, the expression of genes and proteins related to syncytialization (i.e. Syn-2, E-cad, GCM1, HCG-β) and angiogenesis (i.e. PLGF) showed significant changes, which indicated the

trophoblast syncytialization. Exposure to 50 μM PFAS showed no significant effects on cell activity, but significantly suppressed the trophoblast syncytialization. Perfluorosulfonic acid (PFSA) showed higher suppressing effects compared to perfluoroalkanoic acid (PFAA). Among PFSA, PFOS has a higher suppressing effect compared to other PFSA with shorter chain. F53B, an alternative of PFOS, showed an even higher suppressing effect than PFOS. Among PFAA, the suppressing effects on syncytialization had a decreasing trend with increasing in carbon chain from C4 to C8. In summary, the results highlighted higher toxicity of F53B and short-chain PFAA compared to legacy PFAS on placental trophoblast syncytialization, which plays an important role on placental and fetal development.

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High Resolution Mass Spectrometry Based Nontarget Screening and Risk Assessment of Emerging Pollutants in Surface Water of the Hai River and the Yellow River in China

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Abstract

Increasing numbers of Emerging Pollutants (EPs) are released into surface water bodies, and many of them become potential threat to the environment. While the current knowledge on the occurrence and ecological risk of the full range of EPs are limited. Accordingly, we established a high-throughput approach for screening EPs in surface water based on target, suspect and non-target screening strategies of liquid chromatography high resolution mass spectrometry (LC-HRMS), and to study EPs comprehensively in the Yellow River （YR） and Hai River（HR）. The main work focus on: ① A sample pretreatment and instrumental analysis method matching the high-throughput identification of EPs by LC-HRMS based on target, suspect and non-target screening strategies was established; ② Sample collection, analysis and EPs identification of YR and HR was accomplished, and the occurrence and distribution of the full range of EPs was studied，in the end, 106 EPs were identified, including 37 pharmaceuticals, 33 pesticides, 21 industrial compounds, 9 personal care products, 4 food addictives and 2 transformation products. 79 and 84 EPs were detected in HR and YR respectively, and 58 were overlapped. The detection rate of 23 and 39 EPs is higher than 70% and 50% respectively. The detection rate of 1H-benzotriazole, phenazone, 2-hydroxyatrazine, desethylatrazine and creatinine were 100%. 84 EPs was quantitative analyzed and the concentration range was 0.07- 3538.10 ng/L. The characteristics of EPs with high detection rate and concentration in the YR and HR were different, and the distribution characteristics of EPs are related to the space and the surrounding environment. The overall cumulative concentration of EPs in YR was higher than HR, in the tributaries is higher than that in the main stream and in the middle and downstream samples were higher than those in the upstream.③ The ecological risk

assessment of 67 EPs was performed to three trophic model species by calculating Hazard Quotient combining EPs concentration and bioavailability in the environment, 21 and 19 priorization EPs in the YR and HR were selected respectively. The results show, we provide a high throughput LC-HRMS approach for target, suspect and nontarget screening which could be used for screening full range of EPs in surface water samples without prior knowledge. It is not only fast and accurate, but also provides an important basis for subsequent ecological risk assessment and priorization of main chemicals.

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Occurrence and prioritization of organic micropollutants in river water of Korea

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Abstract

In this study, we investigated the occurrence, distribution, and contamination characteristics of river water in South Korea. Simultaneous identification and semi-quantification of 538 chemicals were conducted using liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (LC-Q-TOF/MS) with sequential window acquisition of all theoretical fragment-ion spectra (SWATH) method developed by Kadokami and Ueno in 2019. A total of 538 compounds from 19 different classes were categorized: 296 pesticides (85 fungicides, 101 herbicides, 106 insecticides, and 4 other pesticides), 196 PPCPs (6 antiarrhythmic agents, 4 antidepressants, 8 antidiabetic drugs, 7 antihistamines, 19 antihypertensive drugs, 41 anti-infective agents, 23 nonsteroidal anti-inflammatory drugs [NSAIDs], 6 antineoplastic agents, 6 antipsychotic agents, 7 cardiovascular agents, 6 UV filters, 6 vasodilating agents, and 57 other daily use substances), 29 industrial chemicals, and 13 other product-derived chemicals. These contaminants were subjected to an accurate mass database and library for identification. Water samples were collected in December 2023 and May 2024 to prioritize the major pollutants by section of the river and to confirm the appearance of pollutants before and after the agricultural season. The highest proportions of PPCP residues were detected midstream in the river, while the highest proportions of pesticide residues were observed downstream, in proximity to agricultural land. The list was set by applying the ToxPi mechanism, which calculated optimal weights for matrix such as lowest PNEC, log K_{ow}, detection frequency, and highest concentration. The detailed information on the priority chemical list and contamination patterns of major emerging contaminants will be presented during the conference.

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Assessment of Contaminants in an Anthropogenic-impacted Watershed Using Non-targeted Screening and *In Vitro* Bioassays

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Abstract

Emerging and persistent contaminants (EPC) pose a significant challenge to water quality monitoring efforts. Monitoring the EPC prevalence is crucial for managing water resources effectively, particularly in light of growing population densities worldwide and the increasing production of chemical compounds associated with most industries. In this study, we combine the use non-target screening (NTS) and *in vitro* bioassays to study the EPC presence the upper Ping River Catchment, northern Thailand.

We conducted four sampling campaigns to collect surface water at sites covering different land-use types (Uban, agriculture, rural-remote), as well as additional subsurface water samples. For NTS, samples and methanol blanks were run in MS1 scan in positive mode using an Agilent G6550A iFunnel Q-ToF LC-MS with a dual AJS-ESI source. For bioassays, cytotoxicity using HepG2 cells was assessed followed by four different fluorescence reporter cell assays were performed, which detect estrogenic activity (ERα assay), glucocorticoid activity (GR assay), peroxisome proliferator-activated receptor gamma (PPARγ) activation pathways (PPARγ assay), and CYP1A1 induction (CYP1A1 assay), respectively.

NTS revealed a large number of entities identified individually at each site but a relatively limited number of entities throughout the Ping river transect. Out of the 532 entities identified, 70% were found in agriculture sites, slightly higher than in urban sites (61%). A total of 78 entities (~15%) were found exclusively in agriculture site waters.

More than half of the samples showed some cytotoxicity. Estrogenic compounds were detected in 82% of samples but only 15 had concentrations > 1 ng/L E2 EQ, 14 of which were urban.GR assay showed negative response for all but 17 samples, among which 12 were from urban areas, four from agricultural lands, and one from a subsurface well. Most samples were negative in CYP1A1 assay, yet few sites including canals, road runoff and a subsurface sample showed moderate to high signals. All but 11 samples showed low responses in PPARγ assay.

Shortlisted NTS entities were screened for cytotoxicity, estrogenic receptor (ER) binding, and glucocorticoid endpoints using the OECD QSAR toolbox and compared to the bioassays results for all sites. The combination of toxicological effects and the qualitative identification of compounds through NTS will lead to a better targeted EPC list for water quality monitoring.

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Discovery of antimicrobial drugs and their transformation products in a swine farm by target, suspect, and nontarget screening

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Abstract

Swine farms contaminated the surrounding environment through manure application and biogas slurry irrigation, hence causing the wide residual of multiple antimicrobial drugs (ADs) and their transformation products (TPs). This study performed target, suspect, and nontarget screening methods to comprehensively investigate the pollution profiles of ADs in a typical swine farm, and characterize the potential transformed pathway of TPs and distinguish specific reactions of different catalog of ADs. Samples of fresh feces, compost, biogas slurry, topsoil, column soil, groundwater and plants were analyzed using the database containing 98 target analytes, 679 suspected parent ADs, and ~107 TPs. In total, 29 ADs were quantitively detected, and tetracyclines (TCs) were mostly frequently detected ADs with the concentrations up to 4251 ng/g in topsoil. Soil column investigation revealed that doxycycline (DOX) and tetracycline (TC) in soil could migrate to depths of approximately 1 m in soil. Suspect screening identified 75 parent ADs, with 10 being reported for the first time in environmental media. Semi-quantification of ADs revealed that one of the less-concerned ADs, clinafloxacin, was detected to exceed 5000 ng/L in biogas slurry, suggesting that significant attentions should be paid to these less-concerned ADs. Moreover, 314 TPs was identified, and most of them were found to undergo microbial/enzymatic metabolism pathways. Overall, our study displays a comprehensive overview of ADs and their TPs in swine farming environments, and provides an inventory of crucial list that worthy of concern. The results emphasize the need to quantify the levels and distribution of previously overlooked ADs and their TPs in livestock farms.

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Regional Neonicotinoid Pollution in Wastewater Treatment Plants and Point Source Emissions

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Abstract

Neonicotinoids, currently the most widely used insecticides, pose ecological risks to aquatic systems through runoff into waterways. While non-point source emissions have been studied, the spatial patterns of their point source emissions within watersheds remain poorly understood. Here, we quantified neonicotinoid residues in the influents, effluents and various treatment stages of wastewater treatment plants (WWTPs) in the Yangtze River Delta, China. Results showed influent concentrations were significantly higher than those typically found in surface waters, with municipal WWTPs exhibiting lower removal rates (53.1±20.8%) compared to industrial ones (83.3±4.36%). WWTP influent neonicotinoid concentrations were positively associated with precipitation and population. The study identified the hydrolysis acidification process in industrial WWTPs and the aerobic sludge stage as key to higher neonicotinoid degradation, with Nitrospirota and Chloroflexi as the dominant microbial degraders. Using these quantitative relationships and empirical degradation rates, we constructed a point source emission model. This model estimates an annual emission of neonicotinoids via WWTPs at 5.27 tons/year (95% CI: 5.24-5.30 tons/year) in the studied region, with municipal WWTPs accounting for approximately 90%, especially during June and July. This study accurately assesses secondary point source emissions, offering critical data for basin-wide neonicotinoid pollution control.

2. Computational Toxicology, Machine Learning, and Environmental Big Data Analysis

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Quantifying Influence Factors for Multi-Metal Stabilization: A Machine Learning Approach

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Abstract

There is an urgent need to analyze the importance and interaction effect of influence factors for the multi-metal stabilization effect comprehensively. We integrated machine learning and spectroscopic analysis to analyze importance of influence factors in Pb, Cd and Zn stabilization process, and elucidate the mechanisms underlying their stabilization. The results illustrated that the random forest (RF) exhibited outstanding performance in predicting the concentration of Cd, Pb and Zn ($0.52 \leq R^2 \leq 0.75$). The Shapley algorithm was applied to explain RF model and quantify the importance and interactions of the influence factors (stabilizer application rate (SAR), soil moisture (SM), particle size, and types of stabilizers selected in this study). The results revealed that the stabilization process is primarily influenced by two dominate factors: SAR and SM, with stabilization efficiency exhibiting an upward trend with increasing SAR or SM. The interaction between SAR and SM has the greatest influence on the stabilization of heavy metals. This study proposes an approach to quantify the importance of influence factors and further find out the optimal experimental conditions for multi-metal stabilization.

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Digital Tools To Automate Environmental Risk Assessment for Plant Protect Products

Jing Ma

Tobias Gutgesell, Germany. Horatio Meyer, Germany. Anne Grimbs, Germany. Michael Boeckers, Germany

Abstract

Developing an environmental risk assessment (ERA) package for a plant protection product registration is a complex process which normally requires many months of work from multiple experts. Challenges associated with traditional MS Excel-based ERA tools and higher-tier models are time consuming, resource intensive, and human error prone, often resulting in delays and inefficiencies. Development of an digital solution was needed to address these continuing challenges. Scientists from Bayer Crop Science have developed and validated a new set of tools which incorporate guideline-based equations and higher-tier exposure models to streamline the risk assessment process. This “one click” tool provides significant efficiencies and y which also would benefits non-experts for allowing them to screen potential ideas and products. The guideline-based equations tool utilizes KNIME Analytics Platform to upload the GAPs (Good Application Practice), the endpoints of compounds from a Bayer online database, and implements the calculations based on the integrated Python code of guideline equations. The higher tier exposure models tool uses the ReisWolf Platform to generate input files for and extract outputs from behind models running in cloud computation. Through this automation, the time of tier 1 screening ERA is reduced at least~ 50%. The automation provides a digital transformative solution for China ERA screening and submissions and as well as the pioneer of risk assessment automation in broader APAC for internal safety evaluation and potentially external risk assessments required by authorities in dynamic regulation., by all of these significantly contributing to a faster portfolio decision making within Bayer as well as advocacy with the authorities who want to adopt ERA and automation to manage PPP scientifically.[LM1]

[LM1]These sentences I think are more for an internal audience and not appropriate for an external poster because it describes how it helps Bayer engage with regulators and gives us a business advantage. Instead you can replace these sentences with something more simple like, “In the future, this tool may be of use to regulatory authorities in China and in other countries in the region.”

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Development potential of nanoenabled agriculture projected using machine learning

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Abstract

TTe controllability and targeting of nanoparticles (NPs) offer solutions for precise and sustainable agriculture. However, the development potential of nanoenabled agriculture remains unknown. Here, we build an NP-p lant database containing 1,174 datasets and predict (R2 higher than 0.8 for 13 random forest models) the response and uptake/transport of various NPs by plants using a machine learning approach. Multiway feature importance analysis quantitatively shows that plant responses are driven by the total NP exposure dose and duration and plant age at exposure, as well as the NP size and zeta potential. Feature interaction and covariance analysis further improve the interpretability of the model and reveal hidden interaction factors (e.g., NP size and zeta potential). Integration of the model, laboratory, and ffeld data suggests that Fe2O3 NP application may inhibit bean growth in Europe due to low night temperatures. In contrast, the risks of oxidative stress are low in Africa because of high night temperatures. According to the prediction, Africa is a suitable area for nanoenabled agriculture. TTe regional differences and temperature changes make nanoenabled agriculture complicated. In the future, the temperature increase may reduce the oxidative stress in African bean and European maize induced by NPs. TTis study projects the development potential of nanoenabled agriculture using machine learning, although many more ffeld studies are needed to address the differences at the country and continental scales.

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Interpretable ai: data driven and mechanistic modeling for chemical toxicity and drug safety evaluations

Hao Zhu

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Abstract

Addressing the safety aspects of new chemicals has historically been undertaken through animal testing studies, which are expensive and time-consuming. Computational toxicology is a promising alternative approach that utilizes machine learning (ML) and deep learning (DL) techniques to predict toxicity potentials of chemicals. Although the applications of ML and DL based computational models in chemicals toxicity predictions are attractive, many toxicity models are “black box” in nature and difficult

to interpret by toxicologists, which hampers the chemical risk assessments using these models. The recent progress of interpretable ML (IML) in the computer science field meets this urgent need to unveil the underlying toxicity mechanisms and elucidate domain knowledge of toxicity models. In this new modeling framework, the toxicity feature data, model interpretation methods, and the use of toxicity knowledgebase in IML development advance the applications of computational models in chemical risk assessments. As a result, our recently developed artificial intelligence approaches and relevant modeling studies answered the above challenge by providing new solutions to chemical toxicity evaluations based on big data modeling and mechanistic analysis. The resulted chemical toxicity provided deep insights to the continuum from chemical structure, in vitro, to animal/human toxicity outcomes. The relevant novel big data mining, analysis, and modeling techniques provided critical support to the current drug risk assessments. The challenges and future directions of IML modeling in toxicology are strongly driven by heterogenous big data and newly revealed toxicity mechanisms. The big data mining, analysis, and mechanistic modeling using IML methods will advance artificial intelligence in the big data era to pave the road to future computational chemical toxicology and will have a significant impact on the risk assessment procedure and drug safety.

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Mitigation of soil acidification alleviates the public dietary risks of cadmium in China

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Abstract

The daunting challenges of heavy metal pollution and soil acidification seriously threaten human health and the development of sustainable agriculture worldwide. However, effective approaches for identifying and controlling the public health risks on a large geospace are urgently needed. Here, we proposed a proof-of-concept machine learning-based food risk (MFR) framework and accurately recognized that soil pH is the key driver affecting cadmium accumulation in wheat and rice at the national scale. From the 1980s to the 2000s, under soil acidification, the dietary risk of cadmium through rice and wheat increased approximately 10% in Central-South China and East China. Geospatial trades increase the uncertainty of risks. In contrast, the mitigation of soil acidification alleviated the cadmium accumulation in crops and the public dietary risks from the 2000s to the 2010s. The dietary risk of cadmium was higher for children than for adults, 1.61 times for rice and 1.59 times for wheat. Given that the dietary risk of cadmium for rice is 3.38 (adults) and 3.41 (children) times higher than that for wheat, grain-based dietary structure adjustment is a possible pathway for reducing public health risks. Taken together, soil-based solutions for controlling soil acidification and optimizing dietary structures are large geospatial strategies for alleviating public dietary risks of heavy metals (*e.g.*, cadmium).

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Ecological Status Assessment in Large Watersheds Through Multispecies Edna Sequencing and Environmental Monitoring

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Abstract

The watershed ecological quality assessment aims to predict the health status of ecosystems within a watershed. Large-scale ecological quality assessment requires extensive biological data collection, significantly increasing the costs and challenges associated with assessment and analysis. This study, employing environmental DNA (eDNA) technology, successfully addresses the challenges in environmental sample collection and proposes a method based on environmental and pollutant parameters to predict the overall ecological quality of the Yangtze River basin. Results from eDNA data analysis reveal significant alterations in biological integrity under the influence of human activities and environmental changes, with benthos and microbial communities predominantly driving changes in overall biological integrity. The predictive approach incorporates random forest and structural equation models to ascertain the impact weights of environmental parameters and pollutants, further resolving challenges in ecological quality computation and analysis. This study predicted the changes in ecological quality at 67 different points in the Yangtze River Basin across various seasons, and found that nearly 60% of these points experienced ecological quality degradation. This innovative methodology offers a comprehensive solution for predicting ecological quality across large watershed scales, offering new perspectives for protecting watershed ecosystems and formulating solutions for watershed sustainability.

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Application of Machine Learning to Balance the Functionality and Biocompatibility of Materials

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Abstract

The rational design of molecules with the desired functionality presents a significant challenge in chemistry. Moreover, it is worth noting that making chemicals safe and sustainable is crucial to bringing them to the market. To address this, we propose a novel deep learning framework developed explicitly for de novo design of molecules with both functionality and biocompatibility. This innovative approach comprises two predictive models and one generative model, facilitating the targeted screening of novel molecules from created virtual chemical space. Our method's versatility is highlighted in the inverse design process, where it successfully generates molecules with specified motifs or composition, discovers synthetically accessible molecules, and jointly targets functional and safe properties beyond the training regime. The utility of this method is demonstrated in its ability to design ionic liquids (ILs) with enhanced antibacterial properties and reduced cytotoxicity, addressing the issue of balancing functionality and biocompatibility in molecular design.

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Identifying candidate persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances based on machine learning approaches

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Abstract

Identifying persistent, mobile and toxic (PMT) substances or very persistent, very mobile (vPvM) substances among global synthetic chemicals is of primary importance for reducing contamination of drinking water. This study aims to develop a machine learning model to allow one-step prediction of candidate PMT/vPvM substances. We built and compared 960 machine learning models by combining different molecular description methods, data balancing approaches and machine learning algorithms. The optimal model achieved a high accuracy of 92% for PMT/vPvM identification (i.e. positive samples) on an internal test set, and also resulted in a commendable accuracy of 90% for an external test set of chemical pollutants detected in Taihu Lake, China. Additionally, the optimal machine learning model was applied to identify the candidate PMT/vPvM substances in shale gas drilling fluids and COVID-19 related chemicals. Furthermore, we utilized Shapley additive explanations (SHAP) and causal inference to explore the relationship between PMT/vPvM properties and molecular structures. This work presents an advance of big data in-silico screening models for the identification of substances that potentially meet the PMT/vPvM criteria.

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Prediction and Modeling on Bioaccumulation of Chemicals in Aquatic Organisms

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Abstract

The bioaccumulation of chemicals, which is related to their internal exposure and hazards, is an important element in evaluating the ecological and human health risks of the chemicals and in identifying priority pollutants for control. Conventional assessment of the bioaccumulation relies on laboratory simulation exposure experiments and field monitoring studies, which face limitations such as the availability of authentic chemical standards, high costs, ethical considerations, and time constraints. As a result, developing prediction models for chemical bioaccumulation has become a pressing need. The prediction models for bioaccumulation can be categorized into two main types: mechanical toxicokinetic models and data-driven quantitative structure-activity relationship (QSAR) models. We have developed physiologically-based toxicokinetic (PBTK) models to describe the absorption, distribution, metabolism, and excretion (ADME) process of antibiotics in sea cucumbers and benzotriazole ultraviolet stabilizers in zebrafish. Additionally, we have employed sophisticated machine learning techniques, including multi-task learning, ensemble learning, transfer learning, and graph neural networks, to establish QSAR models for predicting bioaccumulation parameters. Future research should focus more on developing PBTK models for invertebrates and various types of chemicals, expanding the datasets of bioaccumulation parameters, and constructing multimodal models. This will help address the limitations of traditional approaches and meet the growing demand for chemical risk assessment.

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Multimodal Model to Predict Tissue-to-Blood Partition Coefficients of Chemicals in Mammals and Fish

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Abstract

Tissue-to-blood partition coefficients (P_{tb}) are key parameters for assessing toxicokinetics of xenobiotics in organisms, yet their experimental data were lacking. Experimental methods for measuring P_{tb} values are inefficient, underscoring the urgent need for prediction models. However, most existing models failed to fully exploit P_{tb} data from diverse sources, and their applicability domain (AD) was limited. The current study developed a multimodal model capable of processing and integrating textual (categorical features) and numerical information (molecular descriptors/fingerprints), to simultaneously predict P_{tb}

values across various species, tissues, blood matrices, and measurement methods. Artificial neural network algorithms with embedding layers were used for the multimodal modeling. Corresponding unimodal models were developed for comparison. Results showed that the multimodal model outperformed unimodal models. To enhance reliability of the model, a method considering categorical features, weighted molecular similarity density, and weighted inconsistency in molecular activities of structure-activity landscapes was used to characterize the AD. The model constrained by the AD exhibited better prediction accuracy for the validation set, with determination coefficient, root mean square error, and mean absolute error being 0.843, 0.276, and 0.213 log units, respectively. The multimodal model coupled with the AD characterization can serve as an efficient tool for internal exposure assessment of chemicals.

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Enhancing Environmental Modeling Through Multimodal Learning: Methodology, Applications, and Future Directions

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Abstract

The environment faces increasing anthropogenic impacts, resulting in a rapid increase in environmental issues that undermine the natural capital essential for human wellbeing. These issues are complex and often influenced by various factors represented by data of different modalities. While machine learning (ML) provides data-driven tools for addressing environmental issues, the current ML models in environmental science and engineering (ES&E) often neglect the utilization of data from diverse modalities.

Data modalities in ES&E studies include, but are not limited to, numerical vectors, graphs, text sequences, visual data (images and videos), and audio data. With the advancement in deep learning, multimodal learning (MML) holds promise for comprehensive descriptions of environmental issues by harnessing multimodal data. MML methods can be divided into those based on feature fusion or modal interaction and those relying on interaction networks, which can be effectively employed to fuse multimodal data and construct MML models.

MML models have extensive potential applications in ES&E research, including environmental quality assessment, prediction of chemical hazards, and optimization of pollution control techniques, among others. For instance, when assessing environmental quality, factors like pollutant concentrations and land use patterns can be represented as numerical vectors or visual data. Predicting health hazards of chemicals requires consideration of not only numerical vectors and molecular graphs for characterizing chemical structures, but also biological system networks disrupted by chemicals (graphs).

The efficacy of e-waste recycling is influenced by waste quantity and treatment processes, which can be represented by visual data (videos recorded by monitors) and audio data (mechanical sounds during the process). The applications showcase the significant potential of MML in addressing environmental issues,

providing enhanced solutions for environmental modeling tasks. Nevertheless, as an emerging methodology, successful application of MML in ES&E studies still faces challenges, such as data acquisition and issues with MML fusion, which are expected to be further improved.

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Investigation of Eco-efficient Ternary Blended Cement Mortar Using Response Surface Methodology (RSM): Strength Development and Carbon Dioxide Emissions

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Abstract

Concrete production encounters significant challenges, mostly due to the increasing demand for cement and the depletion of natural resources, which has raised environmental concerns. For instance, each tonne of Ordinary Portland cement (OPC) production contributes to approximately 6% of all manufactured carbon emissions, while the global consumption of sand in concrete is around 1000 million tons annually, leading to scarcity and limitations. To mitigate these associated environmental impacts, sustainable alternative materials have been proposed. Local waste from industry such as fly ash and steel slag are well-known examples. This study specifically aims to investigate the effects of fly ash (FA) and steel slag powder (SSP) as cement substitutes and steel slag sand (SSS) as sand substitutes in ternary blended cement mortars (TBCM). Various ratios of FA, SSP, and SSS, ranging from 0% to 20%, were incorporated to analyze the influence on the strength performance of TBCM through compressive strength tests. Response surface methodology (RSM) was used as historical data design to analyze the complexity effects of the TBCM, with FA (0-20%), SSS (0-20%), and SSP (0-20%) as input variables and compressive strength as the output variable. The results demonstrated that FA, SSS, and SSP exert both singular and interactive influences on the compressive strength development of TBCM. Three quadratic models were found to best fit the data, yielding a high adjusted R^2 value of 0.976, 0.994 and 0.998. Statistical values (F-value, 40.86, 79.51 and 165.77; p-value, < 0.05) for the model confirmed its significance and capability to predict the compressive strength of TBCM. Notably, the most significant improvement in compressive strength was observed for TBCM with 20% SSS and 20% FA + 20% SSP. The optimum TBCMs were determined to be those containing 20% FA + 20% SSS and 10% FA + 10% SSP + 20% SSS. Additionally, it was found that partial substitution of cement by 20% FA and 10% FA + 10% SSS can reduce carbon dioxide emissions for each m^3 of material produced. On the other hand, the incorporation of SSS could reduce the use of natural resources.

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Anthropogenic terrestrial loads of sediment and nutrients entering the Great Barrier Reef lagoon, Australia: A case study in science supporting policy direction and change.

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Abstract

Like many receiving waters around the world, the Great Barrier Reef (GBR) lagoon is exposed to multiple stressors including climate change, extreme weather events, direct and in-direct use, and reduced water quality. Nutrients and sediment have been identified as key stressors that can affect the growth and survival of corals and decrease the overall health and resilience of GBR ecosystems. The Australian and Queensland governments have been addressing the decline in water quality since 2003, through several iterations of the Reef Water Quality Improvement Plan (Reef Plan). A key monitoring and evaluation component of the Reef Plan is the Great Barrier Reef Catchment Loads Monitoring Program (GBRCLMP), which provides a long-term and dense dataset to validate and calibrate Source Catchment models that report on progress towards pollution reduction targets. The GBRCLMP, which has operated for 16 years, has calculated over 3500 annual loads for total suspended solids and nine forms of nitrogen and phosphorus. The loads data are used directly in education programs and in determining if changes in land management practices are having measurable effects. Calculated loads are also used in the 5-yearly Reef Scientific Consensus Statement, underpinning data for the water quality targets in the Reef 2050 Water Quality Improvement Plan, and funding prioritisation that support management practice change. The GBRCLMP works directly with landholders, Traditional Owners, extension officers, catchment management groups and researchers in a 'bottom up' approach that allows for data-driven catchment improvements. A recent international review of the GBRCLMP noted its ability to generate real water quality improvements through dynamic engagement and translation of science to action. This presentation will discuss key findings of the GBRCLMP including a comparison of measured annual average loads to modelled 'natural' annual loads and where these data sets have made a difference in policy and legislation. It will also discuss the elements of the GBRCLMP success story that could be applied to environmental assessment frameworks globally.

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An integrated approach for *in vitro* to *in vivo* extrapolation of multiple toxicities for plastic additives

Jingyuan Yang, Xuehua Li, Peiling Han, Jingwen Chen

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Abstract

Over 10,457 chemicals with various functions used in plastic production may be released from plastics, causing toxic effects on organisms and posing risks to human health. However, the relationship between environmental exposure and internal levels in biological target tissues of plastic additives remains unclear, making it challenging to obtain *in vivo* toxicity for additives. A physiologically based toxicokinetics (PBTK) model is regarded as a potential tool for associating internal levels and *in vivo* toxicity of plastic additives through *in vitro* to *in vivo* extrapolation (IVIVE), but the absence of biochemical parameters for plastic additives hinders the development of PBTK models. Thus, this study aims to establish a PBTK model and further create an IVIVE model for multiple toxicities of plastic additives. Firstly, a machine learning (ML) prediction model for the fraction of the chemical unbound in plasma (F_{up}) in mammals was developed to fill gaps in the biochemical parameters of PBTK models (R_{test}^2 = 0.78). Then, an eight-compartment PBTK model was established to predict internal levels at specific tissues of rats by integrating the above ML prediction model into it. Validation results showed that the PBTK model accurately predicted the concentrations of plastic additives in various organs of rats. Subsequently, a PBTK-based IVIVE approach was created and used to derive adverse outcome pathway (AOP) - specific equivalent administered doses (EADs) for nine plastic additives to explore the association between *in vitro* and *in vivo* toxicity, such as reproductive, hepatic, and metabolic toxicity. Comparing predictions with *in vivo* toxicity data indicates the potential of using *in vitro* bioactivity to approximate *in vivo* EADs for the same toxicity (78% of data points within 5-fold differences, N = 58). Therefore, the presented PBTK-based IVIVE approach could provide credible AOP-specific EADs and be suitable for prioritizing risks posed by chemicals lacking *in vivo* toxicity data. Future studies should extend this approach to include other additives and toxicities.

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Degradation Mechanism of Layered Black Phosphorus in Aqueous and Influence of Proteins

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Abstract

Layered black phosphorus (LBP), a new type of two-dimensional nanomaterial, draws increasing attentions because of excellent properties. So far, migration and transformation mechanisms of LBP in the environment are not clear yet. To evaluate potential ecological risks caused by mass productions and uses of LBP, this study clarified the influence of environmental factors on the transformation behavior and biological effects of LBP through experiments combined with quantum chemical calculations. Research results can provide basic data for ecological risk assessment of LBP.

This study found that compared with the weak physical adsorption of water molecules or protons on LBP, a strong chemical adsorption occurred between hydroxide ions (HO^-) and LBP, which can induce disproportionation reaction on the surface of LBP. This process could be divided into three stages. Firstly, HO^- was adsorbed on the surface of LBP to form a P-O single bond; secondly, two thirds of the negative

charge of HO- were transferred to LBP, meanwhile, one of the three P-P bonds originally connected to the attacked P atom was broken; finally, the unbonded P atom was attacked by HO^- or H_2O to generate hypophosphite.

The sorption of human serum albumin (HSA) on the surface of LBP was not only concentration-dependent, but also exfoliated LBP. The oxidation process of LBP influenced by HSA could be divided into three stages. Firstly, excepting promote oxidation by oxygen when HSA was adsorbed on the oxidation site of LBP, HSA adsorbed on other sites of LBP would slow down the oxidation of LBP by oxygen and HO^-; secondly, HSA was continuously adsorbed on the surface of LBP to exfoliated LBP and exposed a new surface, which caused by exposing the edge of LBP as rapidly oxidized and broken; finally, the exposed new surface on the one hand adsorbed a large amount of HSA, on the other hand was degraded, making the degradation faster.

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Synergizing domain knowledge, experimental data, and active learning for modeling environmental processes

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Abstract

As machine learning (ML) modeling has been widely recognized as a powerful tool for environmental process modeling, we continue to face challenges with sparse data in building robust, widely applicable predictive models. To address this limitation, we combined expert knowledge, experimental data, meta-analysis, and ML techniques such as active learning to model the fate and transformation of numerous organic compounds (OCs) in different environments. We used anaerobic biodegradation and soil sorption as case studies.

First, anaerobic biodegradation rates of OCs are pivotal for environmental risk assessment and remediation. Traditional experimental evaluations, constrained by prolonged, oxygen-free conditions, struggle to keep pace with emerging contaminants. We focused on key features for both chemicals and experimental conditions, curating two datasets: one for sediment/soil and another for sludge. We then built two ML models for half-life predictions and validated the models with expert knowledge.

Second, the environmental detection of various OCs has highlighted the limitations of conventional soil sorption models, which oversimplify complex environmental factors and often overlook OCs with polyfunctional and ionizable structures. After compiling a comprehensive soil sorption dataset encompassing 20,945 data points, we conducted a meta-analysis and built ML models to estimate the sorption of diverse OCs on a global scale under real environmental conditions.

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Identification of Hazardous Chemicals and Molecular Design of Green Alternatives Based on Machine Learning

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Abstract

While bringing benefits to the economy and improving human livelihoods, chemicals may be inevitably released into the environment during their life cycles and pose risks to human and ecological health. The rapid growth in the variety and production volume of chemicals can inevitably lead to chemical pollution that exceeds the planetary boundary. Therefore, it is necessary to identify hazardous chemicals, and design green alternative chemicals for sustainable development.

Machine learning (ML) is an important tool for identifying hazardous chemicals. Based on advanced algorithms such as graph attention networks (GAT), ML models were successfully utilized to predict physicochemical and environmental behavior of chemicals and facilitate high-throughput identification of environmentally persistent, bio-accumulative, and toxic (PBT) chemicals.

When confronted with datasets with limited data volume, transfer learning (TL) provides a strategic advantage by transferring knowledge from extensive source domain datasets to the target domain dataset, thus improving performance and generalization of ML models on small datasets. Specifically, TL was employed to leverage knowledge from PBT chemical datasets to support training of GAT models on limited datasets of environmentally persistent, bio-accumulative, mobile, and toxic (PBMT) chemicals, ensuring an accurate PBMT chemical identification with limited data.

Beyond identifying hazardous chemicals, ML can also bring innovative solutions for molecular design of green alternative chemicals. Multi-constraint generative ML models can be employed to design chemicals with desired properties, balancing their functionalities with hazards. For instance, generative ML models were developed to design molecular structures of fluorinated surfactants that simultaneously exhibit low surface tension and low toxicity. Integrating ML algorithms in the molecular design of green alternatives can yield a sustainable and responsible way that both promotes the benefits of chemicals and simultaneously minimizes their adverse impacts on humans and the environment.

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Priority Screening List of 5-hydroxytryptamine Reuptake Inhibitors: Improved CNN-GRU Deep Learning Model

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Abstract

Background and aims. There is a rapid increase in the prescription and consumption of 5-hydroxytryptamine reuptake inhibitors (5-HT-RIs), which are detected in aquatic environments and have biological targeting effects. However, the targeted detection and analysis is difficult, and lacking systematic studies to capture various characteristics and toxicological endpoints. Therefore, we focus on multi-directional selectivity of functionalities (efficacy and resistance) and human health interferences (olfactory toxicity, neurotoxicity and gut microbial interference), which address the limitations of traditional screening lists.

Methods. A total of 29 molecular characteristics are calculated by the Gaussian 09 and ChemBioDraw 12.0 software. The main characteristics are screened as independent variables by the variance threshold-Pearson's correlation coefficient methods. The key receptors are obtained based on the adverse outcome pathway framework. The binding energy are characterized by the molecular dynamics and weighted information weighting methods. The improved convolutional neural network-gated recurrent unit (CNN-GRU) models are constructed using PyCharm software. The key characteristics and factors are analyzed by sensitivity analysis, surface electrostatic potential distribution, molecular polarity index and polar surface area.

Results and discussion. Ten main characteristics with strong rationality were screened. The binding energies showed several 5-HT-RIs have strong interferences. The evaluation of improved models indicated the robustness and accuracy were favorable. The proposed priority screening list identified seven 5-HT-RIs as high-priority (vesvenlafaxine, rac-trans-sertraline, (s)-fluoxetine, citalopram, (s)-citalopram, nefazodone and venlafaxine). Compared with random forest and GRU methods, the improved CNN-GRU models creatively enhanced data input and improve network adaptability. Five key characteristics (dipole moment, quadrupole moment Qyy and Qxz, infrared and boiling point) related to molecular polarity and hydrogen bonds. We inferred high-priority 5-HT-RIs had stronger polarity and weaker electronegativity.

Conclusion. An internal architecture of improved CNN-GRU model was designed for targeted reinforcement to propose the priority screening list. Additionally, molecular polarity and electronegativity had great influence on priorities. This study provided a scientific support for the risk assessment of emerging pollutants.

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Screening, Assessment and Control Technology System for Managing Emerging Contaminants Based on Computational Toxicology

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Abstract

Chemicals represent a major source of emerging contaminants. The primary task in managing emerging contaminants involves screening hazardous chemicals, assessing chemical risks, and implementing preventative control measures. Given the vast number of chemicals, relying solely on experimental methods to measure chemical exposure and hazard parameters and to identify hazardous chemicals is impractical for chemical sound management. The necessity leads to the rapid development of environmental computational toxicology.

Conventional computational methods involve molecular simulation techniques and quantitative structure-activity relationship models, which can be used to predict parameters related to environmental exposures, hazards, and risks of chemicals. Additionally, force fields based on machine learning can increase the speed of quantum chemical simulations while maintaining modeling accuracy. Computational toxicology models based on machine learning algorithms like graph attention networks facilitate the integrated identification of hazardous chemicals.

By integrating advanced AI techniques, environmental computational toxicology can contribute to chemical risk assessment and preventative control of emerging contaminants. Specifically, AI-empowered environmental computational toxicology holds promise in predicting environmental exposures, hazards, and risks of chemicals and molecular design of green alternative chemicals.

The rapid developments in multimodal learning techniques have made it possible to reveal complex patterns behind multimodal big data. Utilizing multimodal learning techniques, computational toxicology models can integrate multimodal data, including molecular structure, experimental conditions, and high-content screening results. By extracting complementary features from multimodal data, the models can achieve precise predictions for target endpoints.

Apart from the immense potential of discriminative AI, generative AI technologies pave innovative avenues for the molecular design of green alternative chemicals. Generative AI algorithms can be employed to design chemicals with specific properties. Multi-constraint molecular generation models can be employed to design chemicals that possess necessary functionalities while exhibiting low environmental hazards. The application of AI techniques in environmental computational toxicology is poised to control emerging contaminants from the sources, minimizing adverse impacts of chemicals.

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Forwarding maturation of Species Sensitivity Distributions using Machine Learning

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Abstract

Introduction

The characterization of impacts of chemical pollution in ecosystems is amongst others performed by a combination of exposure data with insights from Species Sensitivity Distributions (SSDs). SSDs are the statistical description of patterns in observed ecotoxicity endpoint metrics, such as NOECs, EC50s and LC50s. Despite the versatile application of this approach, we do not yet make full use of the available collections of ecotoxicity data to generate SSDs and to fill current datagaps. This presentation ventures into a Machine Learning based alternative approach to the derivation of SSDs from currently available data, and presents a suite of high-utility applications of outcomes of such SSDs derived by ML.

Methods

Despite a wealth of information on chemical hazards there are still severe data gaps for many chemicals and the already available data has not yet been used to identify the sensitivity patterns regarding chemicals and species in the broadest sense of the word. In our innovative versatile approach, we investigate the hidden patterns in the available ecotox data sources and these patterns can be applied to a wide variety of use cases.

In the heart of the employed methods, we use Machine Learning (ML) to address, and potentially solve, the issue of data gaps for various use cases. This core set consists of routines for i) data curation steps, ii) data enrichment steps, iii) model/algorithm validation steps, iv) model version management steps, and v) application routines.

The data itself consists of response data of a wide variety of species, chemicals, exposure durations and experimental settings/descriptors, which are further enriched with additional information (like fingerprints, physchem and MoA data, species similarity, etc.), and includes various endpoints. Depending on the purpose various validation routines are available for various model algorithms (e.g., Factorization Machines, Randam Forest, eXtreme Gradient Boosting, Neural Networks, etc.). In addition, various routines are developed to apply and visualize the models/results.

Applications and use cases

The core routines can be applied to predict SSDs, which have many different uses ranging from the earliest uses in the derivation of protective, regulatory environmental quality standards (such as the Predicted No Effect Concentration), the characterization of the degree of harm caused by unintended ambient mixtures and its application for Safe and Sustainable by Design.

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Computational toxicology in the era of Artificial Intelligence

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Abstract

Production of chemical compounds doubled since begging of this century. While chemical agencies continuously register new compounds, their characterization cannot be fully done due to absence of experimental data, which are limited by high experimental costs but as well as ethical issues with animal testing. Computational toxicology can allow fast and cheap alternative to such studies, provided that the predictions are sufficiently accurate to substitute the experimental tests.

Modern Machine Learning (ML) based on deep neural networks (DNNs) are becoming increasingly more powerful and steadily overcome conventional approaches, in particular if large big data are available. DNNs using representation learning, such as graph neural networks (GNN) or natural language processing (NLP), frequently show similar or higher accuracy than descriptor-based methods for structure-activity/property relationship studies. Representational learning methods are particularly powerful when they are used to combine information from similar endpoints via multi-task learning as will be exemplified by animal toxicity study. However, combination of both types still contributes the highest accuracy at least for simple endpoints as demonstrated by Kaggle solubility challenge results.

The novel developments, such as contrastive learning, can use rich information from assay data, such as high-content imaging, to suggest Mode of Action of chemical compounds. It can be a promising approach to characterize Adverse Outcome Pathways (AOPs) for complex chemicals, such as mixture, complexes, polymers, etc., for which more traditional computational toxicology approaches can have limitations.

Being considered for a long time as black boxes, DNNs are becoming interpretable via eXplainable AI (XAI) including both agnostic and method-specific approaches. In combination with Large Language Models (LLM), which can explain the reasoning of the methods using natural language, these approaches open new perspectives for use of interpretable and trustworthy Artificial Intelligence(AI) in computational toxicology.

I will recapitulate these and other recent developments of ML/AI and will discuss their impact on computational toxicology as showcased in the studies performed within the AIDD (https://ai-dd.eu) and AiChemist (https://aichemist.eu) projects, as well as special issue: AI Meets Toxicology published by Chemical Research in Toxicology.

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Are new phthalate ester substitutes safer than traditional DBP and DiBP? — Comparative endocrine-disrupting analyses on zebrafish using *in vivo*, transcriptome, and *in silico* approaches

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Abstract

Although previous studies have confirmed the association between phthalate esters (PAEs) exposure and endocrine disorders in humans, few studies to date have systematically assessed the threats of new PAE alternatives to endocrine disruptions. Herein, zebrafish embryos were continuously exposed to two PAEs [di-*n*-butyl phthalate (DBP) and diisobutyl phthalate (DiBP)], two structurally related alternatives [diisononyl phthalate (DINP) and diisononyl hexahydrophthalate (DINCH)], and two non-PAE substitutes [dipropylene glycol dibenzoate (DGD) and glyceryl triacetate (GTA)] and the endocrine-disrupting effects were investigated during the early stages (8~48 hpf). For five endogenous hormones, including progesterone, testosterone, 17β-estradiol, triiodothyronine (T_3) and cortisol, the tested chemicals disturbed the contents of at least one hormone at environmentally relevant concentrations (≤3.9 μM), except DINCH and GTA. Then, the concentration-dependent reduced zebrafish transcriptome analysis was performed. Thyroid hormone (TH)- and androgen/estrogen-regulated adverse outcome pathways (AOPs) were the two types of biological pathways most sensitive to PAE exposure. Notably, six compounds disrupted four TH-mediated AOPs, from the inhibition of deiodinases (molecular initiating event, MIE), a decrease in T_3 levels (key event, KE), to mortality (adverse outcome, AO) with the quantitatively linear relationships between MIE-KE ($|r|$=0.96, p=0.002), KE-AO ($|r|$=0.88, p=0.02), and MIE-AO ($|r|$=0.89, p=0.02). Multiple structural analyses showed that benzoic acid is the critical toxicogenic fragment. Our data will facilitate the screening and development of green alternatives.

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In Vitro to *In Vivo* Toxicity Extrapolation Approach for Next Generation Risk Assessment

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Abstract

To reduce the reliance on animals for toxicity testing of chemicals, governments and research organizations are trying to develop new technologies. One representative example was the Next Generation Risk Assessment Program. As the core of this program, *in vitro* to *in vivo* extrapolation (IVIVE) aims to mobilize a mechanism-based understanding of toxicology to translate bioactive chemical

concentrations obtained from *in vitro* assays to corresponding exposures likely to induce bioactivity *in vivo*. This conversion can be achieved via physiologically based toxicokinetic (PBTK) models and machine learning (ML) algorithms. The aim of this work was to gain a deeper understanding of IVIVE research trends, compile and summarize relevant literature, and propose future research directions. The PBTK- and ML-model-based IVIVE studies published in the past 5 years were comprehensively summarized. Compared to previous studies, PBTK-based IVIVE studies in recent years have focused more on the use of mechanistic *in vitro* data, validation of the PBTK model, and incorporation of new approaches such as toxicogenomics, while ML-based IVIVE studies have paid more attention to the incorporation of knowledge on adverse outcome pathways. To further promote the development of IVIVE, future research directions were proposed from the perspectives of "expanding the application scope of IVIVE" and "integrating new technologies in IVIVE". First, in terms of expanding the application scope of IVIVE, it was proposed to (1) focus on toxicity IVIVE studies of metabolites, (2) develop quantitative ML-based IVIVE models, and (3) explore ecological effects extrapolation. Second, in terms of integrating new technologies in IVIVE, the combinations of systems biology, multi-omics, and adverse outcome networks with IVIVE were proposed to enable more comprehensive toxicity prediction. This work highlights the important value of IVIVE in next-generation risk assessment, with the goal of providing confidence for its use in chemical prioritization, hazard assessment, and regulatory decision making.

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PBScreen: A Server for the High-Throughput Screening of Placental Barrier–Permeable Contaminants Based on Multifusion Deep Learning

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Abstract

Introduction

Contaminants capable of crossing a placental barrier (PB) adversely affect female reproduction and fetal development[1]. A high-throughput screening tool is urgently required for the rapid screening of PBpermeable chemicals[2]. We built a high-throughput screening tool to identify PB-permeable chemicals using deep learning. The model was further implemented in a web server (http://www.datascihub.net/service/pbscreen) to provide a highly efficient screening service.

Structural alerts analysis show the hydrophobic moieties and halogen functional groups might be primarily responsible for the enhanced PB permeability, whereas the hydrophilic regions contributed negatively.

Discovery of PB-Permeable Substances and Development of Web Server

The performance of the multifusion model was further validated using ten compounds by in vitro monolayer transport model. The model accurately predicted 90% of experimentally verified substances without false negative results.

Acknowledgement

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Environmental tipping points for global soil carbon fixation microorganisms

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Abstract

Carbon fixation microorganisms (CFMs) are important components of the soil carbon cycle. However, the global distribution of CFMs and whether they will exceed the environmental tipping points remain unclear. According to the machine learning models, total carbon content, nitrogen fertilizer, and precipitation play dominant roles in CFM abundance. Obvious stimulation and inhibition effects on CFM abundance only happened at low levels of total carbon and precipitation, where the tipping points were 6.1 g$kg1and 22.38 mm, respectively. The abundance of CFMs in response to nitrogen fertilizer changed from positive to negative (tipping point at 9.45 kg ha1$y1). Approximately 46% of CFM abundance decline happened in cropland at 2100. Our work presents the distribution of carbon-fixing microorganisms on a global scale and then points out the sensitive areas with significant abundance changes. The previously described information will provide references for future soil quality prediction and policy decision-making.

3. Applications of Stable Isotopes in Environmental Studies

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Characterization of Sulfamethoxazole Direct Phototransformation through Multi-Element Compound-Specific Isotope Analysis

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Abstract

The direct phototransformation of sulfamethoxazole (SMX) represents a significant dissipation process in wetlands. However, distinguishing phototransformation from concurrent processes such as microbial and plant transformation in these environments presents a challenge. Therefore, our objective was to employ novel isotope concepts to characterize and differenciate the specific mechanisms involved in phototransformation processes. The GC-IRMS method developed for SMX includes carbon, hydrogen, and nitrogen isotope analysis, while the GC-MC-ICP-MS method specifically caters to sulfur isotope analysis. SMX exhibits varying protonation states at different pH levels, significantly affecting its transformation kinetics. We conducted direct phototransformation of SMX in simulated sunlight (>280nm) at pH 3 and pH 7. Transformation was faster at pH 3 than at pH 7. We observed normal carbon and sulfur isotope fractionation, yielding carbon isotope fractionation values (ε_C) of -2.0 ± 0.2 at pH 7 and -2.8 ± 0.4 at pH 3. The sulfur isotope fractionations (ε^{34}_S) were -3.8 ± 0.5 at pH 7 and -6.4 ± 1.2 at pH 3, while ε^{33}_S values were -6.3 ± 0.5 at pH 7 and -7.2 ± 1.3 at pH 3. In contrast, an inverse nitrogen isotope fractionation was observed, with ε_N = 3.0 ± 0.2 at pH 7 and 3.6 ± 0.1 at pH 3. Moreover, a mass independent fractionation was obersved for ^{33}S. These results support the idea of an involvement of carbon, nitrogen, and sulfur in the bond cleavage during the rate-limiting step. However, insignificant changes in the hydrogen isotopic compositions of SMX during transformation suggest that either hydrogen was not significantly involved in the bond cleavage or the transformation realted to the hydrogen bond cleavage played a minor role in the overall transformation process. At pH 7, the dominant transformation products were sulfonilic acid, 3-amino-5-methylisoxazole (3A5MI) from N-S bond cleavage, 5-methylisoxazol-3-yl)sulfamate from C-S bond cleavage, and sulfanilamide from C-N bond cleavage, which aligned with the observed isotope fractionation data. Conversely, at pH 3, different dominant transformation products, including sulfonilic acid, 3A5MI and SMX isomerization, suggest that transformation pathways differed from those observed at pH 7. Altogether, the specific isotope fractionation signatures derived from multi-element CSIA for direct phototransformation of SMX represent a unique reference enabling future comparisons with other transformation pathways.

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Pesticide degradation in an integrated constructed wetland: Insights from compound-specific isotope analysis and 16S rDNA sequencing

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Abstract

Carbon isotope analysis and the 16S rDNA sequencing were adopted to investigate the degradation process of chlorpyrifos during its transport in the integrated constructed wetland (ICW). Firstly, the extent of concentration decrease of chlorpyrifos was examined, and the removal efficiency in the first 36 h was found to be the highest. The removal rate reached 96.83 % after 96 h, and this process fit to the first-order kinetic model, with a kinetic constant (k) of 0.066 h^{-1}. A significant carbon isotope fractionation was observed, with a change of the $\delta^{13}C$ values from −26.54 ± 0.07 ‰ to −25.41 ± 0.08 ‰. The average chlorpyrifos biodegradation proportion reached 71.23 % (60.42 %–85.04 %), and it was predicted that about 11.79 %–36.41 % of chlorpyrifos removal in the ICW was attributed to abiotic factors. The outlet of the subsurface flow constructed wetland saw the highest D^*/B^* value(1.38–3.88), indicating that the remaining fraction of dilution was much more significant than that of degradation in this period. The top 20 phyla of microbial community were identified in the ICW. Proteobacteria was the most dominant phylum, accounting for > 40% of the bacterial communities in all sampling locations. Acidobacteria and Bacteroidetes were the second and third dominant phyla. At the genus level, the microbial community composition differed more greatly in every stage of the ICW, and the spatial distribution difference was quite significant in the ICW. This study is important to figure out the migration and transformation of chlorpyrifos when the ICW was adopted as a removal tool for organic micro-pollutants, and more similar studies could be carried out in the future to promote the evaluation of pollutant removal capacity of the ICWs, and to further develop the application of stable isotope analysis of compounds in the natural environment.

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The challenges of CSIA application in emerging contaminants research

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Abstract

Emerging contaminants (ECs) are the substances that have appeared newly or whose presence was identified earlier but the hazards were not known. Fundamental examples of ECs are Pharmaceuticals and personal care products (PPCPs), flame retardants, plasticisers, perfluorinated compounds, nanoparticles, pesticides, etc. With low concentrations and complex structure, the risk assessment of ECs is the challenges around the world. Compound-specific isotope analysis (CSIA) is not only able to show that contaminant transformation occurs, but also points to how these processes happen(ed). In this study we will explore the challenges in CSIA study for the emerging pollutants such as perfluorinated compounds (PFCs) and polybrominated diphenyl ethers (PBDEs). The chemical properties of compounds such as PFCs and PBDEs suggest that microbial degradation or chemical transformation processes in natural environments may lead to significant differences in isotopic fractionation. Furthermore, the influence of physical processes such as diffusion and transport of contaminants, as well as the complexity of the environment and the limitations of the research methodology, may introduce additional environmental variables and uncertainties for isotope analyses under field conditions. The research indicate that the application of CSIA in the study of emerging contaminants requires a comprehensive consideration of the

effects of sample handling, analytical techniques, microbial mechanisms of action, and environmental factors to ensure the accuracy and reliability of the study.

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Stable Carbon Fractionation of Volatile PFAS Caused by Soil-air partitioning

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Abstract

laboratory experiments were conducted to evaluate isotope Carbon fractionation caused by soil-air transfer process for a selection of Volatile PFAS. A selection of 6:2 Fluorotelomer Alcohol (6:2FTOH), 8:2 Fluorotelomer Alcohol (8:2FTOH), 10:2 Fluorotelomer Alcohol (10:2FTOH), N-Methyl perfluorooctane sulfonamide (MeFOSA), N-ethyl perfluorooctane sulfonamide (EtFOSA), N-Methyl perfluorooctane sulfonamidoethanol (MeFOSE) and N-Ethyl perfluorooctane sulfonamide (EtFOSE) were evaluated to determine isotope enrichment factor related to respective phase transfer process. We validated compound-specific isotope analysis (CSIA) methods for $\delta^{13}C$ of seven selected volatile PFAS and developed a solid-phase extraction (SPE) method to minimize matrix interferences during preconcentration of soil and air (Amberlite XAD-2) samples. The SPE recovery ranged from 80% to 115% and the SPE-CSIA procedure showed negligible isotope fractionation for $\delta^{13}C$ ($\leq$0.5‰). For carbon, the magnitude of isotope fractionation is small, but was consistently reproduced over the soil-air partitioning simulation experiments. The results of this study contribute to expand the list of emerging contaminants that can be assessed by the CSIA method deployed in the frame of mass-transfer studies to accurately assess the fate and contaminant transport.

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Elucidating the Photodegradation Mechanism of Ametryn Using Compound-Specific Stable Isotope Analysis (CSIA)

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Abstract

Ametryn, a triazine herbicide, is valued for its broad-spectrum control, cost-effectiveness, and adaptable application timing. Despite these advantages, its chemical stability, toxicity, and environmental persistence raise concerns due to its frequent detection in aquatic ecosystems, threatening both biodiversity and human well-being. This study leverages Compound-Specific Stable Isotope Analysis (CSIA) to dissect the photodegradation dynamics of Ametryn, examining key factors and pathways that influence its degradation kinetics and isotopic signatures. Our objective is to enhance existing methodologies and furnish a solid evidential basis for future pesticide photodegradation studies via CSIA. Key findings include:

1. The photodegradation of Ametryn in pure water, influenced significantly by initial concentration and pH, shows a negative correlation between concentration and degradation rate, with pH variations substantially affecting the process.
2. The role of photosensitizers—NO_3^-, CO_3^{2-}, and DOM—was scrutinized across different Ametryn concentrations. At lower concentrations, NO_3^- enhances degradation, while at higher levels, it inhibits it. The impact of CO_3^{2-} and DOM on degradation is dependent on their concentrations, with an optimal degradation concentration identified under constant NO3- levels.
3. CSIA revealed distinct isotopic fractionation patterns during Ametryn's direct photodegradation, with carbon and nitrogen isotope enrichment factors varying with pH. Neutral conditions led to isotopic depletion, contrasting with the normal enrichment observed under neutral to alkaline conditions.
4. Indirect photodegradation studies via CSIA indicated nitrogen isotope reverse fractionation under direct exposure, with minimal effects in indirect scenarios. Notable variations in isotope enrichment factors across different pathways suggest isotopic fractionation as a distinguishing feature.

The study confirms that Ametryn photodegradation follows first-order kinetics, with factor influences on degradation rates hinging on experimental system compositions. The isotopic signatures, combined with degradation pathways, facilitate the elucidation of photodegradation mechanisms.

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Sources Identification of Polycyclic Aromatic Hydrocarbons in Pohang New Harbor Sediments Based on Compound-Specific Carbon and Hydrogen Isotope Analysis

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Abstract

Polycyclic aromatic hydrocarbons (PAHs) are widespread ecological hazards in the environment. Generated primarily by anthropogenic activities, identifying sources of PAHs is crucial. This study aimed to evaluate the distribution characteristics and potential pollution sources of PAHs in the surface sediments of Pohang New Harbor. Sediment samples from Pohang New Harbor (n = 26) and potential pollution sources (n = 9) were collected in April–May 2022, and a total of 28 PAHs were analyzed using

GC/MSD. The carbon and hydrogen stable isotope ratios of individual PAH compounds were analyzed using GC/IRMS after thin-layer chromatography purification. Significant carbon and hydrogen stable isotope ratios were obtained for 6 PAHs (Phe, Fl, Py, BaA, Chr, and BbF). The source identification of PAHs was conducted using diagnostic ratios, modeling based on concentrations and compositions, and dual compound-specific isotopes ($\delta^{13}C_{PAHs}$ and $\delta^{2}H_{PAHs}$). In the study area, PAHs ranged from 470 to 54,000 ng g^{-1} dw in source areas, while harbor sediments ranged from 390 to 8,200 ng g^{-1} dw, with some points exceeding the Canadian sediment guidelines (4,000 ng g^{-1} dw). Diagnostic ratio and PMF model results indicated that the PAHs in Pohang New Harbor originated from mixed sources of fossil fuel combustion and petroleum sources. The dual-CSIA results showed that $\delta^{13}C_{PAHs}$ ranged from –25.8 to –21.5‰ (mean: –23.1‰) and $\delta^{2}H_{PAHs}$ ranged from –143.6 to –67.6‰, with a mean of –122.8‰. Compared to previous studies, dual-CSIA results indicated a mixed origin of coal and petroleum combustion. Using carbon and hydrogen stable isotope ratios to identify pollution sources, the inner area of Pohang New Harbor was identified as originating from petroleum combustion and spills, while the outer area was identified as originating from coal combustion. The distinct $\delta^{13}C_{PAHs}$ and $\delta^{2}H_{PAHs}$ values for each pollution source demonstrated that dual-CSIA could effectively identify PAH pollution sources.

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Seasonal Variations in the Sources of Particulate Organic Matter in the Estuarine Systems of the Han River, Nakdong River, and Yeongsan River: An Approach Using GDGTs and *n*-alkanes

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Abstract

Estuaries serving as interfaces between rivers and the ocean play a crucial role in the carbon cycles. The characteristics of organic matter (OM) in estuarine systems and their seasonal variations significantly impact coastal ecosystems and related carbon cycle. This study investigates the seasonal differences in the characteristics of particulate organic matter (POM) in the Han River (HR), Nakdong River (NDR), and Yeongsan River (YSR). POM samples were collected from three estuarine systems in the summer and winter of 2022 and 2023 with salinity changes, and analyzed for their carbon concentrations, stable isotope ratios, and lipid biomarkers (glycerol dialkyl glycerol tetraether lipids (GDGTs), *n*-alkanes). The results indicate that the carbon stable isotope ratios in winter (HR: -29.06±3.35 ‰, NDR: -28.2±4.35 ‰, YSR: -27.16±2.9 ‰) were lower than in summer (HR: -28.22±2.78 ‰, NDR: -26.45±4.23 ‰, YSR: -22.78±2.29 ‰). Additionally, the terrestrial aquatic ratio (TAR) index, calculated using *n*-alkanes, was higher in winter (HR: 15.35±10.04, NDR: 9.69±5.05, YSR: 9.22±4.49) than in summer (HR: 6.23±5.23, NDR: 1.46±2.56, YSR: 2.19±2.35). These two results suggest that the influence of terrestrial organic carbon is higher in winter than in summer. However, the branched isoprenoid tetraether (BIT) index, calculated using GDGTs, was higher in summer (HR: 0.71±0.27, NDR: 0.63±0.35, YSR: 0.54±0.36) than in winter (HR: 0.56±0.3, NDR: 0.49±0.32, YSR: 0.43±0.4), showing the influence of terrestrial organic carbon is higher in summer than in winter. This difference is attributed to the origin of the lipid biomarkers; terrestrial *n*-alkanes mainly originate from higher terrestrial vegetation, whereas terrestrial GDGTs are predominantly derived from soil archaea. In summer, rainfall-induced erosion contributes to the higher BIT index, while the elevated TAR index is likely due to wind influence and the increased seasonal input of OM from terrestrial higher vegetation (e.g., dead leaves) in

winter. In this study, carbon stable isotope ratios and lipid biomarkers were used to identify the sources of POM. This study suggests that employing various biomarkers can provide valuable insights into the sources of OM and its seasonal dynamics. In addition, the results of 14-carbon measurements are further interpreted in comparison to those of stable carbon isotope as well as lipids biomarkers.

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The Application of Compound-Specific Stable Isotope Analysis in the Study of Environmental Transformation of Halogenated Organic Pollutants

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Abstract

Halogenated organic pollutants (HOPs) are widely present in natural environments such as organisms, sediments, and the atmosphere. Environmental transformation processes are important ways for pollutants to be reduced in the environment. However, there are many challenges in tracing the environmental transformation processes and mechanisms of HOPs, such as complex transformation processes and the lack of reliable analytical techniques. Therefore, this study pioneers the use of compound-specific multi-element (C-/Cl-/Br-) stable isotope analysis to explore the environmental transformation processes and mechanisms of typical HOPs, providing a basis for scientifically evaluating the environmental transformation processes of HOPs in real environments.

The study developed methods for purifying and separating target compounds in large samples, overcoming technical bottlenecks in CSIA analysis of typical HOPs like polychlorinated biphenyls (PCBs) and polybrominated diphenyl ethers (PBDEs). It established Compound-Specific carbon stable isotope analysis (C-CSIA) methods for PCBs and PBDEs in environmental samples and organisms, as well as GC-qMS-based Cl-/Br-CSIA methods for these compounds. Using C-/Cl-/Br-CSIA technology, it was discovered that after photoexcitation, C-Cl/Br bonds of PCBs and PBDEs broke, with PCBs showing masking effects and site-specific dechlorination during C-Cl bond breakage. Multiple evidence from CSIA helped reconstruct the emission history of HOPs at polluted sites. Indoor simulations of anaerobic degradation revealed that PCBs degrade via meta-dechlorination and PBDEs via para-debromination, but C-Cl/Br isotope fractionation phenomena differed from field study results, likely influenced by habitat and microbial community structure. In human liver microsome systems, PCBs metabolized into hydroxylated products, with molecular docking indicating that PCB exposure can lead to abnormal enzyme expression and endocrine disorders. During PCB136 metabolism, isotopic fractionation initially enriched then depleted, suggesting a shift in enzyme-catalyzed metabolism mechanisms. The AKIE (1.043-1.061) of PCBs during in vitro metabolism significantly differed from the AKIE (1.006-1.038) during photodegradation and microbial degradation, highlighting the potential of ME-CSIA in studying biological and abiotic transformation mechanisms of PCBs and PBDEs.

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Assessing Fatty Acid and Sterol Biomarkers as Tracers for Identifying Organic Matter Pollution Sources in the Sediments of Southeast Ports of Korean Peninsula, South Korea

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Abstract

Ganggu Port and Masan Bay are significant southeast maritime hubs in South Korea, face organic matter pollution from industrial and urban runoff, threatening marine ecosystems and requiring effective monitoring and management strategies. The lack of specificity and ambiguity in understanding pollution processes obscures the environmental pollution footprint in marine research. However, the application of specific lipid biomarkers and compound-specific isotope analysis (CSIA) offers significant insights on the sources of organic matter pollution. Sediment samples were collected from 14 stations in Ganggu Port and 8 source locations: urban dust, water pipeline, tributaries, agriculture, port, fishery (market), and forest soil. In Masan Bay, samples were collected from 24 stations and 4 source locations. Sediments were analysed using lipid biomarker techniques, CSIA and bulk organic carbon analysis. A Bayesian mixing model (MixSIAR) used to estimate the relative contribution of sources to sediment samples. Total organic carbon (TOC) in Ganggu port sediments showed that certain stations had significantly high values: station 4 (15.36 µg/mg), station 5 (19.48 µg/mg), station 6 (26.51 µg/mg) and station 13 (12.09 µg/mg), which rendering them as potential reservoirs of organic matter and highlights them as prime targets for the pollution source investigation. Mixing model source discrimination suggested that the highest relative contributions of the sources to the sediments of Ganggu port were: 40% from tributary 1, 25% from tributary 2, 17% from port, 11% from agriculture, and the lowest contributions were: 3% from forest soil, 2% from fishery, 0.9% from the water pipeline, and 0.2% from urban dust. TOC results from Masan Bay ranged from 1.0 to 3.9 µg/mg. Terrestrial source fatty acids contributed significantly to the total fatty acids (from 20% to 50%). Coprostanol concentrations were notably high in most stations, particularly at the stations 1 (0.816 µg/g) and 5 (0.670 µg/g), which are the closest to urban and industrial areas, sterol ratios also confirmed a significant anthropogenic pollution. Pearson correlation showed a strong correlation between TOC and terrestrial source fatty acids ($p<0.01$), suggesting a substantial contribution of terrestrial organic matter. This study confirms that the application of multiple lipid biomarkers and compound-specific isotope signatures can effectively trace and identify different sources of organic matter in coastal sediments.

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Different response of microalgae Phaeodactylum tricornutum upon exposures to crude oil water-accommodated fraction (WAF) and chemically enhanced WAF: A case study coupled with stable isotopic signatures

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Abstract

Increasing use of chemical dispersants for oil spills highlights the need to understand their adverse effects on marine microalgae and nutrient assimilation because the toxic components of crude oil can be more bioavailable. We employed the crude oil water-accommodated fraction (WAF) and chemically enhanced WAF (CEWAF) to compare different responses in marine microalgae (*Phaeodactylum tricornutum*) coupled with stable isotopic signatures. The concentration and proportion of high-molecular-weight polycyclic aromatic hydrocarbons (HMW PAHs), which are key toxic components in crude oil, increased after dispersant addition. CEWAF exposure caused higher percent growth inhibition and a lower chlorophyll-a level of microalgae than those after WAF exposure. Compared with WAF exposure, CEWAF led to an enhancement in the self-defense mechanism of *P. tricornutum*, accompanied by an increased content of extracellular polymeric substances. ^{13}C-depletion and carbon assimilation were altered in *P. tricornutum*, suggesting more HMW PAHs could be utilized as carbon sources by microalgae under CEWAF. CEWAF had no significant effects on the isotopic fractionation or assimilation of nitrogen in *P. tricornutum*. Our study unveiled the impact on the growth, physiological response, and nutrient assimilation of microalgae upon WAF and CEWAF exposures. Our data provide new insights into the ecological effects of dispersant applications for coastal oil spills.

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Recent applications of compound-specific isotope analysis (CSIA) in environmental forensic and pollutant bio-magnification studies

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Abstract

Many countries have guidelines for assessing and managing pesticide pollution, for farming in diverse environments, as crops and cultivating soils are exposed unintendedly to the pesticides. However, the unintended pollution of pesticide in soil, crops, and adjacent environments has caused several issues for both pesticide users and consumers. The stable isotope approach has been a useful technique to find the source of organic matter in diverse field related to aquatic ecology and environmental sciences. In this presentation, we discuss commonly used analytical methods using compound-specific isotope analysis (CSIA) for tracing organic pollutants and understanding chemical reactions (mechanisms) in real environments. It shows great applicability for the issues on unintended pesticide pollution in several environments. We also show the preliminary study on how stable isotope values may vary in pesticide depending on manufacturers and degradation process. In addition even though many investigations have been carried out to elaborate trophic magnification factor (TMF) and biomagnification factor (BMF), such as normalizing the concentration of pollutants and averaging diet sources, the uncertainty of the indexes still need to be improved to assess the bioaccumulation of pollutants. This study introduces an improved BMF (i.e., BMF′) applied to mercury bioaccumulation in freshwater fish from four sites before and after rainfall. The diet source and TP of each fish were identified using nitrogen stable isotope of amino acids (δ15NAAs) combined with bulk carbon stable isotope (δ13C). The BMF′ was calculated normalizing with TP and diet contributions derived from MixSIAR. The BMF′ values (1.3–27.2 and 1.2–27.8), which are representative of the entire food web, were generally higher than TMF (1.5–13.9 and 1.5–14.5) for both total mercury and methyl mercury, respectively. The BMF′ implying actual mercury transfer pathway is more reliable index than relatively underestimated TMF for risk assessment. The ecological approach for BMF calculations provides novel insight into the behavior and trophic transfer of pollutants like mercury.

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Carbon and hydrogen isotopic evidence for atrazine degradation byelectro-activated persulfate: Radical contributions and comparisons withheat-activated persulfate

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Abstract

The activation ways of persulfate (PS) were dominate for pollutant degradation and energy consumption. This research compared electro-activated PS and heat-activated PS from the perspective of isotope fractionation, in order to “fingerprinted” and precisely interpretate reaction contributions and degradation

pathways. As results, PS can be electrochemically activated with atrazine (ATZ) removal rates of 84.8% and 88.8% at pH 4 and 7. The two-dimensional isotope plots ($\Lambda_{C/H}$) values were 6.20 at pH 4 and 7.46 at pH 7, rather different from that of $SO_4^{\cdot-}$ -dominated process with $\Lambda_{C/H}$ value of -4.80 at pH 4 and -23.0 at pH 7, suggesting the weak contribution of $SO_4^{\cdot-}$. ATZ degradation by electro-activated PS was controlled by direct electron transfer (DET) and ·OH radical, and $\cdot OH_{PS}$ (derived from PS activation) played the crucial role with contributing rate of 63.2%~69.1%, while DET and $\cdot OH_{BDD}$ (derived from electrolysis of H_2O) contributed to 4.5~7.9% and 23.0%~30.8%, respectively. This was different from heat activation of PS, of which the latter was dominated by $SO_4^{\cdot-}$ with contributions of 83.9%~100%. The discrepant dominating reactive oxygen species should be responsible for their different degradation capabilities and pathways. This research provided isotopic interpretations for differences of PS activation mode, and further efforts can be made to realize the selective degradation by enhancing the specific reaction process.

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Atmospheric Inorganic Reactive Nitrogen Deposition Pattern in the South China Sea Changed by the Chinese Government Controlling NOx Emissions: Evidence from Field Cruise Observation

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Abstract

Oceanic nitrogen deposition has attracted much attention because it could affect marine primary productivity and even cause eutrophication. A previous modeling study indicated that the global oceanic nitrogen deposition pattern changed greatly from 1970 to 2018, i.e., ammonia-related nitrogen (NHx) deposition increased and exceeded oxidized nitrogen (NOx) deposition in a few coastal regions, including the China Sea. However, there have been no field observation studies in recent years to check this result. Here, we carried out three field cruises in the South China Sea (SCS), the largest China marginal sea, in 2021 to study the latest atmospheric nitrogen deposition pattern and their sources changes by using isotopes of nitrate ($\delta^{15}N\text{-}NO_3^-$) and ammonia ($\delta^{15}N\text{-}NH_4^+$) linked mixing model. The results demonstrate that the $N\text{-}NH_4^+$ deposition generally exceeded $N\text{-}NO_3^-$ deposition because the NOx emission from the coal combustion decreased and NHx emission from agriculture sources increased. The deposition differences between $N\text{-}NH_4^+$ and $N\text{-}NO_3^-$ increased from the coast to offshore, i.e., $N\text{-}NH_4^+$ becomes the main contributor to oceanic nitrogen deposition, especially in the offshore background region. Source apportionment results showed that agricultural sources' contribution to $N\text{-}NH_4^+$ has increased and become the main contributor, especially in the offshore background area (fertilizer 52% and livestock 17%). Although coal combustion's contribution to marine atmospheric $N\text{-}NO_3^-$ is still the largest, it has reduced to 22% (Northern Coast)–35% (background area) due to the Chinese Government effectively controlling NOx emissions. Along with the decrease in coal combustion's contribution, vessel and marine biogenic emissions would play a more and more critical role.

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Insights into Tissue-Specific Bioaccumulation of Nanoplastics in Marine Medaka as Revealed by a Stable Carbon Isotopic Approach

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Abstract

Despite the high bioavailability and potentially extensive presence of nanoplastics in aquatic environments, the biological fate of nanoplastics is largely unknown because of analytical limitations in detection and quantification. Fluorescently labeled nanoplastics are widely used to detect bioaccumulation, but this method is prone to false-positive results due to the leaching of fluorescent dyes. Here we propose a novel stable carbon isotopic approach to detect and quantify nano- and microplastics in a complex organic matrix. Because carbon is the major component of plastics (>87% in polystyrene), it is possible to investigate tissue-specific bioaccumulation of nano- and microplastics in the medaka *Oryzias melastigma* by quantifying the contribution of plastic particles as an end-member in the composition of stable carbon isotopes in different tissues. In addition to the digestive organs (e.g., the gut and intestines) that are constantly exposed to the water column via ingestion, nanoplastics were shown to selectively bioaccumulate in the gills and ovary, implying a unique mode of action of bioaccumulation based on the physicochemical properties of the nanoparticles. These findings should improve our understanding of the tissue-specific bioaccumulation of nano- and microplastics in aquatic organisms.

KEYWORDS:Nanoplastic, Microplastic, Fish, Carbon isotope, Bioaccumulation, Isotope ratio mass spectrometry

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Application of stable isotopes in characterization of microbial degradation of brominated flame retardants

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Abstract

PBDEs in anaerobic environment, whereas the underlying reaction mechanisms remain elusive. Dual-element stable isotope analysis was recently recognized to distinguish different reaction mechanism for degradation of organic pollutants. In this study, the dual carbon-bromine isotope effects associated with the anaerobic microbial degradation were first investigated to characterize the reaction mechanisms for BDE-47 and BDE-153. Presence of lower brominated congeners indicated stepwise debromination as the main degradation pathway, with the preferential removal of bromine in para position > meta/ortho position. The pronounced isotope fractionation was observed for both carbon and bromine, with similar carbon (ε_C) and bromine isotope enrichment factor (ε_{Br}) between BDE-47 (ε_C = -5.98‰, ε_{Br} = -2.44‰) and BDE-153 (ε_C = -5.57‰, ε_{Br} = -2.06‰) during the microbial degradation. Compared to ε_C and ε_{Br}, the correlation of carbon and isotope effects ($\Lambda_{C/Br} = \Delta\delta^{81}Br/\Delta\delta^{13}C$) was almost the same between BDE-47 (0.436) and BDE-153 (0.435), indicating the similar reaction mechanism. The calculated carbon and bromine apparent kinetic isotope effects ($AKIE_C$ and $AKIE_{Br}$) were 1.0773 and 1.0098 for BDE-47 and 1.0716 and 1.0125 for BDE-153, within range reported for degradation of halogenated compounds following nucleophilic substitution. Combination analysis of degradation products, $\Lambda_{C/Br}$ and *AKIE*, all the results pointed to that the anaerobic reductive debromination of BDE-47 and BDE-153 followed the nucleophilic aromatic substitution, with the addition of cofactor to the benzene ring concomitant with dissociation of carbon-bromine bond via the inner-sphere electron transfer, and the cleavage of C-Br bond was the rate-determining step. This study contributed to the development of dual carbon-bromine isotope analysis as a robust approach to probe the fate of PBDEs in contaminated sites.

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Model-Based Interpretation of Triclosan's Photodegradation and Isotopic Effects

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Abstract

Photodegradation is a primary pathway to remove triclosan (TCS) in surfacewater. Laboratory experiments were conducted to simulate photodegradation of TCS under day-night shifts. Compound-specific carbon and chlorine isotope analysis were applied to identify different bond-cleavage pathways. Also, a numerical model was developed to simulate and describe temporal variations of concentration and stable isotopic signals of TCS. Notably, in presence of sulfate ions in aqueous solutions, different predominant bond-cleavage pathways were observed. To end, we proposed a realistic framework to investigate sunlight-induced natural attenuation of TCS in water, and providing mechanistic interpretation of TCS's bond-cleavage pathways.

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Advancements in Compound-Specific Isotope Analysis (CSIA): Enhancing Understanding and Management of Halogenated Contaminants in Environmental Systems

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Abstract

In environmental science, Compound-Specific Isotope Analysis (CSIA) techniques, particularly Chlorine and Bromine CSIA, have become indispensable for understanding the dynamics of halogenated compounds. Over the past two decades, continuous advancements in CSIA methodologies have significantly enhanced precision and applicability. These improvements have expanded the scope of CSIA, making it a vital tool for investigating organic contaminant behavior across diverse environmental matrices.

The integration of CSIA with complementary analytical techniques, such as molecular biology methodologies, has provided comprehensive insights into chlorine compounds' fate and transport processes in various environmental settings. Multi-element CSIA approaches have enabled researchers to discern degradation pathways within field settings, informing targeted environmental remediation strategies.

Furthermore, the synergistic integration of CSIA with Water Safety Plans (WSPs) has proven crucial for ensuring the safety and quality of drinking water supplies. Numerous case studies conducted on contaminated sites have demonstrated the efficacy of integrated isotope analysis, coupled with groundwater modeling and statistical methodologies, within the framework of WSPs. Stable isotope analyses, including ^{13}C-CSIA and ^{37}Cl-CSIA, have played a pivotal role in accurately identifying contaminant sources, delineating their spatial distribution, and evaluating natural attenuation processes. In summary, the amalgamation of CSIA techniques with the strategic frameworks of WSPs offers a holistic and robust approach to managing water resources within urban locales. By integrating isotope applications with hydrogeological investigations, comprehensive conceptual models essential for effective water resource management can be developed. These endeavors are essential for implementing proactive prevention and mitigation measures, ultimately safeguarding public health and environmental integrity.

This review synthesizes seminal findings from diverse research articles, furnishing a detailed exposition of cutting-edge techniques and applications of CSIA, with a particular emphasis on chlorine isotopes. Encompassing assessments of biodegradation pathways, contaminant tracing, and transformation elucidation in varied environmental matrices, this review serves as a foundational resource for advancing environmental contaminant characterization and management.

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Combining CSIA and Enantiomer Fractionation for Evaluation the Transformation of α-HCH: from Field to Lab

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Abstract

Technical hexachlorocyclohexane (HCH) mixtures and Lindane (γ-HCH) have been produced in Bitterfeld-Wolfen, Germany, for about 30 years until 1982. We studied the natural attenuation of HCH in these groundwater systems through a combination of enantiomeric and carbon isotope fractionation to characterize the degradation of α-HCH in the areas downstream of a former disposal and production site in Bitterfeld-Wolfen. The concentration and isotope composition of α-HCH from the Quaternary and Tertiary aquifers were analyzed. The carbon isotope compositions were compared to the source signal of waste deposits for the dumpsite and highly contaminated areas. The established model for interpreting isotope and enantiomer fractionation patterns showed potential for analyzing the degradation process at a field site with a complex history with respect to contamination and fluctuating geochemical conditions. In addition, in order to understand the correlation between isotope fractionation and enantiomer fractionation, experiments with different biomass were conducted. Constant enantiomer selectivity was observed in experiments employing (i) cell suspensions, (ii) crude extracts, or (iii) LinA1 and LinA2 enzymes of strain B90A for α-HCH degradation in enzyme activity assay buffer. The variability of enantioselectivity and the ε_c were discussed based on the effect of mass transport and degradation rates. Our study demonstrates that enantiomer and isotope fractionation of α-HCH are two independent processes and both are affected by underlying reactions of individual enzymes and mass transport to a different extent.

4. POPs Analysis and Regional Alerts

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Single-cell metabolomics uncovers the toxic mechanism of HFPO-DA exposure in embryonic stem cells

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Abstract

Abstract: Hexafluoropropylene oxide dimer acid (HFPO-DA) is widely used in surfactants, food packaging, and lubricants as a substitute for perfluorooctanoic acid (PFOA). It possesses strong chemical stability and can spread through air, water, soil, and the food chain. Many studies have shown that HFPO-DA exhibits various toxicities, such as hepatotoxicity and neurotoxicity, *etc*. However, there are still significant gaps in the toxicological information related to reproductive development, especially the molecular toxic mechanism and the safety assessment is not yet comprehensive. In this study, we established a single-cell metabolomics mass spectrometry analysis platform for investigating the toxicological mechanisms of HFPO-DA exposure on mouse embryonic stem cells (mESCs). Initially, cell viability experiments were conducted to explore the impact of 0-10 mmol/L HFPO-DA on the proliferation of mESCs. The results indicated that low concentrations of HFPO-DA had minimal toxicity on mESCs after 24 hours of exposure, while high concentrations significantly inhibited mESC proliferation. Furthermore, single-cell metabolomics analysis was used to study the effects of mESCs exposed to different concentrations of HFPO-DA for 24 h, comparing small molecule metabolites and lipid levels. The study found that exposure of mESCs to HFPO-DA affected levels of metabolites such as choline, cytidine, uridine, thymidine, guanine, and succinic acid, disrupting pathways including purine, pyrimidine, tricarboxylic acid cycle, and methylbutanoic acid metabolism. The single-cell metabolomics mass spectrometry analysis platform established in this study revealed the toxicological mechanisms of mESCs exposed to HFPO-DA at the molecular level, providing a unique research platform and new research ideas for environmental toxicology studies.

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The stable soil organic carbon pool controls the burden of persistent organic pollutants in background soils

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Abstract

Persistent organic pollutants (POPs) tend to accumulate in cold regions through processes known as 'cold condensation' and 'global distillation.' Soil organic matter serves as the primary reservoir for POPs following their deposition and subsequent repeated air-surface exchanges. This study investigates the influence of physicochemical properties and environmental factors on the accumulation of POPs in soils from the Qinghai-Tibet Plateau, as well as the Antarctic and Arctic regions. Our findings reveal a significant correlation between the soil burden of most POPs and stable mineral-associated organic matter (MAOM). By integrating the proportion of MAOM with physicochemical properties, we can elucidate much of the soil distribution characteristics of POPs. Estimating the background levels of POPs using a global soil database suggests that stable soil carbon pools are crucial determinants in the global distribution of POPs, counteracting the 'cold-trapping' effects. We propose that future multimedia

environmental models of POPs should incorporate the composition of soil carbon pools to better assess the risk of secondary POPs release from soils under changing climate conditions.

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Atmospheric pesticides in Bangladesh: source apportionment and health risk assessment

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Abstract

Context/Purpose: Organochlorine pesticides (OCPs), often known as persistent organic pollutants (POPs) due to their persistent nature, have hazardous effects on both people and the environment. Thus, the study aimed at detection and quantification of OCPs in Bangladesh using non-power-driven polyurethane foam passive air samplers (PUF-PASs).

Methods: A total of 24 pairs of PUF-PAS samplers were successfully deployed, including 8 urban, 5 industrial, 4 highway, 3 dumping, 1 sub-urban, and 3 rural sites for three seasons during December 2017 to September 2018. The PUF disks were spiked with ^{13}C labeled trans-chlordane as the recovery surrogate and extracted in a Soxhlet apparatus for 24 h with DCM and then GC-MS/MS (Agilent 7890A/7000A) with a CP-Sil 8 CB column (50 m×0.25 mm×0.12 μm) was employed for analysis.

Results: Mean air concentrations of $\sum_{27}$OCPs were ranging from 102 to 6051 pg/m^3 over the study area. Highest concentration of $\sum_{27}$OCPs (2.23 ng/m^3) was found at urban area, while lowest was found at rural area (3.57 ng/m^3). Seasonal distribution of $\sum_{27}$OCPs were higher in the monsoon (average: 0.75 ng/m^3) than those of the winter (0.73 ng/m^3) and pre-monsoon (0.64 ng/m^3) at most of the sites. Among the OCP congeners, p,p'-DDT, o,p'-DDT, p,p'-DDE, o,p'-DDE, p,p'-DDD and o,p'-DDD along DBP and DDMU were significantly contributed the total concentrations of OCPs in all the seasons. Concentrations of $\sum_6$DDT were within a range of 49- 97%, 78 - 98% and 18 - 97% in the winter, pre-monsoon and monsoon, respectively.

Discussion/Interpretation: High concentrations of $\sum_{27}$OCPs have been identified in areas with chemical pesticide storage warehouses. The non-scientific use of chemical pesticides in Bangladesh is also the main source of this POPs family in Bangladeshi environment.

Conclusion: According to spatial distribution of OCPs, air in industrial areas, metropolitan areas and solid waste disposal sites was found to be highly contaminated with OCPs.

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Antibiotic Distribution, Risk and Source Apportionment in Mountainous Rivers of Chongqing, China

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Abstract

Antibiotics as the widespread drug in human society, whose massive use could stimulate the evolution of antibiotic resistance, thereby threatening global health. The spatial and temporal distribution of antibiotics had been widely studied in various water bodies, however, those studies rare conducted in rivers among the regional scale, which limits the management efficient of antibiotic control. Therefore, this study conducted an investigation of the concentration, distribution, risk and source identification of 54 antibiotics in different environmental water bodies and polluted water bodies in Chongqing. The results showed that the concentrations of antibiotics detected in surface water, water sources, effluent of wastewater treatment plant sewage, hospital sewage, livestock sewage and aquaculture sewage were 0.13-290 ng/L, 0.13-151.23 ng/L, 2.17-590 ng/L, 6.58-2.16×105 ng/L, 4.5-7.4×105 ng/L and 4.41-7490 ng/L, respectively. In the water systems investigated, results showed that the order of total antibiotic concentrations was Laixi River > Changshou Lake > Longxi River > Fujiang River > Jialing River > Qiongjiang River > Yangtze River > Wujiang River > Qijiang River. The results of the risk quotient showed that ofloxacin and lincosamide showed high risk among the investigated water bodies. The positive matrix factorization model was used to identify the main sources of antibiotics in surface water and water sources, with aquaculture accounted for 30.7% of the former and hospital sewage represent 33.3% of the latter. This work can provide a valuable regional scale dataset of antibiotics in the mountainous rivers, which promise valued insights for controlling antibiotic contamination.

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Tissue Distribution of Emerging Per- And Polyfluoroalkyl Substances in Multi-Species Wild Fishes From Qiantang River, East China: Comparison of 6:2 CL-PFESA With PFOS

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Abstract

This study argued for the first time that 6:2 chlorinated polyfuorinated ether sulfonate (6:2 Cl-PFESA) and Perfluorooctanesulfonic acid (PFOS) might have different tissue distribution mechanisms in wild fishes. We investigated the distribution and sources of nine emerging and legacy per- and polyfluoroalkyl

substances (PFASs) in Qiantang River, and noticeably high mean concentrations of perfluorooctanoic acid (PFOA) (213 ng/L) and ammonium salt of hexafuoropropylene oxide dimer acid (HFPO-DA) (55 ng/L) were detected in water samples. Target PFAS were further measured in matched muscle, liver, bile, heart, and spleen of multi-species wild fishes collected from Qiantang River, PFOS was observed to be the predominant PFASs contaminant, and was particularly enriched in bile with significantly higher concentration compared to other tissues, which was similarly observed for perfluorobutane sulfonate (PFBS) and perfluorohexane sulfonate (PFHxS). 6:2 Cl-PFESA was the second predominant PFASs contaminant in tissues, and showed no significant enrichment in a particular tissue, but relatively high level in liver, similarly for PFOA, HFPO-DA, perfluorohexanoate (PFHxA) and perfluorobutanoate (PFBA). Concentrations were observed to be highly linear correlated between matched tissues for 6:2 Cl-PFESA, whereas exponential correlations were observed for PFOS, suggesting that they may have different tissue distribution mechanisms. Tissue: water concentration ratios were calculated to estimate bioaccumulation potentials of target compounds, 6:2 Cl-PFESA was observed to be even more bioaccumulative than PFOS in liver, spleen and heart of wild fishes, additionally, comparing to 6:2 Cl-PFESA, PFOS occurrence was observed to vary widely between tissues, but also individually within the tissue, especially in bile.

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Monitoring Concentration Fluctuation Scenarios of Trace Organic Pollutants in Water by Passive Sampling

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Abstract

Considerable pollutant loads can enter surface waters during rain events or effluent discharge, therefore, fluctuating concentrations of trace organic pollutants in water (such as persistent organic pollutants), present a substantial challenge in obtaining representative samples for monitoring and risk assessment. Passive sampling techniques are gaining popularity with low detection limits and time-integrated sampling. However, time-weighted average concentrations from passive samplers in fluctuating concentration scenarios may not reflect the true concentrations accurately. Therefore, evaluating passive sampling performance under variable conditions is essential.

Concentration fluctuation scenarios were modeled and experimentally validated based on three primary characteristics: fluctuation intensity, occurrence timing, and duration time, using two types of passive samplers in a flow-through calibration system, the triolein-embedded cellulose acetate membrane (TECAM, for hydrophobic pollutants) and the hydrophilic-lipophilic balance sorbent-embedded cellulose acetate membrane (HECAM, for polar pollutants), respectively. Sampling errors due to the various 27 concentration fluctuations are influenced by two main factors: release rate constant (k_e) of the pollutant and fluctuation dynamics., The sampling error approached zero as k_e decreased, and reliable sampler performance under fluctuating conditions could be obtained for pollutants with $t_{1/2} > 7$ days (the error

reduced to below 25%). The sampling error was correlated with fluctuation intensity and duration time. Start or mid-period fluctuations led to underestimation, while end-period fluctuations caused overestimation. Mid-period fluctuations resulted in the smallest errors, while end-period fluctuations had the most significant impact. Prolonged fluctuation duration correlated with increased error. Our study also innovatively utilized the characteristic of performance reference compounds (PRCs) to qualitatively characterize the various fluctuation scenarios. Across the tested 27 scenarios, time-weighted average concentrations calibrated by passive sampling with PRCs could effectively reflect concentration fluctuation trends in water and address the feasibility of practical sampling designs. This approach enables passive sampling to provide comprehensive exposure data of trace organic pollutants in water with simplified sampling frequency.

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Aged Organic Contaminants as stratigraphic marker in the Anthropocene: Evidence from Tibetan Lake sediments

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Abstract

Persistent organic pollutants (POPs) and polycyclic aromatic hydrocarbons (PAHs) serve as markers of agricultural and residential activities, but it remains unclear whether their sediment records in the Anthropocene are affected by aging-induced formation of bound residues. In this study, the concentration of rapid desorption, slow desorption, and bound residue fractions were determined for dichlorodiphenyltrichloroethane (DDTs) and PAHs in dated sediment cores from edge to central Tibet using multi-step sequential extraction method. The temporal variations of total DDTs (sum of three fractions) in sediments from southern and eastern Tibet reflected different DDT usage histories in India and mainland China. However, their simultaneous increase in sediment concentrations since the 1950s suggested widespread agricultural practices across Asia. Similarly, the stratigraphic records and estimated source contributions of PAHs in different areas of Tibet also exhibited a coherent change in the mid-20th century, corresponding to the Holocene-Anthropocene transition. Although the relative abundance of bound residue fraction could reach 70% of the total concentrations, the sedimentary DDTs and PAHs displayed a comparable pattern when the bound residue fraction was not accounted for, suggesting their effective retainability under natural aging conditions. This may be elucidated by the enduring forward and back conversions between slow desorption and bound residue fractions, which manifested similar time-dependent variations across organic contaminants. The distinct conversion tendencies of different congeners were predicted by the binding affinity of congeners to surface/inner regions of organic matter using molecular docking simulations. Our findings

demonstrate the persistence of sedimentary POPs and PAHs records under natural aging and validate their use as documentary evidence for investigating the Anthropocene.

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A high-throughput analysis workflow to characterize Pharmaceuticals and personal care products in aquatic environment

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Abstract

Pharmaceuticals and personal care products (PPCPs), emerging environmental contaminants due to their release from human and veterinary medicine, accumulate in urban wastewater treatment plants (WWTPs). These conventional WWTPs inadequately remove PPCPs, posing concerns in water reuse, especially in places like Singapore. With their potential to affect humans and ecosystems, monitoring and analyzing diverse PPCPs demand advanced analytical methods.

Current PPCP detection methods rely on targeted approaches involving complex purification and expensive chemical labeling. While these methods excel with known PPCPs, they fall short in identifying unknown ones. Non-Targeted Analysis (NTA) offers broader coverage but sacrifices sensitivity. Recently, chemical isotope labeling coupled with LC-MS has shown promise in enhancing sensitivity and identifying unknowns, offering a potential solution for PPCP analysis.

In our research, we established a robust method for profiling PPCPs (Pharmaceuticals and Personal Care Products) based on stable isotope derivatization. This innovative method offers significantly improved sensitivity and selectivity compared to existing techniques, effectively addressing common challenges in PPCPs profiling, such as low sensitivity, complex sample preparation, high isotope standard costs, and limited throughput.

To label PPCPs containing hydroxyl, amine, and carboxyl functional groups – which are commonly found in PPCPs – we utilized 12C/13C2-dansyl chloride and 12C/13C2-p-dimethylaminophenacyl bromide. This labeling, combined with streamlined analysis procedures, not only provides a cost-effective means of tagging PPCPs for accurate quantification but also dramatically enhances signal intensity, particularly in electrospray ionization. Furthermore, this approach facilitates the identification of untargeted PPCPs by selecting paired peaks with a predefined mass tolerance.

Additionally, we established an extensive PPCPs database encompassing MS and MS/MS information for over 1400 compounds, drawing from previous studies involving water samples. To streamline operations, we incorporated computational tools for automated database management. With this platform, we successfully profiled 26 PPCP candidates from a 1L recycled water sample.

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Source Identification and Marine Groundwater Discharge of Perfluoroalkyl Compounds in Typical Estuarine Bay in Fujian Province

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Abstract

Per- and polyfluoroalkyl substances (PFAS) are emerging persistent organic pollutants attracting significant international concern due to their persistence and potential ecological and health risks. Widely used in various industrial and consumer products, PFAS are prevalent in the environment. This study addresses the challenge of understanding PFAS pollution in Jiulong River-Xiamen Bay and Zhangjiang Estuary mangrove wetland in Fujian Province, focusing on pollution characteristics, sources, and submarine groundwater discharge.

We conducted a comprehensive analysis of PFAS contamination in surface water and groundwater in these regions. We employed principal component analysis and positive matrix factorization to identify pollution sources and utilized a three-end-member mixing model incorporating basic parameters and stable isotopes to quantify input contributions from river water, seawater, and groundwater.

Key findings include:

1. **PFAS Levels**: PFAS levels in Jiulong River-Xiamen Bay (surface water: 23.70±22.00 ng/L, groundwater: 64.12±53.92 ng/L) are significantly higher than in Zhangjiang Estuary (surface water: 6.58±5.50 ng/L, groundwater: 13.29±9.17 ng/L).
2. **Seasonal Variations**: Seasonal variations in PFAS concentrations differ between the two regions, with Jiulong River-Xiamen Bay showing higher levels in summer and Zhangjiang Estuary in winter.
3. **Pollution Sources**: In Jiulong River-Xiamen Bay, major sources include upstream industrial discharge (32.80%), wastewater treatment plant effluents (28.23%), and fire-fighting foam contamination (30.87%). In Zhangjiang Estuary, sources include residential and industrial wastewater (22.14%) and upstream wastewater treatment plants and petrochemical factories (77.86%).
4. **Submarine Groundwater Discharge**: Submarine groundwater discharge is a significant PFAS input pathway, accounting for 19.1% of PFAS input in Jiulong River-Xiamen Bay and 36% in Zhangjiang Estuary.

The findings underscore the importance of submarine groundwater discharge in PFAS pollution, particularly in Zhangjiang Estuary. This study provides a scientific basis for developing effective PFAS pollution control and management strategies in estuarine and bay ecosystems, advancing our understanding of PFAS environmental behavior in these critical habitats.

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Analysis of Persistent Toxic Substances in Fine Particulate Matter from Industrial Sources and Their Atmospheric Emissions

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Abstract

Industrial production activities serve as the cornerstone of human societal development. However, frequent industrial activities inevitably release fine particulate matter (PM) and the persistent toxic substances they absorb, which adversely affect human health. Due to the lack of comprehensive assessment of industrial emissions, the analysis and atmospheric emissions caused by large-scale industrial activities remains incomplete.

In this study, we comprehensively characterized and quantified the toxic organic pollutants and heavy metals in PM from 118 actual industrial production activities. Regarding the particle size distribution characteristics of industrial particles, we found that 97.9% of PM had a diameter less than 2.5 μm, with 79.0% having a diameter less than 1 μm. Emerging contaminants including hexachlorobutadiene, polyhalogenated carbazoles, and other persistent organic pollutants were identified by GC/MS. Their atmospheric emissions were quantified based on the derived emission factors. Concerning the distribution characteristics of various heavy metal concentrations, the major elements in particulate matter released by different industrial activities vary, exhibiting distinct distribution patterns. Compared to other industrial activities, metal smelting sources are significantly richer in various elements. Particulate matter (PM) generated during secondary metal smelting is a rich carrier of heavy metals such as zinc, lead, arsenic, and copper. Among these, zinc has the highest concentration. Additionally, we estimated the atmospheric emissions of Fe and heavy metals (including As, Cd, Cr, Cu, Ni, Pb, Zn) contained in fine particulate matter from global industrial activities using emission factor methods, which were 51,161 tons and 69,591 tons, respectively. These emissions pose potential health risks to residents. We also identified electric arc furnace steelmaking and iron ore sintering as the main sources of Fe and heavy metal emissions, while secondary non-ferrous metals also require attention, providing theoretical guidance for precise emission reduction. This study is of significant importance for the sustainable development of industry and the assessment of health risks associated with industrial emissions.

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Quantification of 2-chlorohydroquinone based on interaction between N-doped carbon quantum dots probe and photolysis products in fluorescence system

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Abstract

As a member of chlorophenolic compounds, 2-chlorohydroquinone (H_2QCl) has been widely used as intermediates in various chemical industries and leaded to serious threat on the environment. It is urgent to develop simple and robust analytical method for sensitive and selective determination of H_2QCl. Carbon quantum dots (CQDs), a promising photoluminescence nanomaterial, have gained sufficient concern as optical sensors owing to their outstanding photochemical properties. In this work, nitrogen doped carbon quantum dots (N-CQDs) were successfully synthesized by a simple secondary hydrothermal method and applied as a fluorescent probe for the quantitation of H_2QCl. A new fluorescence region centered at excitation wavelength of 310 nm and emission wavelength of 390 nm appeared after nitrogen doping. It was found that the N-CQDs exhibited a high selectivity towards H_2QCl with sensitive fluorescence response and the fluorescence quenching of N-CQDs was linear with the concentration of H_2QCl in the range of 30–90 μM ($Y = 0.0049X + 0.1255$, $R^2 = 0.996$). This is the first time that the dual role of excitation light was observed in the fluorescence detection system. The ultraviolet light acted as not only the excitation energy source for N-CQDs photoluminescence, but also the light source for photolysis of H_2QCl. In the detection process, H_2QCl was degraded to p-benzoquinone by light, and then the CQDs combined with p-benzoquinone through Michael addition reaction under the action of doped nitrogen. The electron transfer from N-CQDs to the linked p-benzoquinone caused the quenching of fluorescence originated from the edge state of N-CQDs. Furthermore, this established method can be applied for the quantitative determination of H_2QCl in environmental water samples with satisfactory recoveries between 94.31 and 105.51%.

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Size-Resolved Pollution Characteristics, Absorption Spectra and Gas-Particle Partitioning of Polycyclic Aromatic Hydrocarbons

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Abstract

As a typical kind of semi-volatile organic compounds, polycyclic aromatic hydrocarbons (PAHs) have the capability for solar radiation absorption related to climate forcing. The gas-particle partitioning can influence the environmental behaviors and health effects of PAHs. Herein, pollution characteristics and

absorption spectra of size-resolved PAHs in atmospheric particles, and the size-resolved gas-particle partitioning of PAHs in a cold megacity were comprehensively investigated. The mean concentrations of Σ_{18}PAHs in all the 11 particle size ranges were $3.95 \pm 4.77 \times 10^4$ pg/m^3 and $2.17 \pm 1.54 \times 10^3$ pg/m^3 in heating period (HP) and non-heating period (NHP), respectively. Except for most PAHs with 2 and 3 benzene rings in NHP, other PAHs showed a unimodal particle size distribution pattern with the peak at 0.56–1.0 μm in both periods. The particulate PAH-related climate forcing was mainly caused by the solar radiation absorptions at ~325 (~330) nm and ~365 nm. In general, the absorption intensities were higher in HP than NHP. The absorption intensity in the particle size range of 0.56–1.0 μm was the highest, and benzo[e]pyrene was the dominant contributor. In colder periods in HP, higher particulate PAH concentrations caused more intensive PAH-related climate forcing. The logarithm of size-resolved gas-particle partitioning quotient (log K_{Pi}) values of PAHs for fine particles were higher than those for coarse particles, indicating that particle sizes could have influence on log K_{Pi}. Three prediction equations of gas-particle partitioning quotient were compared in this study. Wherein, the empirical model based on the ambient temperature matched much better with the measured log K_{Pi}. A new prediction equation including particle sizes was established. For the log K_{Pi} related to most particle size ranges, the new equation showed better prediction performances than the three previous equations. In summary, this study provided new insights for pollution characteristics and absorption spectra of size-resolved PAHs in atmospheric particles, which will be useful for better understanding PAH-related climate forcing. In addition, the study established a new prediction equation of size-resolved gas-particle partitioning quotient, which also provided new insights for related fields in future.

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High Dichloromenthane Emissions from Ethanol Gasoline Vehicles with Chlorinated Paraffins in Lubricating Oil

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Abstract

An increase in CH_2Cl_2 emissions from industrial activities, a type of unregulated Very Short-Lived Substances, have offset some benefits of the Montreal Protocol. The discrepancy in CH_2Cl_2 emissions between the top-down and bottom-up estimates, indicating potential unidentified sources, especially considering the limited natural sources. We found that Ethanol gasoline vechiles (EGVs) with chlorinated paraffins (CPs) in lubricating oil emit CH_2Cl_2 at an average of 64.9±32.9 mg kg^{-1}, influenced by the emission standard, cumulative mileage and driving speed, with highest emissions under the China V emission standard reaching 114 mg kg^{-1}. Averagely, CH_2Cl_2 emissions from EGVs are 1-3 orders of magnitude higher than those from traditional gasoline vehicles. The substantial generation of CH_2Cl_2 is due to the high combustion efficiency of EGVs facilitating the decomposition of CPs in lubricating oil. Our results highlight EGVs as significant sources of CH_2Cl_2 emissions, they should not be overlooked.

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Assessment of Persistent Organic Pollutants in River Water and Their Health Risk: A Case Study of Shitalakshya River in Bangladesh

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Abstract

Water is the crucial substance to humans and the architect of life. Different hazardous substances such as industrial and agricultural chemicals, heavy metals, pesticides, cosmetics, and pharmaceuticals released into the environment and appearing as menacing things for human beings due to pollution of aquatic bodies like ponds, lake, canals, rivers, sea etc. The present study aims to assess the levels of peristent organic pollutants (POPs) present and their health risk assessment in the Shitalakshya River, surrounding the capital Dhaka city to understand the extent of environmental contamination and potential risks to human health and aquatic life. The method was validated in terms of calibration (0.10-5.00 μgL^{-1}), linearity (R^2 = 0.995-0.999), accuracy (recovery), precision (repeatability), specificity, selectivity, LODs and LOQs. Out of 60 samples, POPs found as alpha-BHC (0.01-0.19 μgL^{-1}) in 5, delta-BHC (0.01-0.27 μgL^{-1}) in 10, chlordane (0.01-0.23 μgL^{-1}) in 8, endosulfan (0.01-1.56 μgL^{-1}) in 16, 4,4$^{/}$-DDE (0.01-2.14 μgL^{-1}) in 11, dieldrin (0.03-0.58 μgL^{-1}) in 5, endrin (0.01-2.96 μgL^{-1}) in 12, 4,4$^{/}$-DDD (0.01-4.07 μgL^{-1}) in 30, endrin aldehyde (0.01-3.72 μgL^{-1}) in 22, 4,4$^{/}$-DDT (0.01-0.02 μgL^{-1}) in 3 and endosulfan sulfate (0.03-2.05 μgL^{-1}) in 5 samples. The quantified OCPs were below the standard guideline values set by WHO and EPA, except four organochlorine pesticides such as 4,4$^{/}$-DDE in W_6 (2.14 μgL^{-1}) in 1 sample, dieldrin in W_4 (0.10 μgL^{-1}), W_7 (0.12 μgL^{-1}), W_8 (0.45 μgL^{-1}), W_9 (0.58 μgL^{-1}) and W_{10} (0.03 μgL^{-1}) in 5 sample, endrin in W_{10} (2.96 μgL^{-1}) in 1 sample and 4,4$^{/}$-DDD in W_1 (1.63 μgL^{-1}), W_2 (0.69 μgL^{-1}), W_3 (1.95 μgL^{-1}), W_5 (1.05 μgL^{-1}), W_6 (0.57 μgL^{-1}), W_7 (1.02 μgL^{-1}), W_8 (2.51 μgL^{-1}) and W_9 (4.07 μgL^{-1}) in 8 sample during the late autumn/2022. The POPs were found mostly in late atumn, autumn and somewhat in summer and spring seasons in Bagladesh. The risk assessment studies in terms of cancer risk ($C_r<10^{-6}$), intake exposure level ($P<10^{-4}$), life average daily dose ($R<10^{-6}$), and hazard quotients ($H_q<1.0$) shows no significant negative impact of POPs detected in this study.

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Environmental Risk Analysis for Chemicals with Exposure Model of SWAT-KM: A Demonstrative Study with bis(2-ethylhexyl) phthalate in the Weihe River Basin

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Abstract

Hydrological process is one of the governing processes for chemical transport in an environmental system, contributing most of uncertainties thereof. The Soil and Water Assessment Tool (SWAT) is a renowned semidistributed hydrological model on watershed-scale. The model is capable of simulating a wide range of physical processes involving soil, water/vapour, vegetation, etc. at an explicitly high spatial and temporal resolution, and we have used the model to develop a novel model of chemical environmental exposures, SWAT-KM. By differentiating the dissolved species from the sorbed, and the vapor counterpart of a chemical, its intra- and intermedia transport are delineated along with various processes in SWAT-KM, which is enabled after integrating a simplified atmospheric module into, and overhauling the vegetation module of the SWAT model. Hence, the SWAT-KM model will concertedly simulate the fate of a chemical and present the series of its daily concentrations in the environmental multi-media system including soil, surface water and its sediment, atmosphere, vegetation and shallow aquifer for each subbasin of the watershed. This paper reports a demonstrative simulation of bis(2-ethylhexyl) phthalate (DEHP) by SWAT-KM for a big watershed in Weihe River Basin of China. The simulation results revealed the spatiotemporal differentiation and coordinated variation of the multi-media DEHP concentrations, and notified the strong association between these concentrations and meteorological and hydrological events. This demonstrative case study corroborates the competence of SWAT-KM to technically support environmental exposure assessment, and consequently to assist the risk assessment and risk mitigation for a targeted chemical.

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Monitoring and Capacity Building on POPs in Plastic Recycling in Low- & Middle-Income Countries – Science Contribution to the Stockholm Convention

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Abstract

The rapid growth of plastics production has exacerbated the triple planetary crisis of habitat loss, plastic pollution and greenhouse gas (GHG) emissions and crossed planetary boundaries. The challenges were recognized by the United Nations Environment Assembly, which initiated the development of a global plastic treaty. Plastics can contain a wide range of hazardous additives, including several POPs listed in the Stockholm Convention, such as hexabromocyclododecane (HBCDD), polybrominated diphenyl ethers (PBDEs), short-chain chlorinated paraffins (SCCP), Dechlorane Plus (DP), and UV-328, which although regulated, are present in stocks (e.g. electronics, vehicles, building materials, textiles) and require global management. While many studies have been published on POPs in major products, there is a lack of data

on POPs in plastic recyclates in low- and middle-income countries (LMICs). Therefore, activities were conducted from February to June 2023 with support from UNEP/GEF POPs global monitoring plan and the International Panel on Chemical Pollution (IPCP). The project had 3 major components (i) to develop a webinar series to strengthen capacities on POPs monitoring in plastics; (ii) to assess the state of knowledge and gaps on monitoring POPs in plastic in major use sectors, and (iii) to monitor selected POPs in plastic pellets and shreds of plastic recycled. Plastic pellets and shreds from recycled plastic have been collected in Asia, Africa, Latin America and the Caribbean region. Samples were sent to partnering laboratories of IPCP for analysis of selected POPs, including NIES (Tsukuba, Japan), Fraunhofer Institute (Freising, Germany), IDAEA-CSIC (Barcelona, Spain), and MTEC (Bangkok, Thailand). Selected recyclates used to produce food- or skin-contact products were screened by bioassays for genotoxicity, cell toxicity, or endocrine effects (Bio Detection Systems; The Netherlands). More than 300 recycled pellets and shreds samples used to produce new plastic products in LMICs of different polymers (e.g. PVC, ABS, HIPS, PS, EPS, XPS, HDPE, LDPE, PP, PA, PC, PET) were sampled with an initial assessment of plastic recycling in some countries. Samples were prescreened for bromine/chlorine content by XRF. Selected samples were analyzed for PBDEs, HBCD, SCCPs/MCCPs, PFASs, DP and UV-328. The capacity building Webinar on POPs in plastic was recorded and is online (https://www.ipcp.ch/activities/ipcp-webinar-series-pops-in-plastic-and-monitoring-approaches).

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National Inventory of Soil Contamination with Obsolete Organoclorine Pesticides in Kazakhstan in 2023-2024

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Abstract

Obsolete pesticides remain one of the major environmental and health problems in Kazakhstan. People come in contact with DDT and other organochlorine pesticides, contaminated soil, and empty pesticide containers. But the information about such exposures and locations of contaminated areas and remaining pesticides stocks was very scarce.

A national inventory of sites contaminated with obsolete pesticides was implemented in 2022-2023 as part of the project “Lifecycle Management of Pesticides and Disposal of POPs Pesticides in Central Asian countries and Türkiye,” implemented by FAO and funded by GEF. The study was done using the Rapid Environmental Assessment (REA) protocol. REA is a tool developed by FAO to prioritize pesticide contaminated sites for further intervention.

The project team visited 15 regions of Kazakhstan and managed to identify and conduct 159 assessments of pesticide contaminated sites according to REA protocol. The project team took topsoil samples at each site and recorded the coordinates for each sample. The samples were analyzed in the laboratory for the presence of suspected pollutants (persistent organochlorine pesticides). Based on the collected

information the REA database automatically assigned a human health risk level for each site and 4% of the investigated sites received high risk scores. It was found that the main sources of pesticide contamination were former pesticide warehouses – 68%.

The conducted work led to following conclusions and recommendations:

1. The inventory work should be continued in order to identify all sites contaminated with pesticides in the country. There is information that there were over 700 former warehouses of obsolete pesticides in the country, but only 108 were identified and assessed during this inventory. This means that possibly only 15% of all contaminated sites were identified and assessed in Kazakhstan.

2. It is necessary to improve the REA database for its further use in Kazakhstan and other countries.

3. The results of the inventory should be used to prioritize sites for conducting detailed assessments, planning and implementing cleanup (remediation) projects.

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Characteristics and Sources of PAHs in Soils from the Fuling Shale Gas Field, China

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Abstract

With the rapid development of shale gas development, shale gas reservoirs in China are mainly distributed in the Sichuan Basin, which is a typical karst environment and a relatively fragile ecological environment. However, waste from shale gas production contains Polycyclic Aromatic Hydrocarbons (PAHs) that may pose the risks to the environment and human health. In order to clarify the impact of related activities in the Fuling shale gas exploitation on 16 priority PAHs in the surrounding environment, the distribution characteristics and source analysis of PAHs in soils from the shale gas exploitation area were studied. The concentrations of 16 priority PAHs ranged from 22.2 to 594 $ng \cdot g^{-1}$, 11.5 to 1798 $ng \cdot g^{-1}$, 21.8 to 153 $ng \cdot g^{-1}$ in the background soils, the soils surrounding the platforms, and the soils surrounding the blowout pond, respectively. The average concentrations of PAHs were shown as follows: Soils around the platform (99.1 $ng \cdot g^{-1}$) > background soils (73.4 $ng \cdot g^{-1}$) > soils around the blowout pond (56.4 $ng \cdot g^{-1}$), indicating that shale gas exploitation increased the PAHs pollution level in the surface soils of the area, but the impact degree was not significant, and the PAHs in the soils around the platform was seriously affected by shale gas exploitation activities and directive release. The dominant monomers of PAHs in

different soil types were different. Shale gas exploitation increased the proportion of high molecular weight PAHs in platform surrounding soils. According to the results of source analysis, the PAHs in surface soils were generally affected by oil and gas combustion sources, traffic sources, and biomass combustion sources. And the contributions of oil leakage and traffic emission sources in the soils surrounding the platform reached 74.7%. The influence of a single shale gas platform on PAHs in the surrounding surface soils showed that wind speed was not the main factor, and distance was an important index affecting the distribution of PAHs in the surrounding surface soils. The concentrations of PAHs in the surface soils gradually decreased with the distance between the platform increased. Combined with the analysis of composition characteristics, the distance at which the single shale gas platform affected the concentrations of PAHs in the surrounding surface soils was about 100 meters. This study will provide a theoretical basis and reference significance for the supervision and management of shale gas exploitation in the future.

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Enhanced secondary formation of organophosphate esters in winter in South China

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Abstract

Organophosphate esters (OPEs) have been regarded as a group of widely used contaminants with a variety of adverse environmental and health effects, and thus received considerable attention worldwide. However, the physical processes and chemical mechanisms responsible for atmospheric OPEs formation remain poorly understood. Here we combine field measurements and partitioning models to suggest that hydrophobic OPEs are absorbed favorably into the organic phase, whereas hydrophilic OPEs preferably partition into the aqueous phase. We report direct field evidence that enhanced aqueous secondary formation of hydrophilic OPEs occurred in winter, with the magnitude strongly depending on aerosol water content. The dissolved inorganic salts and transitional metals in aerosol have positively potential impacts on particle-bound hydrophilic OPEs formation through facilitating their aqueous partitioning or oxidation. Our findings highlight the increasing importance of such aqueous oxidation chemistry in OPEs formation with the enhancement of hygroscopicity and oxidation capacity in atmosphere, motivating refinements to future chemical management of OPEs and air pollution control strategies.

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Tire Wear Chemicals in the Urban Atmosphere: Significant Contributions of Tire Wear Particles to $PM_{2.5}$

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Abstract

Tire wear particles (TWPs) are of global concern due to their large emissions and potential toxicity, which contain tire wear chemicals (TWCs). However, TWP contributions to urban fine particles are poorly understood. Here, 72 paired gas-phase and $PM_{2.5}$ samples of ambient air were collected in an urban area in the Pearl River Delta, China, in 2018. The concentrations of 54 compounds were determined, and 28 TWCs were detected with total concentrations of 3130–317000 pg/m^3. The TWCs were mainly (73±26%) in the gas phase. 2-OH-benzothiazole contributed 82±21% of the gas phase TWCs and benzothiazole-2-sulfonic acid contributed 74±18% of the TWCs in $PM_{2.5}$. Guangzhou and Foshan were “hotspots”. Most TWC concentrations significantly correlated with the length of road nearby. The measured gas–particle partition coefficients were higher than coefficients predicted using models, probably because of sampling artifacts, burial in particles, and TWC re-release from TWPs. Source apportionment combined with characteristic molecular indicators indicated that TWPs contributed 13±7% of urban $PM_{2.5}$. TWPs are important contributors of urban air pollution that could pose risks to humans. There is an urgent need to develop strategies to decrease TWP emissions along with broader urban air quality improvement strategies.

5. Levels and Fate of Persistent Organic Pollutants and Chemicals of Emerging Concern in the Arctic

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Polycyclic Aromatic Hydrocarbons (PAHs) in the benthic organisms from the West Spitsbergen fjords (Hornsund, Kongsfjorden, Adventfjorden).

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Abstract

Changes in environmental conditions linked to climate, such as reduction of sea ice, extensive glacier retreat, and escalating summer precipitation, exert a direct impact on the Arctic marine ecosystem and the organisms inhabiting it. Benthic organisms, play a crucial role as food source for organisms from higher trophic levels, constitute a significant component of the Arctic's intricate trophic network.

Additionally, the long lifespan and limited mobility of certain benthic species render them ideal indicators for investigating the spatial and temporal variations of contaminants. In this study, polycyclic aromatic hydrocarbons were measured in benthic organisms collected in different part of Hornsund, Kongsfjorden and Adventfjorden.

Quantitative and qualitative analysis of PAHs was conducted using a gas chromatograph equipped with a flame ionization detector (FID). Compound identification relied on their retention time, utilizing both internal and external standards. Analyte concentrations in the samples were determined via external five-point calibration curves established for each compound within the linear range of the detector's response.

Concentrations of Σ12 PAHs measured in benthic organisms were up to 6.4 μg/g w.w. PAH concentrations were significantly higher in Hornsund than in Kongsfjorden. The levels of PAHs were higher in the central areas of the fjord away from the direct influence of the glaciers outflows. Research results show effective accumulation of PAH by Arctic benthos from seawater. Depending on the compounds analyzed and fjord, biomagnification occurs for even 100% of the predator-prey pairs of studied benthic organisms.

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Local Sources of man-made Organic Pollutants in the Arctic: Sources – Characteristics – Consequences

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Abstract

Since the early 1990s the Arctic Monitoring and Assessment Programme (AMAP) a working group under the Arctic Council, has monitored anthropogenic pollutants in a circum-Arctic perspective, including human exposure. The AMAP Expert Group on Persistent Organic Pollutants (POPs) has compiled circum-Arctic information on POPs in the Arctic environment and assessed temporal trends, biological effects, transport patterns and most recently, the influence of climate change on POPs in the Arctic. This work has resulted in numerous reports throughout the past 3 decades, including science-based policy recommendations. A central finding was that POPs are mainly released into the environment in mid-latitude industrial and agricultural regions and reach the Arctic regions via long-range environmental transport.

New sensitive analytical methods and a strong international research focus on Arctic pollution issues has led, during the past decade, to the discovery of many Chemicals of Emerging Arctic Concern, (CEACs), which includes all chemicals of concern not regulated as POPs. The first AMAP report on CEACs

indicated that many of these substances are not as persistent and bioaccumulative as POPs and they may also be released into the Arctic from local sources. A first assessment of the importance of local sources for the release of organic pollutants has now been conducted by AMAP experts. Several significant local contamination pathways into the Arctic environment were identified. The general lack of appropriate sewage handling, open waste disposal, garbage burning as well as local industrial and military sites were identified as being among relevant contaminant sources in the Arctic regions. A variety of legacy POPs along with many CEACs were local contaminants or contaminants with a local emission component.

Distribution pathways, environmental implications as well as recommendations for regulators and scientists will be discussed in the presentation.

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Long Term Temporal Trends of Chlorinated, Brominated and Fluorinated POPs in Landlocked Char in High Arctic Lakes; Evidence for Continuing Global Sources

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Abstract

Landlocked Arctic char (Salvelinus alpinus) are the only top predators in most high Arctic lakes and they serve as a sentinel species for changes in atmospheric inputs of persistent organic pollutants (POPs) to remote freshwater environments. Legacy POPs have been declining in Arctic air over the past 20 years. An exception is hexachlorobenzene (HCB) which has increased in concentrations in air sampled in Svalbard and Iceland. Polybromodiphenyl ethers (PBDEs) showed no decline in air sampled at Alert in the Canadian High Arctic from 2002 to 2015. Air measurements and studies of ice cap snow/firn/ice cores have shown continuing and, in some cases, increasing, inputs of perfluoroalkyl substances (PFAS) to the high Arctic. Therefore, we were interested to see if the trends of HCB, PBDEs and PFAS were reflected in the landlocked char. Data are available for char from two very remote lakes (Amituk and Hazen) and two (Resolute, Char) near the hamlet of Resolute Bay (pop 150), spanning up to 23 sampling years from the early-1990s to 2023, with sample sizes ranging from 3 to 10 fish per year. Σ13PBDEs significantly increased in Hazen (6.4%/y) and Amituk (3.0%/y) from the early 2000s to 2018. The increase of PBDEs contrasts with phase out of PBDEs in the mid-2000s and modelled predictions of a decline of global in-use and waste stocks. HCB also showed increasing concentrations from 2001 in all 4 lakes ranging from 1.8%/y in Resolute Lake to 8.1%/y in Amituk. In Lake Hazen perfluorocarboxylates (ΣC8-C14-PFCAs) in char increased from 2014 to 2022 (20%/yr) after declining from 2003 (-17%/yr). In Amituk Lake PFCAs showed increasing concentrations (7.7%/yr) from 2009 to 2019. Perfluorooctance sulfonate (PFOS) in Amituk Lake char reached a maximum in 2019 and has since declined, while in Hazen Lake

PFOS has declined from a maximum in 2011 (7%/yr). The trends for PFCAs and PFOS do not reflect the predicted decline in global emissions with the phase out of PFAS precursors. Climate related factors could be an important influence on trends of all these POPs. A huge increase of glacial meltwater inputs to Lake Hazen, occurred from the mid-2000s to 2013 resulting in increased fluxes of POPs to the lake. The ice-free area of the lakes is increasing leading to shifts in the abundance and timing of emerging chironomid larvae and zooplankton, key components of char diets. The increase of HCB may reflect revolatilization from increasing summer ice-free areas of the Arctic Ocean.

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Temporal and spatial shifts in the ecological impact of legacy organochlorine pesticides and polychlorinated biphenyls in the global ocean over the past two decades

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Abstract

Increasing effort has been put on monitoring persistent organic pollutants (POPs) in the global ocean, following the Stockholm Convention's ban or restriction on the production and uses of legacy POPs. The effectiveness of source regulations on reducing POP exposures and risks in marine environments can only be assessed when considering all the data gained since then. In this study, we compile numerous measurements (7446 data points) of individual organochlorine pesticides (OCPs) and polychlorinated biphenyls (PCBs) over the past two decades in both coastal seas and open oceans. The data were analyzed to reveal temporal and geospatial trends which reflect the influence of chemical regulations. Measurements in seawater were more conducted in coastal seas (57%), especially in Western Europe and East Asia. In contrast, data for coastal regions in South and North America, India, and Australia are limited. A declining trend in concentrations of OCPs and PCBs has been observed in the coastal of China, Japan sea, Malacca and Singapore Straits, Indian Ocean, and Mediterranean Sea reflecting the positive impact of source regulations. An increasing trend in OCP and PCB concentrations was noted in the Arctic Ocean, marginal sea of the Arctic Ocean, and Nordic Sea, indicating oceanic current carrying historically emitted pollutants from the mid-latitude to the polar regions. Exposures of the polar marine ecosystem to the legacy POPs can become a concern due to the increasing trend and the vulnerability of the marine ecoregions. Risk assessment on the OCP mixtures reveals a high risk in the coastal seas of China and Malacca and Singapore Straits, primarily driven by *p,p'*-DDT and *p,p'*-DDD, while in the marine ecoregions of the open ocean, the risk is moderate to low. The current data gap merits further research on the biogeochemistry of OCPs and PCBs in the seawater column, sediment in coastal and marginal seas, and organisms in vulnerable regions. It is also essential to understand the impacts of climate changes and human activities on the environmental fate of POPs in the oceans.

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Tracing the Impact of Emerging Bisphenols in the Norwegian Arctic: From Local Pollution Sources to Abiotic and Biotic Environments

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Abstract

Local source has become a significant reason for the pollution in Norwegian Arctic−Svalbard. The residing organisms are under threats due to potential transport of organic compounds into the food chain. Bisphenols (BPs), a class of emerging compounds with a variety of analogues, are known for their toxicity to living organisms and have attracted worldwide attention due to their presence in the environment. This work assessed the profile of 32 BPs compounds in altogether 134 abiotic and abiotic samples from Svalbard. Overall, the total concentrations in soils (1.8-56 ng/g dw) were higher compared with the sediments (0.073-0.86 ng/g dw), with BPF and BPA as predominant compounds, respectively. The total concentration of S_9BPs in leachate was 39 ng/L. The BP profiles near the firefighting training site (FFTS) and landfill in Svalbard were assessed. The FFTS was identified as a source of the abundance of 2,4,6-TBP nearby, but no evidence linked the landfill directly to surrounding BP pollution. Overall, SBPs in different organs of polar bear (216-1396 ng/g ww) are higher than those in consumers with lover trophic levels. However, the examination of food web showed that neither polar bears nor glaucous gulls share the same food web as marine organisms. resulting in distinct patterns, with TBBP-DBPE the dominant in polar bear and lower level in glaucous gulls compared with species with lower trophic level. The bioavailability of BPs to **s**ediment-dwelling organisms and their tendency to the accumulate in higher trophic levels of the marine food web was assessed with similar impacts from BPA and 2,4,6-TBP. The tropical levels were calculated in agreement with the order of the SBPs concentration of these species. A higher trophic magnification factor (TMF) for BPA (79) compared with the 2,4,6-TBP (4.0) indicates a stronger tendency for BPA to biomagnifying in the marine food web.

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Summer Alert: Tracing Currently Used Organic Pesticides in the Arctic Ocean

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Abstract

In recent Arctic expeditions, we have analyzed the presence of Tracing Currently Used Organic Pollutants (CUOPs) in the atmosphere and seawater. The primary regions of our study span from the northwest Pacific to the Bering Sea, the Chukchi Sea, and the high-latitude areas of the Arctic Ocean. Over 100 types of CUOPs were investigated, including organophosphate and organoamine pesticides, as well as other novel types of pesticides. The presence and spatiotemporal distribution of these pesticides in the Arctic suggest that during the Arctic summer, the concentration of CUOPs tends to increase with latitude, with local peak values observed in the high-latitude regions of the Arctic. The sources of atmospheric CUOPs are predominantly from mid to low latitudes of the Northern Hemisphere, but changes in the summer climate of the Arctic can have a negative feedback effect on these regions. Surface seawater CUOPs exhibit complex source characteristics, including air-sea exchange, riverine input, and ocean current contributions. However, one of the key factors affecting the environmental fate of CUOPs in the surface waters of the Arctic Ocean is the variability and melting processes of sea ice. Regions such as the Laptev Sea and the East Siberian Sea show local accumulation zones of CUOPs, which are closely related to sea ice movement and ocean currents in spatial analysis. We have also conducted an ecological risk assessment for trace amounts of CUOPs in the summer seawater of the Arctic Ocean. Multiple CUOPs in the surface seawater, such as Phorate and Paraoxon, exhibit characteristics of high ecological risk. Therefore, in the summer Arctic region, CUOPs demonstrate a Summer Alert impact, whether it is the higher concentrations found, the influence on mid to low latitudes, or the formation of regional high ecological risks.

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GLOBAL SUPPLY CHAIN RELOCATION AND ITS ENVIRONMENT AND CLIMATE CONSEQUENCES IN THE ARCTIC

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Abstract

Modern economic globalization has speeded up since the mid-1980s. Many industries and services have been relocated from developed countries to less developed countries, notably China and Southern and Southeastern Asian countries. Industry relocation, and North-South trade have profoundly shifted the locations where raw materials and industrial products are obtained and the ways that commodities are produced, traded, and consumed. These trends, in turn, affect the magnitude and distribution of global greenhouse gases and air pollutant emissions across the globe. The shift of industries from northern developed countries proximate to the Arctic to southern developing countries also relocate emission sources from north to south, which may help reduce or promote POPs across different regions of the Arctic. We found that global supply chain (GSC) relocation reduced significantly BaP contamination in the European and Asian Arctic but enhanced BaP

loading in the North American Arctic. The GSC relocation has also triggered changes in arctic sea ice and atmospheric circulation, which are important drivers of POPs cycling in the polar region.

778

Fractionations of POPs in Global Surface Soils

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Abstract

The concept of fractionation of persistent organic pollutants (POPs) was first proposed by Wania and Mackay in 1993 as global fractionation, or latitudinal fractionation, suggesting that POPs can be enriched within spatial temperature gradients. This pioneering work has made a great contribution to the understanding of the transport of POPs to the Arctic. According to the authors, the concept of global fractionation or latitudinal fractionation contains two major elements: latitudinal transect and airborne temperature gradient, which were treated undistinguishable. In 2010, von Waldow and co-workers suggested that latitudinal transect and airborne temperature gradient are two different mechanisms.

In this study progress in fractionation of POPs are comprehensively reviewed. All distribution patterns and fractionations of POPs can be divided into primary and secondary types. The results of analysis suggest that the transfer of low molecular weight (LMW) POPs from air to soil is mainly through gas diffusion and particle deposition, whereas high molecular weight (HMW) POPs mainly via particle deposition. HMW-POPs tend to be trapped near the source whereas LMW-POPs are more prone to undergo long range atmospheric transport, thus explaining the main reason for their primary fractionation, which is temperature independent. The secondary distribution and fractionation, however, can be only observed along a temperature gradient, such as latitudinal or altitudinal transects. An animation is produced by a one-dimensional transport model to simulate conceptively the transport of PCB-28 and PCB-180, well revealing the similarities and differences between the primary and secondary distributions and fractionations.

Our suggestion is that the decreasing temperature trend along latitude is not the major reason for POPs to be fractionated into the polar ecosystems, but drives the longer-term accumulation of POPs in cold climates, or polar cold trapping. We suggest that only a small number of light POPs, such as a-HCH, b-HCH, PCB-28, and BDE-28 can produce a secondary distribution pattern in the surface soil, and many other POPs with higher K_{OA} cannot. The former POPs that can be polar cold trapped (PCT) are called the PCT-POPs. Thus, it could be an important task to clarify these PCT-POPs in protecting our Arctic and Antarctic from contamination by these chemicals.

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Quantify the Sampling Efficiency of a Polyurethane Foam Air Sampler: Effect of Temperature, Sampling Rate and the Level of Breakthrough

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Abstract

Effective monitoring of atmospheric concentrations is vital for assessing the Stockholm Convention's effectiveness on persistent organic pollutants. This task, particularly challenging in polar regions due to low air concentrations, requires robust sampling techniques. The Flow-Through Sampler (FTS) is an efficient wind-powered active sampling device, enabling the collection of a significant air volume within a short duration. Throughout the actual sampling process, the air temperature and the sampling rate of FTS experience continuous fluctuations, highlighting the need for an in-depth investigation into their impacts on breakthrough and the temperature dependence of PUF/air partitioning. Here we employ the polyurethane foam (PUF) column of FTS coupled with different types of active pumps to collect air samples at varying temperatures, sampling rates and volumes. We delved into breakthrough profiles of key pollutants, such as polycyclic aromatic hydrocarbons (PAHs), polychlorobiphenyls (PCBs), and organochlorine pesticides (OCPs). We investigated the impacts of temperature and sampling rate (expressed as linear wind velocity through the cross-section of FTS tube, u) on the theoretical plate number (N), breakthrough volume (V_B). It revealed that N and $\log V_B$ of compounds on the FTS-PUF exhibit linear relationships with the inverse of absolute temperature and wind velocity (1/T and $1/u$). Significant linear relationships exist between temperature or wind velocity dependence coefficients (K_{TN}, K_{TV}, and K_{Nu}, $K_{VB\text{-}u}$) and compound volatility ($\log P_L$). While distinct trends are noted for PAHs, PCBs, and OCPs in K_{TN}, K_{TV} values exhibit similar patterns across all chemicals. Wind velocity exerts a stronger influence on V_B for low-volatile compounds. Empirical linear solvation energy relationship (LSER) analysis further confirms a significant positive correlation between N and $\log V_B$ across different temperatures and wind velocities. Therefore, the collection performance of the FTS-PUF sampling column for all types of compounds can be predicted under varying temperatures and wind

velocities/sampling rates. For chemicals with severe breakthrough, the first few PUF disks in front of the FTS were treated as equilibrium passive air samples. The temperature dependence of PUF/air partitioning can be further obtained from the air concentrations and breakthrough levels, which can then be analyzed from multiple comparative perspectives to validate the impact of sampling efficiency.

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Fate of ‘forever chemicals’ in the global cryosphere

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Abstract

The cryosphere, encompassing glaciers, ice caps, and permafrost, serves as a significant sink in the global circulation of organic pollutants, with particular concern for per- and polyfluoroalkyl substances (PFAS), often termed "forever chemicals." This comprehensive study synthesizes existing knowledge on the fate of PFAS within the cryosphere, focusing on their sources, accumulation, release processes, and ecological effects. PFAS are detected widely in the cryosphere due to long-distance atmospheric transport of their precursors, while local activities contribute to regional PFAS pollution. Following the Montreal Protocol's regulation of ozone-depleting substances, ultra-short chain PFAS, especially trifluoroacetic acid, have become predominant, highlighting a future research focus. Components of the cryosphere, such as snowfall, sea ice, and permafrost, act as significant accumulation reservoirs for PFAS. However, under climate warming, processes like air-snow exchange, sea-ice melting, and permafrost thaw lead to the redistribution of these pollutants. During snow and ice melt, short-chain PFAS are released earlier than long-chain PFAS. The PFAS remaining in the proglacial environment exhibit a range of ecological effects on both micro- and higher trophic organisms through the food chain, ultimately leading to biodiversity loss. This study sheds light on the fate of PFAS in the cryosphere under climate warming, emphasizing the urgent need for long-term monitoring and the study of PFAS in glacial regions to protect these fragile environments. The insights presented call for an interdisciplinary approach to address PFAS pollution and its impacts in the context of climate change. The establishment of global observation networks, creation of deposition-release budget models, improved toxicity assessment for ultra-short chain PFAS, and uncovering novel PFAS compounds in snow and ice are proposed as critical future directions.

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POPs and PAHs in Russian Arctic coastal seas

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Abstract

Legacy persistent organic pollutants (POPs) and polycyclic aromatic hydrocarbons (PAHs) are still a pollution issue in the Arctic. While regular monitoring activities have been implemented in most Arctic countries, information from the Russian Arctic is still limited. The objective of this review is to compile and review the existing knowledge on environmental fate and distribution pathways for POPs and PAHs in the Russian Arctic. The review focuses on the Russian Arctic coastal seas; it considers mass exchange processes between environmental compartments including the cryosphere. In the Russian Arctic coastal seas, riverine transport and atmospheric deposition are the main sources of legacy POPs and PAHs, respectively. Northward-draining Russian Arctic rivers has contributed accumulated loads of legacy POPs from historical sources to the Russian Arctic coastal seawater. Ongoing volatilization of low-molecular-weight PAHs from both sediment and seawater in the Russian Arctic coastal seas is likely to be accelerated with ongoing warming climate. The PAH and POPs stored is expected to be released along with the ice/snow melting and permafrost thawing in Russian Arctic in the future. However, more up-to-date information is needed for these chemicals to evaluate these processes and their significance for Arctic pollution.

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Impact of global wildfire biomass burning on POPs in the Arctic

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Abstract

With a unique geographical location and a fragile ecological environment, the Arctic has been a major concern of contamination of persistent organic pollutants (POPs), such as polycyclic aromatic hydrocarbons (PAHs) and dioxin (polychlorinated dibenzo-p-dioxins and dibenzofurans, PCDD/Fs), due to their toxic effects on ecological safety and human health. Extensive efforts have been made to mitigate arctic environmental pollution, as a result, most legacy POPs in the Arctic environment have declined in the past decades. However, unprecedented forest fires in high latitude northern territories occur in recent years and pose new challenges to the effectiveness of elimination and POPs pollution in the Arctic. What extent wildfires in the Arctic Circle and remote sources could perturb Arctic PAH contaminations is poorly understood. In this study, we firstly estimate the global emissions of benzo[a]pyrene (BaP), a congener of PAHs with high carcinogenicity, and PCDD/Fs from forest and grassland fires. A global atmospheric transport model, the Canadian Model for Environmental Transport of Organochlorine Pesticides (CanMETOP), is then used to quantify the relative contributions of worldwide wildfire sources to contaminations of BaP and PCDD/Fs in the Arctic region in the past two decades. We also conduct the multiple emission scenario simulations to identify the impacts of local and distant emissions from wildfires sources on Arctic BaP and PCDD/Fs pollution. The main objective of this study is to provide, the most comprehensive and updated assessment by far of atmospheric transport pathways of wildfire-induced POPs from source regions to the Arctic and seasonal and interannual characteristics in the source-receptor relationships. The results may help fill knowledge gaps in understanding the

sources and transport pathways of POPs pollution in the Arctic and motivate the development of effective mitigation strategies.

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Bioaccumulation and biomagnification of Perfluoroalkyl Substances (PFAS) in a Subarctic Ringed Seal Food Web in Lake Melville, Northern Labrador, Canada

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Abstract

Perfluoroalkyl acids (PFAA) are a type of perfluoroalkyl substances (PFAS) that are highly persistent synthetic fluorinated organic compounds. They have a global ubiquitous presence. Some PFAS have high bioaccumulation potentials. Lake Melville is an oligotrophic semi-enclosed estuarine fjord located in northern Labrador of eastern Canada. This ecosystem has been undergoing environmental changes such as climate warming and hydroelectric power development. We hypothesize that these environmental changes may increase PFAS to water and biota in this estuarine fjord. This is concerning for Lake Melville indigenous populations who consume locally caught seals, fish and invertebrates on a traditionally basis. The objectives of this study are to investigate PFAS concentrations and congener profiles in Lake Melville water and biota, and assess bioaccumulation and biomagnification of these chemicals in ringed seal (*Phoca hispida*) food webs. In total, 18 samples of water, 7 pooled samples of zooplankton, and 54 samples of biota that include invertebrates, fish, and ringed seals were collected. Water, invertebrates, and liver and muscle samples of fish and ringed seals underwent chemical extraction and were analyzed for 17 PFAS using ultra-high performance liquid chromatography tandem mass spectrometry (UPLC-MS/MS). The results show that PFAS are ubiquitous in Lake Melville water and biota. Soluble short-chain PFAS, perfluorobutanoic acid (PFBA), predominates in Lake Melville surface and subsurface water. Other PFAS concentrations in water decreased along the freshwater-marine salinity gradient, likely due to seawater dilution and decreased proximity to riverine sources. PFBA also predominates in freshwater zooplankton. In marine zooplankton, however, perfluorooctane sulfonic acid (PFOS) is the predominant PFAS congener. Perfluoroundecanoic acid (PFUnDA) predominates in fish livers, whereas perfluorononanoic acid (PFNA) and PFOS predominate in ringed seal livers. Trophic magnification factors values > 1 (ranging from 1.35 to 7.44 log ng/g w.w.) showed that long-chain perfluoroalkyl carboxylic acids (PFCA) and PFOS biomagnify throughout ringed seal food webs. This study provides baseline information about PFAS concentrations in Lake Melville water and biota before completion of the hydroelectric power project and is the first to investigate PFAS in a complete food web in Labrador.

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Global Gridded Emission Inventory of Organophosphate Flame Retardants from 2010 to 2020

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Abstract

As a failed alternative of brominated flame retardants (BFRs), the high toxicity, bioaccumulation, and worldwide distribution of organophosphate flame retardants (OPFRs) have raised global concerns. To paint an overall picture of OPFRs in the global environment, the present study develops a gridded global emission inventory of OPFRs on a spatial resolution of 1°×1° from 2010 to 2020. The results indicate a significant increase in global OPFR emissions during this period with an average annual growth rate of 3.31%. The total amount of OPFR released into the atmosphere from OPFR production and consumption reaches 21,324.42 tons for this period. The production process is identified as the major source of OPFR emissions, contributing 55.43% to the total emissions. Consumption processes contribute to the remaining 44.57%. Asia, North America, and Europe are the major sources of OPFRs. The inventory is verified by implementing emissions data to a global atmospheric transport model to predict OPFR concentrations in the global environment and comparing modeled concentrations with field sampled data. The results indicate that the inventory is reliable except for the pristine polar region where the emission inventory and modeled concentrations underestimate OPFR levels in the atmosphere, likely resulted from ignorance of chemical reaction and the secondary derivative of parent OPFRs during their global long-distance atmospheric transport in the model. This model failed to capture OPFR evolution in remote polar region, implying the need of a more comprehensive atmospheric chemistry module that takes photochemical reaction and other chemical processes for OPFR into consideration. The inventory provides a valuable dataset and the most comprehensive view of OPFRs in the global environment, which can help policy making in OPFR emission control strategies and assessment of source-receptor relationships and health risks.

In the future, modeling efforts will focus on integrating atmospheric chemical transformations (photochemical oxidation/degradation) mechanisms of OPFRs into the modules of global atmospheric chemical transport model to accurately quantify global long-range atmospheric transport and deposition based on these global gridded emission inventories, and to depict the atmospheric transport pathways and source-receptor relationships as well as impact of local emissions on Arctic air pollution of OPFRs, which may help to improve the currently underestimate modeled OPFR levels based on simulation of CanMETOP in Arctic.

6. New Approach Methodology in Ecotoxicology and Risk Assessment - Theory and Application

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Data Driven Decision making using advance high-throughput Environmental Risk Assessment of Fragrance Materials.

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Abstract

For the last 20 years, the Research Institute for Fragrance Materials (RIFM) has conducted environmental risk screening and assessments to evaluate the environmental safety of more than 3,000 fragrance materials manufactured and used by its members. Though the RIFM Environmental Framework (Salvito et al. 2002. Environ. Toxicol. Chem., 21: 1301-1308) is an effective tool, in light of rapid growth in global use of fragrance materials, RIFM has updated the framework to expand its geographic scope and to incorporate recent advances in environmental exposure science and ecological hazard characterization. In this presentation we describe the updated Framework, detailing its expanded geographies, real-time access to the most current population and hydrological data, estimated environmental exposure using waste water treatment plant simulation models and biodegradation, material categorization based on mode of action (MoA), application of an MoA-based ecological threshold of concern, and streamlined execution. The tool's methods and outcomes are illustrated through a proof-of-concept exercise. The updated Framework is an enhanced risk assessment tool that enables RIFM and users and suppliers of fragrance materials to perform timely assessments of thousands of fragrance materials in order to maintain a high degree of environmental protection and support science-based decisions related to product formulations.

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Explainable Artificial Intelligence Models for Ecotoxicity Prediction using Adverse Outcome Pathway Framework

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Abstract

Artificial intelligence (AI) models offer a new opportunity to assess the potential toxicity of a vast number of environmental chemicals. However, many toxicity prediction models are inherently 'black boxes,' making interpretation challenging for toxicologists and hindering the

regulatory acceptance of these models. The mechanisms leading to the onset of apical toxicity are complex, and in the absence of process evidence, it is difficult to trust the results, which may, in the worst case, be a mere coincidence. The adverse outcome pathway (AOP) framework holds promise in addressing this issue. AOPs can link molecular toxicity endpoints to human and ecotoxicity endpoints. In response, this study aimed to develop explainable artificial intelligence models for predicting toxicity using ToxCast data within an AOP framework. Initially, we identified AOPs leading to reproductive toxicity from AOP Wiki. We then collected in vitro bioactivity data from ToxCast and in vivo toxicity data from ECOTOX DB. These data were integrated into AOPs, and each assay-AOP pair underwent further assessment to determine relevance to taxa within ecosystems. Finally, machine learning models were developed to predict each mechanistic and apical endpoint-based toxicity. As a result, models for each key event and apical endpoint achieved high performance (F1 score: 87-92%). In a proof-of-concept case study, the model improved the sensitivity of predictions compared to models developed based on in vivo toxicity data alone. This study can serve as a guide for developing explainable machine learning models based on AOPs, addressing the current primary bottleneck in using AI models for chemical risk assessment.

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Integrating In Vivo, In Vitro, and In Silico Approaches to Assess Chemical Toxicokinetics: A Cross-Species Comparative Analysis

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Abstract

Toxicokinetic (TK) data quantitatively describe chemical- and organism-specific processes for absorption, distribution, metabolism, and excretion (ADME). The lack of high-quality measured TK data introduces uncertainty in hazard and risk assessments. Terminal elimination half-lives (HL_T) play a crucial role in inter-species extrapolation of toxicity data and in vitro-in vivo extrapolation (IVIVE) of bioactivity data from New Approach Methods (NAMs). Differences in TK, such as biotransformation half-life (HL_B), between species significantly impact interspecies extrapolation. Allometric scaling and uncertainty factors are commonly used for such extrapolations, but their arbitrary selection may not accurately represent the true uncertainty.

This study aims to analyze HL_B and HL_T differences across various organisms using in vivo, in vitro, and in silico data. In vivo TK data and in vitro biotransformation rate were critically evaluated to identify key sources of uncertainty. Quantitative Structure-Activity Relationships (QSAR) were employed to predict HL_B and HL_T, while allometric scaling based on body mass was used to normalize the data and explore TK differences between species.

The variability in HL_B and HL_T among key species was examined to assess the support for commonly applied uncertainty factors. The study finds general agreement in HL_B and HL_T estimates obtained from different methods for most chemicals. Based on a comparison of 229 chemicals, the mean difference between normalized rat and human HL_T is approximately 2, and an uncertainty factor of about 60 captures 95% of the inter-species variability. This study underscores the necessity for integrated and systematic testing methods to address the significant uncertainty in TK data for numerous chemicals and in the application of hazard data for human and ecological health assessments.

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Random Forest to Predict Ecotoxicity Effects for Pollinators

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Abstract

Available ecotoxicity data for chemicals to pollinators are primarily acute ED50 data. However, exposure levels corresponding to chronic ED10 are closer to reality and aligned with state-of-the-art life cycle impact assessments, but mostly lacking. We address this gap by developing a random forest model trained with a large, comprehensive ecotoxicity-chemical property dataset with 5282 records covering 449 chemicals. The main ecotoxicity data were exported from the ECOTOX database and harmonized to achieve data consistency and uniformity. The dataset was enriched with chemical properties, for example, mode of action, molecular descriptors, chemical categories, etc., from multiple sources. The enriched dataset was split into training and test sets using two splitting schemes: “totally random”, where the dataset was randomly split, and “random by chemical”, where the chemicals present in the training and test dataset were kept distinct. Both splitting schemes were tested on the model training and prediction, applying cross-validation to avoid overfitting. The “totally random”- based model showed a performance with root mean square error (RMSE) of 0.76. However, a decreasing performance with an RMSE of 0.19 was observed when using the “random by chemical”-based model. This indicates that the model was limited in its ability to extrapolate from the existing chemicals to unknown chemicals that were not used for model training. The MACCS fingerprint-based difference was calculated and grouped for each chemical by using K-nearest-neighbors techniques, and it was found to be significantly correlated to the RMSE with an R^2 of 0.75. This demonstrates that a test chemical with a smaller difference compared to the training chemicals has a lower potential to be predicted biased, while a larger difference potentially leads to a higher risk of being biased predicted. The known chemical can always be well-predicted with a lower bias according to the “totally random”-based model’s performance. This study provides an integrated ecotoxicity-chemical property dataset that can be used for different model training and data

analysis. We also trained a random forest model that performs well for the known chemicals. The linear regression between the chemical's difference and RMSE was explored to provide the foundation for determining the applicability domain of the random forest model.

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Analysis of environmental RNA in fish toxicity test with pyrene: a non-invasive approach

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Abstract

Toxicity testing using aquatic animals has been an essential tool for chemical risk assessments. While traditional methods, such as collecting and analyzing tissues or blood samples from animals exposed to toxic chemicals, can provide valuable insights into the molecular mechanisms of toxicity, these methods can also cause pain or death to the animals. Growing concerns over animal welfare have led to calls for New Approach Methodologies (NAMs), which include reducing animal use, replacing it with alternative methods, and refining testing procedures to minimize pain or distress.

Environmental RNA (eRNA) is RNA released by organisms into their surrounding environment such as water, soil, and sediment. Unlike DNA, RNA is produced only for genes that are actively being transcribed, making it a useful tool for understanding the real-time physiological status of organisms. Recent studies have demonstrated that the degradation of eRNA is slower than previously expected. These characteristics suggest that eRNA could serve as a non-invasive measure for assessing the toxic effects on organisms exposed to chemicals; however, this potential remains largely unexplored.

To investigate the potential of eRNA as a non-invasive method for assessing the physiological status of experimental organisms, we conducted toxicity tests using Japanese medaka *Oryzias latipes* as a model fish. The medaka were exposed to pyrene, a polycyclic aromatic hydrocarbon (PAH), for 96 hours. After exposure, eRNA was collected from the surrounding water, extracted, and comprehensively sequenced. Our results showed that 1110 genes were detected in eRNA and the sequenced read counts of these genes correlated with those in fish tissue ($r = 0.50$). Additionally, eRNA detected 86 differentially expressed genes in response to pyrene, some of which were shared by fish RNA, including the suppression of collagen fiber genes. These findings suggest that eRNA can detect changes in gene expression in fish in response to environmental stressors, providing a viable non-invasive alternative to traditional toxicity testing methods.

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Developing Acute to Chronic Ratios (ACRs) for Understanding the Ecotoxic Effects of Surfactants

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Abstract

Surfactants are used in high volumes across various industries. Whilst they are highly removed during wastewater treatment processes, they have the potential to enter the environment. It is essential, therefore, that their environmental impact is assessed. Surfactants are amphiphilic structures containing both hydrophobic and hydrophilic components and are commonly categorised according to the charge of their hydrophilic moieties as anionic, non-ionic, cationic or zwitterionic. Whilst the safety of these substances has been widely investigated, there are still some data gaps to meet regulatory registration requirements and, in particular, to address (fish) chronic toxicity endpoints. Filling such data gaps would require extensive testing. One potential solution to this data shortage lies in the leverage of existing toxicity data, and the development of "acute-chronic ratios" (ACRs). ACRs are empirically derived ratios between the acute and chronic ecotoxicological endpoints which can be used to estimate chronic toxicity where only acute values are available. Previously they have been shown to be robust within certain (non-surfactant) substance classes and non-specific mechanisms of action.

The aim of this investigation was to extend the ACR approach to include a broad range of surfactants. Details of surfactants were obtained from publicly available data sources, and common chemical identifiers were recorded – primarily the Chemical Abstract Service (CAS) number, in addition to names and chemical structures where available. The CAS numbers were used to search for available aquatic toxicity data, which were then recorded and scrutinised to identify representative and robust acute and chronic toxicity endpoints for relevant fish, *Daphnia* and algal species. CAS numbers were compiled for over 1,000 surfactants including anionics, non-ionics, cationics, zwitterionics and miscellaneous groups, such as mixtures. Aquatic toxicity data were available for over 200 substances, from which information was subsequently retrieved to develop reliable ACRs for surfactant classes. The ACRs are fully and transparently documented and will allow the extrapolation of acute toxicity data to chronic values within a defined area of certainty. This increases the efficient use of existing data to support a reduction in the current requirement for testing of vertebrates as part of a Weight of Evidence approach.

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Generic field studies as a method for avian higher tier risk assessment

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Abstract

The registration of plant protection products (PPPs) requires an increasingly extensive multi-tiered risk assessment to ensure environmental safety. The first step of a risk assessment is typically highly conservative, to cover potential uncertainties and filter out non-critical substances. The following steps consider locally relevant and more realistic exposure scenarios. The aim of a higher tier approach is to increase realism and decrease uncertainties in the risk assessment. For birds, this can be done by using generic field studies, which collect data on the exposure of relevant species, i.e., species which are present in the specific crop at the intended time of application of the PPP. Generic field studies have become a valuable tool in countries of the European Union. The conduct of locally relevant studies in Asia should be strived for.

We highlight the implementation of different generic field study methods in a higher tier risk assessment. Studies included are focal species (FS), the proportion of an animal's daily diet obtained in habitat treated with pesticides (PT) and the composition of diet obtained from treated area (PD). Laboratory feeding studies are needed to determine appropriate correction factors which account for differences in digestibility of food items. Video monitoring (VM) can identify birds' feeding behavior and food preferences, to quantify species-specific exposure to PPPs. Generic field studies (FS, PD and VM), which have recently conducted in China on freshly drilled rice fields, serve as an example of the available methods and corresponding challenges.

According to the agricultural practice as well as crop type and crop height, the most appropriate method to identify FS needs to be chosen for the study conduct. The species abundances as well as their frequency of occurrence are used to identify most relevant species within a feeding guild. As soon as FS are defined, their corresponding PT and/or PD can be measured to determine the actual exposure to PPPs. The selection and conduct of the most appropriate study design again requires high expert knowledge.

As a conclusion, generic field studies can substantially help to enhance risk assessments onto a more realistic level, helping the assessor to better understand the actual risks in the field and to reduce uncertainties in assessing the potential exposure of birds to the applied PPPs.

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Construction of ecological safety threshold prediction model for metal elements in typical Chinese soils

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Abstract

The ecological safety thresholds of elements in soil is the main basis for pollution prevention and control, however, obtaining their values through conventional experimental methods is time-consuming and laborious, making it difficult to meet the urgent needs of environmental management. Therefore, it is necessary to establish relevant toxicological data prediction models. This study collected toxicological data of eight elements on five species and three microbial processes in Chinese soils through literature collection, attempting to construct a new model for predicting the toxicity of limited elements in soil data—the Quantitative ion characteristic activity relationship (s-QICAR) model. Firstly, based on the normalization method of soil properties, the toxicity values of eight elements to five species and three microbial processes were obtained under three soil scenarios ($logEC_{10}$). On this basis, the relationship between the structural characteristic parameters of elements and their corresponding biological toxicity values was analyzed, and s-QICAR models were established using the covalent radius (CR) of elements. Furthermore, s-QICAR was used to predict the $logEC_{10}$ of V, As, Se, and Sn for eight species. Combined with the species sensitivity distribution curve, the HC_5 values of these four elements protecting 95% of organisms were calculated, and the ecological risk threshold map for these four elements was drawn. This study establishes a new method applicable to the ecological risk of soil elements in China, providing scientific basis for soil environmental risk assessment and management.

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Drivers of Ecological Risk Released by Biodegradable Plastic in Surface Water: Additive or Microplastic?

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Abstract

Considering as an environmentally friendly alternative to conventional plastics, the production of biodegradable plastics is increasing each year. Studies have shown differences between additives of biodegradable and conventional plastics, and biodegradable material may generate larger amounts of microplastics in environments. These factors cause unpredictable risk on ecosystem thus a systematic assessment is urgently needed. In this work, toxicity induced by additive and microplastic is evaluated separately, after which high-toxicity contribution factors are elucidated with multi-dimension evidence. For additive, key toxicity contribution additives are identified by high-coverage chemical analysis and association analysis between chemical and toxic matrix. For microplastic, quantification and characterization results are analyzed to explore effect of size or type on toxicity.

The results showed that widely used polylactic acid and polybutylene adipate terephthalate shopping bags or trash bags with national certification for biodegradable plastics showing higher toxicity than other plastics that claimed to be degradable in specific condition for multi-level species in aquatic environments. Chemical analysis of high- and low- toxicity samples show significant clustering features, indicating potential high-contribution factors in additives of biodegradable plastics, for example 1-oleoylglycerol, 1,3-diphenylguanidine and 4-dodecylbenzenesulfonic acid. By excluding microplastics in exposure solution, we found that both additives and microplastics exert toxic effect. High-toxicity samples release larger amounts of microplastics than low-toxicity samples. A possible relationship may exist in additive

composition and microplastic release tendency, how this relationship affect toxicity is still need further research in future.

Our research provides systematic risk assessment for biodegradable plastics and may give an answer on whether an overall replacement of conventional plastics by biodegradable plastics is friendly for ecosystem.

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Prediction of Cytotoxicity of Polycyclic Aromatic Hydrocarbons from First principles

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Abstract

Ligand-specific binding interactions of xenobiotics with receptor proteins form the basis of cytotoxicity-based hazard assessment. Computational approaches enable predictive hazard assessment for a large number of chemicals in a high-throughput manner, minimizing the use of animal testing. However, *in silico* models for predicting mechanisms of toxic actions and potencies are difficult to develop because toxicity datasets or comprehensive understanding of the complicated kinetic process of ligand-receptor interactions are needed for model development. In this study, a directional reactive binding factor (DRBF) model based on first priniciples was used to predict cytotoxicity potencies of agonists of the aryl hydrocarbon receptor (AhR) for 16 different polycyclic aromatic hydrocarbons (PAHs). Molecular dynamics were simulated by accounting for the directional configuration factor toward receptor protein and the factor of binding to the Per-Arnt-Sim (PAS) domain. When comparing the experimental results of toxic potencies from *in vitro* bioassays with the predictions among two different *in silico* models, including quantitative structure-activity relationship (QSAR) and molecular docking models, the DRBF model exhibited the highest model performance ($R^2 = 0.90$ and $p < 0.01$). Our results showed that the DRBF model based on first principles and molecular and computational structural biology could serve as novel framework to advance next generation hazard assessment for high-throughput screening of chemical substances.

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New Approach Methodology in Ecotoxicology: Advances and Case Study in Microalgal Bioassays for Environmental Risk Assessments

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Abstract

Microalgal bioassays have become a crucial tool for assessing the potential toxicity of various persistent toxic substances in environmental samples, due to their high sensitivity, short test duration, and cost-effectiveness. With ongoing advancements, these bioassays are being increasingly applied to various environmental matrices. This review encompasses the literature on microalgal bioassays used in environmental assessments, emphasizing the types of samples analyzed, preparation methods, endpoints, and key scientific developments. A bibliographic analysis using keywords like ‘microalgae,’ ‘toxicity,’ ‘bioassay,’ and ‘microalgal toxicity’ led to the review of 89 research articles. Traditionally, water samples (44%) and passive samplers (38%) were predominant, while direct exposure methods (41%) often assessed toxic effects through growth inhibition (63%). Recent advancements include automated sampling, in situ bioanalytical methods with multiple endpoints, and both targeted and non-targeted chemical analyses. Future studies should aim to identify toxicants affecting microalgae and elucidate their cause-effect relationships.

A case study was conducted to identify microalgal toxicants in marine sediments from industrialized areas in South Korea using effect-directed analysis (EDA). Three marine microalgae species (*Dunaliella tertiolecta, Isochrysis galbana, and Phaeodactylum tricornutum*) were tested with various endpoints via flow cytometry. A subsequent study incorporated full-scan screening analysis (FSA) to detect unknown toxicants in Ulsan Bay, revealing toxic responses not fully explained by known compounds, thus indicating the presence of unidentified toxicants. FSA identified thirty-one candidate toxicants, with seven commercially available compounds confirmed in Ulsan Bay, including 2-Nitrophenol, 3-Nitrophenol, and 4-Nitrophenol as potential unmonitored algal toxicants.

An enhanced microalgal bioassay and FSA approach in Gamcheon Harbor highlighted species-specific sensitivities: *D. tertiolecta* was more affected by F2 fractions, while *P. tricornutum* responded more to F3 fractions, likely due to their distinct cell membrane structures. This integrative methodology combining EDA with advanced microalgal bioassays and FSA provides a nuanced understanding of physiological responses beyond traditional endpoints. Further research should explore the distribution, sources, fate, and ecotoxicity of these newly identified toxicants.

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Strategy to deliver a mechanistic based, next generation environmental safety assessment paradigm shift

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Abstract

Historically, regulatory frameworks for assessing environmental and human safety of chemicals were centred around standard information requirements mainly anchored in *in vivo* data generated in a few model species. These traditional approaches were mainly based on apical effects studies performed on whole organisms.

However, we are now seeing a global push towards increased protection, robustness and transparency aiming to deliver enhanced safety for humans and the environment. New Approach methodologies or NAMs are central to this paradigm change due to their ability to offer a greater mechanistic understanding of toxicological responses across species while allowing the generation of points of departure (PoDs) that are useful for safety decision making.

The new knowledge and transparency offered by NAMs will allow further integration of chemistry, biology and toxicology as well as breaking the silos between human health and environmental safety assessment making a more efficient use of available technologies and data.

In this presentation we will discuss examples of relevant NAMs which can be used to inform Environmental Risk Assessment and present a framework guiding the gathering, organization and evaluation of all available data. This will include hazard characterization, mechanism of action, identification of species at risk and Physiologically Based Kinetic (PBK) models, illustrating their use through case studies. Ultimately, we aim to demonstrate that the time is right to move away from the traditional data requirements towards a mechanism-based safety paradigm which considers all available data to improve safety decision making and transparency.

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Laboratory feeding studies to derive appropriate correction factors for avian higher tier risk assessment

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Abstract

The registration of plant protection products (PPPs) requires an increasingly extensive multi-tiered risk assessment to ensure environmental safety. As a higher tier approach for birds, generic field studies have

become a valuable tool in countries of the European Union. Although still hardly conducted in Asian countries, it is noticed that this approach is also becoming more important. In the guidance on environmental risk assessment for pesticide registration by the Ministry of Agriculture of the People's Republic of China, it is explicitly highlighted that when information on birds' behavior is available, these can be used in higher tier assessments.

One of the generic field study method is to quantify the actual exposure of relevant bird species (i.e. focal species) to PPPs is the so-called PD (Portion of Diet) study, which measures the composition of diet obtained from treated area. The derivation of PD needs substantial expertise in the analysis of food remains delivered from the focal species' faeces or their crop content. As different food items are differently digested, factors obtained from laboratory feeding studies with either the same or surrogate species help to correct for these differences.

A laboratory study on correction factors, which has recently been conducted in China serves as an example of the available methods and corresponding challenges, such as the choice of an appropriate model species. We selected the rice finch, as a representative small granivorous species.

Furthermore, the right characteristics of each food component must be examined in order to determine correction factors that can be applied efficiently.

As a conclusion, the derivation of correction factors increase the robustness of generic PD studies. Likewise, robust generic field studies on the composition of the birds' diet substantially help to enhance a risk assessment onto a more realistic level, helping the assessor to better understand the actual risks in the field and to reduce uncertainties in assessing the potential exposure of birds to the applied PPPs.

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Identification of Unmonitored Toxic Substances in the Environmental Samples using Effect-Directed Analysis Combined with Nontarget Screening: A Review

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Abstract

Effect-directed analysis (EDA) combined with nontarget screening (NTS) has established a valuable tool for the identification of unmonitored toxic substances in environmental samples. This approach is designed to identify toxic substances in environmental samples such as sediments, wastewater, and biota, and involves three main steps: identification of highly potent fractions, selection of toxicant candidates, and identification of major toxicants. In the first step, environmental samples are collected and prepared, with organic compounds extracted and subjected to bioassays to screen for potential toxicities. Fractionation helps isolate toxic fractions, reducing sample complexity and enabling more focused

chemical analysis. In the second step, highly potent toxic fractions are further analyzed to select target and suspect analytes relevant to observed toxicity. High-resolution mass spectrometry (HRMS) and data processing techniques are used to select causative agents, narrowing the candidates to a manageable number. In the final step, chemical and toxicological confirmations are performed on the selected candidates. The EDA combined with NTS approach addresses the limitations of traditional monitoring that relies solely on known target chemicals, allowing for the detection of previously unmonitored substances. This study highlights successful applications of this advanced method and discusses its potential to enhance environmental monitoring programs by integrating effect-based monitoring. Challenges include the need for advanced instrumentation, complex data processing, and the necessity of standard materials for confirmation. We provide suggestions for incorporating EDA combined with NTS into environmental management policies, emphasizing the importance of further research to improve the methodology and expand its application. The approach is seen as a significant advancement in identifying and managing environmental pollutants, offering a comprehensive tool for assessing chemical risks in various environmental contexts. This methodology represents a notable improvement in the field of environmental science, potentially addressing how environmental risks are assessed and managed.

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Endocrine Disrupting Chemicals Identification Based on High-throughput Bioassay and Chemical Analysis

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Abstract

In this study, a combination of high-throughput bioassay and chemical analysis was used to identify key toxicants from known and unknown endocrine disrupting chemicals (EDCs) in the environment. Firstly, based on mechanism of competitive binding, reporter gene and cell proliferation assay, we conducted molecular dynamics simulation and molecular docking. In this way, we constructed qualitative- and quantitative-structure relationship on the activity and the type of activity when considering the molecular structure, physicochemical properties and molecular descriptors. We further extrapolated *in vitro* experiments to individual endpoints through the male and female reproductive toxicity pathways, to realize the qualitative and quantitative prediction of male/female reproductive toxicity based on the structure of pollutants. Above virtual screening methods has been officially adopted by the VEGA HUB platform designated by the European Chemicals Agency. The method was then introduced into chemical analysis and bioassay to establish target/non-target identification method for EDCs, revealing the causative toxicants inducing endocrine disrupting effects in source/surface water. For the target pollutants, a mass spectrometry fingerprint-toxicity equivalent database was established targeted different nuclear receptors, which included primary and secondary spectra and toxicity equivalent information. Further, a software for evaluating the toxicity contribution by using the probability density function was constructed, realizing rapid quantitative identification of 500 EDCs and the qualitative screening for nearly thousand EDCs. For non-target compounds, seven golden rules were established to identify mass spectrometry fingerprints and screen molecular formulae. Then, based on correlation between retention indices and molecular formulae, we realized chromatographic fingerprints identification and structure screening. By

combining structure-activity relationship and multivariate analysis, the virtual screening technology for toxicogenic structures was constructed, realizing high-throughput identification of EDCs. This technique was introduced into the actual polluted environments, revealing diisobutyl phthalate, alkylphenols, pyrethroid pesticides and chlorpyrifos as the main contribution of endocrine disrupting effect. This study provides a reliable support for identification of key EDCs and screening of priority control pollutants in complex aquatic environments.

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Integrated Quantitative *In vitro-In vivo* Extrapolation and *In Vitro* Multi-omics Approach Reveals the Pathway-Specific Point-of-departure and Adverse Outcome Pathway Network of Organophosphate Esters

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Abstract

High-throughput *in vitro* assays combined with *for In Vitro-In Vivo* Extrapolation (IVIVE) leverage *in vitro* concentrations associated with bioactivity to an external concentration level associated with a potential hazard (*in vivo*), which play a critical role in development and implementation of reliable alternative methods for systemic toxicity endpoints in animal-free new approach methodologies (NAMs). However, developing non-mammal animal physiologically-based toxicokinetic (PBTK) models for IVIVE in ecological applications is challenging, especially for plausible estimation of internal effective dose (biological equivalent concentration, BEC) linked with complicated biological pathways and adverse outcomes of endocrine disrupting chemicals (EDCs), such as the organophosphate esters in this case. Here, a refined fish PBTK model linked with IVIVE approach for various fish species was established, with parameter optimization of chemical unbound fraction, pH-dependent ionization and hepatic clearance, and integration of temperature effect and growth dilution. The critical biological pathways disturbed by the organophosphate ester (EHDPHP) were explored by integrated analysis of in vitro metabolomics and transcriptomics using zebrafish primary hepatocytes. Other existing *in vitro* bioactivity data and *in vivo* effect data were retrieved from literature. Pathway-specific point-of-departure (POD) and adverse outcome pathway network (AOPN) of EHDPHP were proposed from multi-omics analysis and retrieved data. Sensitivities of metabonomic $mPOD_{pathway}$ and transcriptomic $tPOD_{pathway}$ of EHDPHP were different. $POD_{pathway}$ of EHDPHP associated with reproduction and lipid metabolism were relatively higher than those of common response pathways. The AOP related to reproductive toxicity received a relative high weight of evidence score. The fish-PBTK-IVIVE approach provides not only more precise estimations of tissue-specific concentrations comparing with existing in vivo data (in forward dosimetry) but also reasonable approximations of BEC targeting specific pathways of EHDPHP and other typical EDCs (in reverse dosimetry). Using the available IVIVE-derived BEC with target

pathways was helpful to develop the POD for chemicals with similar mode of action. We conclude that the integrated PBTK-IVIVE and *in vitro* multi-omics analysis approach is capable to provide new insights and solutions to hazard and risk assessment of EDCs.

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Environmental NAMs and NGRA frameworks for chemical safety assessments: Challenges & opportunities

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Abstract

Globally, significant regulatory efforts are underway to advance chemical safety assessments for hazard and risk evaluations. In many regions, these regulatory changes to improve chemical safety for humans and the environment are combined with efforts to generate data with the best available science from New Approach Methodologies (NAMs) rather than traditional, apical-based animal studies. NAMs within next-generation risk assessment (NGRA) frameworks combine effect and exposure including fate information from various tools such as bioassays, grouping & read-across approaches and waiving considerations to assess chemical safety. In the past, human and environmental health safety assessments have operated mostly in silos. NAMs and NGRA frameworks now allow to drive synergies and are based on biological and chemical knowledge which can be used across, envisaging future integrated and intelligent animal-free one health safety assessments.

While there are many opportunities, the scientific availability, regulatory uptake and industrial application of NAMs for chemical safety assessments still lags behind, especially for the environment. Developing NAMs for regulatory data requirements requires relevant and robust approaches with clearly defined applicability domains, robustness, performance and interpretation.

To advance this, multi-stakeholder collaborations between regulators, industry, academia and not-for-profit organizations such as research organizations and NGOs are key. There is increasing momentum and ambition on this particularly within the cosmetic sector with its widespread animal testing bans (e.g. 2013 EU and 2023 Canada). As such, the global non-for-profit organization International Collaboration on Cosmetics Safety (ICCS) focusses on advancing the adoption of animal-free science for human and environmental safety assessment of cosmetics, through science, education & training, and regulatory engagement.

This presentation, supported from the ICCS expert groups, will provide a global overview on the status, challenges and opportunities on uptake of environmental NAMs & NGRAs, covering effects and exposure including fate approaches, for chemical safety assessments with a focus on EU, UK, USA and Canada.

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Towards One Health: Case studies to develop & test an integrated animal-free next generation human and environmental safety framework for cosmetics

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Abstract

There is an increasing momentum and ambition to move towards animal-free chemical safety assessments, particularly for the cosmetic sector with its widespread animal testing bans (e.g. 2013 EU and 2023 Canada).

To increase confidence in, and experience with, non-animal new approach methodologies (NAMs) and next-generation risk assessment (NGRA) frameworks across stakeholders, case studies are required to 'stress-test' the existing tools. This allows a thorough assessment of how the tools can be used together, their applicability in a range of scenarios, and allows the identification of areas of larger uncertainties to inform additional research needs.

While in the past, human and environmental health safety assessments have operated mostly in silos, NAMs and NGRA frameworks give an unprecedented opportunity for a future integrated, intelligent, and iterative animal-free one health safety assessment.

For this, a case studies project will be carried out by the not-for-profit science organization ICCS (International Collaboration on Cosmetics Safety) to develop and test an integrated animal-free next generation human and environmental safety framework for cosmetic and personal care product ingredients. The case studies will span human and environmental health, considering effects and exposure including fate, to foster closer ties between the disciplines through commonalities in biological targets and approaches (e.g., PBK). The project will explore the application of well-established and novel NAMs and NGRA frameworks for safety assessment and regulatory data requirements including registrations (e.g. for US TSCA and EU REACH tonnage data requirements + risk characterisation ratio). If possible, the project will compare the level of protectiveness achieved by NGRA compared with traditional approaches. The learnings will inform best practice guidance further future research efforts, and build support for integrated, one-health, risk assessment approaches.

This presentation will serve as an overview of the planned multi-phase approach for the project, an update on the current status, and an opportunity for stakeholders to provide feedback or share relevant findings in shaping these case studies.

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Incorporating New Approach Methodologies (NAMs) Data Into Risk Assessment of Poly- and Perfluoroalkyl Substances (PFAS) in Consumer Products

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Abstract

Poly- and perfluoroalkyl substances (PFAS) have been widely used in everyday consumer products such as shampoo, mouthwash, and cleaning agent, but their significance as potential exposure sources to PFAS has been overlooked. Also, despite the advantages offered by new approach methodologies (NAMs) data over traditional animal experiment, their applicability for hazard assessment remains uncertain. Therefore, we aimed to evaluate the risk associated with PFAS in consumer products and to explore the integration of NAMs data into the risk assessment of perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS). For hazard assessment, we gathered toxicity data on the hepatic, immune, and developmental toxicity of PFOA and PFOS, representing primary adverse effects of PFAS. Firstly, we selected *in vivo* toxicity values used for health-based guidance value in international regulatory reports. Secondly, *in vitro* toxicity values were collected by systematically reviewing literatures and analyzing ToxCast data, an *in vitro* toxicity prediction program. Thirdly, human equivalent doses (HED) were calculated based on both *in vivo* and *in vitro* data, and we compared *in vivo*-based HED with *in vitro*-based HED. Finally, risk was characterized by considering HED and the results of exposure assessment, conducted through systematic review and the consumer exposure model. This study conducted a comprehensive risk assessment of PFOA and PFOS in consumer products, incorporating both *in vivo* and *in vitro* data. Our findings suggest that *in vitro* data can complement hazard assessment. Future research could extend these findings to the risk assessment of alternative PFAS compounds lacking *in vivo* data.

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Keywords: PFAS, new approach methodologies, next generation risk assessment, consumer product, human equivalent dose

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In silico-In vitro-In vivo Combined Approach for Screening Neurodevelopmental Toxicity of Plastic Additives Based on Adverse Outcome Pathway Network Leading to ASD-Like Behaviors

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Abstract

Autism spectrum disorder (ASD) is a neurodevelopmental disorder for which the environmental causes are still poorly understood. As part of efforts to assess developmental neurotoxicity, an Adverse Outcome Pathway(AOP) framework and battery of assays for regulatory development are being developed. In this context, we identified a putative AOP network associated with ASD-like behavior to gain insight into the ASD potential of environmental chemicals using in silico-in vitro-in vivo combined approach. Frist, we selected human genes (NLGN4X, NRXN1) related to synaptic function mechanism of ASD using SFARI Gene database. Next, we developed the putative AOP network using a database mining approach as previously done, using the Comparative Toxicogenomics Database, AOP Wiki and AOP-DB. Leveraging these AOP network, we screened five environmental plastic additives (bisphenol A(BPA), tetrabromobisphenol A(TBBPA), and hexabromocyclododecane (HBCD), di(2-erhylhexyl) phthalate(DEHP), triclosan(TCS)) by conducting further experiments on specific KEs, such as NMDA receptor binding, calcium influx, BDNF level, cell death, decreased synaptogenesis and decreased learning(measured as development and behavior). For these assays, human embryonic stem cells, human neural stem cells, wildtype Caenorhabditis elegans and C. elegans mutants (nlg-1(lf) and nrx-1(lf) exhibiting decreased synaptogenesis related to ASD) were exposed to plastic additives at 1,10 and 100 μM and molecular docking were performed. First, to screen the chemicals, we observed the locomotive behavior as an Adverse Outcome (AO) of C. elegans (Wildtype, nlg-1, nrx-1) exposed to these plastic additives and NMDA receptor binding as the Molecular Initiating Event (MIE). When exposed to BPA, significant alteration was observed in the AO, late KE (synaptogenesis) and MIE. Next, to evaluate whether BPA can be a stressor of this AOPN, stem cells were exposed to BPA to identify early KEs (calcium influx, BDNF level, and cell death). Among the five chemicals, BPA has the highest ASD-like behavior leading potential, as BPA reacted with all KEs. This study suggests that in silico, in vitro and in vivo integrated approach has the potential to identify causal relationships between BPA exposure and ASD-phenotype.

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AOP-Anchored Transcriptome Analysis Catalogue Accelerates the Discovery of Environmental Toxicants in Zebrafish

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Abstract

Effective toxic screening approaches to evaluate the vast number of environmental chemicals that require assessment are needed. The aim of the present study was to develop an adverse outcome pathway (AOP)-anchored transcriptome analyses (AATA) catalogue to expedite the discovery of environmental toxicants. 437 AOPs from the AOPwiki and 2,280 transcriptomic datasets from NCBI Gene Expression Omnibus (GEO) and EMBL-EBI ArrayExpress (AE) repositories were comprehensively reviewed and analyzed. By using the differentially expressed molecular Key Event (mKE) genes as connection points, we created a large-scale environmental substance- target gene (mKE)- predicted adverse outcomes (SGAs) network that included 78 substances, 1,099 genes, and 354 adverse outcomes (AOs). To validate the reliability of the network, a comprehensive literature verification was conducted. We demonstrated that 164 AOs have been previously characterized in the literatures and the results for 136 AOs were consistent with the predictions of the AATA catalogue, representing an accuracy rate of 82.9%. Besides, distinct patterns in molecular Key Events and AOs among categories of substances, such as biocides and metals, were demonstrated. Moreover, experimental verification were further conducted, with exposures of zebrafish to perfluorooctane sulfonate (PFOS), cresyl diphenyl phosphate (CDP), and lanthanum ($LaCl_3$). Results demonstrated consistency with predictions of the AATA catalogue, with an accuracy rate of 92.3%. Collectively, the present findings support the AATA catalogue as an efficient platform for identifying environmental toxicants to fish and thereby provide novel insights into the understanding of potential risks of environmental substances.

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Wastewater Surveillance Provides Spatiotemporal SARS-CoV-2 and Influenza Virus Infection Dynamics

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Abstract

Wastewater surveillance can leverage its wide coverage, population-based sampling, and high monitoring frequency to capture citywide pandemic trends independent of clinical surveillance. In this study, we developed the sensitive and high-throughput methods for the detection of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) and influenza virus in wastewater samples. Moreover, we conducted the longitudinal monitoring from 12 wastewater treatment plants (WWTPs), covering approximately 80% of the population, to monitor infection dynamics

in Hong Kong. Our findings demonstrate that large-scale intensive wastewater surveillance from WWTPs provides cost-effective and timely public health information, especially when the clinical surveillance is inadequate and costly. This approach also provides insights into pandemic dynamics at higher spatiotemporal resolutions, facilitating the formulation of effective control policies and targeted resource allocation.

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Reproductive toxicity of 6-PPD quinone at environmentally relevant concentrations and underlying mechanisms in *C. elegans*

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Abstract

6-PPD quinone (6-PPDQ), a derivative of tire antioxidant 6-PPD, was reported to have acute toxicity for organisms. However, the possible reproductive toxicity of 6-PPDQ and underlying mechanism are still largely unclear. Using *C. elegans*, we investigated the reproductive toxicity and potential mechanisms after long-term exposure to 6-PPDQ. Firstly, exposure to 6-PPDQ (1 and 10 μg/L) reduced the reproductive capacity. Meanwhile, exposure to 1 and 10 μg/L 6-PPDQ enhanced the germline apoptosis, which was accompanied by upregulation of *ced-3*, *ced-4*, and *egl-1* expressions and down regulation of *ced-9* expression. The observed increase in germline apoptosis in 6-PPDQ exposed nematodes was associated with the enhancement in DNA damage and the induction of cell corpse engulfment. On the other hand, we also observed the association of ferroptosis activation with reproductive toxicity of 6-PPDQ. After 6-PPDQ exposure, Fe^{2+} content was increased, which was accompanied with enhanced lipid peroxidation, increased malonydialdehyde (MDA) content, and decreased L-glutathione (GSH) content. In addition, 6-PPDQ exposure decreased expressions of *ftn-1*, *ads-1*, *gpx-6* and increased *bli-3* expression. RNAi of *ftn-1* decreased *ads-1* and *gpx-6* expressions and increased *bli-3* expression. Meanwhile, RNAi of *ftn-1*, *ads-1*, and *gpx-6* induced susceptibility, and RNAi of *bli-3* caused resistance to the activation of ferroptosis and reproductive toxicity of 6-PPDQ. Moreover, ferroptosis could regulate the expressions of DNA damage checkpoint genes and 6-PPDQ-induced germline apoptosis. Our results demonstrated that 6-PPDQ at environmentally relevant concentrations induced reproductive toxicity of 6-PPDQ through germline apoptosis associated with the enhancement of DNA damage, the induction of cell corpse engulfment, and the activation of ferroptosis in organisms.

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Toxicity Big Data and AI in Chemical Risk Assessment: Potential and Challenge

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Abstract

New Approach Methodologies (NAMs) have emerged as innovative alternatives to traditional animal testing for chemical risk assessment. NAMs leverage *in vitro* and *in silico* techniques to predict chemical toxicity. *In silico* approaches use computational tools such as structure-activity relationship, machine learning, and bioinformatics. Our ongoing projects, "Development of Environmental Diseases Prediction Model Based on Molecular Toxicity Network," aims to develop a platform for predicting toxicity and environmental diseases. By combining chemical and biological databases, we developed a knowledge-based database to refine toxicity data and provide training datasets for AI models. As a case study, ToxCast-based AI models were developed using various machine and deep learning algorithms to predict toxicities. We are also applying these approaches in next-generation risk assessment (NGRA) and safe-by-design (SbD) strategies. For NGRA, we compile NAMs data to compare NAM-derived risk assessment results with those from traditional animal testing, evaluating their applicability and effectiveness. For SbD, our research focuses on nanomaterials and PFAS, examining how physicochemical properties influence toxicity levels. By understanding these relationships, we propose developing safer substances, ensuring new materials are designed with minimal toxicity. Despite their potential, *in silico* approaches face several challenges for regulatory acceptance. Capturing the full range of biological responses, particularly for complex endpoints like carcinogenicity or reproductive toxicity, is a primary challenge. Current ToxCast models may not fully replicate *in vivo* interactions, limiting their predictive capability. Integrating diverse datasets and ensuring interoperability of computational tools is also challenging. Furthermore, addressing the limited availability of high-quality data is essential. While NAMs offer a promising future for risk assessment, significant efforts are needed to address scientific, technical, and regulatory challenges to fully realize their potential.

Keywords: new approach methodologies, risk assessment, toxicity prediction, artificial intelligence, next generation risk assessment

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Key consideration and practice on polymer biodegradation study

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Abstract

The environmental fate of polymers has attracted growing attention in the academic, industrial, and regulatory communities as well as in the public as global production and use of polymers continue to increase. The existing methods have limitation in determining the biodegradability on macromolecules. Moreover, due to the wide usage and application, investigating the key factors for polymer biodegradation become more and more important. The biodegradation of five polymers were studied in this study. No pre-treatment was employed prior to the biodegradation test. The exposure condition as well as the inoculum were refined to make the test closer to real environmental condition. The test duration was extended to 60 days and the long lag-phase time allowed the adjustment for competent microbiota. The increased test volume can improve the biodiversity and increase the biodegradation "lottery". Since the fungi invade capability on petroleum-based polymer in the recent research, the mixed inoculum with both active sludge and soil supernatant was prepared in this study. The results showed that the polymer reference of microcrystalline cellulose attain the pass level of 60% within 28 days. Four testing polymers didn't get the pass level in the standard period. However, all of them were degraded continuously in the prolonged duration and met 60% by day 60. No obvious exponential degradation period was observed in these polymers. It infers that every constituent with various molecular weight has its own degradation kinetics, and the window time is not applicable for the polymer. The biodegradability in the modified OECD 301F is generally higher than the modified OECD 301B results. Two possible reasons are supposed here. 1. The fungi density in all the four testing polymers increased during the OECD 301F test but it was not found in the OECD 301B test. This result support the previous finding that fungi maybe helpful for some polymers biodegradation. 2. The measured total organic carbon and measured chemical oxygen demand were used for the biodegradation calculation in this study. The measured COD is usually a little lower than the theoretical oxygen demand which may overestimate biodegradation in 301F to a little extent. In conclusion, the optimized test condition and mixed inoculum adoption are helpful for the assessment of polymers biodegradation. It can reflect the polymeric compounds' potential biodegradability in the environmental more accurately.

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Can New Approach Methodologies (NAM) and Quantitative Adverse Outcome Pathways (qAOP) Replace Future Fish Toxicity Testing?

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Abstract

A paradigm shift in chemical hazard assessment from conventional laboratory animal-based *in vivo* toxicity testing to better utilization of cost-effective and ethically-sound New Approach Methodologies (NAMs), such as *in silico* predictions, *in vitro* high-throughput screening (HTS) and non-vertebrate models that have strong compliance with the 3Rs (refine, reduce, replace) principle, has been gradually

taking place in the past two decades. Although NAMs are proven to be highly useful for classification and prioritization of chemicals, their relevance for generating hazard information that can be directly used for regulatory decision-making is under discussion, as most NAMs only provide information on lower (e.g., molecular/cellular) levels of biological organization. Adverse Outcome Pathways (AOPs), which causally link toxicological responses across multiple levels of organization, can in this case serve as a translator. Quantitative AOP (qAOP) models may further allow prediction of regulatory relevant hazard information based on NAM data. In this presentation, we will use a case study to demonstrate how NAMs and qAOPs work together to provide useful hazard information and replace conventional fish toxicity testing in the future. The study focuses on energy depletion-associated growth inhibition caused by mitochondrial uncouplers. An AOP network (AOPN) was constructed first and used to guide the generation of *in vitro* key event data (temporal- and concentration-response) from the zebrafish liver (ZFL) cell-line exposed to the model uncoupler, CCCP. We used *in vitro* cell population growth to indicate *in vivo* fish liver growth as the final adverse outcome to avoid fish tests. 105 time-resolved qAOPN models were constructed using piecewise structural equation modeling and ranked based on their predictive abilities. The top qAOPN model was then challenged by additional NAM data generated from ZFL cells exposed to 5 environmentally relevant uncouplers (selected from the US Tox21 HTS program) to evaluate the model performance. The results suggest that the qAOPN model built based on the prototypical chemical (CCCP) is in general able to predict growth for other chemicals with different levels of uncertainties (mainly arise from differences in chemical properties and internal concentrations). Our case study shows a bright future of generating useful hazard information and replacing fish growth tests by a combination of NAMs and qAOPs.

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Coupled modeling for assessing the life cycle environmental risks of shale gas exploration in China

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Abstract

Environmental impacts associated with shale gas exploitation have been historically underestimated due to neglecting to account for the production or the release of end-of-pipe organic pollutants. Here, we assessed the environmental impacts of shale gas production in China and the United States using life cycle assessment. Through data mining, we compiled literature information on organic pollutants in flowback and produced water (FPW), followed by assessments using USEtox to evaluate end-of-pipe risks. Results were incorporated to reveal the life cycle risks associated with shale gas exploitation in both countries. China exhibited higher environmental impacts than the US during the production phase. Substantially different types of organic compounds were observed in the FPW between two countries. Human carcinogenic and ecological toxicity attributed to organics in FPW was 3 orders of magnitude higher than that during the production phase in the US. Conversely, in China, end-of-pipe organics accounted for approximately 52%, 1%, and 47% of the overall human carcinogenic, noncarcinogenic, and ecological impacts, respectively. This may be partially limited by the quantitative data available. While uncertainties exist associated with data availability, our study highlights the significance of integrating

impacts from shale gas production to end-of-pipe pollution for comprehensive environmental risk assessments.

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Soil Ecological Risk Assessment of Various Mines on the Southern Tibetan Plateau: A TRIAD Approach

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Abstract

Soil ecological risks caused by mining activities have attracted global attention. Particularly in remote areas characterized by fragile ecological ecosystems, such as the Tibetan Plateau, the issue of mining-related pollution demands immediate attention. In this study, the TRIAD approach, which integrates three lines of evidence (LoE)–chemical LoE (Chem LoE), ecotoxicological LoE (Ecotox LoE) and ecological LoE (Eco LoE) was conducted to evaluate the soil ecological risk assessment in three mines. Chem-LoE (total metal concentrations) followed the risk order of lead–zinc > chromite > copper mines. Trends were observed for the Ecotox-LoE (the survival rates of earthworms and collembolans) and Eco-LoE (the total vegetation coverage): copper > lead–zinc > chromite mines. In additional, collembolans (*Folsomia candida*) exhibit greater sensitivity compared to earthworms (*Eisenia andrei*) in three mines. Through the combination of three LoEs, soil ecological risk followed the order chromite > lead-zinc > copper mines. Meanwhile, further exploration of the correlations between environmental factors [(*i.e.*, pH, soil organic matter, and cation-exchange capacity and Chem-LoE, Ecotox-LoE, Eco-LoE, and integrated risk revealed that soil organic matter is the dominant factor that control the integrated risk. Overall, the results provide novel insights into ecological risk assessments of mineral deposits and unveil the associated influence factors, helping to provide a basis for government departments and industries to carry out detailed further investigations in mines.

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Hypoxia-associated seasonal shifts of marine community in Jinhae Bay, South Korea: A case study through environmental DNA metabarcoding

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Abstract

Environmental DNA (eDNA) offers non-destructive, accurate, cost-effective, and rapid biomonitoring allowing to overcome practical challenges in traditional biomonitoring. In this study, we investigated the monthly variations in marine eDNA community composition in Jinhae Bay, South Korea, where seasonal hypoxia is prevalent due to anthropogenic eutrophication. Study of eight months of eDNA survey revealed significant changes in community in summer when hypoxia and stratification occurred. This change in composition was largely influenced by the most dominant phylum Arthropoda that showed a negative correlation with hypoxic water mass, especially copepods belonging to the order Calanoida and Poecilostomatoida. These shifts in dominant species under hypoxic conditions likely contribute to alterations in the food web structure of Jinhae Bay, as revealed by weighted gene correlation analysis. Moreover, the recovery of the food web structure following the return to normal oxygen conditions was delayed compared to the losses observed following the onset of hypoxia, highlighting the adverse ecological effects of hypoxia exacerbated by climate change. Our findings underscore the potential impact of hypoxia on marine community dynamics.

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An Artificial Intelligence Approach for Multi-Risk Dynamics of Water Quality Under Anthropogenic Pressures and Climate Change

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Abstract

Water quality serves as a critical determinant of ecosystem health and directly impacts water-use sectors like agriculture and public health. However, the synergistic interactions between extreme climate events and anthropogenic activities can significantly alter water quality dynamics. Furthermore, these impacts are likely to be exacerbated within the context of ongoing climate change and socio-economic development. The main aim of this work is to understand the multi-risk dynamics for water quality by leveraging heterogeneous data at different spatial and temporal scales, e.g. climate data, land-use data, and in-situ water quality measurements by using machine learning techniques and spatio-temporal Bayesian network models. Water quality multi-risk models are developed to explore the synergistic impacts of climate extreme events and anthropogenic pressures on physicochemical water quality parameters (i.e. nutrients, suspended solids, DO, temperature), and other key elements (i.e., biological, chemical, overall ecological status), considering also specific vulnerabilities and exposures of river networks and basins, including the nexus between water quality indicators and the multiple water-dependent sectors (i.e. food and energy production). Land-use and climate change impacts on water

quality are analyzed at different spatial scales in Italy (Adige river basin, Veneto Region, and national level) respectively in three different projects (iNEST, Myriad-EU, and GRINS). These approaches are being developed as potential tools to complement in-situ measurements with additional data sources (e.g. climate, land-use, etc.) for a better understanding of the multi-risk dynamics of water quality at various spatial scales and temporal horizons.

1031

Deriving Aquatic PNECs of Endocrine Disruption Chemicals by Combining Species Sensitivity Weighted Distributions (SSWD) and Adverse Outcome Pathway (AOP) Networks

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Abstract

Endocrine-disrupting chemicals (EDCs), e.g., bisphenols, phthalates, per- and polyfluoroalkyl substances, pose long-term adverse effects on aquatic organisms. The current commonly used ecological risk assessment (ERA) framework mainly focuses on acute and chronic lethal effects of chemicals, rather than reproductive and developmental effects. The mode of toxicity action of EDCs was not fully considered in ERA, which may result in an underestimation of ecological risks. In the study, the species sensitivity weighted distribution (SSWD) models based on adverse outcome pathway (AOP) networks were developed for deriving predicted no-effect concentrations (PNECs) of selected EDCs. Three weighting criteria (intraspecies variation, trophic level abundance, and data quality) and weighted log-normal distribution methods were adopted. This method combined the advantages of both models and provided reliable estimates of PNECs. SSWD models can consider the inter/intraspecies variation and quality of toxicity data of EDCs. AOP network can integrate nontraditional endpoints and muti-biological levels of endocrine disruption effects. For instance, the PNECs of endocrine disruption effects were derived as 8.10 μg/L for BPA, 12.9 μg/L for DBP, and 2.52 μg/L for PFOS, which were more conservative than those derived from the acute toxicity data and were comparable with the values in the literature based on the chronic toxicity data. The long-term effects of EDCs are significant and need to be fully recognized in the ERA. This study provided an ERA framework that can improve the ecological relevance and reduce the uncertainty of PNECs of EDCs.

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Environmental RNA Application in Community Toxicity Testing and Ecological Risk Assessment

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Abstract

Chemical pollution is a global challenge that threatens ecosystem safety. The Kunming-Montreal Global Biodiversity Framework proposed to reduce pollution risks to levels that would not harm biodiversity and its functions. This framework imposed greater demands on the ecological risk assessment of chemical pollution. Conventional ecotoxicity tests focused on species, neglecting genetic diversity and species interactions within communities. Here, we propose a novel strategy using environmental RNA (eRNA) combined with meta-transcriptomic analysis to evaluate chemical pollution across multiple species and biological levels. This study highlights the current state of the science and outlines a path forward for eRNA-based chemical pollution risk assessment. Additionally, it suggests a community toxicity testing strategy and develops a dose-response model of biological impacts from molecule to community. Finally, the study discusses the technical and theoretical challenges associated with eRNA for its application in assessing the ecological impacts of chemicals and mixtures.

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Transgenerational toxicity and risk assessment of neonicotinoid insecticides on natural enemy insects

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Abstract

Neonicotinoids (NEOs) are widely used to control pests and applied on many crops. However, continuous and extensive application often causes contamination in farmland which indicates negative effects on non-target organisms. Natural enemy predators are important regulators to control pests in integrated pest management (IPM) for agricultural systems. To evaluate the neonicotinoid insecticide ecotoxicity in natural enemy which is a crucial focus of IPM programs, however, the study of negative effects on ladybeetle almost focus on acute toxicity, ignoring sublethal effects and intergenerational effects under long-term exposure. Herein, (1) We evaluated the ecological toxicity of 6 neonicotinoid insecticides to the natural

enemy ladybird (*Coccinella Septempunctata L*) by using the leaf residue method to simulate the actual situation in the field; (2) explore the sublethal and transgenerational effects, including development time, longevity, and fecundity were evaluated using the age-stage, two-sex life table theory, in second-instar larvae of ladybeetle exposed to environmentally relevant concentration of NEOs; (3) Transcriptome analysis was used to explore the mechanism of transgenerational toxicity of neonicotinoid insecticides to the natural enemy ladybird

1. Risk assessment results showed that the hazard quotient (HQ) values in field and off-field were all above 2, indicating that 6 NEOs showed potentially harmful to ladybeetle.

1. Under environmentally relevant concentrations of NEOs, adverse effects on survival, development, total longevity, reproductive capacity, and predation ability in ladybeetle were observed. In addition, demographic growth parameters of the F1 generation such as net reproductive rate, and the intrinsic and finite rates of increase were significantly decreased under sublethal dosage LR_{30} (1.91 g ai/hm^2)
2. For transcriptome expression, the mechanism of intergenerational toxicity on NEOs to the ladybeetle were identified pathways related to metabolism of retinol,, biosynthesis of steroid hormone, P450 metabolism, and metabolism of xenobiotics by inhibited

In conclusion, NEOs have potential risk to ladybeetles under sublethal conditions. It has negative effects on survival, bodyweight, predatory ability, and hatchability. development duration of ladybeetles was also prolonged. Therefore, in order to protect the healthy development of ladybeetles populations in the field, we recommend a safe threshold at least LR_{10} (0.93g ai/hm^2). Meanwhile, it is suggested that the risk assessment of pesticides on beneficial non-target natural enemies should be extended to multiple generations

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High-Throughput Omics Approaches in Daphnia: Advancing Precision Toxicology for Chemical Safety

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Abstract

High-throughput omics approaches have emerged as transformative tools for New Approach Methodologies (NAMs) in hazard evaluation of environmental chemicals. High-throughput omics approaches enable to profile biomolecular dose-response changes for qualitative and quantitative assessment of chemicals (e.g. mechanism-of-action characterization, chemical clustering/read-across, and molecular points of departure derivation). Although these approaches appear promising, to date their focus has been limited to human health. Moreover, a long-standing challenge is the regulatory acceptance

of omics due to the lack of standardization. The objective of the present study is to evaluate the ability of high-throughput omics approaches for hazard characterization of environmental chemicals with an invertebrate species. We developed and applied high-throughput omics (transcriptomics, metabolomics, and phenomics) approaches in Daphnia, a widely used invertebrate model in aquatic toxicity testing, to comprehensively investigate molecular perturbations caused by a large set of chemical substances. We used a wild species Daphnia magna (D. magna) resurrected from a biological archive of Lake Ring, Denmark, which demonstrated higher sensitivity than laboratory Daphnia on immobilization. Transcriptomics and metabolomics analysis can identify key biological pathways perturbed in D. magna, which are also conservatively found in other model organisms like Drosophila. High-throughput phenomics platform precisely captured significant mobility changes induced by neuroactive chemicals and environmental pollutants (e.g., PFOA). Lastly, integration of the multi-omics data into an adverse outcome pathway network framework can be used to predict potential apical effects by chemical grouping/read-across. Overall, this high-throughput omics assay with D. magna holds promise for a tiered hazard evaluation and screening strategy utilizing NAMs.

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Dose-dependent Functional Genomics Approach: Enhancing Precision in Chemical Toxicity Assessment

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Abstract

Omics strategies in toxicology, including transcriptomics, proteomics and metabolomics, have shown great performance for unbiased evaluation of the perturbed biological pathways systematically under chemical exposure. However, these traditional omics approaches can only infer the potential molecular toxicity mechanisms indirectly due to the complex interaction of differential expressed genes or proteins. In contrast, the dose-dependent functional genomics approach in *Saccharomyces cerevisiae* offers direct links between chemical exposure and genes across a wide concentration range, thereby identifying the molecular initiating event (MIE) of chemical toxification and yielding point of departure (POD) at genome-wide scale. Moreover, characterization of temporal variability and repeatability has validated the robustness, stability, and reproducibility of the POD results obtained through this approach, as well as the effective identification of the MIE across both short- and long-term exposure scenarios. The platform's utility is underscored by its application in assessing the toxicity mechanisms of a diverse array of chemical substances. For instance, when investigating the toxicity mechanisms of organophosphate flame retardants (OPFRs), this methodology pinpoints the POD for these chemicals and unravels the relationship between biological potency and chemical structures. Furthermore, this approach has been extended to evaluate the synergistic toxicity mechanisms arising from combined pollutants. Regarding the co-exposure scenario involving microplastics alongside triclosan (TCS), the methodology quantitatively compared the POD of affected pathways under both combined and individual exposures, illuminating the molecular mechanisms underlying the altered toxicity profiles in the combined exposure scenario. Lastly, this yeast-based approach offers a high-throughput, cost-effective solution for chemical risk assessment, while the integration of this approach with other omics technologies at multiple biological levels will

further enhance its capabilities in toxicology. Collectively, the yeast dose-dependent functional genomics approach demonstrated great advantages in identifying the MIE perturbed by environmental emerging pollutants and is beneficial for guiding further chemical risk assessment.

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Genetic Modulation of Stereoselectivity of Cytotoxicity of 6PPD and 6PPDQ

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Abstract

As a rubber antioxidant, N-phenyl-N′-(1,3-dimethylbutyl)-p-phenylenediamine (6PPD) and its oxidation product 6PPD quinone (6PPDQ) have received widespread attention for their extensive environmental detection and toxicity. Tire wear particles generally contain high concentrations of 6PPD and 6PPDQ, and 6PPD will be oxidized to be 6PPDQ with higher toxicity. Respiratory exposure is the primary access to 6PPD and 6PPDQ merged in airborne particles, after entering into human lungs and blood circulation. At present, the only literature reporting on the toxicological mechanisms of 6PPD and 6PPDQ focused on oxidative stress and DNA damage. However, their pulmonary toxicity by immune impairment and the underlying mechanism remain unclear. Here, our study aims to identify key genes and pathways mediating pulmonary toxicity of 6PPD and 6PPDQ through functional genomics screening of human alveolar macrophages, and to provide mechanistic understanding of the stereoselectivity of cytotoxicity of 6PPD and 6PPDQ at the systems biology.

7. New Challenges in Chemical Mixture Risk Assessment

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Identification of Toxicants in Treated Flowback and Produced Water from Shale Gas Exploitation Using Effect-Directed Analysis Combined with Nontarget Screening

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Abstract

Shale gas has been regarded as alternative sources to traditional natural gas, however, extensive use of hydraulic fracturing in shale formations has generated substantial amounts flowback and produced water (FPW). Environmental safety of FPW that are highly complex with various chemicals has raised great concerns. Herein, an effect-directed analysis (EDA) method, involving zebrafish embryo toxicity tests, fractionation, target and nontarget chemical analysis, and toxicity confirmation using toxic unit (TU) and toxicological priority index (ToxPi) were applied to identify the major toxicants in FPW. Results showed that hydrophilic compounds significantly contributed to the observed toxic effects to fish embryos. An analysis of nearly a hundred target compounds identified 39 compounds in the effect fractionation. Of these, toxicity data were available for 29 toxicants, which contributed to 4.86% of the observed toxicity. Furthermore, nontarget analysis of effect fractionation was performed using a Thermo Scientific (USA) Orbitrap Exploris 240 LC-MS/MS and 583 pollutants were identified at level 2, with risks ranked using ECOSAR and ToxPi considering toxicity, relative abundance, and hydrophobicity. Six suspect toxicants with higher ecological risks than those identified by targeted analysis were identified and were chemically and toxicologically confirmed using reference standards, significantly enhancing the understanding of observed effects. The present study was the first to apply effect-directed analysis in the shale gas FPW.

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The Tip of the Iceberg: Contribution of Anthropogenic Contaminants and Natural Toxins to Species-Specific Seawater Toxicity

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Abstract

The Indo-Pacific finless porpoise and Chinese white dolphin are iconic threatened marine mammals in Hong Kong. Chemical pollution is amongst the multiple stressors that impact their health. Our understanding is lacking of what extent known contaminants contribute to mixture toxic effects of marine water on the porpoise and dolphin. To fill this knowledge gap, for the first time, we developed species-specific cell lines to assess the cytotoxicity of Hong Kong's marine water and identify key toxicity-contributing pollutants. For dissecting the toxicity-driving components in seawater, we profiled the cytotoxic potency of 41 chemicals previously monitored in Hong Kong coastal waters, including persistent organic pollutants (e.g., polycyclic aromatic hydrocarbons, polyfluoroalkyl substances and brominated flame retardants), organotins, ultraviolet filters, and algal toxins. Additionally, we performed mixture-toxicity modeling to assess their quantitative contribution to the cytotoxicity of seawater. The identified toxic chemicals collectively accounted for an average of 30% (range: 5% - 102%) of the overall

seawater toxicity. Pectenotoxin-2, a natural algal toxin produced by *Dinophysis spp*., explained an average of 25% of the mixture effect on porpoise cells (range: 3.4% - 87%). Other algal toxins produced by *Dinophysis spp* like dinophysistoxin-1 (DTX-1) and okadaic acid (OA) also constitute the largest share of mixture toxic potency in the habitats pf finless porpoise and Chinese white dolphin around the China costal waters. The mixture toxicity modelling suggested that algal toxin dominated toxicity to waters were featured by natural factors, such as algal blooms, and there may be remaining anthropogenic pollutants that have yet to be investigated in waters impacted by anthropogenic activities. While further efforts to identify other toxicity contributors and the sources of the key toxicity drivers in different regions, our study approach will facilitate the prioritization of marine contaminants and development of effect-based trigger assessment in order for concerted management of water quality and biodiversity conservation.

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Applying the principles of grouping and read-across to different lines of evidence to support the development of an ecotoxicity testing strategy for hydrocarbon UVCBs

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Abstract

Substance grouping and read-across are commonly employed to reduce the amount of testing required for chemical registrations under the EU REACH regulation (EC 1907/2006). These approaches use relevant information from analogous (‘source') substances to predict the properties of ‘target' substances. While available guidance tends to be tailored for mono-constituent substances, similar concepts can be applied for ecotoxicity testing of more complex UVCB substances (substances of Unknown, Variable composition, Complex reaction products, or Biological origin). In the present effort, we apply multiple lines of evidence, aligned with read-across principles, to design a testing program for hydrocarbon UVCBs.

Petroleum substances (PS) are comprised of complex combinations of hydrocarbons for which the precise identity of all constituents is usually unknown, and the composition is often variable. Despite these uncertainties, PS may be categorized according to their manufacturing process and their broadly similar physical-chemical properties. Using a comprehensive GCxGC analytical program, the composition of each hydrocarbon UVCB substance can be broken down into relative concentrations of groups defined by

carbon number and chemical class, termed hydrocarbon blocks (HCB). Using non-polar narcosis as the common primary mechanism of toxic action for hydrocarbons, toxicity would be correlated with bioavailability. It is then possible to use representative constituents for each of the relevant hydrocarbon blocks to estimate the toxicity of the whole substance.

For the testing strategy, we determine the "worst-case", or most toxic, sample using two independent methods: (i) an experimental biomimetic extraction-solid phase microextraction (BE-SPME) approach which mimics aqueous exposure to PS in the environment; and (ii) the PetroTox QSAR model that utilizes two sub models (i.e., target lipid model and an oil dissolution model) to estimate PS toxicity to ecological receptors. The outcomes of these two exercises allow for the selection of a "worst-case" PS sample for testing and account for the range in compositional variability across samples. The concepts and various lines of evidence applied here will support testing strategies for multiple PS categories and could inform chemical prioritization initiatives or other regulatory assessments of UVCBs.

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Challenges in Screening Global Chemical Inventories for Toxic Substances with Potential Adverse Environmental Impacts

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Abstract

The United Nations 2030 Sustainable Development Goals include the goal of "environmentally sound management of chemicals … in order to minimize adverse impacts on human health and the environment". Knowledge of how many chemical substances are in commerce, their molecular structure, production, uses, phys-chemical properties, and toxicity are key information requirements for sound management. This information is usually available to chemical regulators although it is often incomplete. Globally, about 19 countries have lists of chemicals. Only recently has the global inventory of ~350,000 substances produced at >1 t/yr been developed (Z. Wang et al EST 2020). Including separate registries for pesticides and pharmaceuticals, brings the total number of large volume commercial substances to ~375,000. The objectives of this presentation are to provide an overview of what we know and don't know in terms of the above information, and to suggest some ways to address knowledge gaps. Data on the mammalian and aquatic toxicity of the 375,000 substances are lacking, especially for industrial chemicals. Molecular structures are available for ~238,000 individual compounds but only ~10% have measured toxicity data available. Measurement data indicating which chemicals and transformation products are present in environmental media is also very useful for assessing chemical exposure and risk. However, a survey of all published data from 1970 to 2021 (Muir et al. EST 2023) showed that only ~19,800 chemicals had been reported in environmental media. The majority were pharmaceuticals and pesticides which accounted for 50-60% of substances reported for the period 2000-2021. Screening of chemicals using machine learning approaches is a very promising approach for identifying chemicals and degradation products with potential adverse effects. However, the lack of toxicity and property data for

the vast majority of substances limits the broad application of artificial intelligence approaches. There are thus many challenges for environmental toxicologists and environmental chemists in terms of expanding knowledge on the universe of chemicals in commerce. Development of a publicly accessible global database would help to identify a much wider array chemicals with potential for human exposure or environmental release, as would requiring manufacturers to make available analytical standards of new and existing chemicals in commerce as part of the registration process.

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Assessing Regional Aquatic Ecosystem Risks Using Large Language Models

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Abstract

Chemical mixtures present significant challenges in environmental risk assessment due to the vast number of pollutants and unclear relationships between them and effects. AI techniques like text mining and machine learning can address data gaps. However, high integration and usage barriers hinder their popularization. To help researchers overcome these hurdles and focus on solving environmental problems, we developed AgentEDT, an AI-integrated system for aquatic ecological risk assessment. AgentEDT utilizes GPT-4, integrating named entity recognition, deep learning fingerprint prediction, and experimental data analysis rules. Users can quickly obtain results through prompts. The system, fine-tuned with 480,000 pollution articles, accesses data from sources like NORMAN, ToxCast, and AOPwiki to build a comprehensive knowledge base. AI modules are integrated as toolkits for execution. Predictions and experimental data are processed within AgentEDT. Researchers input natural language, and AgentEDT performs text mining, machine learning model training, and data analysis in a no-code environment. Responses are generated through chain-of-thought (CoT) and retrieval-augmented generation (RAG), ensuring professional and accurate results. To validate the system, we established a time series Transformer model for GPT-4 based on 480,000 articles. PFAS concentrations from over ten regions were collected and total concentrations calculated. Production parameters predicted total concentrations in the environment. Findings indicate a significant gap between measured and predicted PFAS concentrations before 2020, with 2011's total concentration potentially over ten times the measured concentration. To verify AgentEDT's accuracy, we constructed knowledge prompts based on the NORMAN database. Responses in zero-shot, CoT, and RAG modes were tested within 200 chemicals. Accuracy was evaluated in terms of realism, user alignment, and hallucination. CoT improved answer precision (realism from 20% to 60%) and user alignment (55% to 90%). RAG further enhanced realism and user alignment to 95% and 99%. AgentEDT effectively replaces manual searches of literature and database data, deriving risk-relevant conclusions. AgentEDT suits today's big data era in environmental science, facilitating the extraction of vast chemical and effect data from mixtures, enabling researchers to rapidly use advanced tools to address aquatic ecological risk challenges.

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Event driven taxonomy (EDT): Deep learning(DL) links effect-directed analysis (EDA) and non-target analysis (NTA)

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Abstract

The world is composed of complex mixtures. Identifying causative toxicants is critical for understanding mixture risk but there are many gaps among chemical and bioactivity data. Effect-directed analysis integrates chemistry and biological information to identify toxicants, yet conventional bioassays typically rely on an apical and/or single endpoint, providing no mechanistic information with limited diagnostic potential to guide chemical identification. These practices are further challenged because chemical screening analyses are commonly restricted to the available MS libraries. This limitation can be overcome by a novel event-driven taxonomy (EDT) framework for mixture risk assessment that relies on high-throughput screening bioassays and chemical predictions integrated by artificial intelligence. The EDT framework was evaluated using complex sediment mixtures eliciting activation of arylhydrocarbon receptor and oxidative stress response. While mixture prediction using expert knowledge-oriented target analysis explained <10% of observed bioactivity in sediment extracts, a recently developed metadata-driven suspect analysis expanded the fraction explained to >80%. Additionally, deep learning models were developed to cluster fingerprints of bioactive candidates and convert these candidates to MS-readable information for non-target screening with HRMS. Collectively, we present a "bioactivity-signature-toxicant" mixture deconvolution strategy to connect patchy datasets and guide non-target analysis for diverse chemicals for the first time.

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Pesticide Occurrence and Environmental Risks in Chinese Farmlands: Modeling and Monitoring Approaches

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Abstract

To date, about 600 pesticides have been registered and used in China; some of these chemicals may accumulate in the soil, potentially leaching into groundwater and migrating to surface water. Compared with other pesticides, some may pose a higher risk due to their greater persistence in the environment, higher dosage and higher ecotoxicological properties. Their risks to environmental safety from soil accumulation and movement to groundwater and surface water remain unclear. Monitoring data and model predicted concentration can be used to assess the exposure to pesticides in farmland of China. The current study investigated the presence of 50 commonly used pesticides in soil, groundwater and surface water of farmlands from major agricultural zones in China according to a year-round monitoring program. In addition, fate models were used as effective screening tools to estimate the soil exposure, leaching potential, and aquatic exposure of these targets in farmlands of China with a wide range of target crops, climate, topography, soil type, and agricultural practices. The corresponding environmental risks were assessed for exposure to individual pesticides and mixtures to non-target organisms, including earthworms and aquatic organisms, and to human health through consumption of pesticide-contaminated groundwater. In addition, the agreement between monitoring results and modeling results was investigated and the robustness of the modeling assessment was evaluated.

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Next Generation Risk Assessment of Chemicals in Consumer Products Incorporating Mixture Toxicity Assessment: A Case Study on Triclosan

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Abstract

The exposure of humans to various chemicals via consumer products underscores the necessity for comprehensive risk assessment methodologies. Current approaches, reliant on animal testing, face challenges of expense and ethical concerns, necessitating the development of alternative strategies aligned with the principles of Replacement, Reduction, and Refinement (3R). Moreover, there exists a notable gap in evaluation methodologies concerning the combined toxicity of chemicals present within products. This study aims to address this gap by proposing a next-generation risk assessment framework that integrates an analysis of mixture toxicity, demonstrated through a case study on triclosan (TCS). In the first step, a hazard assessment of triclosan was conducted through the integration of in vitro data obtained from ToxCast and literature in Pubmed, categorized across 21 toxicity endpoints. Point of Departure (POD) was calculated utilizing New Approach Methods (NAM) data and the steady-state concentration (Css) determined using the httk model. In the second step, the SEEM3 consensus model provided by ExpoCast was employed to estimate the exposure levels of triclosan, calculate Benchmark Dose, and compare these results with traditional risk assessment results. In the third step, an investigation into consumer products containing triclosan was conducted using Ecolife, a Korean consumer product database, identifying 28 cleaning products. Among the product components, triclosan was primarily identified in combination with 1,2-Benzisothiazol-3(2H)-one (BIT) and Linalool (LNL). In the fourth step, we screened the mixture toxicity effects on cell viability,

reactive oxygen species (ROS) generation, and inflammation using three cell lines (Beas-2b, HepG2, E6-1) for binary combinations of these substances (TCS+BIT, TCS+LNL). This case study offers a novel strategy for assessing chemical substances present in consumer products by integrating in silico and in vitro data into the risk assessment process, while also examining the combined effects of their mixtures.

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Key words: Triclosan, Consumer Products, Next Generation Risk Assessment, Mixture Toxicity, in vitro Screening

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Human Exposure and Risk Prioritization of Current-use Pesticides in Indoor Environments from an Agricultural Region

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Abstract

Despite being regarded as safer alternatives to traditional organochlorine pesticides, current-use pesticides (CUPs) are now identified as emerging contaminants with growing evidence of their toxicity to wildlife and humans. In this study, we collected samples of dust, drinking water, and urine from 81 families in the state of Indiana, United States, analyzing them for a comprehensive list of 96 CUPs, including 61 insecticides, 26 herbicides, and 9 fungicides. Of these, 37, 33 and 17 CUPs were identified in dust, drinking water and urine with a cumulative median concentration of 18 300 ng/g, 101 ng/L and 3.93 ng/mL, respectively. Notably, concentrations of neonicotinoids (NEOs) in dust were substantially higher than those reported in other studies, indicating severe pesticide contamination in Indiana homes. Herbicides were the most abundant CUPs detected in drinking water with a contribution of 59% of total observed contamination. The highest estimated daily intakes (EDIs) from drinking water and dust consumption were observed for imidacloprid, with a median value of 0.99 ng/kg/day. Our results showed that dust ingestion was a more important exposure pathway for most insecticides and fungicides, while drinking water consumption was an important exposure pathway for herbicides. In addition, a toxicity equivalent factor model incorporated with the ToxCast database indicated that imidacloprid poses the greatest toxicity risk and is of top management priority. This study underscores the importance of monitoring the pesticide contamination in indoor environments and sheds light on the health risks associated with CUPs, particularly for residents near agricultural areas.

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Something from nothing? Chemical Cocktails Threaten the Environment and Human Health

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Abstract

An overwhelming number and diversity of organic chemicals are in daily use and enter the environment during or after use and disposal. Chemical pollution is an increasing threat to our environment, to wildlife and to people. The impact of chemical pollution will be amplified by population growth and climate change. However, conventional chemical monitoring and biomonitoring programs have been criticized on the basis that they cannot include the full range of chemical pollutants that could occur in the environment including transformation products, and they do not account for the combined effects of mixtures of chemicals. Bioanalytical tools may therefore complement chemical analysis for cost-efficient and comprehensive (bio)monitoring. Bioanalytical tools are *in vitro* cell-based bioassays that target specific mechanisms of toxicity and give a measure of the toxicity of mixtures of known and unknown chemicals. Bioanalytical tools provide measures of the cumulative effects of mixtures of chemicals that exhibit the same mode of toxic action plus they can give a measure of the cytotoxicity of all chemicals. One of the biggest challenges for the application of *in vitro* bioassays is the comprehensive extraction of organic chemicals from complex and often also organic matrices. A smart combination of passive equilibrium sampling for hydrophobic pollutants together with solid-phase extraction for more hydrophilic and ionizable organic chemicals leads to a defined extraction without changing mixture composition. Using case studies on the continuum from wastewater/surface water via drinking water and food (fish and milk) to biomonitoring of human samples (tissues, blood, milk), I will illustrate how a combination of chemical analysis and bioanalytical tools in conjunction with mixture modelling can help to understand which fractions of the chemical pollution are known and which are unknown. Improved detection of the presence of mixtures of chemicals in people informs chemical risk assessment and management options.

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Comparative Species Sensitivity in Effect-Directed Analysis of Coastal Pollutants Using AhR Recombinant Yeast

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Abstract

With the rapid increase in potential pollutants and the complex state of coastal pollution, there is a heightened focus on developing pollution assessment methods based on biological effects. One notable challenge in effect-directed analysis (EDA) for ecological risk assessment is the scarcity of in vitro detection methods for non-mammalian models. To understand the differences in species sensitivity in EDA (effect-directed analysis) analysis, our research developed The aryl hydrocarbon receptor (AhR) recombinant yeast systems specifically for the scallop Chlamys farreri and zebrafish. The AhR plays a critical role in the recognition and response of metazoans to external compounds. Employing these systems, our effect-directed analysis, supplemented by full-scan screening, successfully identified AhR agonists in both polar and non-polar sediment components from Laizhou Bay and Sanggou Bay of the Bohai Sea. In vitro assays detected active AhR agonistic properties in organic sediment extracts from various locations. Subsequent separation of components led to the identification of 10, 15, and 12 potential AhR agonists at three sites, including substances from synthetic industrial chemicals, pesticides, personal care products, and pharmaceuticals. Noteworthy compounds such as dimethyl cyclohexane-1,4-dicarboxylate, Sodium 2-phenylphenate tetrahydrate, phoxim, ethyl p-tolylacetate, Disulfiram, 2-naphthol, and aprepitant demonstrated significant activity. This study underscores the practicality and relevance of in vitro methods in ecological risk assessment, emphasizing the imperative to further investigate the distribution, sources, and ecotoxicological impacts of AhR agonists in coastal ecosystems.

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Emerging Contaminants in Tap Water: Treatment Challenges and Health Risks

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Abstract

This study delves into the occurrence and treatment of emerging contaminants (ECs) in tap water and drinking water treatment plants (DWTPs), highlighting the exposure and health risks associated with them. ECs, including per- and polyfluoroalkyl substances (PFASs), parabens, bisphenols (BPs), neonicotinoid insecticides (NEOs), strobilurin fungicides (SFs), triclosan & triclocarban (TCs), benzotriazoles & benzothiazoles (BTs), *N,N'*-substituted *p*-phenylenediamines (PPs), benzophenone-type UV-filter (UV-filter), and bisphenol diglycidyl ethers (BDGEs), are prevalent due to their environmental persistence and bioaccumulation potential. The investigation was conducted across two types of DWTPs in China, and included a nationwide tap water assessment from 45 cities. The results indicate that advanced DWTPs (A-DWTPs) have a higher removal efficiency for ECs, with an average reduction of 34%, compared to conventional DWTPs (C-DWTPs), which showed only a 4.15% reduction. Notably, A-DWTPs demonstrated superior removal rates for specific ECs such as SFs (55%), PFASs (49%), and NEOs (41%). However, concerningly, BDGEs and TCs exhibited negative removal rates of -189% and -48%, respectively, in A-DWTPs, suggesting issues with reformation or recontamination. Moreover, the DWTPs under investigation exhibited a notable deficiency in their capacity to effectively mitigate BP concentrations. Nationwide, the median concentration of total ECs (∑ECs) in tap water was 551 ng/L, with BPs, parabens, and PFASs being the most prevalent, contributing significantly to the ∑EC concentration. The dietary risk assessment revealed that the age group of 2 to 7 years had the highest estimated

daily intake (EDI) for ∑ECs, with a median of 4.47 ng/kg·bw/day, indicating a higher risk of exposure relative to body weight for younger children. The findings underscore the urgent need for improved water treatment technologies to address the presence of ECs, particularly for contaminants like BPs that were challenging to remove. Additionally, the study calls for a reevaluation of EC management strategies, enhanced environmental monitoring, and public education to ensure water safety.

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Contamination of Rubber-Derived Chemicals in Road Stormwater Runoff from Various Functional Areas in Megalopolis Cities, South China

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Abstract

Rubber-derived chemicals (RDCs) originating from tire and road wear particles are transported into road stormwater runoff, potentially threatening organisms in receiving watersheds. However, there is a lack of knowledge on time variation of novel RDCs in runoff, limiting initial rainwater treatment and subsequent rainwater resource utilization. In this study, we investigated the levels and time-concentration profiles of 35 target RDCs in road stormwater runoff from eight functional areas in the Greater Bay Area, South China. The results showed that the total concentrations of RDCs were the highest on the expressway compared with other seven functional areas. *N*-(1,3-dimethylbutyl)-*N*'-phenyl-*p*-phenylenediamine (6PPD), 6PPD-quinone, benzothiazole, and 1,3-diphenylguanidine were the top four highlighted RDCs (ND–228840 ng/L). Seasonal and spatial differences revealed higher RDC concentrations in the dry season as well as in less-developed regions. A lag effect of reaching RDC peak concentrations in road stormwater runoff was revealed, with a lag time of 10–90 min on expressways. Small-intensity rainfall triggers greater contamination of rubber-derived chemicals in road stormwater runoff. Environmental risk assessment indicated that 35% of the RDCs posed a high risk, especially PPD-quinones (Risk quotient up to 2663). Our findings contribute to a better understanding of managing road stormwater runoff for RDC pollution.

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Advancing the effect-directed identification of causative toxicants in waters with combined pollution: Mediation by pathway effects

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Abstract

Although bioassays and chemical analysis have been widely applied to waters with combined pollution, the difficulty in establishing relationships between pollutants and mixture effects leads to significant challenges in the identification of causative toxicants in combined pollution. To this end, an effect-directed analysis method mediated by pathway effects was developed. First, key molecular mechanisms of apical effects were identified via analysis of the concentration-dependent transcriptome. Then, for sensitive pathways, a pathway suspect database containing 2793 chemical-pathway interactions was established to enable suspect screening of causative toxicants, and a non-targeted screening method of causative toxicants corresponding to 72 KEGG pathways was developed based on pathway active fragments. The developed method was applied to two different types of wastewater, textile wastewater and municipal wastewater. Merely through apical effects, including mortality, mutagenicity and behavior profiles, the pollution type could not be well discriminated. Further evaluation using the concentration-dependent transcriptome revealed that the pathway effects were quite different in these two wastewaters. For OB-in, a textile wastewater, pathways related to cardiotoxicity and genetic information processing were significantly enriched. For HL-in, a municipal wastewater, pathways related to neurotoxicity and environmental information processing were significantly enriched. By suspect and non-targeted screening using chemical-pathway interactions, 37 and 422 causative toxicants were identified in OB-in and HL-in, respectively, and their distributions varied in these 2 wastewaters. Twenty-nine toxicants with at least 3 of the reported pathways matched with pathways enriched in wastewater samples were confirmed to explain 58% and 52% of the mortality observed in OB-in and HL-in, respectively. Mediation by pathway effects advances the effect-directed identification of causative toxicants in combined pollution.

990

Effect driven prioritization of contaminants in wastewater treatment plants across China: A data mining-based toxicity screening approach

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Abstract

A diversity of contaminants of emerging concern (CECs) present in wastewater effluent, posing potential threats to receiving waters. It is urgent for a holistic assessment of the occurrence, distribution, and risk of CECs related to wastewater treatment plants (WWTP) on national and regional scales. A data mining-based risk prioritization method was developed to collect the reported contaminants and their respective concentrations in municipal and industrial WWTPs and their receiving waters across China over 20 years. A total of 10,781 chemicals have been reported in 8,336 publications, of which 1,037 contaminants were

reported with environmental concentrations. While contaminant categories varied across WWTP types (municipal vs. industrial) and regions, pharmaceuticals and cyclic hydrocarbons were the most studied CECs. Contaminant composition in receiving water was closer to that in municipal than industrial WWTPs. Publications on legacy pesticides and polycyclic aromatic hydrocarbons in WWTP decreased recently compared to the past, while pharmaceuticals and perfluorochemicals have received increasing attention, showing a changing concern over time. Detection frequency, concentration, removal efficiency, and toxicity data were integrated for assessing potential risks and prioritizing CECs on national and regional scales using an environmental health prioritization index (EHPi) approach. Among 666 contaminants in municipal WWTP effluent, trichlorfon and perfluorooctanesulfonic acid were with the highest EHPi scores, while 17α-ethinylestradiol and bisphenol A had the highest EHPi scores among 304 contaminants in industrial WWTPs. The prioritized contaminants varied across regions, suggesting a need for tailoring regional measures of wastewater treatment and control.

1010

Application of Nontarget High-Resolution Mass Spectrometry Fingerprints for Chemical Partitioning Determination in Aquatic Environment: A Case Study in the Three Gorges Reservoir

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Abstract

Statistics show that a typical environmental sample consists of 10，000 substances. Target analysis of only one or several types of typical pollutants obveriously cannot exhibit systematic and comprehensive knowledge of environmental pollutantion. This study utilizes LC-HRMS for nontarget analysis of sediment, water and wild fish samples to investigate organic chemical fate and partitioning in the three gorges reservoir (TGR), China. Initially, a total of 126066 features were identified by the nontarget screening (NTS) method. We then established 4243, 10995, and 15,718 phase specific HRMS fingerprints for the water phase, the sediment phase, and the fish phase respectively. Qualitative analysis with Compound Discoverer 3.3 show that 495, 162 and 257 qualitative fingerprints were isolated for water, sediment and fish respectively. Among them, alicyclic ketones, alicyclic acids, unsaturated acids and saturated acids are main chemicals in all three phases in the TGR. Besides, the water phase also contained a large number of aromatic amines, pyridines, quinolines, and alkylphenols, pyrimidines, imidazoles were found in the sediment phase. While in the fish phase, there are more alkylphenols, imidazoles, piperidines, etc..When considered physicochemical properties of this qualitative fingerprints, LogD, KOC and LogP significantly affected chemical partitioning in sediment, water and fish, respectively ($p < 0.001$).These findings present a pioneering instance of applying HRMS fingerprints for chemical partitioning determination in real-world scenarios, which empowers the development of more effective strategies for environmental protection.

1013

Quantitative Identification of the Co-exposure Effects of E-waste Pollutants on Human Oxidative Stress by Explainable Machine Learning

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Abstract

Global electronic waste (e-waste) generation continues to grow. The various pollutants released during precarious e-waste disposal activities can contribute to human oxidative stress. This study encompassed 129 individuals residing near e-waste dismantling sites in China, with elevated urinary concentrations of e-waste-related pollutants including heavy metals, polycyclic aromatic hydrocarbons (PAHs), organophosphorus flame retardants (OPFRs), bisphenols (BPs), and phthalate esters (PAEs). Utilizing an explainable machine learning framework, the study quantified the co-exposure effects of these pollutants, finding that approximately 23% and 18% of the variance in oxidative DNA damage and lipid peroxidation, respectively, was attributable to these substances. Heavy metals emerged as the most critical factor in inducing oxidative stress, followed by PAHs and PAEs for oxidative DNA damage, and BPs, OPFRs, and PAEs for lipid peroxidation. The interactions between different pollutant classes were found to be weak, attributable to their disparate biological pathways. In contrast, the interactions among congeneric pollutants were strong, stemming from their shared pathways and resultant synergistic or additive effects on oxidative stress. An intelligent analysis system for e-waste pollutants was also developed, which enables more efficient processing of large-scale and dynamic datasets in evolving environments. This study offered an enticing peek into the intricacies of co-exposure effect of e-waste pollutants.

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Contamination Characteristic of Pharmaceutical and Personal Care Products (PPCPs) in Wastewater Treatment Plants in Wuhan, China

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Abstract

Pharmaceuticals and personal care products (PPCPs) are a class of compounds commonly used in daily life that may have adverse effects on organisms even at trace concentrations, so PPCPs have become one of the research hotspots in recent years. Understanding the occurrence and removal of PPCPs in wastewater treatment plants (WWTPs) is of great significance for the prevention and control of PPCPs. This study investigated nineWWTPs with different processes in Wuhan and used high performance liquid chromatography tandem-mass spectrometry (HPLC-MS/MS) to study the occurrence and distribution of 75 PPCPs in three media (dissolved phase, suspended particle phase, and sludge) in the WWTPs. The main conclusions are as follows:

In the nine WWTPs, the concentration ranges in the influent dissolved phases, effluent dissolved phases, influent suspended particle phases, effluent suspended particle phases and sludges were 666 - 3585 $ng \cdot L^{-1}$, 103 - 1287 $ng \cdot L^{-1}$, 196 - 8473 $ng \cdot L^{-1}$, 4.51 - 130 $ng \cdot L^{-1}$ and 2479 - 14224 $ng \cdot g^{-1}$ (dry weight), respectively. Antibiotics were the PPCPs with the highest concentrations, followed by nonsteroidal anti-inflammatory drugs and β-blockers. The distribution patterns of PPCPs in the three media were related to the physicochemical properties of the target substances, with hydrophobic PPCPs having higher concentrations in the suspended particle phase or sludge.

The results of removal efficiencies of different PPCPs in different WWTPs showed that the nine WWTPs in Wuhan had relatively high removal efficiencies for target substances, with an overall average removal efficiency of 70.8%. Biological treatment is the main unit for removing PPCPs, which is mainly achieved through microbial degradation and sludge adsorption. Different biological treatment processes have different removal efficiencies on target PPCPs, with the anaerobic-anoxic-aerobic and membrane bioreactor processes having higher removal efficiencies than the oxidation ditch and sequencing batch reactor processes.

The total mass loadings of PPCPs in the influents and the total emissions in the effluents ranged from 39.7 (W9) to 2604 (W1) $g \cdot d^{-1}$ and 7.16 (W9) to 397 (W1) $g \cdot d^{-1}$, respectively, with antibiotics being the PPCPs with the highest mass loadings. The mass loadings per inhabitant of total PPCPs in the influents and the emissions per inhabitant of total PPCPs in the effluents ranged from 264 (W9) to 3364 (W1) $\mu g \cdot per^{-1} \cdot d^{-1}$ and 47.7 (W9) to 300 (W7) $\mu g \cdot per^{-1} \cdot d^{-1}$, respectively.

1088

Potential ecological risks of dissolved synthetic musks and organic UV absorbers in freshwaters of China

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Abstract

Pubic concerns are rising on the chemical additives in consumer products due to chronic exposure of organism from huge consumption amounts and unexpected adverse effects. Lakes and reservoirs are key components for the global freshwater ecological system. However, the data on the occurrence and ecological risks of these chemical additives in lakes and reservoirs of large scale are scarce. To address

this issue, the present study conducted two sampling campaigns with passive samplers to measure the dissolved synthetic musks and organic UV absorbers (OUVAs) in freshwaters across China. An *in situ* biological exposure was performed with passive sampler at some selected sites for assessing the relationship between accumulated amounts of target compounds in two model organisms and passive samplers. Results showed that the detection frequencies of polycyclic musks was up to 95%, whereas those of OUVAs were 5–56%. Higher concentrations of polycyclic musks and OUVAs were observed in densely populated Mid, East, and South China compared to less populated West and Northeast China, indicating the significance of anthropogenic activities for these chemicals additives. Significant correlations were found between the dissolved concentrations of two main components for polycyclic musks (HHCB and AHTN) and their lipid-normalized concentrations in co-exposed fish and calm. However, this significant relationship was not observed for OUVAs, probably due to degradation of OUVAs. The estimated ecological hazard quotients for dissolved HHCB, AHTN, UV-326, and EHMC from the non-effect concentration in the sampling sites of Yangtze River Basin were greater than 0.1, but less than 1, indicating the potential ecological risks for these compounds in aquatic environment.

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Learning from Ionizable Pharmaceuticals: Bioaccumulation of Mixtures of Per- and Polyfluoroalkyl Substances in Aquatic Model Organisms

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Abstract

Bioaccumulation approaches have traditionally focused on nonionizable persistent organic pollutants, but diverse groups of substances fall outside of the applicability domains of these models. Our focus on pharmaceutical bioaccumulation in aquatic life has aimed to understand influences of pH on accumulation of ionizable contaminants. From these efforts, we have embraced comparative pharmacology, and identified the utility of employing apparent volume of distribution (V_D) during bioaccumulation studies with fish. Though V_D presents a useful parameter for studying ionizable contaminants, empirical values for this proportionality factor is limited in fish. More recently we have considered bioaccumulation kinetics of mixtures of per- and polyfluoroalkyl substances (PFAS) in aquatic organisms across environmental gradients. This PFAS mixture, which consisted of short and long chain perfluoroalkyl carboxylic acids (PFCAs) and perfluoroalkyl sulfonates (PFSAs), a sulfonamide, and fluorotelomer sulfonates, was introduced to experimental units from the bottom to simulate groundwater contaminated systems. We typically observe V_D below 1 L/kg, indicating PFAS were more distributed in plasma than in tissue; in addition, V_D generally decreased with increasing chain length for both PFCAs and PFSAs. We expect these efforts will contribute to the development of predictive bioaccumulation models for PFAS.

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New environmental monitoring technique for "new" pollutants in the new era

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Abstract

Environmental Monitoring is essential for understanding the water quality, particularly the emerging organic pollutants (refers to ‘new’ pollutants under the national ‘action plan for controlling emerging pollutants’ launched in 2022 in China). Passive sampling has several advantages over active methods: providing time-weighted average (TWA) data and saving time and costs, which is particularly attractive in the new era of the ‘dual carbon’ goal. A typical and novel passive water sampler (called o-DGT) for organic chemicals based on diffusive gradients in thin-films (DGT) has been developed and tested to overcome some drawbacks of current samplers, such as the hydrodynamic controls on the sampling rate. Since first introduced in our lab back in 2012, this sampler has been developed and validated for a wide range of emerging organic contaminants (> 200), including pharmaceuticals and personal care product ingredients (PPCPs), household chemicals, pesticides, perfluoroalkyl substances (PFAS), illicit drug, some persistent mobile and toxic (PMT) chemicals. Although o-DGT was developed primarily for waters, this technique has been further applied to soils for in situ measurement of the concentrations and fluxes of antibiotics in soils and for understanding the desorption kinetics from the soil particles together with the DIFS (DGT-induced fluxes in soils) model. With further development and calibration, particularly with the aid of start-of-art artificial intelligence - machine learning techniques, o-DGT might also be applied to nontarget screening analysis for all possible emerging organic pollutants, which will enhance our understanding of the whole picture of chemicals in the environment, better their risk assessment and management.

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Humic-Like Substances: Potential Risk Drivers of Apoptosis in $PM_{2.5}$ Particulate Matter

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Abstract

Globally, among the various environmental media that may pose a risk to human health, air pollution (PM) ranks first. Among atmospheric particulate matter, $PM_{2.5}$ poses the greatest risk, as it can enter the lungs through respiration, causing harm to human health, with pulmonary diseases being the primary type of illness induced by $PM_{2.5}$. Identifying the main risk-driving factors in atmospheric particulate matter is a prerequisite for accurate prevention and control of air pollution. However, the complex and variable composition of $PM_{2.5}$, coupled with a large number of unknown organic compounds, presents a significant challenge in this field.

This study, incorporating the principles of Environmental Design Analysis (EDA), utilizes advanced environmental chemical analytical techniques to explore the main pollutants in $PM_{2.5}$ samples from ten large cities across the country that induce cytotoxicity in human cells. It investigates the structure, composition, and source information of the target compounds, and selects the molecular formulas of the target compounds. Flow cytometry is used to analyze cytotoxicity, various mass spectrometry methods are employed to detect the content of multiple $PM_{2.5}$ pollutants, electrospray ionization source Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (ESI-/ESI+ FT-ICR-MS) technology is used to collect structural and compositional information of HULIS components, nuclear magnetic resonance (NMR) technology and three-dimensional fluorescence spectroscopy are used to analyze structural information, dual carbon isotope technology with radiocarbon dating ($\Delta^{14}C$ and $\delta^{13}C$) is applied to analyze the source information of pollutants, and gene chip sequencing and BMD (Benchmark Dose) methods are used to screen biomarkers of HULIS, exploring the toxic action patterns of HULIS.

In this study, a correlation analysis between chemical substances and cellular apoptosis data was utilized to identify the HULIS (Humic-like substances) fraction as the toxic compounds inducing apoptosis. Subsequent experiments on HULIS samples from PM2.5 were conducted, employing Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS), Nuclear Magnetic Resonance (NMR), radiocarbon dating ($\Delta^{14}C$ and $\delta^{13}C$), and three-dimensional fluorescence (EEM) to ascertain the molecular formula, structural characteristics, and potential sources of toxicity of the effective toxic compounds within HULIS. Further exploration of the quantitative biomarkers of apoptosis for the effective toxic constituents was conducted through gene sequencing and BMA (Benchmark Analysis). The results indicate that HULIS originating from coal combustion emissions and biomass burning are the primary contributors to apoptosis in PM2.5 within the same volume of air. Nitrophenols and nitropolycyclic aromatic hydrocarbons within HULIS are identified as the types of effective toxic compounds, with potential molecular formulas such as $C_{22}H_{20}O_8N$.

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Less is More: Challenges in Identifying High-Potency, Low-Concentration Toxic Components in Airborne Particulate Matter Pollution

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Abstract

Identifying the risk drivers in complex chemical mixtures has significantly advanced water quality monitoring and management. However, the extent to which chemical and microbial components and their sources contribute to the toxicity of airborne fine particulate matter ($PM_{2.5}$) remains elusive.

We developed a fractionation scheme to investigate the joint effects of different $PM_{2.5}$ fractions on IL-8 induction, a measure of inflammatory response. The fractions studied included water-soluble, polar, non-polar, and insoluble components. Our assessment demonstrated that the joint effect of different $PM_{2.5}$

fractions could be explained by the concentration-addition model, meaning the summed toxic unit of individual fractions approximated that of the whole $PM_{2.5}$ sample. This foundation allows for a quantitative dissection of the contributions of individual toxic components and mixtures to $PM_{2.5}$ toxicities.

For ambient $PM_{2.5}$, we found that endotoxin contributed significantly to $PM_{2.5}$ effects at both locations up to 10%, far exceeding its mass fraction in $PM_{2.5}$ (<0.0005%). The sources of gram-negative bacteria shifted from natural dominance at the coastal site to anthropogenic dominance at the urban site. These anthropogenic sources, such as the built environment, sewage treatment works, and humans, fall outside the currently regulated source categories. This underscores the need to understand the impact of microbial constituents on $PM_{2.5}$ toxicities and to incorporate biological factors into air quality management strategies.

For source-specific PM, we performed controlled combustion experiments across a range of temperatures and biomass fuels to quantify the component-specific contribution to oxidative stress triggered by emitted PM. From low to high temperatures, the emission factor of organic carbon (OC) was reduced by 20-fold, but the emission factor of OC's toxic equivalent was only reduced by 5-fold. The toxicity reduction was mainly attributable to water-extractable organics and was limited by less polar methanol-extractable organics. The relatively consistent toxicity per unit mass of OC for water-extractable organics across temperatures indicates a proportionality of toxicity reduction to mass reduction, driven by compounds such as methoxylates. However, the toxicity per unit mass of OC for methanol-extractable organics increased tenfold from low to high temperatures, partially explained by the formation of potent polycyclic aromatic hydrocarbon derivatives.

These case studies found that highly potent but low-concentration transformation products and natural microbial components contribute significantly to PM toxicity. Advances in generative AI for mass spectra fingerprinting, bioactivity prediction, and high-throughput screening will enhance effect-directed analyses to identify driving components for PM pollution.

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Combined toxicity assessment of azoxystroin and three kinds of exogenous selenium on zebrafish

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Abstract

A widely applied fungicide of azoxystrobin, is increasingly detected in the water environment. Concern has been raised against its potential detriment to aquatic ecosystems. Selenium is one of the critical elements from the biological contexts because it is essential for human health; however, it becomes toxic at high concentrations. The single acute toxicity of azoxystrobin and three kinds of exogenous selenium (sodium selenite, selenomethionine and nano-selenium), and joint acute toxicity of binary mixtures in equitoxicity ratios on zebrafish (*Danio rerio*) during different life stages were determined, respectively.

Additive index (AI) method, toxicity unit (TU) method, and mixture toxicity index (MTI) method were adopted to evaluate the joint toxicity effects, respectively. The results showed that the sensitivity of three life stages to sodium selenite (96 h-LC_{50}) mg/L, mg is the mass of selenium) were as followed: larvae (1.11 mg/L)> embryo (1.48 mg/L)>adult zabrafish (13.05 mg/L); the sensitivity to selenomethionine were as followed: larvae (0.80 mg/L)> embryo (1.03 mg/L)> adult zabrafish (9.36 mg/L); the sensitivity to nano-selenium were as followed: adult zabrafish (0.48 mg/L)> larvae (1.67 mg/L)> embryo (4.32 mg/L). The consistent conclusion could be drawn from three methods (AI, TU and MTI), that the joint toxicity effects of azoxystroin and three kinds of exogenous selenium (sodium selenite, selenomethionine and nano-selenium) on zebrafish during different life stages (embryo, larvae and adult zabrafish) were antagonistic, except for, the joint toxicity effects of azoxystroin and selenomethionine on adult zebrafish were partially additive by MTI method.

To further investigate the developmental effects of combined exposure of azoxystrobin and selenomethionine on aquatic organisms, the developmental toxicity and related enzyme activity of combined exposure of azoxystrobin and selenomethionine on zebrafish embryo and larvae as aquatic model species were determined. These results showed that: after the combined exposure of azoxystrobin and selenomethionine with different concentrations, frequency of autonomic movement of embryos decreased, hatching rate decreased, mortality increased, heart rate decreased, and body length of hatching larvae was significantly inhibited, with an obvious time-dose-effect relationship. Compared with the control group, the activity of catalase (CAT) was significantly decreased in different combined exposure groups (0.0005+0.001, 0.005+0.01 and 0.05+0.1 mg/L), and high concentration combined exposure group azoxystrobin 0.05 mg/L and selenomethionine 0.1 mg/L was the most significant inhibitory effect (P<0.01), but had no significant effects on the activity of superoxide dismutase (SOD).These results can provide data support for monitoring the concentrations of azoxystrobin and selenomethionine in aquatic environment and the ecological risk assessment of combined exposure in the future.

1118

Fate of organic pollutant mixture and associated human health risks in response to climate change

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Abstract

Future climate change will affect the environmental fate of organic pollutants and associated human health risks, yet the extent of these effects remains unknown. Here, we first study the effect of warming on the bioconcentration and bioaccumulation of per- and polyfluoroalkyl substances by pelagic and benthic organisms in a water-sediment system, as well as the effect of warming on the uptake pathway and accumulation of polycyclic aromatic hydrocarbons in spinach in enclosed soil/water-air-plant microcosms. Then we couple a high-resolution environmental multimedia model with a bioaccumulation model to study the multimedia distribution of 16 priority PAHs and assess future PAH-related human health risks under varying climate change scenarios over China at a continental scale. After removing the effects of PAH emission changes, we find that the total PAH concentrations would decrease in the air,

freshwater, sediment, soil, and organisms, while the high-molecular-weight PAH would increase in the air with climate warming from 1.5 to 4°C. Consequently, the multi-pathway exposure human health risks predominately influenced by dietary ingestion are expected to decrease by 1.7-20.5%, while the respiratory risks are projected to rise by 0.2-5.8% in the future. However, the persistently high multi-pathway human health risks underscore the need for reducing future PAH emissions by 69% compared with 2009 levels in China. Our study demonstrates the urgency of limiting PAH emissions under future climate change for public health and highlights the importance of including the contribution of dietary ingestion in human health risk assessment.

1119

Monitoring and risk control of mycotoxins and pesticide residues in corn：a study in China

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Abstract

Mycotoxins produced naturally by toxigenic fungi and intentionally applied chemical pesticides are major contaminants in corn, posing potential health risks to humans and animals. However, there is a lack of research on the monitoring and risk control of mycotoxins and pesticide residues in major corn planting regions of China, resulting in insufficient measures for effective contamination risk control. To address this gap, we conducted monitoring and risk control studies in typical corn planting regions of China, including: 1) Monitoring the occurrence of multiple pesticide residues and mycotoxins in typical corn planting regions, and assessing associated risks and regional variations. 2) Analyzing the co-contamination of mycotoxins and pesticide residues, and evaluating the correlations and combined exposure risks of mycotoxins. 3) Assessing the effectiveness of chemical pesticides, genetically modified insect-resistant corn, and egg parasitoid wasps in reducing mycotoxin levels in typical corn planting regions. 4) Investigating the optimal timing for chemical pesticide application to control mycotoxins, and optimizing key techniques for pesticide application.

1. A total of 12 mycotoxins and 24 pesticides were detected. At high- exposure levels, pesticide residues posed relatively low risks, whereas potential health risks from mycotoxin exposure were identified in samples from certain regions.
2. 67% of the samples contained more than five contaminants, indicating a high co-contamination rate of mycotoxins and pesticide residues.
3. Control techniques with insecticidal effects demonstrated significant efficacy in reducing fumonisins and other mycotoxins, whereas fungicides were less effective. This discrepancy may be attributed to regional environmental conditions and variations in pest infestations.
4. Applying insecticides and fungicides 4-8 days after corn silking showed the best effects for mycotoxin reduction.

In summary, we identified the occurrence and risk characteristics of mycotoxins and pesticide residues in three typical corn planting regions in China, evaluated the efficacy of mainstream mycotoxin reduction techniques, and optimized key parameters. Our study contributes to the targeted regional prevention and control of mycotoxin and pesticide residue contamination.

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Research progress of mathematical method and assessment model for pesticide dietary risk

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Abstract

Nowadays，dietary exposure has become a global issue that consumers generally facing and it gradually gained the attention from people all over the world. Lots of fearful events happened before were finally found to be caused by the toxic substances contained in the dietary. In 1999, the severe European food crisis was caused by dioxin pollution. In 2008, the melamine-tainted milk powder incident affected nearly 300 thousand infants. These incidents have significantly increased the public attention to dietary exposure. In case similar events happen again, pesticide residue is an essential step just to control the risk of dietary exposure.

The risk assessment of dietary exposure to pesticide residues contains a critical concern within the domains of chemical risk management, food safety, and public health. An effective quantitative model for assessing such risks is indispensable for the accurate determination of dietary exposure to pesticide residues. Based on the advanced research progress of pesticide residue dietary exposure risk assessment both domestically and internationally, this study endeavors to compile an overview of the assessment models about the risk of dietary exposure to pesticide residues, including deterministic assessment model, probabilistic assessment model and cumulative assessment model. According to the model's evolution, applications and the requisite evaluations, we conducted a various analysis of the advantages and disadvantages for various analytical models. The key factors such as model uncertainty, evaluation software and database application were meticulously examined.

According to the assessment purpose, target chemical characteristics, population characteristics and assessment accuracy requirements, dietary exposure assessment software used on large-scale computer simulation is required to calculate dietary exposure. The software such as MCRA, DEEM, SHEDS and LifeLine has been applied in United States and European Union countries. China has developed cDEEMs to evaluate the exposure of chemical contaminants in food, but it's still a work in progress. The development and utilization of evaluation software in China is revelatively slow at present, so it's necessary to selectively absorb the successful experience of foreign countries in combination with China's actual situation and establish an assessment software with Chinese characteristics, gradually integrating with the world.

In response to the current situation of dietary risk assessment of pesticide residues in China, we forecasted the urgency and significance of integrating relevant parameters of the model, thereby offering a scientific reference for improving the construction of dietary exposure risk assessment system of pesticide residues.

1146

Toxicokinetics and freshwater risks of nano-encapsulated imidacloprid: A life cycle perspective

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Abstract

Agricultural applications of nanotechnologies necessitate addressing safety concerns associated with nanopesticides, yet research has not adequately elucidated potential environmental risks between nanopesticides and their conventional counterparts. To address this gap, we investigated the risk of nanopesticides by comparing the ecotoxicity of nanoencapsulated imidacloprid (nano- IMI) with its active ingredient to nontarget freshwater organisms. Nano-IMI elicited approximately 5 times higher toxicity than IMI to zebrafish embryos with and without chorion, while no significant difference was observed between the two invertebrates. Toxicokinetics further explained the differential toxicity patterns of the two IMI analogues. To thoroughly address their environmental impacts throughout the life cycle while considering nano-specific properties and environmentally relevant scenarios, we assessed the “cradle-to-gate” environmental impacts of both pesticides via a life cycle assessment. Meanwhile, we derived ecotoxicity-characterization factors and impact scores for both IMI and nano-IMI, enabling the quantification of ecological risks associated with their end-of-life emissions. The ecological risks of nano-IMI during production (4,631 CTUe) were approximately four times higher than those of IMI (1,177 CTUe). Conversely, the freshwater ecological risks associated with end-of-life nano-IMI release (0.012–6.93×104 CTUe) were at least one order of magnitude lower than those of IMI (1.59×103–6.13×106 CTUe), considering the impacts of rainfall, toxicity data selection, fate, and transport. Under identical rainfall conditions, nano-IMI exhibited substantially reduced integrated life cycle risks compared with IMI, showing potential as an alternative to conventional IMI. Our work provides a novel approach for assessing engineered nanomaterial alternatives considering various possible scenarios and offers valuable insights into the life cycle environmental risk assessment of nanopesticides for the first time.

8. Atmospheric Environmental Chemistry

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Characteristics of nitrogen-containing organics in $PM_{2.5}$ in Ürümqi, northwestern China – differential impacts of combustion of fresh and aged biomass materials

Yijia Ma, Yu Xu, Huayun Xiao

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Abstract

Nitrogen-containing organic compounds (NOCs) are abundant and important aerosol components deeply involved in the global nitrogen cycle. However, the sources and formation processes of NOCs remain largely unknown, particularly in the city (Ürümqi, China) farthest from the ocean worldwide. Here, NOCs in $PM_{2.5}$ collected in Ürümqi over a 1-year period were characterized by ultra-high-resolution mass spectrometry. The abundance of CHON compounds (mainly oxygen-poor unsaturated aliphatic-like species) in the positive ion mode was higher in the warm period than in the cold period, which was largely attributed to the contribution of fresh biomass material combustion (e.g., forest fires) associated with amidation of unsaturated fatty acids in the warm period, rather than the oxidation processes. However, CHON compounds (mainly nitro-aromatic species) in the negative ion mode increased significantly in the cold period, which was tightly related to aged biomass combustion (e.g., dry straws) in wintertime Ürümqi. For CHN compounds, alkyl nitriles and aromatic species showed higher abundance in the warm and cold periods, respectively. Alkyl nitriles can be derived from fresh biomass material combustion associated with the dehydration of amides (the main CHON compounds in the warm period). In contrast, aromatic species were tightly related to aged biomass burning. These findings further suggested different impacts of the combustion of fresh and aged biomass materials on NOC compositions in different seasons. The overall results shed light on the mechanisms by which fresh and aged biomass materials release different NOCs during combustion.

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Novel field evidence for constraints of nearly dry and weakly acidic aerosol conditions on the formation of organosulfates

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Abstract

A global perspective on the abundance and formation of organosulfates (OSs) in the field observations (relative humidity of 53% to 77%) suggested that the investigated particles are generally non-dry and acidic (pH < 6). However, the key factors affecting OS formation in nearly dry and weakly acidic aerosol conditions remain elusive. This topic was resolved by examining the composition and formation of OSs

in PM2.5 collected in Urumqi (dry and dusty) over a one-year period. Anthropogenic OSs accounted for 49 ± 8% of the total OSs, indicating a large anthropogenic contribution to OS formation in Urumqi (particularly in winter). The low aerosol liquid water (ALW) concentration (2 ± 2 μg m-3) and weak particle acidity (pH = 7 ± 2) during summer were important factors limiting anthropogenic OS formation. However, increased ALW (103 ± 71 μg m-3) and particle acidity (pH = 5 ± 1) during winter significantly promoted anthropogenic OS production. The formation of most of isoprene- and monoterpene-derived OSs during summer was also constrained by unfavorable ALW concentration and particle acidity, resulting in biogenic OS levels being lower in summer than in winter. This study provides observational evidence on OS formation constraints by dry and dusty atmospheric conditions.

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Diurnal variations of aminiums in $PM_{2.5}$ during winter in Shanghai: implication for significant anthropogenic origin and differential formation mechanisms

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Abstract

Aminiums are significant components of secondary organic aerosols, primarily driving intense research on aliphatic aminiums. However, the formation mechanisms of aromatic aminiums in urban aerosols remain elusive. Atmospheric fine particles ($PM_{2.5}$) were collected in centre Shanghai (China) during the winter to investigate the relative contributions of biogenic and anthropogenic sources on aminiums and the formation mechanisms of aliphatic and aromatic aminiums. Aliphatic aminiums were the dominant aminium groups, followed by aromatic and alicyclic aminiums. Anilinium is the third most abundant aminium species, whose concentration together with total aminium concentration showed higher levels during the daytime and on weekdays. This finding combined with positive matrix factorization analysis suggested that the daily- and weekly-scale variations of anthropogenic activities (e.g., traffic for commuting) were largely responsible for the fluctuations in aminium concentrations (particularly aromatic aminiums). Moreover, we concretized aminium formation based on the interactions among amines, acidity, and ozone, suggesting that ozone-related processes and subsequent acid-base reactions weakened the abundance of aliphatic aminiums but promoted the formation of aromatic aminiums. The molecular characterization of aromatic aminiums suggested that the oxidative degradation of higher-molecular-weight aromatic amines is an important mechanism for anilinium formation. This study provides novel insights into the formation of aromatic aminiums.

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Characteristics and potential sources of air pollutants in Xi 'an from 2014 to 2022

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Abstract

Characteristics and potential sources of air pollutants in Xi 'an from 2014 to 2022

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Abstract: As a typical city in the Fenwei Plain, Xi'an has always been widely concerned about air pollution issues. This study is based on meteorological data and environmental air quality monitoring data of Xi'an City from 2014 to 2022. Mathematical statistical methods are used to analyze the characteristics and meteorological factors of air pollution in Xi'an City. The results showed that the concentration of five pollutants had a decreasing trend during 2014-2022, while the increase change for O_3. The average monthly concentration of O_3 is "high in summer and low in winter", and January is the most polluted month of PM_{10} and $PM_{2.5}$. The diurnal concentration distribution of O_3 is "single-peak", while the distribution characteristics of PM_{10} and CO are "double-peak and double-valley". From the perspective of spatial changes, the high value areas of $PM_{2.5}$ pollution have been decreasing year by year, since the high value areas of O_3 pollution have shifted from the west to the central region. Meteorological factors (average temperature, relative humidity and precipitation) are strongly correlated with pollutant concentrations. Through backward trajectory clustering and potential source area analysis, it can be concluded that the heavy polluted areas of $PM_{2.5}$ are concentrated in western Henan, northwestern Hubei and southern Shaanxi. The heavy polluted areas of O_3 are concentrated in northern Hunan, southern Hubei, northeastern Sichuan, and southern Shaanxi.

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Investigation of Chemicals Associated with Odours in Singapore

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Abstract

Singapore is an urbanized island nation with a high population density, with scarce land area. In some areas where less pollutive industrial activities are located in closer proximities to residential areas, nuisance such as unpleasant or chemical-like odours could at times be experienced by residents. While the stringent regulations on industrial emissions control air pollutants to safe levels, some chemical levels may still be within odour levels/thresholds which can be experienced by the public.

This study investigates, the Volatile Organic Compound (VOC) profiles at various residential areas of Singapore, including known chemical odour hotspots, to assess the chemicals and associated industrial activities (or sources) which could potentially contribute to the chemical odours which were experienced by the residents.

A sampling strategy involving both active and passive sampling of ambient air using sorbent tubes was devised for this investigation. Sampling was conducted at the industrial premises and spatially strategic locations around it to provide hints to unique chemicals to which the odour may be attributed to. Samples were also collected at various parts of Singapore (Central, Northeast, East, and South) for comparison. Chemical identification and quantification were performed by gas chromatography-mass spectroscopy involving target analysis of known chemicals associated with wafer fabrication processes as well as non-targeted analyses for potential unknown candidates.

Spatial and statistical methods (Principal Component Analysis, PCA) were applied to analyse the results. VOC profiles in different residential areas of Singapore were compared and some unique chemicals were found to be associated with certain industrial activities or sites. Longitudinal monitoring is ongoing to assess longer-term trends and the effects of environmental variables such as wind direction during the different monsoon periods. The results from this investigation could provide deeper understanding of chemicals/VOCs that could be potentially associated to odours experienced by the public and provide insights to guide operations.

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Three pressing topics in current tropospheric aerosol chemistry: Woodsmoke, pathogens and nanoplastics

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Abstract

An overview on recent work of our department on aerosol particle chemistry will be given for the three topics given in the title. Accodingly, the presentation will introduce into aerosol chemistry, then turn towards the three parts and conclude.

First, woodsmoke is a very important constituent of PM because of wildfires in certain regions of the world but also increased household heating with firewood. Initially deemed as a climate-neutral means for houshold heating, particulates from wood combustion now are a major air pollution problems creating substantial PM load in countries such as Germany. I will report about related targeted field campains, chamber experiments and multiphase modelling with CAPRAM.

Second, we have worked to be able to use our aerosol simulation chamber ACD-C for investigations of aerosol-related pathogen transmission and have applied this to aerosol particles containing phages or viruses. First results on this will be presented based on work in two national projects.

Third, micro- and nanoplastics are found to be dispersed into the atmosphere and costitute a non-negligible fraction of OM , here we present some first results from a Leibniz-project we coodinate named AIRPLAST,

A summary and an outlook wil be given, work in these three complexes is in an early stage.

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Contributions of East Asian Emissions to Atmospheric Mercury Pollution in North America from 2010 to 2015

Jingmeng Jin, Lei Zhang, Xia Liu, Jialin Zhang, Yang Zhang

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Abstract

Mercury (Hg) is a toxic element which can undergo long-range transport and bioaccumulation. East Asia has the largest anthropogenic Hg emissions in the world, and is therefore a hot zone for the Minamata Convention. With the increasingly stringent air pollution control policies carried out in China, the impacts of transpacific Hg transport from East Asia to North America and other regions need to be re-evaluated.

In this study, the anthropogenic Hg emission inventories for China in 2010 and 2015 were developed based on the Dynamic Inventory for Mercury Emission (DIME) model. Coupled with the global emission

inventory as the input data, the global atmospheric Hg concentrations and wet deposition fluxes were simulated using the GEOS-Chem model. Results from the model were verified by comparing with observation data from the Atmospheric Mercury Network (AMNet), the Canadian Atmospheric Mercury Network (CAMNet), and Mercury Deposition Network (MDN). By turning the emission in East Asia on and off, four cases were conducted to calculate the impacts of Hg emission from East Asia on North America in 2010 and 2015.

The performance of the updated GEOS-Chem model was improved compared to previous studies. The observed and simulated values of gaseous elemental mercury (GEM) in 2015 were 1.64±0.68 and 1.30±0.58 ng m^{-3}, and the R^2 value reached 0.8, while the observed and simulated Hg wet deposition fluxes were 7.92±4.22 and 5.30±4.33 μg m^{-2} yr^{-1}. The model results show that compared with 2010, the contribution of anthropogenic Hg emissions in East Asia to GEM in North America decreased in 2015, which was mainly driven by the decrease of emissions in China (by 75.3 t from 2010 to 2015). The contribution to Hg wet deposition flux increased, which was probably related to the global climate change. In addition, the main affected areas of GEM in North America in 2010 and 2015 were consistent, mainly in the western and northern parts of North America, especially near the west coast of the Pacific Ocean. The most affected areas of Hg wet deposition flux in North America were concentrated in the eastern coast and Mississippi river basin, which was likely related to their high precipitation and topographic characteristics. The level of contribution of East Asian emissions to atmospheric Hg pollution has been significantly reduced compared to the late 1990s.

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Contribution of the Open Field Burning of Rice Straw to Particulate Matter Air Concentrations in the Red River Delta, Vietnam in 2022

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Abstract

Agricultural field open burning as a source of air pollution remains a big environmental problem in Vietnam. However, the scale of the problem and its contribution to the air pollution load were not very well studied. Such information could help in developing policies and taking actions to reduce and eliminate field open burning. An attempt was made to study the contribution of

the field open burning of rice straw to the increase of ambient Particulate Matter $(PM)_{2.5}$ concentrations as part of a research project implemented by Global Alliance for Health and Pollution (GAHP) and Vietnam Association for Conservation of Nature and Environment (VACNE) with support of the UK's Department for Environment, Food & Rural Affairs (DEFRA). The study aimed to investigate how the daily $PM_{2.5}$ concentrations vary each month and whether they increase during the field open burning season. A statistical model was developed to use the correlation between the satellite-derived Aerosol Optical Depth (AOD) and PM2.5 concentrations in order to assess and map the spatial distribution of PM2.5. This model accounted for some variables that may affect the correlation between AOD and PM2.5 such as air temperature, humidity, air pressure, rainfall, wind direction and speed. The dispersion modelling of PM2.5 concentrations was based on the model of Weather Research and Forecasting with the inputs from the global meteorological data. The data was extracted for the period of January – November 2022 with the spatial resolution of 1°×1° and the temporal resolution of 1 hour.

The results showed that in 2022 $PM_{2.5}$ air concentrations in the Red River delta have increased during the open burning seasons at the end of May – beginning of June and in October-November. In was found through field observations that the increased daily $PM_{2.5}$ concentrations were observed when many local farmers set their paddies to fire. June 6th was the worse day for the air quality in the region when $PM_{2.5}$ concentration reached 142 $\mu g/m^3$. The $PM_{2.5}$ concentration had lowered by June 12th when the rice straw burning had stopped.

The maps showing the changes in air concentrations of $PM_{2.5}$ can be used for demonstration of the scale of the problem to the decisionmakers to develop policies to limit field open burning.

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Understanding the importance of atmospheric transformation in assessing the risks of emerging contaminants

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Abstract

In this talk, I will use a few examples to highlight the importance of atmospheric transformation in assessing the environmental and health risks of emerging contaminants. These examples include (1) Urban air pollution: atmospheric transformation of organophosphate esters (OPEs) in global megacities; (2) Indoor air pollution: indoor emission of liquid crystal monomers (LCMs) and atmospheric transformation chemistry of bisphenols; and (3) Air pollution in polar regions: atmospheric transformation of organophosphite antioxidants (OPAs) to OPEs in the global atmospheric environment including the Arctic and Antarctic.

1132

Characteristics and Environmental Impacts of Full-volatile Organic Compounds from Vehicles

yan liu

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Abstract

Vehicular emission are major contributors to VOCs、I/SVOCs sources in urban areas, while quantification and characterization of the evaporative emission in China are rarely reported. In this study, we performed evaporative emission experiments in a sealed housing evaporative determination (SHED) using eleven new and in-use light-duty gasoline vehicles to investigate the evaporative VOCs and S/IVOCs emission from the China 5 and China 6 vehicles and unravel the deterioration of evaporation control system of in-use ones. Furthermore, consecutive-day evaporation tests were performed on 11 in-use vehicles spanning from China 3 to China 6 emission standards, elucidating the mechanisms and patterns underlying long-term evaporative emissions. A novel set of rapid calculation methods for estimating long-term evaporative emission inventories was developed based on the definition of the residential activity factor, and the inventory results were validated using positive matrix factorization (PMF). Due to COVID-19 lockdowns, there was a further increase of 22% in evaporative emissions, highlighting the long-term significance of evaporative emissions as a neglected source of anthropogenic VOCs.With the implementation of China 6's standard, the evaporative THC emission in China may peak in 2022 and will be cut down by 76% until 2030. Also, the underestimation of evaporative emission was estimated when neglecting the difference of EFs between new and in-use vehicles.

1133

New particle formation modelling: from configurational sampling to cluster kinetics

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Abstract

New particle formation contributes to half of the cloud condensation nuclei and the formation of haze. Therefore, understanding the formation process of atmospheric aerosols is of great significance for

comprehending climate change and air pollution. There already exists a theoretical workflow that proceeds from thermodynamics to kinetics for aerosol nucleation molecular clusters. However, in terms of thermodynamics, it is still challenging to find the most stable minimum of molecular clusters. We designed the basin-hopping configurational sampling algorithm and applied it to various nucleation systems[1,2]. Furthermore, for cluster kinetics, the collision rate coefficients are typically calculated by assuming hard sphere collisions, which neglects the long-range interactions. Here, we developed a general artificial intelligence-driven workflow to enhance the accuracy of collision rate coefficients[3]. We further benchmarked a general machine learning potential called ANI-2x, and its inaccuracy in the forces of nucleation clusters calls for the further design of a specific aerosol nucleation potential[4]. Our introduction of deep neural network techniques into atmospheric aerosol nucleation simulations lays the foundation for accurately describing the new particle formation mechanism in climate change predictions and air quality modeling.

9. Environmental Interfacial Chemistry

185

Probe the reactivity of pyrogenic carbonaceous matter (PCM) using PCM-like polymers

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Abstract

Pyrogenic carbonaceous matter (PCM; e.g., biochar and activated carbon) can promote a broad range of chemical and microbial synergies, from affecting redox-active elements' global biogeochemical processes to influencing environmental remediation and water treatment. However, due to PCM's inherent chemical heterogeneity, it is difficult to identify what critical properties contribute to its reactivity, thus limiting the ability to predict the scope of reaction types or design a PCM for engineering applications. My research group has pioneered employing polymer synthesis to develop a tunable PCM-like polymer (PLP) network that possesses PCM's key attributes. Through controlled polymer synthesis, we delineate the contribution of individual properties (e.g., functional groups, porosity) to the reactivity of PCM. Specifically, we have identified critical properties of PCM that can accelerate surface-enhanced hydrolysis of nitroaromatics and facilitate the complete dechlorination of 1,2,3-trichloropropane. Understanding the critical properties of PCM that enhance contaminant destruction is essential, as it allows for the design of a reactive adsorbent that can simultaneously concentrate and destroy contaminants on the carbon surface, thus significantly reducing the cost of materials replacement.

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Quantitative Insights into Phosphate-Enhanced Lead Immobilization on Goethite

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Abstract

Despite extensive study, geochemical modeling often fails to accurately predict lead (Pb) immobilization in environmental samples. This study employs the Charge Distribution MUlti-SIte Complexation (CD-MUSIC) model, X-ray Absorption Fine Structure (XAFS), and Density Functional Theory (DFT) to investigate mechanisms of phosphate (PO4) induced Pb immobilization on metal (hydr)oxides. The results reveal that PO4 mainly enhances bidentate adsorbed Pb on goethite via electrostatic synergy at low PO4 concentrations. At relatively low pH (below 5.5) and elevated PO4 concentrations, formation of monodentate O-sharing Pb-PO4 ternary structure on goethite becomes important. Precipitation of hydropyromorphite (Pb5(PO4)3OH) occurs at high pH and high concentrations of Pb and PO4, with an optimized logKsp of -82.02. The adjustment of logKsp compared to that in bulk solution allows for quantification of the overall Pb-PO4 precipitation enhanced by goethite. The CD-MUSIC model parameters for both the bidentate Pb complex and monodentate O-sharing Pb-PO4 ternary complex were optimized. The modeling results and parameters are further validated and specified with XAFS analysis and DFT calculations. This study provides quantitative molecular level insights into contributions of electrostatic enhancement, ternary complexation, and precipitation to phosphate-induced Pb immobilization on oxides, which will be helpful in resolving controversies regarding Pb distribution in environmental samples.

470

Concentration profiles of organic chemicals across sediment-water interface: Experimental and modeling approaches in spiked-sediment toxicity tests

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Abstract

Spiked-sediment toxicity tests are essential for assessing the ecological risks of hydrophobic or persistent chemicals in sediment environments. These tests involve exposing benthic organisms to sediment spiked with a test chemical, considering multiple uptake pathways (e.g., diet-borne, water-borne) available to the

organisms. While the freely dissolved concentration (C_{free}) in pore water is generally accepted as a suitable metric for the bioavailable fraction of organic chemicals in sediment, several studies indicate that the fraction bound to dissolved organic matter can increase the uptake by organisms beyond what is expected from C_{free} alone.

Given the complexity of sediment test systems, understanding the partitioning and state (i.e., freely dissolved and bound to dissolved organic matter) of test chemicals is crucial for linking observed toxic effects to bioeffective exposure concentrations. However, there is a notable gap in research on detailed spatial profiles of test chemicals in spiked-sediment toxicity tests, especially in distinguishing between freely dissolved and bound chemical states.

To address this gap, we have performed 10-day and 42-day spiked-sediment toxicity tests using *Hyalella azteca*, a freshwater amphipod, with various organic chemicals, such as polycyclic aromatic hydrocarbons (PAHs), insecticides, and a cationic surfactant. In these tests, we analyzed C_{free} of the test chemicals at multiple positions (within sediment, at the sediment-water interface, and in overlying water) using passive sampling, and compared the results to spatiotemporal concentration profiles simulated by a mechanistic chemical transport model. Both experimental and modeling results indicated a steep concentration gradient within the first few millimeters of the sediment-water interface, with the extent of the gradient dependent on the properties of the test chemicals (e.g., hydrophobicity, neutral or cationic). This concentration gradient is crucial, as epibenthic organisms residing at the sediment-water interface may experience variable exposures to freely dissolved and bound concentrations, potentially influencing measured toxicity based on their behavior.

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Interfacial interaction mechanism between nanoplastics and typical minerals: Insights for the transport and deposition behavior of nanoplastics

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Abstract

The widespread utilization of plastic products ineluctably leads to the ubiquity of nanoplastics (NPs), causing potential risks for aquatic environments. Interactions of NPs with mineral surfaces may affect NPs transport, fate, and ecotoxicity. The interactions of two types of polystyrene nanoplastics (PSNPs), i.e., bare-PSNPs and carboxylated COOH–PSNPs, with iron (hydr)oxides (hematite, goethite, magnetite, and ferrihydrite), aluminum (hydr)oxides (boehmite and gibbsite), and clay minerals (kaolinite, montmorillonite, and illite) were investigated. Investigate systematically the deposition and aggregation behaviors of carboxylated polystyrene nanoplastics (COOH-PSNPs) by the types of clay minerals (illite, kaolinite, Na-montmorillonite, and Ca-montmorillonite) under various solution chemistry conditions (pH, temperature, ionic strength and type). The deposition behaviors of carboxyl-modified polystyrene nanoplastics (COOH-PSNPs) with goethite (α-FeOOH) were systematically investigated under various solution chemistry and organic macromolecule conditions (i.e., pH, ionic type, humic acid (HA), sodium alginate (SA), and bovine serum albumin (BSA)). The results of the present study suggested that the heteroaggregation of PSNPs in environments could be strongly affected by minerals, solution pH, humic acid, and ionic strength. Revealing the deposition behavior and mechanisms

between NPs and minerals under environmentally representative conditions, provides novel insights into the transport and fate of NPs in natural aquatic environments.

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Atmospheric air-water interfacial chemistry

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Abstract

Aerosol microdroplets, ubiquitous in the atmosphere, play a crucial role in climate change and air quality. With a large surface-to-volume ratio, the air-water interface of microdroplets serves as a vital site for multiphase chemical reactions. However, the interfacial physicochemical properties differ significantly from the bulk, posing challenges for traditional characterization methods. This study innovatively applies stimulated Raman scattering (SRS) microscopy for in situ and real-time characterization of the air-water interface in microdroplets. By establishing a droplet-based chemical quantification method using SRS spectra, we achieved three-dimensional quantitative imaging of pH and ion concentrations within individual droplets. The results reveal, for the first time at the micrometer scale, significant chemical heterogeneity inside atmospheric aerosols: both hydrogen ions and other solutes exhibit higher concentrations at the air-water interface compared to the bulk, with the gradient becoming more pronounced as the droplet size decreases. Molecular dynamics simulations confirm that the strong electric field at the interface drives the migration and enrichment of charged species from the droplet interior to the surface. This unique interfacial physicochemical environment can significantly impact atmospheric chemical processes. For instance, the acidity at the air-water interface is much stronger than in the bulk, which can accelerate acid-catalyzed reactions such as metal dissolution and organic degradation. Moreover, the interfacial enrichment of reactive species facilitates their interaction with trace gas-phase compounds. Importantly, the strong electric field at the interface can further enhance the reaction rates of various atmospheric chemical processes, such as the uptake and oxidation of trace gases, ion-molecule reactions, and free radical reactions. These findings challenge the isotropic assumptions in current atmospheric aerosol models, highlighting the importance of interfacial effects and kinetic mechanisms. The SRS methodology established in this study offers new insights for the detailed characterization of atmospheric microdroplet interfacial properties, contributing to an improved molecular-level understanding of multiphase atmospheric chemical processes and the predictive capability of aerosol models.

822

Interfacial Engineering of (Photo)catalytic Nanomaterials for Efficient Air Purification

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Abstract

The leading technology for removing indoor air pollutants is the adsorption using filtration media such as activated carbon. However, it is doubtful whether the adsorption technology is efficient since removal efficiency of adsorbents is remarkably reduced on humid condition. In addition, adsorbed air pollutants can be re-emitted from the media to ambient air. Photocatalytic air purification technology is a promising method for removing indoor volatile organic compounds (VOCs) because it can degrade VOCs completely to harmless CO_2 and H_2O under ambient conditions. In this talk, the principles of photocatalytic air purification, various physicochemical modifications of photocatalysts (nanotubes structures, metal loading, surface fluorination, and exposed facets), and success case of photocatalytic air cleaner will be introduced. Based on in-situ DRIFTs analysis, which measures adsorption and reaction behaviors at the interface between the catalyst surface and VOCs, the optimal modification of catalyst surfaces will be introduced. Finally, the interactions between single atom catalysts (SACs) and VOCs will be discussed.

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Traditional and Novel Organophosphate Esters in Plastic Greenhouse: Occurrence, Multi-media Migration, and Exposure Risk via Vegetable Consumption

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Abstract

Organophosphate esters (OPEs) are commonly utilized as plasticizers and flame retardants in wide range of plastic products. The presence of these chemicals in the environment and their potential toxicity has raised significant concerns. However, the occurrence characteristics of OPEs in the multi-media of greenhouses remain unknown. The study explored the distribution of organophosphate esters across different media in greenhouses.The total concentrations of these OPE-related contaminants in the air ranged from 594 to 1560 pg/m³, and in atmospheric particles, they ranged from 443 to 15,600 ng/g. Moreover, these contaminants were also found in the soils (96.8–9630 ng/g) and vegetables (197–7540 ng/g) within the greenhouses. Plastic films used in the greenhouses were identified as the primary source of these contaminants. The main migration route of novel OPEs was identified as particle dry deposition into the soil and leaves. For traditional OPEs, leaf absorption was found to be the predominant uptake

pathway. A risk quotient assessment revealed a high ecological risk associated with NOPE compounds. Furthermore, total exposure to OPE-associated contaminants through vegetable consumption was estimated at 2250 ng/kg bw/day for Chinese adult residents and a significant ecological risk was identified for novel OPEs, with a median risk quotient of 975.This study is the pioneering effort to demonstrate the distribution of OPE-related contaminants across various media and to highlight the potential risks they pose in agricultural greenhouses.

1139

Electrochemistry-inspired rapid remediation of pollution and recovery of lithium resources

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Abstract

In the presentation, I will discuss how principles of electrochemistry are employed to engineer a triple-phase catalyst design and to extract lithium ions from brine efficiently. This triple-phase configuration substantially accelerates the degradation of organic pollutants, achieving rates over 15,000 times faster than conventional two-phase catalysis. Furthermore, a novel electrochemical configuration has drastically reduced the electrodialysis voltage required for lithium extraction to nearly zero, which is just one tenth of the energy conventionally used. These advancements demonstrate the significant opportunities that electrochemistry presents for advancing environmental science and enhancing resource recovery through innovative designs.

10. Environmental Behaviour of Emerging Contaminants in Soils

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The occurrence of "yellowing" phenomenon and its main driving factors after the remediation of chromium (Cr)-contaminated soils

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Abstract

Chromium (Cr) is a highly toxic element, which is widely present in environment due to industrial activities. One of most applicable technique to clean up Cr pollution is chemical reduction. However, the Cr(VI) concentration in soil increases again after remediation, and meanwhile the yellow soil would appear, which is commonly called as "yellowing" phenomenon. To date, the reason behind the phenomenon has been disputed for decades. This study aimed to introduce the possible "yellowing" mechanism and the influencing factors. In this work, the concept of "yellowing" phenomenon was explained, and the most potential reasons include the reoxidation of manganese (Mn) oxides and mass transfer were summarized. Based on the reported finding and results, the large area of "yellowing" is likely to be caused by the re-migration of Cr(VI), since it could not sufficiently contact with the reductant under the effects of the mass transfer. In addition, other driving factors also control the occurrence of "yellowing" phenomenon. This article provides valuable reference for the academic peers participating in the Cr-contaminated sites remediation.

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Temporal and spatial variability of antibiotics in agricultural soils and the response of microorganisms

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Abstract

The objective of this study was to investigate the residual distribution of antibiotics in agricultural soils of Huang-Huai-Hai Plain, which is a major agricultural producing area and economically developed region in China. In this study, 336 soil samples of greenhouse and open-field including 13 groups of soil profile samples (0-20, 20-40 and 40-60 cm) were collected from four provinces/municipality in 2018-2020. The occurrence of 50 antibiotics and 7 metabolites, including tetracyclines (TCs) and their metabolites (MTCs), quinolones (QNs), sulfonamides (SAs) and macrolides (MLs) were measured. The concentrations of total antibiotics fell in the range of 1.62-4238 μg kg-1. TCs and QNs were dominant

antibiotics in soil. The concentration of MTCs in soil was almost equivalent to TCs, indicating that equal attentions should be paid to MTCs as well as TCs. Regional differences of antibiotic residues in soil were found among the four regions as well as between different cropping systems. The levels of antibiotics in greenhouse soils were higher than those in open-field soils. In soils of greenhouse of 1-6 years old, the levels of antibiotics were higher than those with longer history (7-30 years). Antibiotics were mainly distributed in the depth of 0-20 cm. Higher concentration of antibiotic residues in soil was prone to decrease the diversity and shift the structure and composition of soil microbial community. Antibiotic resistome occurred in soils with antibiotic residues exceeding 300 μg·kg-1. Bacteroidetes and Firmicutes were the top attributors impacting the profile of antibiotics in soil. According to weighted comprehensive pollution index of risk quotient, in 9/32 of soil samples the residual antibiotics presented high ecological risk, whereas in the rest of soil samples (23/32) the ecological risk is medium. The results will enrich the database and provide references for antibiotic contamination control in soils of the region and alike.

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Responses of soil bacterial communities and metabolic function to polyethylene and cadmium combined pollution

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Abstract

Polyethylene (PE) and cadmium (Cd) are emerging contaminants, which have attracted increasing concern about their effect on the soil environment in recent years. However, there is limited research on how soil bacterial communities respond to the combined pollution of PE and Cd. This study investigated the effect of PE and Cd on soil bacterial communities and associated metabolic function using high-throughput sequencing and GC-MS-based metabolomics. The results suggested that the combined pollution of PE and different concentrations of Cd significantly reduced the alpha diversity and affected soil beta diversity. *Proteobacteria*, *Gemmatimonadetes*, and *Actinobacteria* were the predominant phyla, while *Sphingomonas* was the leading genus that significantly enriched in soil treated with PE and Cd. Amino acid metabolism, membrane transport, and carbohydrate metabolism were the three primary metabolic functions. Notably, the remarkable changes in soil bacterial functions were the excretory system, immune system, and signaling molecules and interaction, implying the significant influence of PE and Cd pollution on the soil bacterial functions. Furthermore, PE and PE and Cd combined pollution revealed adverse effects on soil metabolites. Overall, this study provides scientific insights into the response of soil bacterial communities to PE and Cd pollution.

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From Water to Water: Insight into the Translocation of Pesticides from Plant Rhizosphere Solution to Leaf Guttation and the Associated Ecological Risks

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Abstract

Plant guttation is an important source of water/nutrients for many beneficial insects, while the presence of pesticides in guttation has been considered as a new exposure route for nontarget insects. This study aimed to elucidate how 15 diverse pesticides are translocated from growth media to guttation by maize plants through a hydroponic experiment. All pesticides were effectively translocated from the growth solution to maize guttation and reached a steady state within 5 days. The strong positive correlation (R^2 = 0.43–0.84) between the concentrations of pesticides in guttation and in xylem sap demonstrated that xylem sap was a major source of pesticides in guttation. The relationship between the bioaccumulation of pesticides in guttation ($BCF_{guttation}$) and the chemical K_{ow} was split into two distinct patterns: for pesticides with log K_{ow} > 3, we identified a good negative linear correlation between log $BCF_{guttation}$ and log K_{ow} (R^2 = 0.71); however, for pesticides with log K_{ow} < 3, all data fall close to a horizontal line of $BCF_{guttation} \cong 1$, indicating that hydrophilic pesticides can easily pass through the plants from rhizosphere solution to leaf guttation and reach saturation status. Besides, after feeding with pesticide-contaminated guttation, the mortality of honeybees was significantly impacted, even at very low levels (e.g., ∑600 μg/L with a mortality of 93%). Our results provide essential information for predicting the contamination of plant guttation with pesticides and associated ecological risks.

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Effects of Reduced Graphene Oxide Nanomaterials on Transformation of ^{14}C-Triclosan in Soils

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Abstract

Increasing use and release of graphene nanomaterials and pharmaceutical and personal care products (PPCPs) in soil environment have polluted the environment and posed high ecological risks. However, little is understood about the interactive effects and mechanism of graphene on the behaviors of PPCPs in soil. In the present study, the effects of reduced graphene oxide nanomaterials (RGO) on the fate of triclosan in two typical soils (S1: silty loam; S2: silty clay loam) were investigated with ^{14}C-triclosan, high-resolution mass spectrometry, scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), density functional theory (DFT) calculations, and microbial community structure analysis. The results showed that RGO prolonged the half-life of triclosan by 23.6–51.3%, but delayed the formation of transformed products such as methyl triclosan and dechlorinated dimer of triclosan in the two typical soils. Mineralization of triclosan to $^{14}CO_2$ was inhibited by 48.2–79.3% in 500 mg kg^{-1} RGO in comparison with that in the control, whereas the bound residue was 54.2–56.4% greater than the control. RGO also reduced the relative abundances of triclosan-degrading bacteria (*Pseudomonas* and *Sphingomonas*) in soils. Compared to silty loam, RGO more effectively inhibited triclosan degradation in silty clay loam. Furthermore, the DFT calculations suggested a strong association of the adsorption of triclosan on RGO with the van der Waals forces and π-π interactions. These results revealed that RGO inhibited the transformation of ^{14}C-triclosan in soil through strong adsorption and triclosan-degrading bacteria inhibition in soils. Therefore, the presence of RGO may potentially enhance persistence of triclosan in soil. Overall, our study provides valuable insights into the risk assessment of triclosan in the presence of GNs in soil environment.

425

Persulfate Activation with Biochar Supported Nanoscale Zero- valent Iron: Engineering Application for Effective Degradation of NCB in soil

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Abstract

Nitrochlorobenzene (NCB) is very common in pesticide and chemical industries, which has become a major problem in soil environment. However, the remediation of NCB contaminated soil is received finite concern. Using biochar as a substrate for nanoscale-zero valent iron (nZVI/p-BC) to activate peroxodisulfate (PDS), a novel heterogeneous oxidative system had been applied in the current study to remediate NCB contaminants in soil. The degradation efficiencies and kinetics of m-NCB, p-NCB, and o-NCB by various systems were contrasted in soil slurry. Key factors including the dosage of nZVI/p-BC, the molar ratio of nZVI/PDS, initial pH and temperature on degradation of NCB were further examined. The results confirmed that the nZVI/p-BC/PDS displayed the remarkable performance for removing NCB compared with other systems. Higher temperature with nZVI/PDS molar ratio of 2:1 under the acidic condition favored the reduction of NCB. The treatment for NCB with optimal conditions were evaluated for the engineering application. The mechanism of nZVI/p-BC/PDS indicated that electron transfer between p-BC and nZVI was responsible for activation of PDS, generating active species ($SO_4^{\bullet-}$, •OH and $^1O_2$) via both the free and non-free radical pathways. Experimental results

revealed prominent availability of nZVI/p-BC/PDS system in remediation of actual contaminated field by NCB.

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Design of all-solid-state nitrate ion-selective electrode for testing nitrate ions in the wetlands soil of the *Yellow River Delta*

Nan Jiang, Yunzhe Pan, Canyun Meng, Hongyu Cao, Feng Luan, Chunyuan Tian, Yanhong Li, Xuming Zhuang

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Abstract

All-solid-state ion-selective electrodes (ASS-ISEs) have been applied in many fields, such as cellular chemistry, environmental sciences, etc., due to their superior properties including simple operation, small size, low cost, and portability [1-3]. In the field of soil environmental monitoring, it is highly required but still a big challenge for finding a suitable protocol for high stability, reproducible, and reliable production of ASS-ISEs. Moreover, there are fewer reports on the detection of nitrate ion in the wetlands soil of the *Yellow River Delta*.

Herein, we report on a general, facile, and straightforward method for the preparation of robust ASS-ISEs using the bimetallic sulfide material used as ion-electron transducer layer. The optimal volume was conducted by examining the different drip volumes of the transducer layer materials dispersion liquid. By using the nitrate ion as a model, a nitrate ion-selective electrode (NO_3^--ISE) based on bimetallic sulfide materials as ion-electron transducer layer is successfully developed. Results show that the NO_3^--ISE exhibits a good Nernstian slope of -54.2 ± 0.5 mV/dec (R^2 = 0.999, n = 5) in the concentration range from 1.0×10^{-5} to 1.0×10^{-1} M. The introduction of bimetallic sulfide materials transduction layer material improves the stability of NO_3^--ISE, thus yielding a high potential stability of 1.3 ± 0.02 μV/h. In addition, the constructed NO_3^--ISE exhibits good reversibility and selectivity, and is not affected by gas, light and water layers. Moreover, the prepared NO_3^--ISE has been successfully used for accurate analysis of nitrate ion concentration in the wetlands soil of the *Yellow River Delta*. The proposed strategy utilizing bimetallic sulfide materials as a solid contact ion-electron transducer layer is a promising alternative for the fabrication of robust ASS-ISEs.

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Aging and Fraction Distribution of Halogenated Persistent Organic Pollutants (POPs) in Soil based on Sequential Extraction

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Abstract

To investigate the dynamics of distribution and availability of persistent organic pollutants (POPs) during aging processes in dry soil, we conducted a 130-day indoor microcosm experiment. Fourteen halogenated POPs, including three organochlorine pesticides, five polychlorinated biphenyls, and six polybrominated diphenyl ethers with diverse physicochemical properties, were spiked into the soil as target pollutants. We employed a four-step sequential extraction method—comprising oscillating extraction, ultrasonic extraction, silylation, and alkaline treatment—to obtain bioaccessible fractions, stable-adsorbed fractions, and two types of non-extractable residues of the target POPs in aged soil samples. Results showed that the average volatilization rate of pollutants peaked around the 5th day and decreased significantly thereafter, with minimal volatilization observed after the 30th day. By the 130th day, the fractions of bioaccessible, stable-adsorbed, and non-extractable residue ranged from 79.5% to 96.3%, 3.0% to 14.2%, and 0.1% to 8.8%, respectively. Changes in the fractions of halogenated POPs were influenced by temperature and the physicochemical properties of the pollutants. Specifically, the bioaccessible fraction increased while the stable-adsorbed fraction decreased with rising temperatures. POPs with higher molecular weights exhibited higher proportions of stable-adsorbed fractions and lower proportions of non-extractable residues. Throughout the experiment, the bioaccessible fraction consistently remained the dominant form, indicating sustained higher bioavailability and environmental risk of soil-borne POPs in arid conditions over an extended period.

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Genetically encoded fluorescent whole-cell biosensors for real-time detecting estrogens and psychoactive substances

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Abstract

Two biosensors were developed based on the single fluorescent protein-based biosensor theory. The ER-Light biosensor was developed for detecting environmental estrogens by fusing the ligand-binding domain of estrogen receptor (ER) with the green fluorescent protein variant Citrine, and expressing it in the periplasmic of *Escherichia coli*. Similarly, PsychLight was created to detect psychoactive substances by integrating the green fluorescent protein cpGFP into the third loop of the 5-HT receptor HTR2A and expressing it in the periplasmic of *Escherichia coli*. Both biosensors fit the additive effect, and have the advantages of rapid response to target substances, good fluorescence stability, high sensitivity,

satisfactory recovery rate, and no toxicity to target substances. The detection limits and working ranges of ER-Light and PsychLight can meet the application of environmental estrogens and psychoactive substances and show obvious dose-dependent effect. Compared with the current methods such as chemical analysis and reporter gene assays, ER-Light and PsychLight are more suitable for environmental monitoring because of their better environmental tolerance, simpler operation, lower cost, better comparability, and especially higher speed. The design, construction and application of the biosensors is attempt to apply the single fluorescent protein-based biosensor in the field of environmental monitoring, which is expected to provide new design guidelines for the construction of biosensors that can detect more key PPCPs in real-time.

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6-PPD Quinone exposure at environmentally relevant concentrations causes neurotoxicity by affecting dopaminergic, serotonergic, glutamatergic, and GABAergic neuronal systems in *Caenorhabditis elegans*

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Abstract

6-PPD quinone (6-PPDQ), an emerging environmental pollutant, is converted based on 6-PPD via ozonation. However, a systematic evaluation on possible neurotoxicity of long-term and low-does 6-PPDQ exposure and the underlying mechanism remain unknown. In the present work, 0.1–10 μg/L 6-PPDQ was added to treat *Caenorhabditis elegans* for 4.5 days, with locomotion behavior, neuronal development, sensory perception behavior, neurotransmitter content, and levels of neurotransmission-related genes being the endpoints. 6-PPDQ exposure at 0.1–10 μg/L significantly reduced locomotion behavior, and that at 1-10 μg/L decreased sensory perception behavior in nematodes. Moreover, 6-PPDQ exposure at 10 μg/L notably induced damage to development of dopaminergic, glutamatergic, serotonergic, and GABAergic neurons. Importantly, obviously decreased dopamine, serotonin, glutamate, dopamine, and GABA content and altered neurotransmission-related gene expression could be confirmed in nematodes with chronic 6-PPDQ exposure at 10 μg/L. Consequently, 6-PPDQ exposure disturbed neurotransmitter transmission, while such changed molecular foundation for neurotransmitter transmission was related to 6-PPDQ toxicity induction. The present work shed new lights on mechanisms of 6-PPDQ and its possible neurotoxicity to organisms at environmentally relevant concentrations.

706

Contamination status of novel organophosphate esters derived from organophosphite antioxidants in soil and the effects on soil bacterial communities

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Abstract

The contamination status of novel organophosphate esters (NOPEs) and their precursors organophosphite antioxidants (OPAs) and hydroxylated/di-ester transformation products (OH-OPEs/di-OPEs) in soils across a large-scale area in China were investigated. The total concentrations of the three test NOPEs in soil were 82.4–716 ng g^{-1}, which were considerably higher than those of traditional OPEs (4.50–430 ng g^{-1}), OPAs (n.d.–30.8 ng g^{-1}), OH-OPEs (n.d.–0.49 ng g^{-1}), and di-OPEs (0.57–21.1 ng g^{-1}). One NOPE compound, i.e., tris(2,4-di-*tert*-butylphenyl) phosphate (AO168=O) contributed over 65% of the concentrations of the studied OPE-associated contaminants. A 30-day soil incubation experiment was performed to confirm the influence of AO168=O on soil bacterial communities. Specific genera belonging to Proteobacteria, such as *Lysobacter* and *Ensifer*, were enriched in AO168=O-contaminated soils. Moreover, the ecological function of methylotrophy was observed to be significantly enhanced (*t*-test, $p<0.01$) in soil treated with AO168=O, while nitrogen fixation was significantly inhibited (*t*-test, $p<0.01$). These findings comprehensively revealed the contamination status of OPE-associated contaminants in the soil environment and provided the first evidence of the effects of NOPEs on soil microbial communities.

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Assessment of Plant and Earthworm Uptake of Aryl-Type Pollutants in Soil Using Machine Learning Models

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Abstract

With the rapid development of modern industry and urbanization, the release of both traditional and emerging aryl pollutants into the soil has intensified, leading to increased soil contamination. Soil fauna and flora, which are typical components of soil ecosystems, play a vital role in interacting with soil pollutants, either directly or indirectly. However, existing studies on the bioavailability of soil pollutants have predominantly relied on time-consuming experimental methods that lack the ability to offer quick and precise insights. Therefore, the establishment of predictive models has become imperative. Machine learning, renowned for its efficiency and accuracy, has been extensively utilized in environmental research. By integrating soil pollutant studies with machine learning for predictive modeling, it becomes

possible to accurately forecast the bioavailability of pollutants under diverse environmental conditions. This, in turn, can provide more dependable scientific evidence for ecological protection and risk management. The current study utilized various machine learning algorithms to assess the uptake of aromatic pollutants by plant roots and the accumulation capacity of earthworms. The findings revealed that the gradient boosting regression tree model excelled in predicting plant absorption of aryl pollutants in soil (R^2=0.75, MAE=0.11, RMSE=0.22), while the random forest model demonstrated significant effectiveness in predicting earthworm accumulation of aryl pollutants (R^2=0.95). Furthermore, multiple model interpretation techniques were employed to analyze the features, emphasizing the significance of soil organic matter, plant protein and lipid content, animal species, exposure time, and molecular descriptors like xlogP. The study concluded that an increase in organic matter reduces overall absorption rates, with other variables displaying strong correlations within specific ranges. These findings establish a crucial groundwork for future research.

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Emerging contaminants: A One Health perspective

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Abstract

Environmental pollution is escalating due to rapid global development that often prioritizes human needs over planetary health. Despite global efforts to mitigate legacy pollutants, the continuous introduction of new substances remains a major threat to both people and the planet. To confront this challenge effectively, comprehensive research is imperative to understand the sources and potential repercussions of these pollutants on human health, ecosystems, and animals in agriculture, embracing the One Health. Furthermore, evaluating how these contaminants interact with various environmental factors, both living and non-living, is crucial within our ever-changing environments. Leveraging advancements in analytical techniques and artificial intelligence is indispensable for monitoring these emerging environmental pollutants and predicting their behavior within intricate environmental systems. Additionally, careful consideration of the potential risks stemming from advancements in material production across diverse domains, including biotechnology and nanotechnology, is vital for fostering the responsible development of materials for environmental purposes. Addressing environmental pollution demands a paradigm shift in our lifestyles, advocating for policies geared toward minimizing contaminants and implementing coordinated efforts to tackle existing pollutants through global cooperation. This collective endeavor is vital for safeguarding the health and sustainability of our planet for the benefit of both current and future generations, aligning with the principles of One Health.

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Evidence for Historical Emission and Long-Range Atmospheric Transport of Chlorinated Paraffins to the Tibetan Plateau

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Abstract

The Tibetan Plateau, a recognized global sink for Persistent Organic Pollutants (POPs), lies adjacent to two major emitting regions, inland China and India. This unique geographical setting makes it a pivotal site for examining the long-range atmospheric transport characteristics of POPs. This study focused on the current predominant POPs, chlorinated paraffins (CPs). We comprehensively screened 675 homologues of the very short- (vSCCPs), short- (SCCPs), medium- (MCCPs), and long-chain CPs (LCCPs) in six dated sediment cores across the extensive Tibetan area. The findings unveiled pronounced temporal disparities in CP concentrations between Tibet's southern and eastern sectors, reflecting divergent usage and emission chronicles of inland China and India. Notably, the fractionation effect, which intensifies with transport distance from the source regions, may result in varying abundances of vSCCPs, SCCPs, MCCPs, and LCCPs among the six sediment cores. This assumption was supported by their characteristic transport distances—393 km, 776 km, 517 km, and 1303 km, respectively—based on the OECD P_{OV} and LRTP Screening Tool. This study enhances our understanding of the emission inventories and LRAT behavior of these transitional regulatory contaminants, highlighting the Tibetan Plateau's crucial role as an environmental sentinel in global pollution dynamics.

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Foliar Exposure of Deuterium Stable Isotope Labeled Nanoplastics to Lettuce: Quantitative Determination of Foliar Uptake, Transport, Trophic Transfer in a Terrestrial Food Chain

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Abstract

In this study, deuterium isotope labeled ^{2}H-PSNPs were synthesized to serve as a highly sensitive, stable and robust model to evaluate NP exposure in terrestrial food chains at environmentally relevant concentrations. Utilizing this method, we demonstrated dose-dependent absorption of PSNPs by lettuce through foliar application. Specifically, foliar exposure adversely affected lettuce in a dose-dependent fashion, inhibiting photosynthesis and increasing the production of defense metabolites. Dynamic accumulation of NPs in snails fed lettuce leaves exposed to ^{2}H-

PSNPs was also observed, with an overall kinetic TTF value of 0.451, demonstrating trophic dilution in this food chain. Furthermore, feeding on ^{2}H-PSNP-exposed lettuce negatively impacted snail digestion. This impact on the herbivore was due to the accumulation of ^{2}H-PSNPs, which reduced the palatability of lettuce tissues for the snails and to the elevated levels of chemical defense metabolites in lettuce, further disrupting snail digestive function. Overall, deuterium stable isotope labeling provides a reliable method for enhancing our understanding of NPs-plants interactions and shedding light on the potential risks of NPs transfer through food chains to higher trophic levels. This study has some limitations. For example, it utilized a short exposure time and focused on one type of NP at a limited dose range within a short model food chain. Therefore, future research on NP trophic transfer and risk assessment should adopt a more comprehensive approach, exploring low-dose exposure, long-term transfer patterns, diverse NPs, and interacting stressors in more complex food webs. However, the current work provides important insight into NP contamination risk in terrestrial food chains and provides understanding necessary for the development of effective risk management strategies for these emerging contaminants.

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Dissipation of Emerging Organic Contaminants in Soil: The role of Non-Extractable Residue Formation

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Abstract

Removal of organic contaminants from soil is usually recognized by dissipation of these contaminants in soil; however, the dissipation of contaminants does not always mean a complete degradation of the contaminants in the soil, because organic contaminants often form non-extractable residues (NERs, also called bound residues) in soil during the degradation. Using ^{14}C-radiotracer, we studied the dissipation of some emerging organic contaminants, including bisphenolic compounds, polybrominated diphenyl ethers, and sulfonamides, in soils under various conditions. For polar contaminants, their dissipation in soil was mainly attributed to formation of NERs but not degradation, while mineralization (complete degradation) played minor role in the dissipation. NERs of most polar contaminants were formed by sequestration (*i.e.*, physical entrapment and physicochemical adsorption) into soil matrixes and by covalent binding to soil organic matter. Such NERs were not stable in soil and could be released and become available to soil organisms, if the soil redox potential altered, *e.g.*, from anoxic into oxic state. The sequestrated NERs contained both parent and transformation products of the contaminants. Phenolic and anilinic contaminants could formed NERs by binding to soil organic matter via ester- and amide-linkages, respectively, which were instable in soil. In the case of PBDEs, the NER formation was less significant than the phenolic and anilinic contaminants, but almost all NERs were formed by physical entrapment or adsorption. Plants and earthworms could accumulate the contaminants from soil, reduce their NER in soil, and modify transformation pathways of the contaminants in soil resulting in new transformation products. Our results provide detailed information about dissipation of typical emerging organic contaminants in

soil and imply that formation and nature of NERs of both parent and transformation products of contaminants, especially polar contaminants, in soil are crucial in determining the removal efficiency of contaminants, and therefore the risk of contaminants in soil.

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Research on the Crystal Facet Effects Mechanism in the Hydrolytic Conversion of Organophosphate Pollutants Mediated by Nano α-MnO_2.

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Abstract

Organophosphate esters (OPEs) are synthetic derivatives of phosphoric acid, characterized by the substitution of the hydrogen in the phosphate group with three groups, forming triesters. Widely used as flame retardants and plasticizers, OPEs are frequently detected in various environmental media, posing potential threats to ecosystems and human health, thus emerging as notable new pollutants. Hydrolysis is a key natural attenuation mechanism for OPEs. Metal oxides can catalyze OPE hydrolysis at environmental pH, with their catalytic capabilities influenced by intrinsic properties. The effect of intrinsic physicochemical properties, such as exposed crystal facets of manganese oxides, on their catalytic hydrolysis of phosphates, remains to be explored. We synthesized α-MnO_2 materials with primarily exposed {110}, {310}, and {200} facets, systematically studying their catalytic hydrolysis behavior of 4-nitrophenyl phosphate (pNPP), a model OPE, under environmental pH (5-8) conditions and its correlation with exposed facets. Kinetic results indicate facet-dependent catalytic hydrolysis of OPEs by nano α-MnO_2, with α-MnO_2-110 showing the best performance. In situ ATR-FTIR analysis and DFT calculations suggest that unsaturated Mn atoms on exposed facets are adsorption sites, facilitating inner-sphere complexation with phosphate groups, promoting pNPP electron redistribution, activating the P-O bond, and accelerating hydrolysis. This study enhances our understanding of the catalytic hydrolysis mechanism of phosphates by α-MnO_2 and underscores the significant impact of exposed facets on α-MnO_2 catalytic performance, providing valuable guidance for efficient catalysis of organophosphate pollutants.

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Development of the SWAT-KM model to know the dynamic fate of organic contaminants in a watershed: A comparative modeling among three climatically distinct zones

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Abstract

Integration of geo-knowledge into chemicals' environmental behavior modeling has obvious advantages to reveal the environmental exposure discrepancies or hotspots spatially and chronologically. Realizing the prevalent dominance of hydrological processes in water and solid(sediment) transport, we adopted the world famous Soil & Water Assessment Tool (SWAT) model frame in terms its spatial division, its daily timestep, and its fundamental hydrological processes' modelling. Accordingly, we call our model "SWAT-KM" to credit its mother model of SWAT but featured by "KM" which stands for Chemical in a phonatory but concise manner.

The land-water unit-specifical modeling scheme for hydrological modeling in the SWAT modeling system, is invariantly adopted in SWAT-KM. In addition, we developed new models to include air as an important environmental medium which is however disregarded in SWAT. Then the vertical transports between the air, vegetation and soil are interconnected, which is further integrated with the horizontal transports (following SWAT) to make a process based environmental system model with explicit spatial resolution.

Upon each transport process of water, air, or solid(sediment) the authors integrate with it a chemical behavior kinetic equation, which enable the transport of chemical with that of the water air, and/or the solid, and ultimately build a modeling system, i.e., the SWAT-KM, to grasp the multiple media transport of target chemicals in a watershed scale region.

The SWAT-KM was implemented to model demonstrative chemicals in three distinct watersheds in China, namely, the Weihe basin, a semi-arid watershed in the northwestern China, the Beijiang basin, a sub- and tropical watershed in the southern China, and Dalinghe basin, a near-mid-temperate region in northeastern China. For every the three waterwsheds, the SWAT-KM performed reasonably well with its estimated multimedia concentrations agreeing with the literature fairly well. The authors would like to advocate more test and use of the SWAT-KM model with more watersheds and more chemicals.

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Environmental Fate and Risk of Pesticides in Water and Soil

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Abstract

Hydrolysis, photolysis and degradation in soil were three principal degradation pathways of pesticides which might generate toxic chemicals and pose threats to environment and non-target organisms. In the present study, laboratory experiments were carried to study the degradation kinetics, mechanisms and toxicity of the neonicotinoid pesticide imidaclothiz and the triazole fungicide difenoconazole in water and

soil under different conditions. The results showed that imidaclothiz was fairly stable in water and soils under natural condition except in alkaline aqueous solutions or at high temperature. Ten good matched degradation products which reserved the common fragments of parent chemical and conformed to the degradation trend were filtered out using UHPLC-QTOF-MS and UNIFI scientific information system. Then the standards of candidates were synthesized according the structures and analyzed under same condition. The microscopic mechanisms of three degradation reactions (imidaclothiz degraded to M216, M216 degraded to M217 and M216 degraded to M198) were elucidated using theoretical calculation. A total of 14 degradation products of difenoconazole were tentatively identified and six intermediates were further confirmed by self-synthesizing their standards and they were quantified using ultra-performance liquid chromatography with tandem mass spectrometry (UHPLC-MS/MS). Several possible degradation pathways of difenoconazole in water and soil were proposed, which included the cleavage of the ether link, oxidation, hydrolysis, hydroxylation and dechlorination. The toxicity data from experiments and ECOSAR prediction showed that imidaclothiz had low toxicity to Daphnia magna and Danio rerio and had high toxicity to Apis mellifera, 50% of the degradation products exhibited the higher toxicities to aquatic organisms than parent chemical and the degradation products (M149 and M217) deserved more attention in the ecological assessment of imidaclothiz. For difenoconazole, some degradation products that are acutely and chronically toxic to aquatic life may pose a potential threat to aquatic ecosystems, though their toxicities are substantially lower than that of the parent compound difenoconazole. The results of this study are important for elucidating the environmental fate of imidaclothiz and difenoconazole, and provide guidance for further assessing the environmental risks.

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Distribution of antibiotic resistant bacteria in different soil types following manure application

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Abstract

Swine manure is often considered to be an important reservoir of antibiotic-resistant bacteria (ARB). It is commonly used as organic manure. Considering the potential risks of ARB to both environmental and human health, there is an urgent need to understand the distribution and prevalence of ARB in the ecosystem. In this work, we hypothesize that differences in soil type affect the environmental behavior of ARB; their distribution was investigated using three typical soil types including black soil, fluvo-aquic soil and red soil. Experiments were conducted with and without antibiotics in manured soil. Chlortetracycline (CTC) acted as our antibiotic. The results showed that the abundance and diversity of CTC-resistant bacteria (CRB) in black soil was affected by both manures, while they were affected by CTC-manure in both fluvo-aquic and red soils. For the CTC-manure treatment, a more significant shift in the number of OTUs (operational taxonomic units) and the community composition of CRB was observed in fluvo-aquic soil than in black and red soils. Thus, it induced resistance development or an increase in soil indigenous microorganisms (*Streptomyces*, *Pseudomonas*, *Bacillus*, *Rhodococcus*, *Enterobacter*), which was most evident in fluvo-aquic soil. Furthermore, LEfSe analysis specified the key different bacterial genera that

changed significantly between treatments. They were *Microbacteriaceae* in black soil, *Lactobacillus*, *unclassified_c__Bacilli* and *Paenibacillus* in fluvo-aquic soil, and *Dyella*, *Ralstonia* and *Bacillus* in red soil. Moreover, the largest negative influences on *Ralstonia* and *Bacillus* were soil electric conductivity, total phosphorus and organic matter. *Streptomyces* were significantly positively correlated with pH and organic matter. Overall, antibiotic manure application (CTC-manure in this work) would pose a greater influence on a soil's CRB. Taking measures to control antibiotic residues in manure and to conduct proper return methods according to soil types are effective ways of reducing ARB-manure's potential risk to humans and ecosystems. We observed that exposure to raw manure and antibiotic residuals in contaminated manure increased the prevalence and diversity of ARB communities within soils, which has great consequences for safe agricultural practices.

11. Environmental Dehalogenation and Co-transformation of Metals

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Effects of microbial diversity loss on degradation of γ-HCH and methanogenesis in anaerobic soil environment

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Abstract

Anthropogenic activities have led to a general decline in biodiversity in a range of ecosystems. Loss of biodiversity is considered to be detrimental for ecosystem function. A mechanistic understanding, and theoretical support, to clearly explain the loss of ecosystem function under the condition of decreased biodiversity in soil is still lacking. Here, the degradation of γ-HCH (lindane, the gamma isomer of organochlorine pesticide hexachlorocyclohexane) and methanogenesis were track as changes in soil functions under flooding anaerobic environments in which the microbial community diversity had been manipulated through dilution to extinction. 1) In oligotrophic environments, the loss of microbial diversity did not decrease the degradation rate of lindane, but increased the methane production; There is a positive synergistic relationship between lindane degradation and methane accumulation, and dilution treatment may enhance the coupling between reductive dechlorination and methanogenesis; 2) In eutrophic environments, microbial diversity loss reduced the degradation rate of lindane and the methanogenic process in soil, but increased the complexity and the stability of microbial networks. The coupling strength between the reductive dechlorination and methanogenesis weakened with the decrease of diversity; 3) Changes in interspecific interactions could affect the carbon pool storage in soil and the degradation of organochlorine pesticides, causing potential risks for paddy soil management (greenhouse gas emissions) and agricultural green development (long-term residues of OCPs in paddy fields) under biodiversity reduction. In summary, the diversity loss is not the direct reason for the stability change of soil microbial communities; On the contrary, interactions between microorganisms mediated by nutrient conditions have a significant impact on the relationship between community diversity and soil function.

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Chlorinated Organic Pollution Status and Potential Risk in Flooded Environment: Evidence from Meta-Analysis and Case Study

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Abstract

Chlorinated organic pollutants (COPs) are common pollutants in flooded environments. To examine the residual status and effects of COPs on flooded environments, we first applied a meta-analysis to identify the occurrence status, pollution sources, and environmental risk of COPs around the world from 246 peer-published literature, including 25 kinds of COPs from 977 sites. Results showed that the median concentrations of COPs were at the ng g^{-1} level. The environmental risk of COPs on wetlands was higher than in other flooded environments. Correlation analysis indicated a positive and significant correlation between CH_4 emissions intensity and 11 kinds of COPs. Our results highlighted the COP pollution status in wetlands and the potential risk of increased methane emission caused by COPs.

Based on these results, we further surveyed 7 coastal wetlands in Zhejiang, East China. COPs residual level, sediment properties and microbial indicators were measured. Total COP concentrations were detected from 95.69 to 412.76 ng g^{-1} dw. Gamma-HCH and o,p'-DDT posed the greatest risk with exceedance rates of 100% according to sediment quality guidelines. Samples with higher COP pollution had higher microbial diversity, more complex microbial networks, more deterministic community assembly processes and lower microbiome stability. Further analysis using quantitative real-time PCR suggested COP dechlorination interacted with natural redox processes, especially sulfate reduction and methanogenesis. The positive correlation between CH_4 and pentachlorobenzene indicated a potential increase in greenhouse gas emissions caused by COP pollution. Correlation between *dsr* gene and COPs demonstrated the ability of sulfate-reducing bacteria to degrade COPs.

Thus, we try to isolate organohalide degraders from these wetland samples. Two strains were isolated from these wetland samples. The ability of these strains to degrade γ-HCH was demonstrated. And they were identified as *Hungatella* sp. CloS1 and *Enterococcus avium* PseS3. The findings of this study have significant implications for the bioremediation of COP pollution.

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Coupling Effect of Multi-Processes in Soil and the Regulation: Reductive Dechlorination and Methanogenesis

He Yan

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Abstract

Reductive dechlorination mediated by organohalide-respiring bacteria (OHRB), is the most efficient way for depletion of chlorinated organic pollutants (COPs) in anaerobic environment, where the methanogenesis is usually mass-produced. A systematic study is necessary to understand the synergistic associations and mechanisms between reductive dechlorination and methanogenesis, and to develop effective strategies for the simultaneous regulation of both processes.

In this study, we mapped microbial dehalogenation traits and taxonomy across global soil metagenomic samples, highlighting the potential impact of widespread and diverse microbial dehalogenation on organohalide biotransformation and environmental microecology. Our meta-analyses results indicated the accelerated methanogenesis were commonly synergistically coupled with the accelerated removal of COPs. We further emphasized the critical role of extensively distributed OHRBs in natural attenuation of ubiquitous soil residual COPs throughout China, and highlighted the potential risk of methanogenesis due to overlapping ecological niche and positive interaction between OHRB and methanogens. Soil microcosms and culture experiments further verified the syntrophic relationship between γ-HCH dechlorination and methane production, likely due to direct participation of methanogens in dechlorination, and feasible metabolic interaction OHRB and methanogens. Also, methanogenic species could promote some COP dechlorination by regulating cell metabolic functions, e.g., the coenzyme F430 could reduce the activation barrier of reductive dechlorination. Accordingly, we demonstrated the feasibility of simultaneous regulation of conductive materials and acyl-homoserine lactones through microbial electrolysis cells. Collectively, our work provides a novel insight into the multiple environmental function of methanogens that likely contribute to COP dechlorination, and the associations between dechlorination and methanogenesis. Caution is necessary to be paid on the potential risk of increased methane release from flooded soils and sediments polluted with COPs.

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S-ZVI@biochar constructs a directed electron transfer channel between dechlorinating bacteria, *Shewanella oneidensis* MR-1 and trichloroethylene

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Abstract

The technology of combined micron zero-valent iron (mZVI) and microorganisms has received much attention for trichloroethylene (TCE) degradation, however, the electron transfer efficiency between mZVI, microorganisms, and TCE needs to be improved. A sequential chem-bio hybrid process was developed using a composite material (S-ZVI@biochar) prepared by ball milling of sulfurized mZVI and biochar as a chemical remover, and *Shewanella oneidensis* MR-1 and self-isolated dechlorinating bacteria (DB) as a biological agent for TCE degradation. S-ZVI@biochar had better stability, biocompatibility, and TCE removal ability compared to ZVI and S-ZVI. After 30 d of reaction, the removal efficiencies of TCE reached 55.5%, 68.5%, and 93.5% for systems DB, DB + S-ZVI, and DB + S-ZVI@biochar, respectively. MR-1 can not only improve the dechlorination ability of DB, but also improve the dechlorination ability of the composite system of DB and materials. After 30 d of reaction, the removal efficiencies of TCE reached 67.4%, 76.4%, and 96.5% for systems DB + MR-1, DB + MR-1 + S-ZVI, and DB + MR-1 + S-ZVI@biochar, respectively. Combining variation of H_2, evolution of corrosion products, and metagenomic sequencing analysis, the improved dechlorination performance of DB + MR-1 + S-ZVI@biochar was mainly due to the following mechanisms: H_2 and electrons generated by S-ZVI@biochar corrosion were efficiently utilized by DB; MR-1 adjusted the community structure of DB and provided nutrients to enhance the dechlorination capacity of DB; MR-1 converted Fe(III) to Fe(II) in the system and realized the recycling of iron in the system. S-ZVI@biochar constructed electron transport channels in the composite system, thereby improving the overall dechlorination capacity. The increased electron transport efficiency of the composite system enhanced the removal of TCE for the following reasons: Sulfurization modification and biochar modification increased electron transfer efficiency between composites and TCE and chemical dechlorination capacity; DB transferred electrons to TCE through the composite material, which resulted in enhanced electron transfer efficiency and enhanced biological dechlorination capacity; Enhanced electron transfer efficiency between MR-1 and the composite led to enhanced microbial iron reduction and production of more reduced Fe(II) for dechlorination. As a result, iron recycling was enhanced.

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Enrichment of Tetrabromobisphenol A Debrominating Bacterial Consortia: Degradation Characteristics and Bacterial Community Succession

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Abstract

Tetrabromobisphenol A (TBBPA), a widespread and emerging pollutant, adversely affects ecological communities. However, there is little information on the evolution and interactions of microbial communities during the domestication of efficient TBBPA-degrading flora. Therefore, a deeper understanding on the conventional method of enrichment culture is necessary for the development of culture practice and broader application of the microorganisms.

In this study, four dehalogenating flora originating from anaerobic environment polluted by halogenated organic compounds were enriched with 1, 2, 5 and 10 mg L^{-1} of TBBPA by successive and iterative transfers to investigate the degradation characteristics of TBBPA and the changes of microbial community structure during the process. The results showed that the iterative domestication resulted in up to 7.1-fold increase in the degradation efficiency of TBBPA by the flora, and the degradation products were dominated by bisphenol A. Specifically, at the end of the domestication period, the bacterial communities had lower α-diversity, more complex microbial networks, more deterministic assembling processes, lower niche breadth index, more hydrogen production and were predicted to have higher abundance of dehalogenation functional genes. What's more, during the domestication process, the core functional microorganisms that play a key role in the domestication process underwent significant changes, in which genera such as *Sphaerochaeta* and *Proteiniphilum* that are related to hydrogen and acid production were enriched.

All of the above illustrate the shaping of microbial community assembly (structure and interactions) by domestication. This study will contribute to the optimization and development of enrichment culture techniques for the biocontrol and remediation of emerging organic pollutants.

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Pyrolytic carbon enhances microbial anaerobic dechlorination and cadmium co-immobilization

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Abstract

Pyrolytic carbon, acting as an electron shuttle or conductor, plays a significant role in biogeochemical processes such as iron cycling under anoxic conditions, yet its contribution to the reduction-dehalogenation and heavy metal immobilization mediated by iron cycling has been consistently underestimated. The process is likely dominated by the redox and electrochemical activities of pyrolytic carbon, but the specific mechanisms remain enigmatic. This study modulates the redox and electrochemical activities of pyrolytic carbon by controlling the carbonization temperature to explore the underlying mechanisms of pyrolytic carbon in enhancing microbial anaerobic reductive dechlorination coupled with ferrous iron oxidation and cadmium immobilization. The results indicate that high-temperature pyrolytic carbon exhibits the strongest promotion capability for the microbial anaerobic

dechlorination and cadmium immobilization process (after 10 days of incubation, the reduction rates of trichloroethylene and cadmium(II) immobilization reached 77% and 68%, respectively, with cis-1,2-dichloroethylene production at 7.26 mg/L and ethylene at 2.6 mg/L). Low-temperature pyrolytic carbon follows, with a reduction rate of trichloroethene and cadmium(II) immobilization of 50% and 48%, respectively, after 10 days of incubation, and cis-1,2-dichloroethylene and vinyl chloride production at 1.5 mg/L each, with ethylene at 2.2 mg/L. In comparison, medium-temperature pyrolytic carbon shows weaker promotion capabilities for the aforementioned processes. The high-temperature pyrolytic carbon's strong conductivity, attributed to the delocalization of π-electrons in graphitized regions and defects, may function as a geological capacitor, enhancing the electron transfer process in reductive dechlorination coupled with ferrous iron oxidation through charge-discharge; the low-temperature pyrolytic carbon's strong electron-shuttling ability, due to redox-active groups, may act as a geological battery, enhancing the electron transfer process through charge-discharge; whereas the medium-temperature pyrolytic carbon exhibits weaker conductivity and electron-shuttling capacity. This research advances the development of pollutant biogeocatalysis technology based on bacterial-carbon-iron mineral conduction networks.

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Degradation of trichloroethylene by a newly isolated iron-reducing bacterium Escherichia sp. F1 coupled with micron iron powder

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Abstract

Trichloroethylene (TCE) is a common organic pollutant found in soil. The oxide passivation layer covering the surface of micron iron powder prevents the release of its reducing components, resulting in ineffective reduction and purification of TCE in soil. A coupling remediation technology "iron-reducing bacterium-micron iron powder" was developed to improve the degradation effect of TCE in soil. A new iron-reducing bacterium Escherichia sp. F1 was isolated from soil contaminated with chlorinated hydrocarbon, the reduction rate of Fe(III) was 38.7% within 15 days, showing sustained iron reduction ability. Genome sequencing revealed that the strain contained 53 functional iron reduction and 2 dehalogenation genes. Single-factor experiments indicated that the optimal conditions for TCE degradation in soil using the coupling material were as follows: the glucose concentration was 40 mmol/kg, the soil water content was 50%, and the bacterial inoculum was 1% (v:w). Under these optimal degradation conditions, the coupled material reached 86.86% degradation of TCE in soil within 28 days. Further analysis using x-ray photoelectron spectroscopy of micron iron powder, soil Fe(II) concentration, and soil physiochemical properties demonstrated that the addition of strain F1 to soil could destroy the passivation layer of iron oxide on the surface of micron iron powder, promoted the exposure of its reaction sites and internal reducing active components, thus improving the removal rate and achieving complete dechlorination of TCE in soil. Soil microbial high-throughput sequencing revealed that the addition of strain F1 regulated the soil bacterial community, with the relative abundance of Escherichia-Shigella related to iron-reducing function reaching 87.28% in soil. This promotion facilated the degradation of TCE in soil by coupling materials. This study provides a new method for the remediation of TCE-contaminated soil.

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Biogeochemical Regulation for Sustainable Agricultural Soil Remediation

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Abstract

Intensive agricultural activities and high geological background result in widespread heavy metals and pesticides in agricultural soils, exacerbating the global food crisis and thus becoming a barrier to achieve the sustainable development goals. Amongst one of the largest countries in the world, China particularly faces the unprecedent dilemma in restoring over million hectares of croplands, as many field trials have demonstrated with the traditional physicochemical approaches such as immobilization and heavy metal extraction. Hence, there is an urgent need to gain fundamental understanding into the biogeochemical processes of these pollutants in soils. To address this research gap and to resolve the national needs, our group conducted systematic studies from unveiling fundamental understanding into the underlying biogeochemical elements cycles, to developing sustainable technology innovation. Our research reveals that microbially-driven coupling cycling of iron and carbon serves as a key hub for synchronously regulating the migration and transformation of heavy metals and chlorinated phenols in soils. Organic electron shuttling substances are demonstrated to accelerate the reductive transformation of organic pesticides by key functional microorganisms, to achieve dichlorination of these toxic pesticides. In addition, this process can also initiate reduction of ferric iron to consume hydrogen raising soil pH, and subsequently promoting heavy metal passivation, while ferrous iron oxidation activates arsenic oxidation genes, promoting arsenic oxidation and passivation. This achieves synchronous regulation of cadmium/arsenic passivation while blocking arsenic reduction. Accordingly, leveraging this biogeochemical principle for pollutant regulation, biomass-derived carbonaceous materials (e.g., biochar, humic substances) have been developed by incorporating with nano zero-valent iron. Compared to pure zero-valent iron, the number of reactive sites has been greatly increased by two orders of magnitude, leading to substantially improved abatements of diverse pollutants in paddy soils. Compared to pure charcoal, the chemical adsorption constants of cadmium and arsenic have increased by orders of magnitude, with a sound synergistic effect for simultaneous passivation of cadmium and arsenic. Overall, our study paves an avenue towards sustainable agricultural soil remediation.

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Removal of hexavalent chromium and 2,4,6-trichlorophenol from aqueous solution by iron and nitrogen co-doped biochar

Shakeel Ahmad

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Abstract

Research on synthesizing efficient and stable environmental composites and their use in the remediation of halogenated compounds and heavy metals contaminated sites is needed to address water pollution concerns. This research explores iron (Fe) and nitrogen (N) doped biochar (BC) composites for removing heavy metals [hexavalent chromium (Cr(VI))] and halogenated compounds [2,4,6-trichlorophenol (TCP)]. Temperature-dependent Fe-N-BC composites are synthesized with $FeCl_3$ as Fe, melamine and chitosan as N, and pinewood sawdust (PWS) as BC precursors via carbothermal reduction at 300-900 ℃. Characterizations indicating low-temperature incorporates superior N and high-temperature incorporates more Fe species in Fe-N-BC composites. Cr(VI) and TCP are removed with Fe-N-BCs, and experimental results are confirmed with standard isotherm and kinetic models. N species (pyridinic-N, pyrrolic-N, graphitic-N, quaternary-N, and oxidized-N) and Fe species (Fe_3C, Fe^0, Fe $2p_{3/2}$, and Fe $2p_{1/2}$) in temperature-dependent Fe-N-BC composites participate in pollutants removal. Mass ratio of 1:1:1 of Fe, N, and BC is effective, and under optimum conditions, low-temperature and high-temperature composites completely removed Cr(VI) and TCP, respectively. Fe-N-BC is efficient due to Fe, N, and BC synergy for better pollutant interaction and removal. Effects of different operation parameters on pollutants removal with Fe-N-BCs are studied to expose removal mechanisms. According to characterization results of as-synthesized and used Fe-N-BC, TCP removal with Fe-N-BC is attributed to adsorption via pore-filling because of porous structure of Fe-N-BC, H-bonding, electrostatic interactions, and π–π EDA interactions between TCP and Fe-N-BC happened by co-doping of Fe and N species and reduction of TCP by Fe-N-BC. Expected Cr(VI) removal mechanisms by Fe-N-BC are chemical and physical adsorption due to surface pores and N/O functionalities, electrostatic attraction between positively charged Fe-N-BC and negatively charged Cr(VI) ions ($HCrO_4^-$), reduction of adsorbed Cr(VI) to Cr(III) due to surface functional groups on Fe-N-BC, and surface complexation between Cr(III) and N groups on Fe-N-BC in oxidized state. Additionally, Fe-N-BC showed better efficiency for reusability and applicability for multiple pollutants. This study offers a benign approach for synthesizing and applying Fe-N-BCs to remove heavy metals and halogenated compounds and explore reaction mechanisms.

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Screening of tetrabromobisphenol A degrading bacteria and degradation effect study

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Abstract

Tetrabromobisphenol A (TBBPA), a widely used brominated flame retardant in the market, is characterized by persistence, bioconcentration and acute and chronic toxicity, which poses a great threat to ecological environment and human health. In this study, highly efficient aerobic degrading strains of Tetrabromobisphenol A were screened from activated sludge. The preliminary screened strains showed a degradation rate of more than 50% without the assistance of other carbon sources and still had strong degradation ability when the concentration of the target pollutant was 50 mg/L. The results showed that the degradation rate of TBBPA in the activated sludge was higher than that in the activated sludge. The optimal degradation conditions of this strain were explored by controlling the temperature, pH and oxygen content. The present experimental results showed that the optimal degradation effect was achieved in a low concentration, alkaline environment, in which the pH change had a significant effect on the solubility of pollutants and the enzyme activity in the microorganisms.

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Efficient Simultaneous Removal of Cr(VI) and Carbon Tetrachloride from Groundwater by Silicate-Stabilized Green Rust

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Abstract

Green rusts (GRs) are materials with strong reducing ability useful for soil and groundwater remediation. In this study, we synthesized GR_{Cl}-Si with green rust chloride (GR_{Cl}) by using silicate for stabilization and evaluated its capacity for simultaneous removal of Cr(VI) and carbon tetrachloride (CT). Cr(VI) acted as a promoter to accelerate CT removal by GR_{Cl}-Si, while GR_{Cl}-Si could barely degrade CT in its absence. Further analyses of aqueous Fe(II) concentration, Cr(VI) species evolution, and transformations of solid phases showed that Cr(VI) could react with GR_{Cl} and initiate structural changes to form GR_{OX}-Cr(III) precipitates, which exhibited stronger adsorption of silicate than GR_{Cl}. Adsorption experiments showed that GR_{OX}-Cr(III) precipitates might abstract silicate from GR_{Cl}-Si to expose reactive sites of GR_{Cl}. These experiments demonstrated that the GR_{OX}-Cr(III) functions as an adsorbent and promoter to accelerate CT dechlorination by GR_{Cl}-Si rather than as an inhibitor of further redox reactions. This study reveals the positive effect of Cr(VI) on CT dechlorination by stabilized GRs and highlights the importance of Fe(III)-Cr(III) precipitation and environmental behavior during the remediation of contaminated sites polluted with Cr(VI) and chlorinated compounds by using minerals with high iron contents. These findings are valuable for *in-situ* remediation of combined pollution of heavy metals and organic compounds, which is also be implicational for development and diversification of soil and groundwater remediation technology.

621

Interplay of Organohalide Respiration, Sulfate Reduction, and Methanogenesis in Marine Ecosystems

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Abstract

Organohalide pollutants have attracted extensive attention due to their toxicity, bioaccumulation potential and persistence. The marine environment is a major sink of organohalides. But we have limited knowledge about the potential of marine microbes to dehalogenate organohalides and its relationship with the cycling of sulfur and carbon. We investigated the functional microbes catalyzing dehalogenation of organohalides and their interplay with sulfate reduction and methanogenesis.

We found that marine microorganisms use multifunctional reductive dehalogenase (RDase) to dehalogenate diverse organohalides. Enrichment cultures derived from marine samples dehalogenated all tested organohalides. Multiple *Dehalococcoides* and uncultivated Dehalococcoidia were identified in the initial marine microcosms, but only *Dehalococcoides* was dominant in enrichments. Transcription of a gene encoding a PcbA5-like RDase was observed during dehalogenation of different organohalides. When induced by a single organohalide, the PcbA5-like RDase dehalogenated all tested organohalides *in vitro*, suggesting its involvement in dehalogenation of structurally distinct organohalides.

Furthermore, salinity determines performance and microbial ecology in dehalogenating consortia. Marine-derived cultures exhibited higher halotolerance. The dehalogenators in marine cultures shifted from *Dehalococcoides* to *Dehalobium* when salinity increased. Lower microbial diversity, simpler co-occurrence networks, and more deterministic community assemblages were observed under higher salinity. The inhibition of dechlorination by high salinity could be attributed to suppressed viability of *Dehalococcoides* rather than reduced provision of substrates by syntrophic microorganisms. Genomic analyses indicated that the capability of *Dehalobium* to perform dehalogenation under high salinity was owing to the presence of genes associated with halotolerance in its genomes.

We also observed distinct responses of organohalide respiration, sulfate reduction, and methanogenesis to salinity in marine microbial cultures. Sulfate reduction preceeded organoahlide respiration and methanogenesis in the marine microbial cultures under low salinity, whereas the former two microbial processes tended to simultanoeusly occurr and methanogeneiss was inhibited under high salinity. These findings contribute to better understanding the fate of organohalides and its interplay with sulfur and carbon cycling in the marine environment.

669

Lattice-Engineered Nanoscale Fe^0 for Selective Dehalogenation and Long-term Metals Encapsulation

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Abstract

In situ groundwater remediation is in pressing demand for sustainable freshwater supplies. Achieving rapid and highly selective chemical reductions using Fe^0 nanomaterials for groundwater remediation remains challenging. Here lattice-engineered nFe^0 materials with controllable lattice strain and S speciation via a one-step procedure were synthesized to overcome the reactivity–selectivity–stability trade-offs. Chemoselective dehalogenation and hydrogenation at a remarkable activity (up to 956-fold higher than for unmodified Fe^0) outcompete H_2 evolution for >90% electrons from lattice-doped Fe^0, also offering high stability in air and water. The surface accumulation of heavy metals was tuned into intraparticle sequestration via a boosted Kirkendall-like effect. This talk demonstrates the ability to control the local microenvironment in the Fe^0 crystalline structure via lattice engineering, and the tunable geometric and electronic properties constitute a promising platform for the rational design of metallic nanomaterials with robust performance in efficient and selective groundwater remediation.

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Minor chromium passivation of S-ZVI enhanced the long-term dechlorination performance of trichlorethylene: Effects of corrosion and passivation on the reactivity and selectivity

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Abstract

The corrosion and surface passivation of sulfidized zero-valent iron (S-ZVI) by common groundwater ions and contaminants are considered to be the most challenging aspects in the application of S-ZVI for remediation of chlorinated contaminants. This study investigated the impacts of corrosive chloride (Cl^-) and passivation of hexavalent chromium (Cr(VI)) on the long-term reactivity, selectivity, corrosion behavior, and physicochemical properties during the 60-day aging process of S-ZVI. Although the co-existing of Cl^- promoted the initial reactivity of S-ZVI, the rapid consumption of Fe^0 content shortened the reactive lifetime owing to the

insufficient electron capacity. Severe passivation by Cr(VI) (30 mg L^{-1}) preserved the Fe^0 content but significantly interfered with the reductive sulfur species, resulting in an increase in electron transfer resistance. In comparison, minor passivated S-ZVI (5.0 mg L^{-1} Cr(VI)) inhibited the hydrogen evolution while concurrently mitigating the further oxidation of the reductive iron and sulfur species, which significantly enhanced the long-term reactivity and selectivity of S-ZVI. Furthermore, the enhancement effect of minor passivation could be detected in the aging processes of one-step, two-step, and mechanochemically synthesized S-ZVI particles with different S/Fe ratios and precursors, which further verified the advantages of minor passivation. This observation is inspirable for the development of innovative strategies for environmental remediation by S-ZVI-based materials.

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Biochar and Fe-Cr Mineral Interactions: A Novel Approach to Chromium Contamination in Groundwater

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Abstract

Chromium contamination and transport in groundwater is a complex issue in environmental science, especially acute in the context of the prevalence of iron ore. Iron in iron ores affects the morphology of chromium through redox reactions and combines with chromium to form stable minerals, which under certain conditions may release Cr(VI) and exacerbate contamination. Biochar, a widespread carbonaceous component of the environment, interacts with Fe-Cr minerals and participates in their transport and transformation. Although studies have been conducted to explore the role of biochar in the environment where Fe-Cr minerals are present, the synergistic interaction of biochar with Fe minerals with different surface properties and its modulation mechanism on Cr geochemical behavior are still not fully explored. In this study, the surface properties of biochar were modulated by calcination and ball milling under different atmospheres to explore the relationship between these properties and biochar activity and redox properties. Advanced characterization techniques, competitive kinetic analysis and simulation experiments were also applied to reveal the influence of biochar on the reduction and migration of chromium in the presence of iron in groundwater, as well as its interfacial effects and driving mechanisms. The results show that the surface structure of biochar significantly affects the synergistic interaction with iron, probably due to the difference in electrical conductivity of aromatic conjugated carbon structures. The biochar with superior electrical conductivity can act as an electron shuttle to promote the electron transfer in the charcoal-iron-chromium system in water and change the interfacial effect, thus affecting the chromium reduction and migration process. The study also reveals that Fe-Cr migration and transformation in water are mainly regulated by the lactone functional groups on the surface of biochar, and that by altering the

physicochemical properties of biochar and endowing it with different redox activities, it can in turn regulate the electron transfer in iron ore and influence the geochemical cycling of hexavalent chromium. These findings provide a new basis for understanding the environmental behavior of biochar in chromium-containing groundwater and offer new insights into the effects of thermogenic biomass charcoal on pollutants in geochemical cycling.

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Enhanced reductive degradation of trichloroethylene by ball milled nitridation of bimetallic Ni-ZVI: combination effect of electron transfer and catalytic hydrogenation

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Abstract

The performance optimization of zerovalent iron (ZVI) based materials for reductive dechlorination is critical but remains challenging. Combining the advantages of bimetallic modification and heteroatom modification may lead to a novel strategy for reductive dechlorination of chlorinated ethenes (CEs) pollution. In this study, three different types of dual-modified micron zerovalent iron (mZVI) composite particles, namely, pre-bimetallic modified mZVI (Ni/mZVI-N), pre-nitrogen modified mZVI (N/mZVI-Ni), and simultaneously modified mZVI (Ni/N-mZVI), were prepared by adjusting the order of ball milling modification of nickel and melamine, in which ball milling mechanical-chemical interactions contributed to the generation of enriched M-N structures. In terms of combined reactivity and selectivity, Ni/N-mZVI exhibited the best performance, with trichloroethylene (TCE) dechlorination rate and electron efficiency of 0.14 h^{-1} and 8.9 %, respectively, which were 10.7 and 7.5 times higher than those of mZVI. The distribution and percentage of degradation products further illustrated the reductive dechlorination of nickel-nitrogen dual-modified mZVI via both electron transfer and atomic hydrogen (H*) pathways. A series of characterization and mechanistic analyses showed that the enhancement of TCE reductive dechlorination performance could be attributed to the combined effect of Fe−N to accelerated electron transfer and Ni-N to enhance catalytic hydrogenation. In addition to lowering H_2 accumulation, Ni/N-mZVI reduced leaching ions thus mitigating secondary contamination. This double-modification strategy employed to enhance the optimization of mZVI for groundwater remediation establishes a foundation for ongoing progress in the synthesis of reactive materials.

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Study on the effectiveness of an in situ biogenic sulfidated zero-valent iron system for the selective removal of trichloroethylene in groundwater

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Abstract

Impermeable barriers and multiphase extraction are prevalent remediation technologies for purifying groundwater contaminated with chlorinated aliphatic hydrocarbons (CAHs). In recent years, zero-valent iron (ZVI)-based in situ reactive zone technology has emerged as a powerful complement to these traditional methods, facilitating rapid and effective in situ remediation of contaminated groundwater. Site investigation data indicates that the composition of chlorinated groundwater is complex. Nitrate (NO_3^-) acts as the primary natural reductant demand (NRD), competing for ZVI's reduction equivalents and contributing to the formation of toxic vinyl chloride and ammonium. Recent studies have demonstrated that sulfate-reducing bacteria (SRB) can generate biogenic sulfides (S^{2-}, S_2^{2-}) and promote the formation of iron sulfides (e.g., Mackinawite, Pyrite) on ZVI particle surfaces. This process significantly enhances ZVI's reduction selectivity towards trichloroethylene (TCE), a common chlorinated aliphatic hydrocarbon (CAH). Given the common presence of sulfate and sulfate-reducing bacteria (SRB) in aquifers, the in situ biogenic sulfidation of zero-valent iron (ZVI) is proposed as a remedial strategy. However, the effectiveness and sustainability of this approach in environments containing NO_3^- remain poorly understood. To address this, a five-month column experiment was conducted to assess the long-term performance of an in situ biogenic sulfidated ZVI system, targeting TCE as the contaminant. The system's efficacy was compared with both the original ZVI system and a chemically sulfidated ZVI system. Our study revealed that the biogenic sulfidated ZVI system could achieve long-term, complete removal of TCE, with cumulative removal rates 1.57 and 1.16 times higher than those of the other two systems, respectively. The biogenic sulfidated ZVI system also demonstrated the highest complete dechlorination ratio (93.79% ~ 98.69%) and N_2 selectivity (93.92% ~ 97.71%). These results strongly suggest that chemical reduction is the predominant pathway for TCE removal in the system, while biological reduction to N_2 represents the ultimate fate of most NO_3^-. X-ray photoelectron spectroscopy analysis confirmed the presence of the hydrophobic conductive mineral Mackinawite, providing direct evidence of ZVI's biogenic sulfidation. Our findings offer comprehensive and insightful information crucial for selecting remediation schemes in practical applications.

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Prevalence of organohalide-respiring bacteria in sewage sludge and application

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Abstract

Massive amounts of sewage sludge are generated during biological sewage treatment and are commonly subjected to anaerobic digestion, land application, and landfill disposal. Metabolically versatile microorganisms originating from sewage sludge are inevitably introduced to sludge-receiving systems, potentially affecting the fate of POPs. However, there is currently a dearth of comprehensive assessments regarding the capability of sewage sludge microbiota from geographically disparate regions to attenuate POPs and the underpinning microbiomes.

Here, we report the global prevalence of organohalide-respiring bacteria (OHRB) known for their capacity to attenuate POPs in sewage sludge, with an occurrence frequency of ~50% in the investigated samples (605 of 1186). Laboratory tests of 84 sludge microcosms showed extensive attenuation of polychlorinated biphenyls (PCBs) and polybrominated diphenyl ethers (PBDEs) by microbial reductive dehalogenation in 80 (95%) and 82 (98%) microcosms, respectively. Notably, complete debromination of PBDEs to diphenyl ether was observed in 58 (69%) microcosms. Known obligate OHRB (*Dehalococcoides*, *Dehalogenimonas*, and *Dehalobacter*) and several uncultivated Dehalococcoidia populations were implicated in dehalogenation, and it is likely that some of these OHRB employed currently undescribed reductive dehalogenases for PCB and PBDE dehalogenation. Microbial community analyses revealed a positive correlation between biodiversity and dehalogenation activity, whereas there were apparent thresholds of community co-occurrence network complexity beyond which dehalogenation activity decreased.

We also revealed that anaerobic OHRB in consortia could survive under continuous oxygen exposure of up to 24 hours, attributed to the consumption of oxygen by facultative microorganisms and physical protection by sludge flocs. Moreover, we validated that amendment of sewage sludge was an effective approach to remediate POPs in sediments. For example, dechlorination of PCBs was accelerated by 126-544% in a soil microcosm via sludge amendment.

Our findings that sludge microbiota exhibited nearly ubiquitous dehalogenation of PCBs and PBDEs indicate widespread and nonnegligible impacts of sludge microbiota on the fate of POPs in sludge treatment and disposal systems. The existence of diverse OHRB also suggests sewage sludge as an alternative source to obtain POP-attenuating consortia and calls for further exploration of OHRB in sewage sludge.

1050

Microbial Reductive Dehalogenation of Polychlorinated Biphenyls: Pathway and Reactivity

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Abstract

持久性卤代有机物污染不仅破坏自然生态系统，而且严重威胁人类健康。微生物脱卤作为一种经济环保的脱卤途径，在卤代有机物的去除中发挥着重要作用。卤代有机物在脱卤酶上反应的空间选择性及反应活性共同决定了卤代有机物的脱卤途径，从而影响其环境赋存和生态毒性，但该具体机制有待深入研究。因此，我们结合实验及理论计算，开发了一种新的高通量体外酶活筛查方法——HINVARD，其与量子化学及机器学习结合，以多氯联苯（PCBs）作为具有代表性的卤代有机物。我们创新地整合了氯原子电荷和空间效应，使 PCB 脱氯区域选择性合理化（98.3±2.4%的准确率），并与多氯联苯的范德华表面积和溶解度一起进一步阐明了所有 209 种 PCB 同系物的脱氯反应性。值得注意的是，二恶英样多氯联苯同系物易受还原脱氯解毒作用。本研究为了解多氯联苯的环境命运和优化生物修复应用的脱卤模式提供了路线图。

12．Trace Metals in Aquatic Environment

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Co-accumulation of Copper and Zinc in the Eye and Disruption to Visual Pathways in Copper-stressed Zebrafish Larvae

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Abstract

The widespread contamination of aquatic ecosystems with metals is concerning as they accumulate in biota causing adverse effects. This study uses copper (Cu)-stressed zebrafish embryos and larvae to identify regions of accumulation of elevated Cu, the impact of Cu on these regions and any effects on biomolecules present. Embryos at 24h post fertilisation were exposed to excess Cu (<11 μg L^{-1}) and healthy larvae were collected after 48h and 96h of exposure. High-resolution elemental maps from synchrotron X-ray fluorescence microscopy (XFM) revealed increases in the concentrations of Cu and also zinc (Zn) in the retinal tissue of exposed larvae, compared to controls, despite no Zn being added to the medium. Further analysis using X-ray absorption near edge spectroscopy (XANES) showed that the local atomic environment of the accumulated Zn in the eye of the larvae exposed to 10.7 μg L^{-1} of Cu for 96h differed from the controls. Moreover, Fourier transform infrared microscopy (FTIR) revealed changes in the relative amount of aldehyde and Schiff-base molecules in the retinal pigment epithelium at 96h of Cu exposure. However, it was only at the earlier time point of 48h that exposure to 10.7 μg L^{-1} of Cu caused the differential expression of proteins involved in retinol synthesis and the visual cycle, including rhodopsin. This study shows that environmental Cu accumulates in the eye and may disrupt visual processing and key visual behaviours necessary for survival.

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Bioimaging Techniques for Quantitative Monitoring of Label-Free Metallic Nanoparticle in a Unicellular Alga

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Abstract

Simultaneously quantitatively monitoring label-free metallic nanoparticles (MNPs) and their corresponding ionic counterparts is critical to determining the exact contribution of MNP toxicity. Herein, we propose a novel bioimaging technique by coupling the aggregation-induced emission (AIE)-based bioimaging with label-free scattered light imaging, which allows for quantitatively visualizing the unlabeled MNPs and their corresponding metal ions in *Chlamydomonas reinhardtii* (*C. reinhardtii*). The proposed bioimaging method was first confirmed using the commercialized bioimaging and quantification techniques. The detection limit of the proposed method towards the intracellular unlabeled MNPs and metal ions was about 45.63 to 62.55 μg/g and 6.76 to 22.38 μg/g, respectively. Besides, MNPs within 18 to 110 nm can be quantitatively visualized as well as their dissolved ionic counterparts. Further, we confirmed the internalization of MNPs in the algal cells, with more than 90% of the total metal concentrated at the apical zones, the cell wall, and the cytoplasmic regions. The ratio of MNPs and metal ions ranged from 9.52% to 32.03% across different types of MNPs, suggesting the capability of the proposed method for distinguishing and quantifying various types of MNPs and corresponding metallic ions. Contrasting to the biodistribution patterns of MNPs, around 80% of different types of metal ions were consistently detected at the cell nucleus, suggesting that the nucleus can be one of the major intracellular accumulation sites. This study proposes a novel bioimaging and quantification method for quantitatively monitoring the intracellular unlabeled MNPs and their corresponding ionic counterparts, having tremendous implications for exploring the biological behaviours of MNPs and their potential toxic mechanisms.

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Investigating environmental fate of lithium from the Yangtze River to the East China Sea: Distribution, source and bioaccumulation

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Abstract

The application of lithium (Li) has been prospering in the recent decades, which would increase the Li burden in the aqueous environment. However, the environmental fate of Li in the area adjacent to developed Li industry still remains research gap. Here, we investigate the distribution and source of dissolved Li from the lower reaches of Yangtze River to the East China Sea (ECS) inner shelf, and the Li bioaccumulation in the coastal food web. As for the dissolved Li in the lower Yangtze River, the concentrations of the river waters in 2022 were remarkably higher than 2006, while the δ^7Li values were significantly lower. Importantly, the site with the highest Li concentration was impacted by significant anthropogenic Li input, supported by the δ^7Li value close to the wastewater and the relatively substantial registered capital of Li industry in the sampling city. Consequently, anthropogenic disturbance has induced the non-negligible impacts on Li in the Yangtze River. As for the aquatic environment from the Yangtze River Estuary (YRE) to the ECS inner shelf, the behavior of dissolved Li was conservative that the concentrations linearly increased with the salinity and were not strongly impacted by other water parameters. The bioaccumulation of Li in the fish was not principally impacted by trophic transfer, supported by the non-positive correlation between the Li contents and stable nitrogen isotopes. Despite more concentrated Li in the habitat, the high salinity and benthic fish did not have significantly higher contents of Li, and the bioaccumulation factors (BAF) were significantly lower. In addition, the contents of Li displayed strong positive correlation with the Na contents in the fish, which can be explained by the cell transport of Li associated with Na^+/H^+ exchangers. The high salinity can decrease the bioavailability of Li via inhibiting transmembrane transport of Li rather than altering the metal speciation, thus leading to the lower contents and BAF of Li observed in the benthic fish. Therefore, our results illuminate that the salinity is the pivotal factor on dissolved Li distribution in the aquatic environment and Li bioaccumulation in the food web, which facilitate the precaution of ecological risk under the escalating Li industry.

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Stimulating and toxic effect of chromium on growth and photosynthesis of a marine phytoplankton

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Abstract

Marine phytoplankton can interchange trace metals in various biochemical functions, particularly under metal-limiting conditions. Here, we investigate the stimulating and toxicity effect of chromium (Cr) on a marine Chlorophyceae Osetreococcus tauri under Fe-replete and Fe-deficient conditions. We determined the growth, photosynthesis, and proteome expressions of Osetreococcus tauri cultured under different Cr and Fe concentrations. In Fe-replete conditions,

the presence of Cr(VI) stimulated significantly the growth rate and the maximum yield of photochemistry of photosystem II (F_v/F_m) of the phytoplankton, while the functional absorption cross-section of photosystem II (σ_{PSII}) did not change. Minor additions of Cr(VI) partially rescued phytoplankton growth under Fe-limited conditions. Proteomic analysis of this alga grown in Fe-replete normal and Fe-replete with Cr addition media (10 μM Cr) showed that the presence of Cr significantly decreased the expression of phosphate-transporting proteins and photosynthetic proteins, while increasing the expression of proteins related to carbon assimilation. Cr can stimulate the growth and photosynthesis of O. tauri, but the effects are dependent on both the Cr(VI) concentration and the availability of Fe. The proteomic results further suggest that Cr(VI) addition might significantly increase starch production and carbon fixation.

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Environmental processes-exposure mechanism-ecological health of arsenic in nearshore waters

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Abstract

Arsenic pollution has become a serious environmental problem in China, South Asia, Southeast Asia and other places. Arsenate [As(V)] mainly exists in marine environment, which has high toxicity, teratogenicity, carcinogenesis and other hazards. Arsenic is bioaccumulated and passed along the food chain, resulting in risks to seafood safety and marine ecology and potential health threats to consumers.

Salinity and arsenic species play a major role in arsenic migration, and salinity is the key controlling factor. Dietary absorption is the main way of arsenic accumulation in marine fish. The transport and transformation rules of arsenic between different tissues and organs of marine fish were revealed, and the synthesis of arsenobetaine (AsB) in the gut and the storage of AsB in the muscle were the main reasons for the high arsenic enrichment in marine fish, and the exposure mechanism of arsenic in the metabolic organs-intestines and target organs -muscles was revealed. AsB had a weak ability to pass through the intestinal membrane and was slowly absorbed and eventually stored in the muscle, while As(V) showed a rapid ability to pass through the intestinal membrane, transport and discharge quickly. Marine fish could convert toxic As(V) in the environment into non-toxic AsB to achieve the purpose of detoxification. It was first reported that *bhmt*, *mat2aa* and *gstt1a* were the key genes involved in AsB synthesis in marine medaka, which provided the key evidence for AsB synthesis. It is explained that AsB is more easily transferred and absorbed along the food chain than inorganic arsenic during the transfer process of different arsenic forms, and the transfer efficiency along the food chain of AsB is 4-9 times higher than that of inorganic arsenic, and the bioavailability of AsB is higher than that of inorganic arsenic. The bioavailability of arsenic in marine fish has been verified, which solves the scientific question of the transfer of different arsenic forms along the food chain. Mice can degrade non-toxic AsB to As(V) raises

significant health concerns about the long-term intake of arsenic from seafood and calls into question the reasonableness of limiting only inorganic arsenic in seafood. Therefore, the mechanism of high arsenic enrichment in marine fish and the potential risks to human health were analyzed, which provided important theoretical and technical support for the bioavailability, food safety, and human health risks of arsenic.

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Cultural Considerations of Trace Elemental Seafood Safety Following Volcanic Eruption at Whakaari White Island

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Abstract

Whakaari (White Island) is a continuously active volcano located 50 km offshore from the town of Whakatane, Te Moana a Toi, Aotearoa New Zealand. A major eruption in late 2019 resulted in the deaths of 21 visitors to the island and life-changing injuries to many more.

The local iwi/ tribe, Ngāti Awa, placed an immediate rāhui/ restriction in the area to prohibit taking seafood and as a sign to acknowledge the lives lost in the tragedy. A 1km exclusion zone (rāhui) surrounding Whakaari has been put in place to prohibit fishing.

In response to the eruption, local iwi were concerned regarding the safety of consuming kaimoana/seafood near Whakaari, due to geothermal emissions of toxic trace elements, and a project has been undertaken to understand trace element bioaccumulation in seafood in the vicinity of the volcano. This presentation focuses on this research from an indigenous perspective.

To address this potential health problem, environmental management from Te Rūnanga o Ngāti Awa/ tribal council co-developed a research PhD project with The University of Waikato to investigate contamination by toxic trace elements in finfish and shellfish at Whakaari. The project encompasses traditional Māori knowledge from Ngāti Awa to align with their values and to ensure that the outcomes of the research will be relevant for their community. The target species encompass a range of fish and shellfish species at different trophic levels and were selected because they are tāonga/culturally significant species. To effectively work with iwi, it was important to follow customary protocols wherever possible and show respect to the people and the environment. With guidance from Kura Paul-Burke, we held an initial ceremony before work began and invited elders of the iwi to participate in the planned fishing trips. Attempts were made to time seafood collection with the Māori fishing calendar (Maramataka). We have hosted a workshop with youth/rangitahi to share some of the laboratory processes of sample analysis and have held wānanga/meetings to share and discuss this research with iwi. When this research is completed, we hope to disseminate the results with Ngāti Awa which will inform

tribal elders to help keep their community safe and provide valuable information to inform future iwi-led marine development in Te Moana a Toi.

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Trace Element Bioaccumulation in Marine Biota from an Active Marine Volcano; Whakaari White Island

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Abstract

Whakaari/White Island is one of several continuously active volcanoes situated in the Bay of Plenty off the north-east coast of New Zealand. In 2019, an eruption tragically killed 21 people visiting the island, and the ejection of volcanic material raised concerns for local people about the safety of consuming seafood in the vicinity of the volcano. In addition to periodic eruptions, discharges of geothermal fluids to the adjacent marine environment continuously occur from the crater lake and submarine vents. Emissions from Whakaari are known to contain elevated concentrations of several toxic elements including mercury, cadmium, lead and arsenic.

We investigated the bioaccumulation of potentially toxic trace elements in several species of finfish and shellfish from the volcano and within the wider Bay of Plenty Region, which also receives geothermal inputs via rivers draining inland geothermal regions. The species were chosen to represent commonly consumed seafood and across several trophic levels from algal grazers (urchin) to large predatory fish (yellowtail kingfish).

Fish species resident at Whakaari White Island displayed elevated concentrations of mercury and cadmium with concentrations tending to be higher in reef-resident species close to geothermal emissions. Bioaccumulation of elements varied significantly between species and, as expected, some elements showed relationships with fish size or age, especially for species with long life-spans. Large variability was observed between individuals of the same species at the same sites which complicates advice for consumers regarding safe levels of consumption.

Results of this study will be shared with the local population, especially Maori (Ngāti Awa), to provide recommendations for customary and commercial fishers within the Bay of Plenty, and to inform how local trace element concentrations might affect proposed aquaculture development in the area.

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Predicting Sedimentary Toxicity Using DGT-Induced bioavailable Metals within a Toxicokinetic-Toxicodynamic (TKTD) Model Framework

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Abstract

Quantitatively predicting heavy metal bioaccumulation and toxicity is crucial for understanding the the ecological risks of contaminated sediment. However, existing toxicokinetic-toxicodynamic (TKTD) models that describe the adverse biological effects of heavy metals face challenges when applied to contaminated sediments, particularly in distinguishing complex exposure pathways (i.e. aqueous and dietary exposure). The technique of diffusive gradients in thin films (DGT) enables measurement of metal concentrations from both porewater and those loosely bound to sediments. Using DGT-induced bioavailable metals to characterize metals accumulated by organisms through various complex pathways in TKTD model appears feasible. In this study, benthic clams (*Ruditapes philippinarum*) were exposed to sediments spiked with varying concentrations of copper, while measuring metal accumulation and observing their survival. To further simplify model construction, we assumed that parameters such as the efflux rate constants (k_e), internal threshold concentration (C_{IT}), and killing rate (k_k) are controlled soley by the physiological processes of the organism and remain independent of the exposure medium. These parameters were thus obtained independently from aqueous exposure tests. Our finding indicated that predicting copper bioaccumulation and toxicity in sediments is effectively done using DGT-measured bioavailable metal concentrations and parameter values from aqueous exposure tests. Overall, this approach provides a reliable method for predicting metal bioaccumulation and toxicity in contaminated sediments, enhances the assessment of ecological risks associated with metal-contaminated sediments, and offers insights for environmental risk management.

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Incorporating Passive Sampling Data into a Toxicokinetic-Toxicodynamic (TKTD) Model for Predicting Sedimentary Metal Toxicity

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Abstract

Developing kinetic models, such as the toxicokinetic-toxicodynamic (TKTD) model, to predict the bioaccumulation and toxicity of metals in sediments is crucial but challenging. The primary difficulty lies in delineating the contributions of metal uptake through different pathways (i.e. aqueous and dietary exposure). The diffusive gradients in thin-films (DGT) technique, a passive sampling method, can capture metals from both porewater and those loosely bound to sediments, which are potential pools of bioavailable metals. Using DGT-labile metal concentrations as a surrogate in the TKTD model appears promising. To test this approach, we exposed the benthic clam species, *Ruditapes philippinarum*, to sediments amended with varying levels of Cu, while measuring metal bioaccumulation and monitoring their temporal survivorship. To further simplify model construction, we assumed that parameters such as the efflux rate constants (k_e), internal threshold concentration (C_{IT}), and killing rate (k_k) are controlled soley by the physiological processes of the organism and are independent of the exposure medium. These parameters were thus obtained independently from aqueous exposure tests. Our study demonstrated that both Cu bioaccumulation and toxicity can be effectively modeled by the TKTD model using DGT-labile concentrations and parameter values from aqueous exposure tests. Overall, the results highlight that developing the sedimentary TKTD model can benefit from the DGT passive sampling measurement and the existent aqueous toxicity model database, making it a valuable tool in assessing the ecotoxicity risk of metal-contaminated sediments.

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Room-temperature Synthesis of Defect-Rich Hierarchical Porous UiO-66-NH_2 for Enhanced Arsenate Removal

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Abstract

As(V)-contaminated drinking water has affected millions of people worldwide. Zr-based metal-organic frameworks (Zr-MOF) are attractive for removing arsenic from water due to its high chemistry stability and tunable active sites. However, the practical feasibility of Zr-MOFs is limited by low adsorption kinetics and difficulties in achieving deep removal. In this work, we developed an advanced synthesis route by coupling room-temperature method and modulator-

induced strategy to fabricate the rich-defected hierarchically porous Zr-based metal-organic frameworks (UiO-66-NH_2) at room temperature for highly efficient As(V) removal from water. The optimized UiO-66-NH_2 showed high crystallite, abundant mesopores and rich defect sites, and outstanding deep adsorption performance towards As(V). Specifically, at low As concentration (50-1000 ug/L), As(V) levels can be reduced to below 10 ug/L at neutral pH using the rich-defective UiO-66-NH_2 as adsorbent (0.25 g/L). Batch adsorption experiments showed that the defective UiO-66-NH_2 exhibited adsorption capacity of 180.3 mg As/g and achieved adsorption equilibrium within 60 min. moreover, the obtained UiO-66-NH_2 showed strong anti-interference towards common co-existing ions and humic acid. The adsorption mechanism suggested that the strong coordination between As(V) an Zr cluster and the hierarchically porous structure played a critical role in boosting As(V) uptake performance. It's worth noting that high As(V) concentration (co >10000 ug/L) promoted the release of the component belonged to UiO-66-NH2 due to the competing coordination between As(V) and organic ligand to Zr cluster, whereas very small amount of the component could be detected when exposed to low As concentration (co < 1000 ug/L). In fixed-bed experiments, the treatment volumes of As(V) spiked natural surface water reach about 3 L using column packed with UiO-66-NH2-8 (co =191 ug/L, 100 mg of adsorbents in each column). This study offers a new strategy for design high performance Zr-MOF adsorbents for purification of practical As(V)-contaminated drinking water.

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Neurotoxicity and Behavioral Effects of Dietary Selenium in Zebrafish

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Abstract

Selenium (Se) is an essential trace metal for animals, but toxicity occurs at higher concentrations than those needed for normal development and growth. Fish behaviors are important for their survival and population stability in the wild. Swimming performance, locomotion, aggression, courting, feeding, and predator avoidance can all be impacted by exposure to toxicants. Fish behaviors are often controlled by neurotransmitters secreted from areas of the central and peripheral nervous systems. However, mechanisms and key events associated with the effects of selenium on neurotransmitters and the associated behaviors in fish are unclear. Therefore, we exposed adult zebrafish to dietary selenium at environmentally relevant concentrations for two months. Targeted metabolomics, histopathological, and transcriptional endpoints were compared to behavioral metrics to evaluate the effects of dietary exposure to selenium. We found that mitochondrial damages and decreased activities of the mitochondria respiratory chain complexes in the neurons. In addition, dietary selenium influenced neurotransmitters, metabolites, and transcripts of the genes associated with the dopamine, serotonin, gamma-aminobutyric acid, acetylcholine, and histamine signaling pathways in zebrafish brains. The swimming behaviors were

altered. These results provided more data on the effects of selenium-affected ultrastructure of the zebrafish brain, neurotransmitters, and fish behaviors. These data would help enhance adverse outcome pathways for neurotransmitter-behavior events in fish.

451

Research on Detection/Monitoring of Different Species of Trace Metals in Coastal Seawater

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Abstract

Trace metals in the marine waters play an important role in the growth of phytoplankton and human health. The morphology, bioavailability, and relationship with algae of trace metals have always been a hot topic in marine science. Our research group has established electrochemical detection methods for dissolved and labile metals in seawater. Relevant instruments have also been developed for the study of the speciation analysis, spatio-temporal distribution, and relationship with algal absorption of trace metal in coastal seawater of China.

468

Assessment of Metal Concentrations in Macroinvertebrates along the Longitudinal Gradient of the Apies River, South Africa

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Abstract

The Apies River drains a catchment characterized by urbanization, wastewater work, and industrial and agricultural activities. The river is regarded as one of the most polluted systems in South Africa. Therefore, the present study aims to assess the concentrations of As, Cr, Cu, Fe, Pb, Ni, and Sr in macroinvertebrates from the Apies River. Water and macroinvertebrates samplings were conducted between December 2019 – March 2020, and February 2021 – December 2022 at the headwaters, a site after Pretoria town and a site further downstream. The water exhibited

neutral to slightly alkaline pH at all sites throughout the study ($p>0.05$). Arsenic, Fe, and Sr in the water showed significant differences between sites whereas Cr, Cu, Pb, and Ni were below detection levels. There was a significant shift of macroinvertebrate community structure from the headwaters, through to urbanized and further downstream stretches. Sensitive taxa such as Atyidae and Aeshnidae were observed in the headwaters with tolerant taxa such as oligochaetes, leeches, chironomids, and caddisflies being observed in polluted sites. A site immediately after the wastewater effluent discharge point showed relatively higher metal concentrations for oligochaetes and leeches, and vice versa for caddisflies and coenagrionids. In contrast, Potamonautidae was recorded at the headwaters and further downstream with those collected from downstream exhibiting relatively higher concentrations for most metals ($p<0.05$). Taxa occupying higher trophic levels exhibited relatively higher metal concentrations compared to those at the lower levels. These findings provide guidance on which taxa to be considered for biomonitoring and risk assessment in metal-impacted streams.

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The differences on the bioavailability between light and heavy rare earth elements in *Daphnia magna*

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Abstract

Rare earth elements (REEs) have recently emerged as contaminants in the environment, but the their bioavailability to the zooplankton is still under scrutiny. We assessed the bioaccumulation of light (Nd) and heavy (Y) rare earth element via different exposure pathways. The uptake rate constants (k_u) of Nd and Y from the dissolved phase did not show any significant changes, ranging between 2.48 and 2.75 $L \cdot g^{-1} \cdot h^{-1}$. In terms of dietary exposure, there was a notable variation in the assimilation efficiency (AE) of Nd and Y in daphnids. The elimination rate constants (k_e) of Nd and Y were ranging between 0.23 and 0.33 d^{-1} in daphnids. We found that when the concentration of Nd and Y in the aquatic environment is more than 3×10^{-8} M, the main uptake pathway is through the water, making up to 98% of the total accumulation. We also investigated the uptake and elimination of fifteen rare earth elements in daphnids. The elements Nd and Sm were the most abundant in the daphnids, whereas La and Y were the least abundant. This indicated an enrichment of light REEs compared to heavy REEs in the daphnids.

495

Trophic Level Bioaccumulation of Cadmium in Macrobiota of the Geothermal Te Arawa Lakes, New Zealand

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Abstract

Freshwater environments may become enriched with potentially toxic, non-essential trace elements through natural or anthropogenic processes, and New Zealand has experienced anthropogenic enrichment with cadmium through the use of phosphate fertilizers in pastoral agriculture. In addition to anthropogenic sources, New Zealand aquatic environments also receive geothermally sourced inputs of cadmium. The unique and varied geochemistry of the thirteen Te Arawa Lakes in the Rotorua Region serves as an excellent natural system to examine processes associated with bioaccumulation of geothermally derived trace elements. Non-essential heavy elements such as mercury and lead are generally assumed to progressively biomagnify with increasing trophic level. However, cadmium appears to exhibit a much more complex trophic association. Cadmium levels in fish from cadmium-enhanced environments may be significantly elevated in some species and not in others. Analyses were undertaken of macroinvertebrates (crayfish/kōura and unionid mussels/kākahi) representing important traditional foods (mahinga kai) for local Māori, and rainbow trout, an important local sports fishery. Wherever possible, all species were sampled from each of the Te Arawa Lakes, and the results showed lowest bioaccumulation of cadmium in trout and the highest levels in koura, with this pattern being consistent across many lakes with highly variable cadmium concentrations. A strong correlation was seen between tissue zinc and cadmium. With the exception of one lake (Rotorua), a strong association was also observed between cadmium in koura and the trophic status of the lakes. Further understanding of trophic distribution of cadmium and other potentially toxic trace elements in New Zealand freshwater environments is required to fully understand ecological threats and human consumption risks associated with harvested species in geothermally associated aquatic environments.

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Zinc Availability Can Regulate Dimethylsulfoniopropionate (DMSP) Production by a Coastal Diatom

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Abstract

The DMSP (dimethylsulfoniopropionate) and its enzymatic products DMS (dimethyl sulfide) have important physiological functions in phytoplankton, including osmotic stress protection, cryoprotection, and ROS (Reactive Oxygen Species) scavenging. They are also considered to play a pivotal role in regulating Earth's climate. The DMSP production by marine phytoplankton was known

to be light and temperature dependent, and potentially can be affected by the availability of trace metals such as Zn, which regulates various essential biological pathways involved. Here we investigate how Zn availability impacts DMSP production by phytoplankton under different temperatures. We exposed the coastal diatom *Phaeodactylum tricornutum* to a wide range of Zn concentrations (0.0798 to 39900 nM) under their optimal growth light intensity (190 μmol photons m^{-2} s^{-1}) and two temperature conditions (17°C and 25°C). The optimum growth rates were found at 79.8 nM under 17°C and at 7.98 nM at 25°C, indicating that the diatom might have lower Zn requirements under higher temperature (half saturation constant under 25°C versus 17°C: 0.00394 < 0.02558). Zn limitation (0.0798 nM) led to an over 30% reduction in growth rates under both temperatures. Zn toxicity (39900 nM) caused a 44% decrease in growth rates under 25°C, while only 23% reduction was found under 17°C. Compared to lower temperature condition, higher temperature (25°C) in this study led to a dramatically lower production of DMSPt+DMS in phytoplankton across all Zn treatment groups, but no significant difference was observed between Zn treatments. Zn limitation appears to significantly promote the production of DMSPt+DMS (up to nearly 4 fmol/cell), whereas excess Zn decreased their production to below 2.5 fmol/cell under 17°C. Our study highlights the importance of Zn availability in regulating DMSP production by marine phytoplankton that was dependent on temperature, which might be linked with phytoplankton Zn requirements under different temperatures.

502

Unraveling Metal Allometry by Toxicokinetics in Hong Kong Oyster: Critical Role of Age

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Abstract

Allometry of metal concentrations in marine bivalves challenges the assumptions of prevailing biomonitoring programs, which assume a direct relationship between metal concentrations in organisms and the ambient environment. While the allometric effect of body size is easily observed, the influence of age is often overlooked, despite its importance. This study aims to elucidate the intertwined effects of body size and age on metal concentrations in Hong Kong Oyster. By analyzing oysters of varying ages and sizes, we determined metal bioaccumulation capacity across and within age groups. For most metals studied (Cu, Zn, Cd, Pb, Ni, and Ag), metal concentrations generally increase with body size across age groups. Age-dependent metal uptake rates (aqueous rate constants k_u and dietary rate constants k_f) emerged as the primary driver of this trend, while size-dependent uptake playing a lesser role. Additionally, factors such as age-dependent effective exposure time and size-dependent growth dilution, particularly for metals with slower elimination like Cu, also influenced metal uptake. These factors weakened the negative correlation between metal concentration and body size. Overall, the results

underscore the importance of incorporating age data into biomonitoring programs for more accurate assessments of metal contamination in marine bivalves.

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Speciation, distribution and relationship of zinc and cadmium in summer coastal seawater of northern China

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Abstract

Considering that zinc (Zn) is essential for marine phytoplankton growth and cadmium (Cd) can replace Zn as a cofactor of mutual conversion and regulate the effect of carbonic anhydrase, we here presented the concentration, chemical speciation and relationship of Zn and Cd collected from three consecutive voyages (2019–2021) in summer coastal seawater of northern China. Dissolved Zn and Cd concentrations were determined using inductively coupled plasma mass–spectrometry (ICP–MS) and ranged from 0.37 to 3.09 μM and 1.88–13.66 nM, respectively. Natural labile Zn and Cd were determined using a highly automated electrochemical detection system and ranged from below detection limit-1.11 μM and below detection limit-5.23 nM, respectively. The speciation, distribution and interrelationships of Zn and Cd were compared with the distribution of the diatoms community, and studied by the correlation with pH and dissolved inorganic carbon (DIC). Finally, the Zn and Cd labile and inert chemical species concentrations were compared with those of the open sea and the coast. The results indicated that the dissolved Zn and Cd concentrations in surface seawater were higher than those in bottom seawater, possibly due to the dominance of exogenous inputs compared to phytoplankton uptake. Higher phytoplankton abundance was associated with lower natural labile Zn and Cd concentrations, but this was not the main factor affecting the distribution of natural labile Zn and Cd. Unlike the open ocean, there was no potential for Zn limitation of certain phytoplankton groups in this region, but both Zn and Cd played important roles in the fixation of carbon dioxide, and Cd might result in mitigating Zn uptake. Activities such as ocean currents, which bring limiting nutrient trace metals (e.g., Zn) from the coast into the open ocean, could regulate the structure of primary producers. This study has great potential for the investigation of the biogeochemical cycling of Zn and Cd and their role in marine carbon fixation in coastal seawater.

538

Temperature and Salinity Modulate Thallium Accumulation in a Coastal Snail: Insights from Toxicokinetic Modeling

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Abstract

Thallium (Tl) concentrations in water bodies are typically low, resulting in limited bioaccumulation data and challenging ecological risk assessments. However, previous investigations have found high background concentrations of Tl in *Reishia clavigera*, a common coastal snail species ideal for biomonitoring due to its wide temperature tolerance. Given that it also inhabits areas with varying salinity levels, it is crucial to understand the impact of salinity and temperature on Tl accumulation. This study used metal stable isotope tracing to determine the toxicokinetics of Tl in *Reishia clavigera*under varying salinity and temperature conditions. Results showed that within a salinity range of 15 to 30, Tl accumulation decreased as salinity increased. The uptake rate constant (k_u) decreased from 0.287 ± 0.017 L g^{-1} d^{-1} to 0.132 ± 0.012 L g^{-1} d^{-1}, while the efflux rate constant (k_e) remained consistent at 1.812 ± 0.148 d^{-1}. Within a temperature range of 7-28°C, the highest Tl concentration was observed at 21°C (0.138 ± 0.019 µg g^{-1} dry weight, N = 64). Both k_u and k_e increased with rising temperature, but k_e increased more significantly. Overall, the study demonstrates Tl accumulation in *Reishia clavigera* is influenced by salinity and temperature. Salinity primarily affects the uptake phase, while temperature variations significantly impact the elimination phase. These findings enhance our ability to accurately interpret biomonitoring data and assess the ecological risks of Tl contamination.

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Aquatic ecotoxicology of metals in the environment: A perspective

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Abstract

Aquatic ecotoxicology of metals has an enriched history spanning half a century. It first started with measurements of metal concentrations and speciation in aquatic systems, followed by examining their impacts on aquatic ecosystems as well as conducting environmental risk assessments. With a diversity of metals (metalloids) and organisms, both fundamental and applied research have been conducted over the past decades. Modeling is often the highlight of ecotoxicology given the complexity of different chemical and biological processes involved. In this talk, I will discuss some of the perspectives in the field, in particular, 1) developing new technologies to studying many of the ‘unsolved’ mysteries of metals in both environmental and biological systems; 2) studying the real environmental impacts of metals on aquatic systems.

619

Utilizing modified Nanoscale Zero-valent Iron (nZVI) for Cr(VI) Removal with High Efficiency

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Abstract

As a kind of trace metal in aquatic environment, Cr(VI) poses a threat to human health and freshwater systems due to its high toxicity and superior mobility. Several modifiers have been used to prepare modified nanoscale zero-valent iron (nZVI) to enhance the efficiency for Cr(VI) removal. However, the modification performance and mechanism of different types of modifiers have never been compared in depth. In this study, four typical modified-nZVIs, including pyrogallic acid modified nZVI (pyGA-nZVI), ethylenediamine modified nZVI (EDA-nZVI), sodium dihydrogen phosphate modified nZVI (MSP-nZVI) and sodium persulfate modified nZVI (PS-nZVI) were prepared by directly adding modifiers during the synthesis of nZVI. pyGA-nZVI presented the highest efficiency for Cr(VI) removal (complete removal within 8 min), followed by MSP-nZVI (81.7% within 30 min), EDA-nZVI (77.1% within 30 min) and PS-nZVI (55.1% within 30 min). The addition of modifiers reduced hydrogen generation, boosted the electron selectivity and prolonged the life of modified nZVIs. Fe^0 was the main contributor to Cr(VI) removal by nZVI, EDA-nZVI and PS-nZVI, while Fe(II) was mainly responsible for Cr(VI) removal by pyGA-nZVI and MSP-nZVI. The decrease of P and S element demonstrated the direct participation of MSP and PS in Cr(VI) removal, while the same content of N before and after reaction indicated the indirect involvement of EDA. This research provided a perspective on the performance enhancement mechanisms of different nZVIs and might regulate the utilization efficiency of modified nZVI in subsequent application.

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Spatial Distribution of Heavy Metals and Ecological Risk Assessment of Wetland Soils in Rara National Park, Central Himalaya

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Abstract

The potential threat of heavy metal pollution to the environment in high-elevation wetlands underscores the need for a thorough understanding and strategic management to protect these distinct ecosystems and their biodiversity. Understanding the levels and consequent ecological risks linked to heavy metals is essential for the sustainable preservation and management of the Lake Rara basin, a significant Ramsar wetland. We analyzed heavy metals such as iron (Fe), chromium (Cr), copper (Cu), lead (Pb), manganese (Mn), cobalt (Co), nickel (Ni), and cadmium (Cd) across 20 soil sampling locations in the catchment just near Rara Lake. Extraction and quantification were performed using inductively coupled plasma - Optical Emission Spectrometry (OOS). The average metal concentrations were as follows: Cr (161.124 $mgkg^{-1}$), Mn (904.671 $mgkg^{-1}$), Co (30.2775 $mgkg^{-1}$), Ni (37.738 $mgkg^{-1}$), Cu (21.6545 $mgkg^{-1}$), Pb (11.05 $mgkg^{-1}$), Cd (0.0975 $mgkg^{-1}$), and Fe (4621.526 $mgkg^{-1}$). The results showed that the order of the mean concentrations of heavy metal was Fe > Mn > Cr > Pb > Ni > Cu > Cd. Correlation and principal component analyses revealed shared geological origins for Mn, Cu, Cd, and Ni, while Pb and Cr originated from anthropogenic sources. Pollution assessment employed various indices, such as the enrichment factor (EF), index of geoaccumulation (Igeo) and risk indices for individual metals and the environment (& RI). Among the heavy metals, manganese (Mn) had the highest enrichment, while the Igeo results indicated exceptionally high average levels of Mn and Fe, except for Ni and Pb. For other heavy metals, the study indicated light to moderate pollution for Co, Cd, and Cu, with a moderate level of contamination for Co and Cr. The ecological risk index (RI) associated with individual metals surpassed the combined risk of multiple heavy metals, indicating heightened signatures of heavy metal contamination attributed to anthropogenic influences within the lake catchment. These influences include extensive littering from cattle and horse activities, solid waste pollution, and inadequate drainage infrastructure. Notably, the direct discharge of wastewater into wetland soil emerges as a significant contributor to the observed ecological risks. These findings underscore the pressing need for effective environmental management strategies to mitigate the impact of anthropogenic activities on the ecological health of the surrounding areas in the Rara Lake basin.

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Bioavailability-based environmental risk assessment approaches for nickel: Considerations for determining ecosystem impacts of critical raw materials

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Abstract

Metals like nickel are increasingly acknowledged as playing a role in the green energy transition given their role as cathode materials in batteries used to fuel electronic vehicles. Nickel's role has led to increased global production, particularly in Southeast Asia. This increase in production raises concerns

about nickel's impact on ecosystems. Ecosystem protection involves a wide range of tools, including the derivation of threshold concentrations that can be used as the basis for emission limits and in various stages of environmental risk assessment, e.g., the establishment of clean-up goals. This is challenging for naturally occurring substances like nickel, as threshold concentrations need to be at once protective of ecosystem structure and function while avoiding situations where standards are set at concentrations occurring below those that occur naturally. One approach that has received global attention is *bioavailbility-based approaches*. Nickel toxicity to organisms is influenced by the naturally-occurring constituents of different environmental matrices like water, sediment, and soil. For example, nickel toxicity to aquatic organisms is determined by toxicity modifying factors (TMFs) including pH, water hardness (calcium and magnesium concentrations), and dissolved organic carbon concentrations, such that effects of nickel can vary considerably from one system to another. Likewise, the TMFs affecting nickel toxicity to soil organisms are Cation Exchange Capacity (CEC) and soil pH. The basis of these bioavailability models comes from laboratory toxicity tests where TMFs are varied, and where modeling parameters or statistical relationships can be determined. The bioavailability-based approaches for nickel that have been demonstrated to be equally protective for temperate and tropical ecosystems, and have been validated using natural waters and soils in laboratory toxicity tests, and in field and mesocosm studies. Our validation work includes studies on Chinese species in Chinese waters and soils. These approaches are based on extremely diverse ecotoxicity databases and bioavailability normalization processes that yield local- and regional-level thresholds that are adaptable to the desired level of ecosystem protection. The basis of metal-specific environmental risk assessment approaches will be reviewed, and the specific relevance to Asia will be emphasized.

932

Elucidating the Impact of Microbially Mediated Organic Matter Transformation in Sediments on the Multiphase Distribution of Heavy Metals in the Yangtze River Estuary

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Abstract

The intense hydrodynamic conditions in the Yangtze River Estuary result in the substantial deposition of fine-grained, organic-rich sediments associated with metals in the turbidity zone. The mobility of sediment metals across different phases is influenced by hydrodynamic conditions, physicochemical factors, and microbial activities, potentially posing further threats to aquatic organism health. However, the relationship between the phase mobility of sediment heavy metals and dissolved organic matter in pore water and bottom water remains unclear, especially under microbial mediation. In this study, the optical and molecular characteristics of dissolved organic matter, as well as the taxonomy and functions of microbial community were characterized in the Yangtze River Estuary by excitation-emission matrix, Fourier transform ion

cyclotron resonance mass spectrometry and metagenomic sequencing. The results indicate that microbial activity, gene abundance, sediment heavy metal concentrations, and the composition and abundance of organic matter are higher at turbidity zone sites in the Yangtze River Estuary compared to marine sites. The distribution of heavy metals in surface sediments is mainly controlled by total organic carbon content and grain size, while the components and abundance of dissolved organic matter and specific microbial groups are key factors regulating heavy metal concentrations in pore water and the partitioning coefficients of heavy metals between sediments and pore water. Identifying the key factors influencing the multiphase distribution of sediment heavy metals is crucial for accurately understanding metal diffusion fluxes at the sediment-water interface and the ecological toxicity of water bodies in estuarine regions.

976

Monomethylmercury Bioaccumulation in Macrobiota of a Complex Group of Geothermal Lakes in New Zealand

Nicholas Ling, Adam Hartland, Grace-Lynn Chong

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Abstract

The Taupo volcanic zone in the central North Island of New Zealand is a highly active geothermal region. Geothermal fluids are often enriched with toxic trace elements including mercury, and anaerobic conditions in aquatic sediments and waters lead to the biotransformation of elemental mercury into monomethyl mercury (MMHg). The thirteen lakes of the Te Arawa lakes in the Rotorua region vary considerably in their geothermal inflows, their geomorphology, and their trophic states, and present an interesting case study for methylmercury biomagnification in aquatic systems. We examined total mercury and MMHg in rainbow trout throughout the Te Arawa lakes to compare recent values with historical studies in some lakes to determine whether changes in the trophic status of some lakes has contributed to greater bioaccumulation of MMHg. We also measured mercury concentrations in freshwater mussels and crayfish as additional significant edible biota of cultural importance to local Māori.

Lakes with a large proportion of geothermal inflows had highest mercury concentrations in macrobiota, and concentrations in rainbow trout have worsened in some lakes corresponding with a deterioration in lake trophic state (more eutrophic), possibly caused by more prolonged periods of hypolimnetic anoxia during summer stratification. However, recent efforts to improve lake trophic state appear to have a positive impact on mercury bioaccumulation. Concentrations in edible flesh of trout in some lakes are sufficiently high to pose a risk for human consumption, although mercury concentrations vary considerably between individual fish.

Trout and freshwater mussels showed a strong inverse relationship between MMHg as a proportion of total mercury and tissue selenium concentration, supporting the protective function of selenium on bioaccumulation of mercury.

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The influence of arsenic speciation on the trophic transfer of arsenic in marine food chains

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Abstract

Arsenic is a highly hazardous environmental pollutant, causing serious environmental issues in coastal areas. However, the factors responsible for arsenic biomagnification in marine ecosystems remain unclear. Our study initially explores the trophic transfer of arsenic in various marine food chains/webs to determine the prevalence of arsenic biomagnification in marine ecosystems. It was evident that arsenic tends to undergo biomagnification when arsenobetaine is dominant in the organisms within the food chains. Furthermore, indoor experiments revealed that arsenobetaine exhibits higher bioavailability and trophic transfer efficiency compared to arsenate, arsenite, and methylated arsenic species. These findings contribute to our understanding of the ecotoxicology and biogeochemistry of arsenic, helping to assess the ecological risks associated with arsenic and protect marine ecological safety.

1020

Metal Risks in Turbid Coastal Waters

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Abstract

In coastal waters, high turbidity leads to a significant fraction of metals existing in particulate forms. This study investigates the bioavailability and toxicity of particulate metals in turbid coastal environments.

Using the estuarine clam *Potamocorbula laevis* and suspended particulate matter from the Jiulong River estuary, we conducted experiments to compare the bioaccumulation of Cu under "dissolved only" and "dissolved + particulate" conditions. A toxicokinetic-toxicodynamic model was employed to quantify the processes of Cu uptake, ingestion, assimilation, egestion, and elimination, and to relate mortality risk to tissue Cu concentrations. The findings revealed that particulate Cu significantly contributes to the overall bioaccumulation of Cu and increases the toxicity to organisms. To refine water quality criteria, modifying factors were calculated, suggesting that criteria based on dissolved metal exposure should be adjusted to provide adequate protection in turbid waters. Further site-specific assessments using suspended particulate matter from various coastal sites in China demonstrated variations in metal bioavailability, which were well-predicted by the total organic carbon and iron content of the suspended particulate matter. This study provides a scientifically sound framework to better manage the risks of metals in turbid coastal waters and proposes modifications to current water quality criteria to account for the significant contribution of particulate metals.

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Understanding the biogeochemical controls of toxic methylmercury across aquatic and terrestrial ecosystems

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Abstract

Mercury (Hg) is a metal of global concern, mainly due to its atmospheric emission, long-range transport, and deposition into both aquatic and terrestrial environments. Once deposited, Hg exists predominantly in its inorganic form [Hg(II)] and is not very toxic. However, a small fraction of Hg(II) can be microbially converted to highly toxic and bioavailable methylmercury (MeHg), which can strongly bioaccumulate and biomagnify in all natural food webs, leading to elevated levels for the chronic exposures to human and wildlife. Here, we compiled our previous and ongoing studies across different aquatic and terrestrial environments, and attempted to better understand the biogeochemical controls on the MeHg levels in sediments and soils across ecosystem types, including aquatic vs. upland ecosystems, freshwater vs. saltwater ecosystems, etc. The ranges of MeHg in these solid phase matrices can vary over three orders of magnitude differences, even though total Hg levels varied much less than that, and MeHg can range from 0.01-10 ng/g dry wt., which can have both spatial and temporal variations within each ecosystem. This keynote presentation will provide an overview of these data and an assessment of key factors influencing these environments variations of MeHg, which ultimately control the biological uptake and risk of this toxic compound globally.

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Toxicity mechanisms of copper to freshwater mussel: cellular and molecular vulnerable perspectives from a model species *Anodonta woodiana*

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Abstract

Introduction: Copper (Cu) is the most polluted heavy metal in the freshwater fishery ecological environment of China (Johnson et al., 2020; Yan et al., 2024). The toxicity of Cu to aquatic animals should be paid special attention. *Anodonta woodiana* is a globally distributed freshwater mussel (Yan et al., 2024). Unfortunately, its resources in China have declined sharply in recent years. Therefore, we propose the scientific hypothesis that the vulnerability to toxic effects of Cu is the key factor contributing to the sharp decline in the resources of this model species.

Materials and Methods: A comparative study of Cu toxicity vulnerability of *A. woodiana* at different life history stages (early juvenile, late juvenile, and adult mussels) was carried out; then a cytotoxicity study of Cu was conducted by using primary cultured hemocytes (the most vital component of mussel immune system) as a model cell; in addition, a transcriptomic analysis of Cu toxicity to gills (the target organ for Cu accumulation) was performed.

Results: The 96-h median lethal concentration (96-h LC_{50}) of Cu was the lowest for early juveniles (0.012 mg/L) but the highest for adults (22.1 mg/L). Exposure of hemocytes to Cu over 0.001 mg/L for 3 h caused a significant increase in reactive oxygen species ($P < 0.05$); over 0.01 mg/L disrupted the cellular membrane, decreased mitochondrial membrane potential, and caused DNA damage ($P < 0.05$), but did not induce significant changes in the stability of lysosomal membrane even as high as 10 mg/L ($P > 0.05$); while more than 0.1 mg/L, it significantly increased hemocyte mortality ($P < 0.05$). Exposure of the mussel to 2.0 mg/L Cu (approximately 1/10 of the 96-h LC_{50} of the adults) for 72 h produced 3160 differentially expressed genes (DEGs) in their gills. GO enrichment analysis showed that cellular processes, metabolic processes, and biological regulation contained the most DEGs in the biological processes; KEGG pathway analysis showed that DEGs mainly enriched in the apoptosis, arginine and proline metabolism, and the toll-like receptor signaling pathway ($P < 0.05$).

Discussion and Conclusion: The earlier the mussel is in its life history, the higher its vulnerability to copper. Even Cu at environmentally relevant concentrations (0.01 mg/L) could still cause molecular, cellular, and early juvenile toxicity damage. Cu produces toxic effects on mussels by disrupting gene expression, altering cellular function, and triggering cell apoptosis/death. Therefore, it is important to emphasize the toxic effects of Cu on the most vulnerable early juveniles in the conservation or restoration of *A. woodiana* and other freshwater mussel resources. In future, it is necessary to reveal the mechanism of high vulnerability of early juveniles to Cu toxicity at the cellular-subcellular-single cell molecular levels.

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"Freshwater Mussel Watch": An innovative approach for metal biomonitoring and toxicological assessment on aquatic environments

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Abstract

Introduction: Freshwater environment is the critical basis of sustainability of the fishery and biodiversity conservation. Unfortunely, it has fallen victim to water pollution in the worst case scenario due to related aquatic- and land-based human activities. It is urgent to establish a targeted biomonitoring and toxicological assessment system to diagnose and warn the pollutants /impact factors, and then to propound the effective solution for pollution control and ecological protection. Consequently, we innovatively proposed a distinctive approach of "Freshwater Mussel Watch" (FMW) system in 2003 using Chinese pond mussel *Anodonta woodiana* as a model species and unique bioindicator (Yang et al., 2005; Yang et al., 2008). It is believed that this systematic approach has great applied potentials to bio-monitor, assess, early warn various inorganic (e.g., heavy metals)/organic pollutants in freshwater environments (e.g., lakes, rivers) and interpreter the toxicological/vulnerable mechanism.

Materials and Methods: So far, our "Freshwater Mussel Watch" approach has been mainly investigated and applied over the past 21 years on the fields of passive/active biomonitoring, tissue/living individual "Specimen Bank" construction, model animal (with similar biotic variability, germplasm strains, and low background contamination)/cell pool establishment, and individual-/tissular-/cellular-/molecular-biological level toxicological assessment of aqueous pollutants (especially heavy metals).

Results: The spatial/temporal backgrounds and trends over time of heavy metals in various lacustrine/riverine environments have been successfully revealed by passive/active biomonitoring. Corresponding pollutant toxicology, bioaccumulation kinetics and water purification functions have been

possibly understood through application of the “Specimen Bank”, related individual-/tissular-/cellular-/molecular-level toxicological/vulnerable mechanisms have been effectively interpreted by the model animal (e.g., glochidia, early juvenile)/cyto-materials (e.g., hemocyte and gill cells) pool. In addition, *A. woodiana* was discovered to be an unusual Mn hyperaccumulator.

Discussion and Conclusion: Heavy metals (e.g., Cu) in the aquatic environment are constantly accumulating in the mussels of FMW, resulting in substantial differences in metal backgrounds and toxicological impacts in mussel samples collected from different water bodies. FMW approach clearly demonstrates that the mussels at early life history stages are the most vulnerable to aqueous metal contaminations (even at environmentally relevant levels). The FMW-based approach is exactly instrumental in metal biomonitoring and toxicological assessment on aquatic environments. Further studies are necessary to extend this approach on regional and international pollutant monitoring and develop more “standardized” methods for evaluation of bioaccumulation, biotoxicity and ecotoxicological risk assessment of traditional/emerging pollutants in aquatic ecosystems by means of *A. woodiana* materials at different early life history stages or biological structure levels.

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13. Mercury Biogeochemistry, Biotransformation, and Planetary Health

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Recent advances in Hg biogeochemistry in the rice-paddy system

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Abstract

Hg biogeochemistry in the rice-paddy system is critical, given that rice is the primary source of MeHg exposure for Asians and infants. Over the past 3 years, we have conducted a series of studies in this field, including the MeHg analysis method, Hg methylation, and MeHg demethylation. We propose alkaline extraction (KOH-CH_3OH) is an optimal choice for paddy soils, with negligible MeHg artifacts and consistently high extraction efficiency. In contrast, acid extraction, i.e., $CuSO_4$/KBr/H_2SO_4-CH_2Cl_2, is not suitable for paddy soils, given the low extraction efficiency (21.3–70.8%). For Hg methylation, we identify the supply of Hg as the limiting factor of Hg methylation in paddy soils at a national scale. Although the sulfate-reducing bacteria (SRB) are the dominant microbial Hg methylator, soil *Geobacteraceae*, mainly iron-reducing bacteria (FeRB), could predict MeHg accumulation in rice. This is concluded from the facts that the hgcA-containing *Geobacteraceae* have the highest abundance, their activities are significantly correlated to soil MeHg production, and rice MeHg accumulation is more sensitive to *Geobacteraceae* activity than Hg input via deposition or irrigation. We also find that soil selenium (Se) could impact *Geobacteraceae* activity and thus propose an approach to mitigate Hg risk by regulating *Geobacteraceae* in soils. For MeHg demethylation, we report a light- and microbe-independent pathway in plants. This pathway is mediated by the *in vivo* generated singlet oxygen, which attacks the C-Hg bound with the aid of thiols, reducing MeHg accumulation in rice by 58–79% and avoiding an IQ decrement of 0.01–0.51 points/newborn in major rice-consuming countries (equivalent to economic losses of US$30.7–84.2 billion globally). In addition, MeHg photodegradation, a critical natural pathway of MeHg degradation in aquatic systems, is an overlooked process mitigating Hg risks, which reduces MeHg concentrations in water and rice by 82% and 11%, respectively. Without photodegradation, paddy water could be a significant MeHg source for downstream ecosystems, with an annual export of 178–856 kg MeHg. The above findings broadly advance our understanding of Hg global cycling and provide insights into Hg risk mitigation.

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Mechanism of methylmercury photodegradation in the Yellow Sea and East China Sea: dominant pathways, and role of sunlight spectrum and dissolved organic matter

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Abstract

Methylmercury (MeHg) is the major form of Hg that accumulates along the food chain and poses threat to humans and wild life. Photodegradation is the dominant process that MeHg is eliminated from freshwater

system and upper ocean. The formation of MeHg-dissolved organic matter (DOM) complexes and a variety of free radicals (FR)/reactive oxygen species (ROS) have been previously proposed to be involved in MeHg photodegradation. However, most of these studies were conducted in freshwater, and the mechanism of MeHg photodegradation in seawater remains unclear. In this study, the main pathways of MeHg photodegradation in the seawater of Yellow Sea (YS) and East China Sea (ECS) were investigated using FR/ROS scavenger addition and DOM competing-ligand addition techniques. The results showed that direct photodegradation of MeHg-DOM complexes is the major pathway of MeHg photodegradation in the YS and ECS, while indirect photolysis of MeHg by hydroxyl radical (·OH) also plays a certain role at some sites. MeHg photodegradation was found to be mainly induced by ultraviolet (UV) light rather than visible light in YS and ECS seawater, and the contribution of UV-B was higher than UV-A which was opposite to that previously reported in freshwater. The energy for breaking the bond of C-Hg in MeHg-Cl complexes formed in seawater is higher than that in MeHg-DOM complexes and this may cause the relatively greater contribution of UV-B with higher energy to MeHg photodegradation in seawater. In addition, MeHg photodegradation in various fractions of natural DOM with different molecular weights, hydrophilicity/hydrophobicity and acid-base was tested. MeHg photodegradation rates (k_d) varied in these fractions and k_d in high molecular weight DOM and hydrophobic Acid (HOA) fractions were faster than that in the other fractions. A significantly positive correlation was observed between k_d and thiol concentrations while there was no significant correlation between k_d and other measured parameters representing the composition of DOM (specific UV absorbance at 254 nm ($SUVA_{254}$), spectral slope (SR), chromophoric dissolved organic matter (CDOM), humification index (HIX), biological index (BIX) and fluorescent components). These results indicate that thiol may be the key functional group in DOM affecting the photodegradation of MeHg in the YS and ECS.

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Forest mercury network: from tropical rainfall forests to Tebitan forests

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Abstract

Mercury is a global pollutant regulated by a United Nations convention. Currently, the scientific dilemma of mercury compliance and emission reduction is difficult to accurately assess whether the risk of mercury pollution in ecosystems decreases with the reduction of anthropogenic mercury emissions. This is because the large knowledge gaps in how to link the atmospheric mercury depositions into ecosystems, ecosystem mercury cycle, and ecological impact. Therefore, this project aims to understand the whole processes of mercury cycle in forests of multiple climatic zones, and model the mercury cycling to evaluate ecological risk assessment in forests. Our project will break through the lack of scientific understanding and effective model tools in the evaluation of compliance effectiveness, and sets a typical example to evaluate the effectiveness of the Minamata Convention on controlling Hg pollution. Hence, we plan to construct a field observation network of forest mercury cycle from the southwest tropics of China to the Tibet Plateau, and integrate new techniques such as mercury isotope tracing tools and micrometeorological mercury flux measurements to establish a new "three-positional and two-

dimensional" observation system for quantifying the cycling of atmospheric elemental mercury in forest systems. Additionally, we will use the end-member labeled mercury isotope tracing tools to quantify the oxidized mercury fates in forests. Moreover, we will assess the how the spatiotemporal pattern of climate and vegetation to shape the atmospheric mercury depositions, biogeochemical cycling and mercury pollution risk of birds in multiple forests from tropical regions to Tibet Plateau. Finally, we will construct a new forest mercury model which containing the whole mercury biogeochemical processes and assessment of mercury pollution risk in forests. Overall, our projects would meet the need of regulation of the Minamata Convention for the government.

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Ferrous sulfide nanoparticles controls mercury speciation and bioavailability to methylating bacteria in contaminated groundwater

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Abstract

Mercury speciation in groundwater affects its removal effectiveness and methylation potential. Yet, most studies focus on the removal of inorganic dissolved Hg(II) and few studies explored the mercury methylation before and after the treatment. This study comprehensively explored the removal performance of three model mercury species, namely, dissolved inorganic divalent Hg (Hg(II), including free Hg^{2+} and Hg^{2+} complexes with Cl^- and OH^-), Hg^{2+} bound to dissolved organic matter (Hg-DOM), and HgS nanoparticles by FeS nanoparticles and further investigated the resultant impacts on the microbial methylation of Hg. The nanoparticles efficiently immobilized the three mercury species within 20 h. The sorption isotherm data of Hg(II) and Hg-DOM were well fitted by the dual-mode isotherm model and the maximum sorption capacities were 3358.28 and 2396.38 mg/g, respectively. Hg(II) and Hg-DOM were predominantly removed via ion exchange, chemical precipitation, and surface complexation whereas HgS was mainly immobilized through heteroaggregation. The simple treatment greatly reduced the bioavailable Hg species, thereby diminishing the net MeHg production by 70.2%, 32.7%, and 11.3%, respectively. This study provides compelling evidence that FeS nanoparticles efficiently removed various mercury species in groundwater and remarkably inhibited the microbial methylation of mercury.

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The mechanism of foliar physiological parameters restricting foliar assimilation of atmospheric mercury in typical forest ecosystems

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Abstract

The accumulation of gaseous elemental mercury (Hg(0)) on foliage represent a pivotal mechanism for atmospheric Hg deposition into terrestrial ecosystems. However, the mechanism of foliar Hg(0) uptake is poorly understood, limiting our understanding of foliage accumulation of atmospheric Hg. In this study, we conducted in situ measurements of the crucial foliar physiological parameters, including photosynthetic rate (A), stomatal conductance (gsw), transpiration rate (E), water vapor deficit (VPD), of eight dominant tree species across China's typical tropical rainforest, tropical sparse shrub, and subtropical evergreen broad-leaved forest. Our aim was to gain insights into the limiting factors affecting the foliar uptake of atmospheric Hg^0 by combining these physiological parameters with the net accumulation rate, spanning from leaf emergence to senescence. The results indicate that the foliar Hg concentration of various tree species in different ecosystems exhibits a linear upward trend during leaf growth. However, it is noteworthy that the rate of this increase varies significantly among species. (1.76 ng g^{-1} $month^{-1}$ ~ 4.94 ng g^{-1} $month^{-1}$). Model result infers that atmospheric relative humidity shows the dominant positive effects on foliar Hg(0) uptake in the three forest ecosystems. It promotes Hg(0) uptake by increasing physiological activity of leaves. Among these physiological parameters, the net photosynthetic rate has the most primary positive influence on atmospheric Hg(0) uptake by subtropical forest leaves, while the positive impact of stomatal conductance is more significant in tropical forests, due to the inhibited uptake of atmospheric Hg(0) by stomates under high VPD conditions. Additionally, multiple linear regression models of net Hg(0) uptake rate and environmental factors, foliar physiological parameters and atmospheric Hg concentration during the leaf growth cycle are established, so as to quantify the effects of temporal and spatial dynamics of foliar physiological parameters on global Hg cycle in future model assessment.

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Biogeochemical controls on methylmercury production and degradation in the environment

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Abstract

The neurotoxin methylmercury (MeHg) is a global health and environmental concern due to its bioaccumulation and biomagnification in the food chains. The concentration of MeHg in the environment is governed by the processes of MeHg production and degradation, which depends on the bioavailability of mercuric ion [Hg(II)] and the microorganisms involved. Hg(II) is known to complexed with organic ligands such as natural organic matter (NOM). The binding strengths and configuration of Hg^{2+}-ligand complexes are key factors controlling Hg(II) bioavailability. By devising a stepwise reduction approach using ascorbic acid (AA) and stannous tin [Sn(II)], we observed dynamic, competitive ligand exchanges for Hg^{2+} from weak carboxylate to strong thiolate, and then to stronger functional groups within NOM. Additionally, via forming heteroleptic coordinated Hg(II)-S_3/S_4 complexes, Hg(II) complexes with NOM was more reducible in the presence of thiolate ligands, which strongly enhanced microbial methylation potential of Hg(II). Interestingly, we found that, in addition to the conventional mer-mediated pathway, phytoplankton and methanotrophs also showed strong ability to degrade MeHg despite no mer operons presented. These findings suggests that microbial methylation and demethylation of mercury is more complicated than previous thought and underscores improved modelling and assessment of the biogeochemical cycling of mercury.

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New Insights into MeHg Accumulation in Rice (*Oryza* sativa L.): Evidence from Cysteine

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Abstract

The intake of methylmercury (MeHg)-contaminated rice poses immense health risks to rice consumers. However, the mechanisms of MeHg accumulation in rice plants are not entirely understood. The knowledge that the MeHg−Cysteine complex was dominant in polished rice proposed a hypothesis of co-transportation of MeHg and cysteine inside rice plants. This study was therefore designed to explore the MeHg accumulation processes in rice plants by investigating biogeochemical associations between MeHg and amino acids. Rice plants and underlying soils were collected from different Hgcontaminated sites in the Wanshan Hg mining area. The concentrations of both MeHg and cysteine in polished rice were higher than those in other rice tissues. A significant positive correlation between MeHg and cysteine in rice plants was found, especially in polished rice, indicating a close geochemical association between cysteine and MeHg. The translocation factor (TF) of cysteine showed behavior similar to that of the TF of MeHg, demonstrating that these two chemical species might share a similar transportation mechanism in rice

plants. The accumulation of MeHg in rice plants may vary due to differences in the molar ratios of MeHg to cysteine and the presence of specific amino acid transporters. Our results suggest that cysteine plays a vital role in MeHg accumulation and transportation inside rice plants.

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Predictions of global distribution in vegetation and soil mercury and their implications on air-surface exchange processes

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Abstract

Foliar assimilation of elemental mercury (Hg^0) from the atmosphere plays a critical role in the global Hg biogeochemical cycle, leading to atmospheric Hg removal and soil Hg insertion. Meanwhile, soil stores a large amount of Hg that has adverse effects on human health and ecosystem safety. Recent studies have estimated global foliar Hg assimilation and soil Hg accumulation; however, large uncertainties remained due to coarse accounting of observed foliar Hg concentrations and soil Hg concentrations, posing a substantial challenge in constraining the global Hg budget especially air-surface exchange processes. Here, we integrated a comprehensive observation database of foliar Hg and soil Hg concentrations and machine learning algorithms to predict the spatial distribution of foliar Hg concentrations and soil Hg concentrations on a global scale. The global average of foliar Hg concentrations was estimated to be 24.0 ng g^{-1} (7.5−56.5 ng g^{-1}) and the global total in foliar Hg pools reached 4561.3 Mg (1455.2−9062.8 Mg). Hg content in surface soils ranges from 3.8 to 618.2 μg kg^{-1} with an average of 74.0 μg kg^{-1} across the globe. Our prediction of the distributions highlights the hotspots in East Asia, the Northern Hemispheric temperate/boreal regions, and the tropical areas, while the coldspots in arid regions. Importantly, predictions of global distribution in vegetation and soil mercury have significant implications on air-surface exchange processes of Hg. For instance, a range of 2268.5−2727.0 Mg yr^{-1} was estimated for annual foliar Hg assimilation accounting for the perennial continuous assimilation by evergreen vegetation foliage. Meanwhile, compared to previous studies, lower Hg emissions from wildfires and higher soil Hg emissions were estimated based on the new global distribution of foliar Hg concentrations and soil Hg concentrations. The new predictions of foliar Hg and soil Hg distributions may aid in understanding the global biogeochemical cycling of Hg, especially in the context of climate change.

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Health effects and economic benefit of ecological remediation in typical mercury contaminated area

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Abstract

Methylmercury (MeHg) exposure via rice consumption poses health risk to residents in mercury contaminated areas, such as the Wanshan Hg mining area (WSMA) in southwest China. Making use of the published data for WSMA, this study developed a database of rice MeHg concentrations for different villages in this region for the years of 2007, 2012, 2017, and 2019. The temporal changes of human MeHg exposure, health effects, and economic benefits under different ecological remediation measures were then assessed. Results from this study revealed a decrease of 3.88 μg/kg in rice MeHg concentration and a corresponding reduction of 0.039 μg/kg/d in probable daily intake of MeHg in 2019 compared to 2007 on regional average in the WSMA. Ecological remediation measures in this region resulted in the accumulated economic benefits of $38.7 million during 2007-2022, of which 84% was from pollution source treatment and 16% from planting structure adjustment. However, a flooding event in 2016 led to an economic loss of $2.43 million (0.38% of regional total Gross Domestic Product). Planting structure adjustment generates the greatest economic benefits in the short term, whereas pollution source treatment maximizes economic benefits in the long term and prevents the perturbations from flooding event. These findings demonstrate the importance of ecological remediation measures in Hg polluted areas and provide the foundation for risk assessment of human MeHg exposure via rice consumption.

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Challenges of Microbial Hg Methylation and MeHg Degradation Studies with one East Texas Lake as a Case

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Abstract

Microorganisms affect MeHg production directly by methylating inorganic mercury (Hg) to methylmercury (MeHg) and by degrading MeHg. Therefore, the exploration of Hg biotransformation mechanisms will facilitate remediation strategies to control MeHg production in the environments and thus protect the health of humans and wildlife. Martin Lake Steam Station located along Martin Lake in east Texas was reported to be the highest mercury emission

polluter in USA, and emissions from coal-fired power plants are the leading cause of Hg contamination in Texas fish and wildlife. This study investigated Hg contamination in the sediment, lake water, and pore water samples and explored microbial Hg methylation activities by focusing on Hg methylation gene analyses and potential MeHg degradation in this lake from 2019 to 2023. The biogeochemical analyses indicated that the THg and MeHg levels in the lake environments were higher in the sampling sites following the annually dominant wind direction, and the sediments were featured with high-sulfate and high-Fe(III) matrices. However, bioinformatic analyses of Hg methylation *hgcA* genes by Illumina sequencing revealed that, rather than typical SRB and FeRB occurring in freshwater lakes or rivers, the microbial MeHg-synthesizing species in Martin Lake benthic ecosystems were dominated by the methanogens, bacteria from class *Desulfuromonadales*, diverse unclassified novel groups, and *Syntropales*. The most widespread order of microbes throughout all the sample sites was *Methanomicrobiales* which constituted the largest composition (>50%) of the genomic DNA extracted from the South Island Road sediment. The novel Hg methylating community in this lake suggests that the biotic Hg methylation be led by unconventional mechanisms, although the actual pathways are warranted for further exploration. This presentation will also extend discussions of the general challenges in microbial Hg methylation and MeHg demethylation studies, considering the broadly distribution of novel Hg methylators found among anaerobic microbial taxa in diverse anoxic environments, and uncertain linkages of the detected operational taxonomic units (OTUs) in environmental Hg methylation gene assemblages to Hg methylation capabilities.

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Technologies for Safe Utilization of Mercury-Contaminated Farmland Based on Oxygen Regulation

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Abstract

Mercury (Hg) is a highly toxic heavy metal, especially methylmercury (MeHg) is extremely neurotoxic. MeHg is produced by microorganisms under anaerobic conditions. Rice paddies are seasonally flooded constructed wetlands, which are anaerobic, and are considered as "hot spots" for MeHg production. MeHg contamination in rice fields has led to severe contamination of rice with MeHg. Rice consumption can lead to MeHg exposure health risks to human at Hg mining regions, threatening health residents at Hg mining regions. Therefore, the development of techniques to control MeHg risks in paddy fields, achieving the safe use of paddy fields are great significance. Increasing soil redox potential by increasing soil oxygen content is a key pathway to inhibit soil Hg methylation. Controlling soil oxygen content by periodically draining rice fields can reduce the total mercury (THg) and MeHg content in rice to a certain extent, but this method is limited due to its effect on rice yield. To address this, we have developed two strategies for increasing oxygen in paddy fields: (1)Slow-release oxygen fertilizer (SOF): with CaO_2 as the fertilizer core, urea phosphate as buffer, attapulgite as

filler, sodium alginate as adhesive, and polyacrylate as the coating agent, which can not only slowly release oxygen in soil, but also provide nutrients to rice, achieving a simultaneous remediation and use of Hg-contaminated paddy fields. Our results demonstrate that after adding slow-release oxygen fertilizer, the THg content in the soil solution was reduced by 54%-93% and the MeHg content by 41%-95%. (2) Man-made aerenchymatous tissues (MAT): increase soil Eh by mimicking O_2 release from wet plant roots. Our results show that MAT inhibits the activation and methylation of Hg in the soil, significantly reducing the accumulation of THg (26%-35%) and MeHg (31%-42%)in rice grains. Inhibiting the reductive dissolution of iron and manganese oxides and decreasing the relative abundance of anaerobic mercury-methylating microorganisms in soils are the main reasons for the reduction of dissolved Hg and MeHg content after oxygenation. This work offers a low-cost and sustainable method for mitigating Hg release in rice paddies by addressing the issue of soil Eh management.

Key words: Slow-release oxygen fertilizer; Man-made aerenchymatous tissues; Mercury-contaminated paddy field remediation; Mercury speciation transformation; Rice methylmercury contamination; Health risks

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A synthesis on air-surface exchange of atmospheric mercury over the global terrestrial ecosystem

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Abstract

Mercury is a globally distributed toxic metal regulated by the United Nations Environmental Programme (UNEP). Both human activities and natural processes release mercury into the atmosphere where mercury undergoes long-range transport and subsequently deposits in terrestrial and aquatic ecosystems. Under anoxic conditions, the deposited mercury can be transformed into highly toxic methylmercury in water and sediments and bioaccumulated in the food chain, causing significant concerns for human health and ecosystems. To protect human health and the environment from the impacts of anthropogenic mercury emissions, UNEP's Minamata Convention on Mercury, a legally binding international treaty, entered into force in August 2017. However, significant knowledge gaps in global mercury cycling, coupled with the forcing of changing climate, challenge our ability to assess the effectiveness of the Convention in reducing human and wildlife exposure to mercury. This paper provides a state-of-the-science synthesis based on theoretical analysis, field observations, and environmental modeling of air-soil, air-foliage, and air-water exchange of atmospheric mercury vapor, with a focus on the processes governing the transport, transformation, accumulation, translocation and sequestration in tropical and alpine forests. The collective

effect of these transport processes on the mercury mass budget of air-forest exchange in the global terrestrial ecosystem will be discussed.

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Illuminating microbial taxa responsible for methylmercury degradation by tracking carbon consumption

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Abstract

Methylmercury (CH_3Hg^+) is a potent neurotoxin that threatens human health and wildlife due to its significant ability to bioaccumulate through the food chain. While microbial demethylation has been recognized as a crucial pathway of CH_3Hg^+ degradation, the microbial communities accountable for CH_3Hg^+ degradation in environments have remained elusive. Using ^{13}C-labeled CH_3Hg^+ and combined analyses of ^{13}C-enriched DNA and shotgun metagenomics, here we explored microbial taxa and associated biochemical processes involved in CH_3Hg^+ degradation in the soils with distinct background mercury levels. The qPCR analysis of ^{13}C-derived 16S rRNA genes revealed that soil microorganisms assimilated $^{13}CH_3Hg^+$ after 14 days of incubation. We identified *Arenimonas*, *MM2*, and *Dechloromonas* as the most significant genera potentially engaged in the consumption of $^{13}CH_3Hg^+$ in the paddy soil characterized by high Hg contamination. We further validated considerable ability of putative taxa (e.g., *Dechloromonas denitrificans* and *Methylovorus menthalis*) to degrade CH_3Hg^+ by pure culture assays. Furthermore, reconstructed metagenome-assembled genomes from the ^{13}C-labeled DNA unveiled functional genes associated with processes including Hg reduction, Wood-Ljungdahl pathway, dicarboxylate-hydroxybutyrate cycle, methanogenesis, denitrification, and nitrate reduction. Collectively, these findings provide unprecedented new insights into the soil microorganisms responsible for CH_3Hg^+ degradation and offer a novel avenue for the development of bioremediation strategies targeting CH_3Hg^+ contamination.

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Mercury Transformations in Organisms: The Occurrence, Mechanisms and Significance

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Abstract

Mercury (Hg) is a global pollutant showing potent toxicity to living organisms. The transformations of Hg are critical to global Hg cycling and Hg exposure risks, considering Hg mobilities and toxicities vary depending on Hg form. Though currently well understood in ambient environments, Hg transformations are inadequately explored in non-microbial organisms. The primary drivers of in vivo Hg transformations are far from clear, and the impacts of these processes on global Hg cycling and Hg associated health risks are not well understood. This hinders a comprehensive understanding of global Hg cycling and the effective mitigation of Hg exposure risks. Here, we focused on Hg transformations in non-microbial organisms, particularly algae, plants, and animals. The process of Hg oxidation/reduction and methylation/demethylation in organisms were reviewed since these processes are the key transformations between the dominant Hg species, i.e., elemental Hg (Hg0), divalent inorganic Hg (IHgII), and methylmercury (MeHg). By summarizing the current knowledge of Hg transformations in organisms, we proposed the potential yet overlooked drivers of these processes, along with potential challenges that hinder a full understanding of in vivo Hg transformations. Knowledge summarized in this review would help achieve a comprehensive understanding of the fate and toxicity of Hg in organisms, providing a basis for predicting Hg cycles and mitigating human exposure.

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Gaseous Elemental Mercury Exchange Fluxes over Air-Soil Interfaces in the Wetland of Eastern China

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Abstract

Natural source emissions of mercury have become a major source of atmospheric mercury, but there is currently a high degree of uncertainty in estimates of emissions from natural sources, especially from landscape-covered surfaces, as well as a lack of field observations. Wetland is among the most ecologically sensitive and landscape-complex systems, and the source-sink relationships of atmospheric Hg in wetlands are poorly defined. Understanding the mechanisms controlling gaseous Hg flux from wetland is important to predict the retention of Hg and project the impact of ecology on the global Hg cycle. To reveal the characteristics of mercury exchanges in wetlands, we conducted field in-situ monitoring experiments in the Baguazhou wetland (BWL) in eastern China. This study investigated GEM exchange fluxes over two land cover types (including mudflats and shallow waterfront) using a dynamic flux chamber attached to an automatic mercury vapor analyzer (namely, Tekran 2537X) in three seasons from September 2022 to July 2023.

The surface–air fluxes of GEM were −0.12 (mudflat) and −0.08 (waterfront) ng m^{-2} h^{-1} in spring, 0.39 (mudflat) and 0.42 (waterfront) ng m^{-2} h^{-1} in summer, and 1.72 (mudflat) and 0.81 (waterfront) ng m^{-2} h^{-1} in fall. The mean ambient GEM concentrations were 1.04, 2.94 and 2.63 ng m^{-3} in spring, summer and fall, respectively. The diurnal pattern of GEM flux is characterized by high daytime level and low nighttime level with a peak in the midday. GEM fluxes were found to be positively correlated with solar radiation and air or soil temperatures. Soil Hg reduction driven by solar radiation and soil moisture and Hg re-emission driven by soil temperature could be the most likely sources of GEM fluxes. Plants play a comprehensive role in wetland surface–air Hg exchange. Emergent macrophytes have been found to promote GEM emissions through evaporation from vascular tissues in previous studies. However, the dwarf aquatic plants at BWL in this study acted more as a sink of Hg through stoma uptake, which highly compromised soil Hg emission in spring and summer with lush vegetation. Fall, with strong solar radiation and withered plants, exhibited strong Hg emission fluxes. Overall, a typical wetland in eastern China acts as a strong source of atmospheric Hg in summer and fall, while as a weak sink in spring.

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Molecular insights into the oxidation of Hg^0 in the leaves of *Oryza sativa* L.

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Abstract

The molecular mechanism of Hg^0 assimilation in plant's leaf is rarely studied. Such knowledge gaps limit our abilities to deep understanding Hg^0 cycle between air-leaf interface, and maintain the safety of crops via genetic modification. Here we studied underling Hg^0 oxidation molecular mechanism and potential key genes in response to Hg^0 exposure in rice's leaf using a combination of spectral and transcriptomic tools under chamber condition. Exposure to Hg^0 for 24 h led to a noticeable rising of total Hg concentration in rice's leaf, in which most Hg presented as $Hg(cysteine)_2$ complexes as characterized with Hg L_3-edge X-ray absorption near-edge structure spectroscopy (XANES). Transcriptomic results showed that genes for stomatal aperture might control Hg^0 entering into inner tissue of leaf. The genetic network of antioxidant process (e.g., catalase) likely mediated Hg^0 oxidation to Hg(II). The transcription factors i.e., NAC (NAM, ATAF1, 2 and CUC2) and ERF (ethylene-responsive transcription factor) acted as upstream regulators to regulate catalase, and consequently on Hg^0 oxidation. The upregulation of genes for cysteine metabolism showed a vital role of cysteine in response to Hg exposure, consistent with the formation of $Hg(cysteine)_2$ complexes. Further, *OsHIPP29*, *OsZIFL1*, and *OsCRK10* genes might be involved in Hg^0 exposure and detoxification. These results improve our molecular understanding of Hg^0 cycle at air-leaf interface, and are essential for genetical modification of crops to achieve a sustainable development of global Hg-contaminated soils.

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Mercury isotope fractionation for tracing the uptake and metabolism of Hg by earthworms

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Abstract

Mercury stable isotopes have emerged as a powerful tool for tracing Hg biogeochemical cycling, and has been applied to trace the metabolism and trophic transfer of Hg in aquatic food chains, but the Hg isotope fractionation in terrestrial biota was rarely studied. The goal of this study is to elucidate Hg isotope fractionation during the uptake, metabolism, and elimination of Hg in earthworms, a model terrestrial invertebrate, and provide new insight for the biogeochemical cycling of Hg in terrestrial environment.

Pheretima guillelmi was exposed to Hg-contaminated soils. Total Hg (THg) and methylmercury (MeHg) concentrations as well as THg isotope compositions of soils and different tissues of *Pheretima guillelmi* (intestinal contents, epidermis, castings) were analyzed. All tissues displayed more negative $\delta^{202}Hg$ (representing mass-dependent fractionation, MDF) than that in the bulk soils. Among different tissues of *Pheretima guillelmi*, Hg of intestinal contents ($\delta^{202}Hg_{intestinal\text{-}contents}$) were isotopically heavier than epidermis ($\delta^{202}Hg_{epidermis}$) and lighter than castings ($\delta^{202}Hg_{castings}$), suggesting preferential accumulation of lighter Hg isotopes and excretion of heavier isotopes by earthworms. The MeHg/THg ratio in earthworms is relatively low, indicating that Hg isotope fractionation is not induced by methylation. A positive correlation between $\delta^{202}Hg$ and $\Delta^{199}Hg$ in all experimental groups was observed, with a slope about −0.08, suggesting that Hg may have undergone mass independent fractionation (MIF) in internal tissues. We also found that Hg speciation can significantly affect Hg isotope fractionation between different tissues. Overall, our results revealed significant Hg isotope fractionation during the uptake and metabolism of Hg in earthworms, and the fractionation pattern is different from that in aquatic organism, which typically exhibit little MIF and preferential accumulation of heavier Hg isotopes.

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Improved Anthropogenic Mercury Emission Inventories for China from 1980 to 2020: Towards Effectiveness Evaluation for the Minamata Convention

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Abstract

Anthropogenic mercury (Hg) emission inventories are crucial for the effectiveness evaluation of the Minamata Convention on Mercury. Existing inventories for China still suffer from problems such as untimely update of inter-decadal inventories and inconsistency in the methodology of the inventories. In this study, we developed an integrated Dynamic Inventory for Mercury Emission (DIME) model and improved the accuracy of emission estimates for primary sources in China. Long-term historical speciated Hg emission inventories for China were established.

For coal-fired power plants (CFPPs), DIME uses a probabilistic technology-based emission factor method regarding the impacts of coal quality on Hg removal efficiencies of air pollution control devices (APCDs), which contains a sub-model for the transformation and synergistic removal of different Hg forms across APCDs. Results show that the probabilistic model solves the emission overestimation in the deterministic model due to the skewed probability distribution of Hg content in coal, and the consideration of coal quality results in a significant reduction of the uncertainty in the emission inventory of CFPPs. Another key improvement in the methodology is the quantitative estimation of the effectiveness of synergistic Hg removal by ultra-low-emission (ULE) retrofit measures in CFPPs, coal-fired industrial boilers (CFIBs), cement clinker plants (CCPs), and iron and steel plants (ISPs).

Results of DIME show that the total Hg emissions increased from 217.0 t in 1980 to 357.8 t in 2020 with a peak value of 506.6 t in 2010. Three stages with distinct leading drivers were identified. At Stage 1 (1980–1997), Hg emissions doubled with the rapid growth of economy; the driver was offset by the increase of dust and SO_2 control measures at Stage 2 (1997–2010) except for cement production; and co-benefits from strict control measures induced the decoupling of Hg emissions from the economy at Stage 3 (2010–2020). The ULE retrofits in key industries had pronounced Hg removal efficiencies. Large emission reduction potential still exists in CCPs. The improved emission estimation methods for key sectors in China, the consistency in methodology for historical Hg emission inventories, and the improvement of spatial distribution of speciated Hg emissions in this study provide a practical toolkit for more accurate effectiveness evaluation of the Minamata Convention.

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Mercury Reduction by Black Carbon under Dark Conditions

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Abstract

An accurate depiction of mercury (Hg) reduction is important to predict Hg biogeochemistry in both aquatic and soil systems. Although the photoreduction of Hg is well documented, reduction in the dark is poorly known and is thus the focus of this work. Black carbon (BC), an important constituent of organic matter in environments, can reduce Hg^{2+} in dark and oxygen-deficient conditions. Fast removal of Hg^{2+} in BC/Hg^{2+} solution was observed, with 4.99 – 86.88 L $mg^{-1}h^{-1}$ of the reaction rate constant, which could be ascribed to the combined actions of adsorption and reduction. Meanwhile, slow Hg reduction was obtained, compared to Hg removal, with 0.06 – 2.16 L $mg^{-1}h^{-1}$ of the reaction rate constant. Thus, in the initial stage, Hg^{2+} removal was mainly triggered by adsorption, rather than reduction. Afterward, the adsorbed Hg^{2+} on black carbon was converted into Hg^0. Dissolved black carbon and aromatic C-H on particulate black carbon were dominant triggers of Hg reduction for black carbon. During Hg reduction, the intastable intermediate, formed in the complex between aromatic C-H and Hg^{2+}, behaved as persistent free radicals, which could be detected by in situ electron paramagnetic resonance. Subsequently, the intastable intermediate was mainly converted into C-O on black carbon and Hg^0. Corresponding results of the present study highlight the important role of black carbon in the Hg biogeochemical cycle.

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Physiochemical controls on the multi-size distribution of total mercury in the Yangtze River Estuary

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Abstract

The spatial variations of total mercury (THg) distribution in water collected along the Yangtze River Estuary (YRE) – East China Sea (ECS) in 2023 were investigated. Six fractions of THg distribution were obtained via sequential filtration processes, including truly dissolved (<10 kDa), colloidal (10-100 kDa, 100 kDa-0.2 μm, 0.2 μm-0.7 μm), and particulate (0.7 μm-2 μm, >2 μm) fractions. The THg concentrations in the six fractions and dissolved organic matter were measured by trace Hg analysis, TOC analysis, fluorescence emission-excitation matrix (EEM) analysis, UV–Vis absorption spectrophotometer and asymmetric flow field-flow fractionation method. From freshwater sites to marine sites, it was observed that the total dissolved THg concentration generally remained constant (except at one site that highly impacted by coastal currents) and colloidal fractions were the dominant carriers, while particulate THg levels decreased. Specifically, at the maximum turbidity zone, the extremely high suspended particle concentration led to a 348% and 584% rise in particulate and 10-100 kDa colloidal THg concentration, respectively, compared to the adjacent landward site, which highly associated with the elevated autochthonous protein-like organic matter. At the 30-m isobath, the elevated Cl- concentration and reduced terrestrial humic-like organic matter greatly controlled the total dissolved THg partitioning in the truly dissolved fraction (73%). Meanwhile, a noticeable portion of terrestrial-derived particulate THg shifted from >2 μm to 0.7 μm-2 μm phase due to flocculation/precipitation processes, which further transported into the open shelf of ECS. To further the impacts of estuarine mixing process on the multi-size distribution of THg, we conducted mixing experiments using in situ collected freshwater and seawater end member samples (both unfiltered and filtered water samples). The results further proved

that high salinity induced coagulation of colloidal and particulates, and increased the proportion of truly dissolved THg. Overall, our results demonstrated the importance of physiochemical gradients (especially salinity and organic matter) on controlling the environmental fate of Hg in fluctuating estuarine environment.

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Importance of algal biomass on regulating Hg accumulation and trophic transfer in planktonic food chain in subtropical freshwater lakes

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Abstract

Algal biomass can significantly impact mercury (Hg) accumulation and transfer in planktonic food chain, but the underlying mechanisms are still controversial. We investigated bioconcentration and bioaccumulation of total mercury (THg) and methylmercury (MeHg) in size-fractionated plankton, including bacterioplankton, phytoplankton, meso-zooplankton and macro-zooplankton, which were sampled from six subtropical freshwater lakes during autumn in the Yangtze River Delta, China. Across the six lakes, there were large gradients of water characteristics, such as pH, dissolved organic carbon (DOC) and algal biomass (indicated by chlorophyll-*a* (Chl-*a*)). We observed significantly negative relationships between Chl-*a* and Hg bioconcentration factor (BCF) in phytoplankton, as well as Hg bioaccumulation factor (BAF) in zooplankton, suggesting lower waterborne Hg bioavailability at higher productive lakes. Such phenomenon was highly associated with the elevated levels of allochthonous humic-like substances with high molecular weight. Additionally, higher %MeHg in bacterioplankton was observed in two deep reservoirs (with lower trophic status) among the six lakes, which was correlated with the lake-to-lake variations of Hg-methylation microorganisms based on metagenomic data, implying the impacts of algal biomass on in situ MeHg production and further trophic transfer. Although the underlying mechanisms still require further investigations, the low Hg BCF and BAF driven by allochthonous humic-like substances and spatial variations in mercury methylation potential, which are both highly related with algal bloom, are important driving forces for Hg accumulation and trophic transfer in planktonic food chain in subtropical regions.

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Response of rice seed endophytic fungi to Hg-contamination

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Abstract

Rice is a methylmercury (MeHg) hyperaccumulator, and the consumption of rice is one of the main routine of human MeHg exposure. Endophytes have great effects on host plants heavy metal absorption, transportation and accumulation. However, little is known about the community structure and function of endophytes of rice seeds from Hg-contaminated areas. In the present study, Illumina sequencing method was used to compare the fungal community of rice seed endophytes from 3 different Hg-contaminated areas (SK, Hg heavily contaminated areas, followed by GX; HX, Hg-uncontaminated area). Totally, 608 OTUs was obtained from 9 seed samples, and they were assigned into 9 phyla and 204 genera. The most dominant phylum of rice seeds from 3 sites was Ascomycota (HX: 99.54%, GX: 98.86%, SK: 98.44%). However, the most dominant genera of rice seeds from 3 sites were different, they were *Microdochium* (33.60%), *Microdochium* (22.10%) and *Gibberella* (23.72%) for HX, GX and SK, respectively. Although *Microdochium* was also found in SK rice seeds, but it only accounted 4.87%. Interestingly, the relative abundance of Ascomycota and *Microdochium* in seeds decreased with increasing Hg content. The relative abundance of *Coniothyrium* and *Saccharomycopsi* in SK was significantly higher than in GX and HX, while *Epicoccum* and *Edenia* were significantly lower than that in GX and HX. The diversity and richness of seed fungal endophytes in Hg contaminated areas were lower than those in non-contaminated areas. Although there was no significant difference, the diversity decreased with increasing Hg concentration. Notably, dominant endophytes in seeds differ significantly from those in the other tissues. Moreover, endophytes ubiquitously present in roots, stalks, and leaves during various stages do not necessarily proliferate in seeds, suggesting a selective colonization that may occur independently from their abundance in earlier plant growth phases. The function of these selected endophytes needs to be further studied in future, especially their effects on seeds MeHg hyperaccumulation and the mechanism.

Keywords: Rice, methylmercury (MeHg), Hg, heavy metal, seed endophyte, diversit

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Abstract

Mercury emissions from human activities persist in the environment, posing risks to humans and ecosystem, and are regulated by the Minamata Convention. Understanding the historical emissions of mercury is critical for explaining the presence of mercury in the environment. In recent years, some studies have looked at the historical trends of atmospheric emission inventory. The spatial resolution of inventories for relatively recent years have improved. However, limited inventories have combined both long time scales and high spatial resolution, which is essential for evaluating the legacy impacts of anthropogenic mercury emissions, particularly in regions with high levels of mercury emissions. Here we compile a new comprehensive point source database by fusing multiple data source, and integrate it with previous China Atmospheric Mercury Emission Model to create an annual point source and gridded emission inventory for China covering 1978-2021. Integrating point source emission inventory (P-CAME) improves the accuracy of the gridded emissions, reducing the normalized mean error for all grids by 108% compared to not using point sources in the most recent year of 2021. The improved gridded emissions inventory notably enhances the simulation of atmospheric mercury concentrations, particularly in urban areas. P-CAME inventory resulted in a 20-23% reduction in the normalized mean bias. The improved gridded emission data identifies potential polluted grids characterized by high cumulative emissions. It indicates that 20% of cumulative emissions originate from just 0.3% of the grids, primarily distributed in Gansu, Yunnan, and Hunan Provinces. These areas are predominantly dominated by non-ferrous metal smelters or a mix of emissions sources including coal-fired industries and cement production. With the improvements in simulation accuracy and the identification of highly polluted regions, this updated inventory would greatly facilitate the assessment of mercury exposure, legacy impacts, and effective management of cross-media mercury pollution.

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Algal Biomass Regulates Mercury Bioaccumulation and Trophic Transfer in Anthropogenic-impacted Subtropic Lakes in the Yangtze River Delta, China

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Abstract

Mercury (Hg) contents in fish are commonly lower in more productive lakes, but the driving mechanism still remain controversial in subtropical regions. Based on more than 5 years field surveys, we conducted comprehensive studies on the bioconcentration, bioaccumulation and trophic transfer of the Hg across six anthropogenic lakes that spanning large gradients of algal biomass in the Yangtze River Delta, China. The total Hg (THg) and methylmercury (MeHg) contents in wild fish captured from mesotrophic deep lakes were much higher than other eutrophic lakes, although the dissolved Hg concentrations were lower. The less efficient transfer of Hg (from water to high trophic level fish) in more productive lakes could not be

explained by the impacts of food chain length on Hg biomagnification, but highly attributed to the less efficient entering of Hg into plankton, while the trophic transfer efficiency above plankton showed less lake-to-lake variations. Therefore, we further investigated the bioaccumulation and trophic transfer of Hg in planktonic food webs across the six lakes. In accord, we observed lower Hg bioaccumulation in size-fractionated plankton samples at more productive lakes/sites, which could not be explained by algal bloom dilution, but attributed to the impacts of physiochemical characteristics of lake water and plankton communities. Especially, the lower Hg bioconcentration and bioaccumulation in plankton at more productive lakes were highly associated with the lower Hg bioavailability (driven by higher dissolved organic matter) that hampered the dissolved uptake in plankton, while the smaller body-size of zooplankton also contributed to its lower Hg bioaccumulation. In addition, higher algal biomass associated with reduced proportion of MeHg in THg (% MeHg) in bacterioplankton and phytoplankton, and further transferred to zooplankton and fish along pelagic food chains, which are important but yet underestimated driving forces for the low Hg contents in pelagic fish in eutrophic lakes. Overall, our results highlight the important and complex impacts of algal biomass on controlling Hg bioaccumulation and trophic transfer in anthropogenic-impacted subtropic lakes.

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Tracing the biogeochemical cycling of mercury in polar regions by stable mercury isotopes

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Abstract

Polar regions, with minimal anthropogenic impacts, are ideal locations for studying mercury (Hg) pollution as background areas. To clarify the global circulation of Hg and its environmental impacts on the fragile ecosystems in the Antarctic and the Tibetan Plateau, the transport and accumulation of Hg from atmospheric to aquatic ecosystems were investigated from an isotopic perspective.

The annual variations in isotopic compositions of total gaseous Hg (TGM) at the Chinese Great Wall Station (GWS) were examined to trace the sources and environmental dynamics of atmospheric Hg in the western Antarctic. The positive δ^{202}Hg (0.58 ± 0.21‰, mean ± 1SD) and negative Δ^{199}Hg (-0.30 ± 0.10‰, mean ± 1SD) observed in TGM suggested minimal influence from vegetation−air exchange in the Antarctic. Intensified katabatic winds transporting inland air masses to the continental margin increased TGM Δ^{199}Hg in the austral winter, while marine surface emissions controlled by sea−ice dynamics lowered TGM Δ^{199}Hg in the austral summer. Meanwhile, the isotopic compositions of Hg in an aquatic food chain from GWS, involving sediment, mollusks and fish, provided insights into the histories of methylmercury (MeHg) in polar waters.

Total gaseous Hg (TGM) at an urban and a forest site on the Tibetan Plateau was collected respectively, and isotopic compositions were measured to clarify the influences of landforms and monsoons on the

transboundary transport of atmospheric Hg to the Tibetan Plateau. The transboundary transported anthropogenic emissions mainly originated over Indo-Gangetic Plain and carried over the Himalayas by convective storms and mid-tropospheric circulation, based on the binary mixing model of isotopes. In contrast, during the transport of TGM from South Asia with low altitude, the uptake by evergreen forest in Yarlung Zangbo Grand Canyon largely decreased the TGM level and shifted isotopic compositions in TGM at the Nyingchi forest site, which are located at the highaltitude end of the canyon. Our results provided direct evidence from Hg isotopes to reveal the distinct patterns of transboundary transport to the Tibetan Plateau shaped by landforms and climates, which is critical to fully understand the biogeochemical cycling of Hg in the high-altitude regions.

14. Carbon Neutrality and Ecosystem Health

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Tipping points of marine phytoplankton to multiple environmental stressors

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Abstract

Importance of the work:

Globally, anthropogenic climate change is threatening marine species. However, whether and how global marine phytoplankton, which represent the base of marine food webs, will exceed their tipping points under multiple climate factors remains unclear. Here, by establishing machine learning models, we identified the tipping points of global marine phytoplankton production and resistance under eight environmental stressors.

Objectives:

We aim to demonstrate the effectiveness of machine learning, specifically ensemble machine learning, in studying ecological responses to global climate changes with multiple stressors. Our next goal is to investigate the productivity, resistance, and biodiversity tipping points of phytoplankton that are threatened by intensifying climate changes. We intend to build models to analyze the relationships between extreme disturbances, environmental factors, and phytoplankton production, resistance, and richness. Lastly, we aim to identify and predict the tipping points of global marine phytoplankton production and resistance under multiple environmental stressors using machine learning models.

Methodologies:

We collected and identified extreme events of nine environmental variables describing the key dimensions dominating global marine phytoplankton responses. This study provides a framework for

building robust machine learning models and identifying the critical tipping points of phytoplankton during multiple climatic and environmental disturbances using reliable machine learning models.

Main results:

Phytoplankton production and resistance are affected by multiple factors and the temperature and partial pressure of carbon dioxide dominate the risks for reaching their tipping points. If the current emission scenario continues, 50% (40-61% at 90% confidence) and 41% (2-80% at 90% confidence) of tropical areas would reach the tipping points of ongoing phytoplankton production and resistance decline, respectively, in 2100.

Conclusion

Compared with single- or few-factor studies, machine learning (for example, ensemble machine learning) provides a powerful and realistic solution for policy-makers facing large-scale ecological responses to global climate changes under multiple environmental stressors.

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Development and Application of the Compound Indicators for Vulnerable Ecosystems (CIVE): A Multidimensional Approach to Assessing Ecosystem Vulnerability

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Abstract

Assessing the vulnerability of ecosystems to environmental stressors, including heat, water, and air-related disasters, presents a complex challenge. These stressors impact the multi-dimensional aspects of ecosystems' exposure, sensitivity, and adaptive capacity. Our research introduces the Compound Indicators for Vulnerable Ecosystems (CIVE), a novel metric designed to capture the intricate dynamics of ecosystem stress responses. The CIVE framework comprehensively integrates responses from various variables including vegetation dynamics, soil conditions, and changes in water, carbon, and energy levels. By employing dimensionality reduction techniques and resilience metrics, we systematically compute the CIVE. This involves normalizing and averaging subindices for each spatial location against specific combinations of stressor and ecosystem variables. Our method identifies and maps 'hot spots' and temporal patterns of vulnerability, termed 'hot moments'. This comprehensive tool facilitates targeted ecosystem management and informs policy-making by pinpointing areas and times of highest risk. This study advances our understanding of ecosystem vulnerabilities and offers practical insights crucial for developing adaptive strategies and enhancing the resilience of ecosystems to environmental changes.

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Widespread Decline in Recent Tree Growth under Climate Change

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Abstract

Tree water use efficiency (WUE) has increased globally in the past 150 years, but this has not been translated into global increases in tree growth consistently in space and time. Complex and dynamic forest ecosystems would respond non-linearly to climate change with multiple factors over a long period, and can have tipping points or critical boundaries / thresholds at which a sudden shift to a contrasting dynamic regime might occur. However, prediction of such critical points / thresholds before they are being reached is extremely difficult. Indeed, our comprehensive studies undertaken in the last 18 years (mostly unpublished) have shown for the first time that long-term tree growth of beech and oak in temperate central Europe (Belgium) responded non-linearly to rising atmospheric carbon (C) dioxide (CO_2) and water (H_2O) limitation. This is due to the increasing mean annual temperature and decreasing summer rainfall during 1840s–1990s. It is ***the initial CO_2 fertilisation*** and ***then warming-induced water limitation*** that ***control tree growth under climate change***. This would result in decreased forest CO_2 assimilation and increasing atmospheric CO_2, ***leading to accelerated global warming and increasing water limitation***. We have tested the CO_2 fertilisation - warming-induced water limitation model globally, and our exciting major findings (unpublished) have highlighted that ***there is a widespread decline in tree growth beyond the tipping points of atmospheric CO_2***: average atmospheric CO_2 tipping point at 321.8 ppm or reached in ca. 1956 for tropical tree species, with the corresponding mean tipping points of 357.8 ppm or 1994 (Mediterranean), 354.7 ppm or 1990 (temperate), 352.8 ppm or 1989 (arid), 354.5 ppm or 1990 (subtropical) and 363.5 ppm or 1996 (boreal). It is interesting to note that the atmospheric CO_2 tipping points for a given biome (such as temperate) would be influenced by both biotic (e.g. tree species and age) and abiotic factors (e.g. water and N availability), but ***there is a global convergence of atmospheric CO_2 tipping point at 353.9 ppm or in 1990***, which is surprisingly close to the theoretical or model-predicted atmospheric CO_2 tipping point of 350 ppm.

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Investigations of the relationship among growth, shells formation and carbon sequestration of marine mussels

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Abstract

Ocean is one of the largest active carbon pools, and the carbonate marine organisms, e.g. mussels, can be one of important parts of the ocean carbon sequestration.

Mussel shells are mainly composed of inorganic calcium carbonate, and the formation process of mussel shells requires the use of carbon in the water, but the specific process and mechanism of shell formation, and the relationship with mussels growth are still unclear.

Key genes related to carbon synthesis in mussel shells were also screened and their expression levels at different growth stages were quantitatively analyzed and compared to imply the potential carbon flux of mussel shells at different growth stages.

In this study, thick-shelled mussels with different growth status were sampled from the aquaculture ranch. Following the basic growth indexes measurements, mussels were dissected into shell and soft tissues for carbon content measurement. Meanwhile, the mantle tissue which was the key tissue for shell formation was also dissected separately for the determination of key molecular regulation of shell formation at transcriptional levels.

The results showed that the changes in dry and wet weights of mussel shells and soft tissues were closely related to their growth stages and the growth capacity of mussels' soft tissues and shells differed in different growth periods depending on particular environmental status, such as water temperature, salinity and food supply. In addition, the carbon content of soft tissues and shells of thick-shelled mussels showed that the carbon content per unit weight of the mussel shells was higher than that of the soft tissues, which was the main contributor to the mussel's carbon content; and that the carbon content changed with the mussel's growth.

Our results provided the scientific basis for the realization of carbon sequestration by carbonate marine organisms, and help to truly understand the potential roles of mussels in carbon sink or source.

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Process and Mass Transfer Intensification Strategies of Ammonia-based CO_2 Capture

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Abstract

Greenhouse gas-induced climate change has emerged as a worldwide environmental concern due to the need to address the excessive CO_2 emissions from industrial sources. The ammonia process is considered as a feasible and pragmatic direction to precipitate CO_2 among several potential CO_2 capture systems. The ammonia-based carbon capture offers excellent CO_2 absorption capacity, prevents solvent degradation, and requires less regeneration energy compared to conventional amine solvent. However, the high volatility of ammonia restricts its utilization due to the need for low-temperature absorption conditions and a relatively low ammonia concentration, resulting in a reduced CO_2 absorption rate. Enhancing CO_2 absorption is essential for decreasing operational and capital expenses by improving absorption efficiency, lowering chemical absorbent circulation, and minimizing the absorber column's size. Implementing a combined system that incorporates both chemical promoters and physical process modifications in ammonia-based carbon capture can be advantageous compared to using either approach individually. The synergistic effects of the combined system enhance CO_2 capture rates, mitigate ammonia loss, and provide flexibility in adapting to different operating conditions. This study analyzes the latest advancements and obstacles concerning the ammonia absorption process, with a specific focus on investigating reaction mechanisms, thermodynamics, process modeling, and techno-economic analysis. The study proposes mass transfer and process enhancement strategies for ammonia-based carbon capture, with the aim of identifying efficient and cost-effective solutions for maximizing CO_2 absorption while minimizing energy consumption. Furthermore, the environmental impact of the technology is also presented. Overall, this study aims to provide valuable perspectives on the potential of the ammonia technique for capturing CO_2 and to propose feasible approaches for improving its efficiency, thus contributing to the global efforts underway to address climate change.

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Ecological Effects and Microbial Mechanisms of Microplastic on Carbon and Nitrogen Cycles in Paddy Fields

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Abstract

The carbon (C) and nitrogen (N) cycles in paddy soils play a crucial role in understanding their contributions to greenhouse gas (GHG) emissions and climate change mitigation within global agriculture and environmental sciences. The accumulation of microplastics (MPs) in agricultural soils has raised significant concerns due to their role as carriers of pollutants and microbial carbon sources, influencing biogeochemical cycles and potentially exacerbating climate warming. However, there remains a substantial knowledge gap regarding the ecological impacts and microbial mechanisms associated with MP enrichment in paddy soils, particularly concerning C/N cycles and GHG emissions. This study systematically evaluated the impacts of polylactic acid (PLA) and polyethylene (PE) MPs on the C/N cycles and GHG emissions in paddy fields through microcosm experiments. The results demonstrated that PLA notably increased methane and nitrous oxide emission fluxes. Compared to PE MPs, PLA exposure showed an increasing trend in plant biomass, C/N accumulation, and enhanced activity of antioxidant enzymes. Further analysis using 16S rRNA amplicon sequencing and metagenomics revealed that PE enrichment significantly reduced the abundance of nitrification/denitrification functional genes in the rhizosphere, while both types of MPs decreased the abundance of genes related to carbon fixation. Conversely, PLA enrichment notably increased the abundance of genes encoding nitrite reductase (Nir). These findings suggest that PLA in paddy soil may enhance denitrification, thereby increasing N emissions and losses, whereas PE MPs influence the C/N cycle by suppressing nitrification/denitrification and carbon-fixing microorganisms in the paddy field system. Additionally, under cadmium (Cd) pollution conditions, the global warming potential of paddy soil was significantly lower than that of soils enriched solely with MPs, mitigating N emissions. Structural equation modeling revealed that dissolved organic matter and soil bioavailable Cd from MPs indirectly impact soil GHG emissions by directly influencing microbial abundance (e.g., Firmicutes, Nitrospirota bacteria). This study provides novel insights into the intricate interactions between microplastics, soil microbes, and biogeochemical cycles in paddy ecosystems, contributing to a broader understanding of environmental sustainability in agriculture.

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An increase in marine heatwaves without significant changes in surface ocean temperature variability

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Abstract

Marine heatwaves (MHWs)—extremely warm, persistent sea surface temperature (SST) anomalies causing substantial ecological and economic consequences—have

increased worldwide in recent decades. Concurrent increases in global temperatures suggest that climate change impacted MHW occurrences, beyond random changes arising from natural internal variability. Moreover, the long-term SST warming trend was not constant but instead had more rapid warming in recent decades. Here we show that this nonlinear trend can—on its own—appear to increase SST variance and hence MHW frequency. Using a Linear Inverse Model to separate climate change contributions to SST means and internal variability, both in observations and CMIP6 historical simulations, we find that most MHW increases resulted from regional mean climate trends that alone increased the probability of SSTs exceeding a MHW threshold. Our results suggest the need to carefully attribute global warming-induced changes in climate extremes, which may not always reflect underlying changes in variability.

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Tree Diversity Affects Soil Carbon and Nitrogen Accumulation

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Abstract

Biodiversity has been shown to be linked to ecosystem services such as ecosystem productivity, particularly in manipulative experiments. However, few have studied such relationships in natural ecosystems. Using a large dataset that includes surveys on plant communities and soils across 18 years (between 2000 and 2017) in Canada's National Forest Inventory program, we tested the relationship between tree diversity and forest soil carbon and nitrogen accumulation over time. The dataset includes 406 plot inventories, covering much of Canada's temperate and boreal forests. We found that soil carbon and nitrogen accumulation increased with tree diversity. More specifically, soil carbon and nitrogen accumulation in the organic horizon was 30 and 42%, respectively, greater in forests with the lowest species evenness than those with the highest species evenness. In addition, soil carbon and nitrogen accumulation in the mineral horizon was 32 and 50%, respectively, greater in forests with the lowest functional diversity than those with the highest functional diversity. Soil properties in the studied forests also played major roles in affecting changes in forest soil carbon and nitrogen stocks. For example, forests with higher initial organic horizon thickness had smaller increases in organic horizon thickness over time, and thus less accumulation of soil carbon and nitrogen in the organic horizon. Through structural equation modelling, our study shows that, after controlling for the influence of background climatic and soil conditions, higher tree diversity was linked to greater soil carbon and nitrogen accumulation in natural forests. Our study suggests that conserving and promoting tree diversity in forests could enhance the contribution of forests in mitigating climate change.

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Advanced CO_2 Capture Using Mesoporous Alumina Enhanced with Alkaline Earth Metals

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Abstract

Abstract

Introduction: The pressing issue of climate change, driven by rising greenhouse gas emissions, especially carbon dioxide (CO_2), has spurred extensive research into carbon capture, utilization, and storage (CCUS) technologies. One promising approach involves using adsorbent materials to capture CO_2 from industrial emissions.

Methods: Mesoporous alumina (MA) adsorbents loaded with alkaline earth metals, including 5M/MA (M = Mg, Ca, Sr, Ba) and xMg/MA (x = 1, 3, 5, 7 wt.%), were prepared using evaporation-induced self-assembly (EISA) and impregnation methods.

Results and discussion: The CO_2 adsorption capacity of the modified mesoporous alumina samples was measured using a thermogravimetric analyzer (TGA). Among them, 5Mg/MA showed the highest CO_2 adsorption capacity, reaching 1.08 mmol/g, which was 2.16 times higher than that of pure mesoporous alumina (0.50 mmol/g). In situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) analysis revealed that CO_2 primarily adsorbed as carbonates on the surface of Mg-modified alumina. Examination of adsorption kinetics indicated that the process was largely chemisorption, benefiting from the basic sites introduced by the Mg modification. Density functional theory (DFT) calculations confirmed that the presence of Mg significantly increased the affinity of the alumina surface for CO_2, corroborating the experimental findings. This strong interaction is attributed to the increased number of basic sites and the enhanced surface basicity of the Mg-loaded mesoporous alumina. The cyclic stability of the 5Mg/MA adsorbent was evaluated through multiple adsorption-desorption cycles. The results showed that the Mg-loaded alumina maintained its high CO_2 adsorption capacity over several cycles, indicating excellent stability and potential for repeated use.

Conclusion: Modification of mesoporous alumina with alkaline earth metals, especially magnesium, greatly boosts its CO_2 adsorption capabilities. The 5Mg/MA adsorbent demonstrates high CO_2 capacity, favorable adsorption kinetics, and exceptional cyclic stability, positioning it as a promising option for CO_2 capture applications. This research offers critical insights into the development and enhancement of advanced adsorbent materials, crucial for effective carbon capture strategies aimed at combating climate change and lowering greenhouse gas emissions.

815

Life-cycle thinking based GREENNESS framework for advancing green chemistry: Case study with typical ionic liquids for cellulose dissolution and regeneration

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Abstract

Due to its abundancy and renewability, cellulose has emerged as a promising candidate to tackle the challenges posed by fossil fuel depletion and global warming impacts in the transition toward green chemistry. In the value-added utilization of cellulose, ionic liquids (ILs) have been increasingly used as green solvents for efficient cellulose dissolution due to their low volatility. However, greenness is a multicriteria concept that has been extensively hyped without comprehensive assessment in chemical processes or final products. Herein, we propose a comprehensive assessment framework, GREENNESS, to quantify the greenness of three typical ILs employed in cellulose dissolution and regeneration, i.e., 1-allyl-3-methylimidazolium chloride (AmimCl), 1-butyl-3-methylimidazolium chloride (BmimCl), and 1-ethyl-3-methylimidazolium acetate (EmimOAc). To prevent burden shifting across life cycle stages or impact categories, this framework adopts a full life cycle perspective, encompassing IL production through to emission, with a focus on (eco)toxicity. Toxicity tests were conducted on three trophic levels to characterize the freshwater ecotoxicity associated with IL fate, transport, and exposure via the USEtox model. Human noncarcinogenic toxicity was also evaluated. The results indicated that AmimCl is superior to BmimCl and EmimOAc across all environmental categories, which differed from the outcomes observed via the CHEM21 solvent selection guide. Overall, the comprehensive framework GREENNESS can also guide the selection of other solvents to promote environmentally friendly chemistry and chemical engineering, thereby decreasing their impacts on the environment.

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Comparative Analysis of the Life Cycle Environmental and Economic Potentials of Various Energy Storage Systems

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Abstract

The deployment of energy storage systems (ESS) plays a pivotal role in accelerating the global transition to renewable energy sources. Specifically, comprehending the life cycle environmental and economic impacts, as well as the necessary conditions and scenarios required for sustainable deployment, is critical in guiding decision-making and supporting sustainable ESS operations. In this study, life cycle environmental and economic impacts of pumped hydro energy storage (PHES), lithium-ion batteries (LIB), and compressed air energy storage (CAES) were initially analyzed. Further analysis was conducted to elucidate the potential for carbon neutrality and sustainability of existing PHES compared to LIB in Guangdong, China, integrating various reduction measures to meet net-zero emission (NZE) scenarios. Regarding environmental impacts, LIB is currently the most environmentally favorable ESS, followed by PHES. Economic analysis indicates that the life cycle cost per MWh for PHES is $66.5, approximately half that of LIB, emphasizing PHES's superior economic benefits. The analysis of various decarbonization measures revealed that transitioning to renewable energy sources is the most effective strategy for carbon reduction, with projected reductions ranging between 75 and 112% in both PHES and LIB systems. When implementing all carbon reduction strategies simultaneously, LIB is expected to achieve carbon neutrality by 2030, whereas PHES is projected to reach this milestone by 2040. With anticipated future energy mix optimizations, carbon emissions are expected to further decrease, potentially dropping to 22.2 kg CO_2/MWh for PHES and 48.7 kg CO_2/MWh for LIB by 2050. Although PHES may achieve carbon neutrality slower than LIB, its overall advantages in environmental and economic make it a more suitable choice in regions where its implementation is feasible.

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Microbiome stimulated degradation of organic carbon and the coupled nutrient cycling during macroalgae decay

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Abstract

Seasonal macroalgae bloom decay in the coastal areas triggered catastrophic impacts on environmental degradation. Marine microbes are the key drivers of biogeochemical cycles in the coastal ecosystems, yet the mechanisms of how marine microbes driving the degradation of organic carbon during macroalgae decay remains unclear. This study investigated the microbial community composition, functions, and metabolic pathways among different areas with or without *Sargassaceae*. By combining high-throughput sequencing of amplication, metagenome and metatranscriptome, we found that the decay of *Sargassaceae* in sediments decreased the α-diversities but increased the biochemical cycling processes. The *Sargassaceae* decay enhanced the microbial gene expression of carbohydrate energy metabolism (glycolysis, citrate cycle, and pentose phosphate), carbohydrate degradation (cellulose, starch), and carbon fixation (CBB cycle, WL cycle). In addition, the progress of denitrification, dissimilatory nitrate reduction, and sulfur oxidation were stimulated by *Sargassaceae* decay, and could lead to the release of N_2O and CH_4. Functional annotation of metagenome-assembled genome indicated that the *Vibrio,*

Pseudoalteromonas, *Lutimonas*, and *Exiguobacterium_A* members were the key players in organic carbon mineralization which coupled with sulfur, nitrogen, and metal biogeochemical cycles. This study enhances our understanding of microbially driven organic carbon degradation and biochemical cycling during the decomposition of macroalgae.

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Core microorganisms drive marine carbon sinks through anabolism in seaweed cultivation areas

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Abstract

Despite the carbon sequestration of DOC and POC in seawater released by macroalgal growth, little attention has been paid to the contribution to carbon sink in on-site sediments after macroalgal decay. In addition, the main metabolic pathways of microorganisms are worth analyzing. There, we assessed DOC flows in seawater and carbon contents in on-site sediments in a sub-tropical macroalgal bed after macroalgae decayed. The increase of carbon content in sediment is the main site for macroalgae to increase marine carbon sinks. Macroalgae has caused changes in microbial species composition, increasing microbial diversity, stability, and network complexity in seabed sediments. Metabolic reconstruction shows that most MAGs have the potential to degrade unstable organic carbon, with limited ability to degrade recalcitrant polysaccharides such as rhamnose and polysaccharides, and utilizing sugars for synthetic metabolic pathways may be another major pathway for marine carbon sinks. This study investigated the progress of microorganisms driving marine carbon sinks through metabolism in seaweed cultivation areas.

1067

Ensemble learning model identifies adaptation classification and turning points of river microbial communities in response to heatwaves

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Abstract

Heatwaves are a global issue that threaten microbial populations and deteriorate ecosystems. However, how river microbial communities respond to heatwaves and whether and how high temperatures exceed microbial adaptation remain unclear. In this study, we proposed four types of pulse temperature-induced microbial responses and predicted the possibility of microbial adaptation to high temperature in global rivers using ensemble machine learning models. Our findings suggest that microbial communities in parts of South American (e.g., Brazil and Chile) and Southeast Asian (e.g., Vietnam) countries are likely to change due to heatwave disturbance from 25 to 37°C for consecutive days. Furthermore, the microbial communities in approximately 48.4% of the global river gauge stations are prone to fast stress inadaptation, with approximately 76.9% of these stations expected to exceed microbial adaptation after heatwave disturbances. If emissions of particulate matter with sizes not more than 2.5 μm (PM2.5, an indicator of human activities) increase by twofold, the number of global rivers associated with the fast stress adaptation type will decrease by ~13.7% after heatwave disturbances. Understanding microbial responses is crucially important for effective ecosystem management, especially for fragile and sensitive rivers facing heatwave events.

1075

Unveiling Microbial Nitrogen Metabolism in Rivers using a Machine Learning Approach

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Abstract

Microbial nitrogen metabolism is a complicated and key process in mediating environmental pollution and greenhouse gas emissions in rivers. However, the interactive drivers of microbial nitrogen metabolism in rivers have not been identified. Here, we analyze the microbial nitrogen metabolism patterns in 105 rivers in China driven by 26 environmental and socioeconomic factors using an interpretable causal machine learning (ICML) framework. ICML better recognizes the complex relationships between factors and microbial nitrogen metabolism than traditional linear regression models. Furthermore, tipping points and concentration windows were proposed to precisely regulate microbial nitrogen metabolism. For example, concentrations of dissolved organic carbon (DOC) below tipping points of 6.2 and 4.2 mg/L easily reduce bacterial denitrification and nitrification, respectively. The concentration windows for NO_3^--N (15.9−18.0 mg/L) and DOC (9.1−10.8 mg/L) enabled the highest abundance of denitrifying bacteria on a national scale. The integration of ICML models and field data clarifies the important drivers of microbial nitrogen metabolism, supporting the precise regulation of nitrogen pollution and river ecological management.

1110

Microbial Direct Interspecies Electron Transfer and Electroautotrophy

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Abstract

Direct interspecies electron transfer (DIET) is a nutritionally dependent behavior between different species of microorganisms, which achieves interspecies metabolic dependence and collaboration through direct electron transfer. This process is generally believed to be mediated through conductive pili and is widely present in various methanogenic habitats, thus contributing to global methane emissions. Here, we first studied DIET in a model system consisting of *Geobacter metallireducens* and *Geobacter sulfurreducens*. In situ Raman and electrochemical Fourier transform infrared (FTIR) spectroscopy indicated that cytochromes are abundant in the electric syntrophic coculture. Cyclic voltammetry and potential step experiment revealed a diffusion-controlled electron transfer process and the electrochemical gating measurements further demonstrated a cytochrome-mediated electron transfer in the DIET coculture. Genetic Mutation revealed two pilus-free *Geobacter* species can form DIET and Gmet_2896 cytochrome of *G. metallireducens* plays a key role in DIET. Furthermore, we studied the DIET coculture between *Geobacter metallireducens* and *Rhodopseudomonas palustris*. The results showed that electrons generated by *G. metallireducens* could transfer to *R. palustris*, thereby providing reducing power and energy for the dark CO2 fixation. Our findings deepen our understanding on DIET and the global carbon cycle under dark, anoxic conditions.

15. Environmental Chemistry and Toxicology of Priority Substances

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Toxicity of Conventional and Biodegradable Plastic Additives on Soil Fauna: A Case Study with the Root Lesion Nematode *Pratylenchus neglectus*

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Abstract

Several traditional additives used in both conventional and biodegradable plastics, such as phthalate acid esters and polybrominated diphenyl esters, have been reported as hazardous, neurotoxic, or otherwise toxic substances. As a result, there is an emerging trend to replace traditional hazardous additives with bio-additives. However, limited information exists on the effect of the emerging bio-additives on the environment and on soil biota health. When assessing additive toxicity, high and often unrealistic concentrations are used to demonstrate their negative impact on a range of soil biota, including soil macrofauna and microbial communities. These studies have clearly revealed a concentration-dependent relationship between additives and the health of soil fauna.

Traditionally, earthworms are used as a model organism in the assessment of soil health, yet very few are found across the arid regions of Western Australia. Whereas nematodes are ubiquitous in Australian soils, but there is limited information about their response to plastic and their additives. The root lesion nematode, *Pratylenchus neglectus*, is a plant parasite extensively researched to mitigate their economic impact in the agricultural sector thus is used as a model soil faunal organism.

A comparison between chronic toxicity of plastic additives found in conventional and biodegradable plastics was investigated in this study, with *P. neglectus* as the model organism. A significant increase in mortality and decrease in reproduction was observed when the concentration of the additives increased to 10000 µg L-1. However, the behaviour and movement of the nematodes were not significantly impacted when exposed. Additionally, the nematodes oxidative stress levels were monitored through the accumulation of reactive oxygen species. When exposed to conventional and biodegradable additives, a significant increase in stress levels was observed compared to the control. Identifying key differences in the toxicity between conventional and biodegradable plastics and the impact of individual plastic additives will aid the development of new safer plastic products.

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Compound- and regio-selective toxicity and metabolism of 6PPD-Quinone

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Abstract

The tire rubber-derived ozonation product of N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD), 6PPD-Q, was recently discovered to cause acute mortality in Coho Salmon (*Oncorhynchus kisutch*). Aiming to identify a potential nontoxic replacement antioxidant for 6PPD, we herein synthesized seven PPD-quinones with distinct side chains to investigate their structure-related toxicities in rainbow trout (Oncorhynchus mykiss). While 6PPD-Q exerted strong toxicity (96 h LC50 = 0.64 µg/L), toxicity was not observed for six other PPD-quinones despite their similar structures. This demonstrated that para-Phenylenediamines (PPDs) are potential replacement commercial antioxidants. We further tested the multiphase gas-surface ozone reactivity of four select PPDs and evaluated the toxicity of their reaction mixtures in Coho Salmon and Rainbow Trout. The viability of Coho Salmon CSE-119 cells was strongly affected by the ozonolysis products of 6PPD, but not by those of the other three PPDs. As with Coho Salmon cells, acute mortality was only observed in juvenile Rainbow Trout that were exposed to the

oxidized 6PPD reaction mixture, suggesting a common mechanism of toxic action in the two salmonid fish species. Compound- and regio-selective formation of hydroxylated metabolites of 6PPD-Q were detected in Rainbow Trout exposed to the 6PPD reaction mixture, which may be related to its selective toxicity. Our studies report the structurally selective toxicity and metabolism of 6PPD-Quinone, which demonstrates that other PPDs are potential alternative antioxidants.

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"Occurrence and time trends in color developers including bisphenols in thermal receipt papers collected in 2015 and 2023 in Korea"

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Abstract

Color developers are used in the thermal printing technology to activate the thermochromic dye under heat condition, transforming it into a colored form. Bisphenol A (BPA), traditionally used for this purpose, has been substituted with alternatives (e.g., bisphenol S, BPA) due to the domestic and global regulations. The present study determined the concentrations of 19 color developers including BPA and its alternatives in thermal receipt papers collected in 2015 (n = 120) and 2023 (n= 200) from Korea to investigate the residue levels and profiles according to regulatory actions. The concentrations of BPA decreased in thermal receipt papers between 2015 and 2023, while the BPS concentrations increased. In this study, different types of thermal paper products (n = 62; shipping labels, lottery tickets, and tickets) were also collected in 2023. In shipping label samples, BPS was a predominant developer with a 93% proportion of total concentrations, while 4,4′-sulfonylbis[2-(2-propen-1-yl)phenol] (TGSA) and 4-[[4-(1-methylethoxy)phenyl]sulfonyl]phenol (D-8) were predominant in lottery ticket samples (96%) and ticket samples (64%), respectively. TGSA and D-8 are known as BPS derivatives. Our findings suggest the change from the BPA to BPS-based developers in thermal paper markets. Thermal receipt papers (n = 87) were additionally collected from China, Japan, Vietnam, the Netherlands, and Austria for a global comparison. BPA was not detected in all samples from Japan with a dominance of BPS and D-8. All samples collected from China and Vietnam contained only BPA. Samples from European countries, such as the Netherlands and Austria, showed the predominance of BPS, Pergafast® 201 (PF201), and PF201. This result suggests the different usage patterns in color developers among countries. Further studies are required to investigate toxicological effects of BPA replacements applied in thermal papers.

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Non-Target Screening of Persistent Chemicals in Swedish Waters based on Wastewater Persistency

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Abstract

The huge variety of chemicals applied and produced threaten environmental health and drinking water safety. Moreover, the majority of registered chemicals have not been monitored in the environment, have uncertain toxicities and environmental persistence, and unknown transformation products. In waters, we are especially concerned about persistent, mobile and toxic substances (PMTs), since they can accumulate in our water resources and can be hard to remove under water treatment. Here, we applied a non-targeted liquid chromatography-high resolution mass spectrometry (LC-HMRS) workflow to characterize and understand chemical persistency with environmental waters big data analysis. Groundwaters (N=63), surface waters (N=147), raw- (N=38) and treated drinking waters (N=73), urban storm waters (N=23), and household-, influent and effluent wastewaters (N=38) were analysed with a comprehensive LC-HRMS workflow, and then pre-processed (i.e. peak picking, data alignment, blank filtering, MS2 deconvolution) in MS-DIAL. To prioritize persistent chemicals, we created a feature-based molecular library based on persistency through wastewater treatment by comparing paired wastewater influent and effluent (N=7). Features with median peak area effluent/influent ratio > 80 % and 50-80% were classified as persistent (N=8081) and semi-persistent (N=1823), respectively, and were added to the library and thus screened for in the environmental samples. For 60 non-target features flagged as persistent/semi-persistent in positive ionization mode, we got a match with MassBank Europe database. Among these, we identified (confidence level 1) 1,3-diphenylguenidine, 1H-benzotriazole, 4/5-methyl-1H-benzotriazole and melamine, which have previously been classified as PMTs. Another four chemicals (level 2a) had previously been classified as PMTs, in addition to seven chemicals (level 1 and level 2a) as potentially persistent, further indicating that this unbiased screening approach is relevant to flag persistent features in environmental waters.

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Non-target Analysis of Persistent Chemicals in Natural Waters using Feature-Based Molecular Libraries

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Abstract

Persistent, mobile and toxic substances (PMTs) are of increasing concern due to their potential to irreversibly contaminate drinking water resources. Under European REACH regulations, chemicals with annual production volumes ≥ 10 tonnes must undergo persistency testing, however there are many exemptions, and the persistence of transformation products is often neglected. Using liquid chromatography - high resolution mass spectrometry we targeted a wide range of recognized PMTs while also aiming to discover unknown PMTs by a strategic non-target workflow. In a nation-wide survey of Swedish waters, we collected and analysed groundwaters, surface waters, drinking waters, storm waters

and wastewaters. A feature-based molecular library was generated from the analysis of paired wastewater influent and effluent, with features ranked on persistence and screened in all water samples. In positive ionization mode, all features classified as persistent were detected in one or more environmental samples, with highest detection frequencies (DF) in surface waters (median DF 80%, 0.6% features non-detected), and lowest detection frequencies in groundwaters (median DF 59%, 8.5% non-detected) and tap waters (median DF 70%, 6.7% non-detected). Sixty nontarget features, categorized as persistent in wastewater, had spectral library matches in MassBank Europe (confidence level 2a) and were detected in environmental waters, including pharmaceuticals, industrial chemicals, UV-filters, organophosphate flame retardants and pesticides. Eight of these had previously been classified as PMTs, or very persistent and very mobile, including 1,3-diphenylguanidine, 1H-benzotriazole, 4/5-methyl-1H-benzotriazole and melamine, which were all confirmed with analytical standards (level 1). Moreover, the majority of the 60 discovered substances were detected in groundwaters (75 %) and tap waters (70%). With this large non-target dataset and a novel persistency-based prioritization approach we show that unbiased screening and characterization of persistent chemicals is possible in high-throughput to discover relevant chemicals of high concern to society.

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Applying Single-Cell RNA Seq to Elucidate Tissue-Specific Responses in PFOS Embryotoxicity and Metabolic Insights in Zebrafish

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Abstract

Perfluorooctanesulfonic acid (PFOS) is a persistent and ubiquitous legacy environmental toxicant and member of the per-and-polyfluoroalkyl substances (PFAS) superfamily, historically used in numerous commercial and consumer products. Epidemiological and animal studies have linked PFOS exposure to several adverse health outcomes, including diabetes, pancreatic β-cell dysfunction and oxidative stress. Previously, we have shown that PFOS exposure during embryonic development in zebrafish can disrupt development of the pancreas, resulting in smaller and mis-shaped islets of Langerhans, truncation of the exocrine pancreas, dysregulation of lipids, and indications of metabolic dysfunction. To gain mechanistic insight into how PFOS exerts toxicity during early life, we used single-cell RNA-sequencing (scRNA-Seq) to identify cell and tissue-specific transcriptomic responses to PFOS exposure. Embryos were exposed to 0 (0.01% DMSO solvent control) or 16 µM PFOS from 3-72 hours post fertilization and were processed for scRNA-Seq. We used 10X Genomics' Loupe Cell Browser to obtain t-SNE and UMAP plots and generated custom annotations for the identified clusters representing different tissue types by comparing marker genes from the ZFIN database and published literature to assess significant differentially expressed genes (DEGs) across clusters. Initial findings among the data indicate numerous tissue-specific differences in processes including apoptosis, epigenetic changes, oxidative stress, calcium signaling, ER stress, and hormone secretion among others. Validation of these mechanistic insights confirmed changes in islet vasculature, insulin biosynthesis, and oxidative stress as examples. A limitation of this approach is that some cell types that are at very low abundance remain difficult to detect and robustly quantify

changes. Overall, scRNA-Seq is a powerful tool to identify tissue-specific changes and novel mechanisms by which toxicants like PFOS disrupt embryonic development.

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Zinc-enriched Yeast Can Improve Acrylamide-induced Cognitive Impairment Through ZnT3/BDNF/TrkB Pathway

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Abstract

Aims Acrylamide (ACR) is an environmental pollutant that is neurotoxic and can cause cognitive impairment. Zinc (Zn) is a trace element critical in many biological processes. Zn deficiency can lead to cognitive impairment. This study investigates whether zinc-enriched yeast (ZnY) can ameliorate acrylamide-induced cognitive impairment through the ZnT3/BDNF/TrkB pathway.

Methods Sprague-Dawley (SD) rats and HT22 cells were used as in vivo and in vitro models, respectively. Rats were divided into four groups: control, ACR (5 mg/kg/day), ZnY (8 mg/kg/day) and ACR + ZnY groups, receiving treatments via gavage for 16 weeks. In HT22 cells, ZnT3 expression was knocked down by small interfering RNA (siRNA) transfection to verify the regulatory role of the ZnT3/BDNF/TrkB pathway mediated by ZnT3 in ACR-induced toxicity.

Results ZnY improved impaired recognition and spatial memory in the novel object test and the mirror water maze in ACR-exposed rats. Additionally, ZnY attenuated ACR-induced histopathological changes in the hippocampus, upregulated Vglut1 and NeuN expression, and ameliorated synaptic plasticity disruption observed via transmission electron microscopy. Inductively coupled plasma mass spectrometry (ICP-MS) showed decreased zinc levels in plasma and brain tissue of ACR-exposed rats, which were restored by ZnY supplementation. TSQ staining revealed ACR decreased zinc levels in the hippocampus and cortical areas, improved by zinc supplementation. Zinc supplementation alleviated the reduction in zinc transporter 3 (ZnT3) protein, as well as its downstream protein brain-derived neurotrophic factor (BDNF) and phospho-tyrosine kinase receptor B (P-TrkB) expression that is induced by ACR. In HT22 cells, compared to the siNC + ACR + Zn group, the expression of P-TrkB and BDNF was not increased in the siZnT3 + ACR + Zn group.

Conclusions The investigation confirms the neuroprotective capacity of ZnY against ACR-induced brain injury, and suggest that ZnT3/BDNF/TrkB pathway mediated by ZnT3 may play an important role. These findings contribute to understanding the neuroprotective role of zinc supplementation in mitigating neurotoxic insults, suggesting further research into cognitive protection strategies in environmental pollutant exposure.

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Key words: acrylamide, zinc, ZnT3, vglut1, BDNF

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Molecular Docking-Based Prioritization of Chemicals in Plastic Additives

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Abstract

Various additives are incorporated into plastic products to enhance their properties and durability. However, the potential leaching of these additives from plastics when they degrade into micro- and nano-sized particles in the environment is suspected to contribute to the environmental and human toxicity of microplastics significantly. This study aims to screen the potential toxicity of additive chemicals commonly used in plastics based on their direct binding to human nuclear receptors. Firstly, we compiled a list of 457 chemicals frequently employed in plastics from the ECHA database. Their potential toxicity was systematically evaluated using molecular docking simulations with selected human nuclear receptors, key transcription factors responsible for regulating diverse physiological functions. The most active nuclear receptors were found to be the constitutive androstane receptor, followed by the pregnane X receptor and peroxisome proliferator-activated γ. These findings suggest potential toxicity mechanisms of additive chemicals that could contribute to conditions such as cancer and developmental diseases. Furthermore, 138 chemicals were prioritized based on their binding affinity with human nuclear receptors (less than -7.5 kcal/mol), among which the top 22 plastic additives were selected for their high binding affinity with a high number of nuclear receptors. Despite being actively used in the US-TSCA with annual production volumes exceeding 1,000 tons, only three of these chemicals are currently regulated in South Korea and Europe, highlighting significant regulatory gaps. While our analysis demonstrated that binding simulation with nuclear receptors can aid in chemical classification, it was not sufficient to predict the most hazardous chemicals. In conclusion, this research highlights both the potential and challenges of employing *in silico* molecular docking simulations as rapid screening tools for industrial chemicals, including additives in plastics.

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Key words: Plastic additive, Nuclear receptors, Molecular docking, Chemical screening, Molecular initiating event

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Prioritization of Organic Micropollutants in Global Waters and Their Contributions to Disinfection Byproduct Formation and Toxicity in Chlorine Disinfection

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Abstract

More than 219,000,000 chemicals have been compiled in the Chemical Abstracts Service Registration, and this number is still increasing by about 15,000 every day. Over 350,000 chemicals and chemical mixtures are registered for production and use, resulting in their continuous release into water environments. We first compiled a total of 83 prioritization case studies using the risk quotient method and select 473 compounds (out of 3466) with risk quotients greater than 0.01. To determine the micropollutants of global concern, we proposed a "weighted average risk quotient", which integrates both risk intensity and frequency of micropollutants in global water environments to achieve a more comprehensive priority determination. Through metadata analysis, we recommended a ranked list of 53 micropollutants, including 36 pharmaceuticals and personal care products. Then, we investigated the contributions of pharmaceuticals (a mixture of ten representative pharmaceuticals) and natural organic matter (NOM) to the overall disinfection byproduct (DBP) formation and toxicity during drinking water chlorination. By innovatively "normalizing" chlorine exposure and constructing a kinetic model, we were able to differentiate and evaluate the contributions of NOM and pharmaceuticals to the total organic halogen formation for source waters that contained different levels of pharmaceuticals. It was found that at a chlorine contact time of 1.0 h, NOM (2 mg/L as C) and pharmaceuticals (total 0.0062–0.31 mg/L as C) contributed 79.8–99.5% and 0.5–20.2% respectively of total organic halogen. The toxicity test results showed that the chlorination remarkably increased the toxicity of the pharmaceutical mixture by converting the parent compounds into more toxic pharmaceutical-derived DBPs, and these DBPs might contribute significantly to the overall developmental toxicity of chlorinated waters. This study highlights the non-negligible role of pharmaceuticals in the formation and toxicity of overall DBPs in chlorinated drinking water.

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Modernizing Persistence–Bioaccumulation–Toxicity (PBT) Assessment with High Throughput Animal-free Methods

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Abstract

The assessment of persistence (P), bioaccumulation (B), and toxicity (T) of a chemical is a crucial first step at ensuring chemical safety. Existing methods for PBT assessment are overly complex and cumbersome, have produced incorrect conclusions, and rely heavily on animal-intensive testing. New-approach methodologies (NAMs) can overcome the limitations of current PBT assessment. The conventional indicators for PBT are recommended to be replaced by two innovative hazard indicators only, termed cumulative toxicity equivalents (CTE) and persistent toxicity equivalents (PTE). The proposed "toxicity equivalents" can be measured with high throughput *in vitro* bioassays. CTE refers to the toxic effects measured directly in any given sample, including single chemicals, substitution products, or mixtures. PTE is the equivalent measure of cumulative toxicity equivalents measured after simulated environmental degradation of the sample. With an appropriate panel of animal-free or alternative *in vitro* bioassays, CTE and PTE comprise key environmental and human health hazard indicators. CTE and PTE do not require analytical identification of transformation products and mixture components but instead prompt two key questions: is the chemical or mixture toxic, and is this toxicity persistent or can it be attenuated by environmental degradation? I will illustrate the new approach with case studies.

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Exploring the Great Unknown: New Tools to Assess Complex Environmental Mixtures

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Abstract

Environmental pollution never occurs as a few discrete substances . Conversly, contaminants occur within extremely complex mixtures of anthropogenic and endogenous substances. Monitoring programs often target a limited subset of contaminants based on their known occurrence and/or harm. However, many pollutants remain unidentified until damage occurrs. Synthetic chemicals have been part of the human experience since the late 19th century with the accidental discovery of the synthetic dye, mauve. Today, over 65 million chemicals are commercially available, many entering the environment both knowingly and unknowingly. From a water exposure standpoint, both the chemicals themselves and their innumerable transformation products formed during water treatment pose risks. Historically, analytical techniques to measure trace levels of environmental pollutants were time-consuming, labour-intensive, and technically-sophisticated. New techniques are

rapidly evolving to measure ultra-trace levels of chemicals with automated and/or minimum sample preparation and detection by tandem and/or high-resolution mass spectrometry. Monitoring indicator compounds by high-resolution quadrupole mass spectrometry (QTOF) coupled to both GC and LC interfaces provides both targeted analytic information and a comprehensive view of the complex chemical mixtures and their transformation products in water. Coupled with high-throughput bioassays, these techniques provide new insights into the complex mixtures occuring in the environment and their potential health impacts. Recently, high performance analytical platforms are coupled with advanced genomics tools which can even encompas pathogen monitoring in environmental samples, such as monitoring the Sars-CoV-2 virus in municipal sewer systems can be normalized to chemical markers to provide population-level evaluations of disease occurrence and transmission. Another recent discovery is that vulcanization agents leaching from tires are among the most toxic substances evaluated on salmonid fish. Our research demonstrated that chlorinatingthe common vulcanization substances found in surface waters results in chlorination byproducts more toxic than the parent compound, as evaluated through several in vitro methods. This presentation will demonstrate the latest findings and provide a view for the future of addressing the unknown world of chemical and biological mixtures in the environment.

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The harmful outcomes and molecular mechanisms of exposure to fine particulate matter

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Abstract

Environmental fine particles can enter the body through respiratory exposure, skin surface, oral and intravenous injection, and be transmitted to distant organs in the bloodstream to cause damage. It is crucial to elucidate the toxic effects and harmful outcomes caused by environmental fine particles at the molecular level.

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Toxic effects and mechanisms of nanoparticles on embryonic brain development using brain organoids model

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Abstract

Nanoparticles can be easily absorbed into the human body through inhalation, ingestion, and skin contact due to their physicochemical property. Despite the numerous studies postulating the potential adverse effects of environmental exposure to nanoparticles on neurodevelopment, the effects of nanoparticles and their regulatory mechanisms have not been specifically elucidated. We focused on the toxic effects of nanoparticles on brain developmental processes by investigating their interactions with brain organoids. Our findings indicated that nanoparticles exposure caused cellular dysfunction and structural disorders. nanoparticles adversely affected critical cells in brain organoids, resulting in the reduction of neural precursor cells and neuronal cells. The expression of neural cadherin was also inhibited, which might lead to impaired axonal extension and formation of synaptic connections. In addition, transcriptome sequencing was performed to study the effects of different concentrations of nanoparticles on the signaling pathway. The qRT-PCR analysis confirmed that nanoparticles exposure resulted in decreased expression of several genes related to the Wnt signaling pathway, suggesting that nanoparticles may adversely affect embryonic brain growth through the suppression of the expression of these genes. Our research findings shed light on the deleterious effects of nanoparticles on embryonic brain development and have significant implications for the field of environmental toxicology.

962

Injury target and component action from local fine particulate matter exposure

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Abstract

China is experiencing the period with most complex air pollution in the world. Fine particulate matter, $PM_{2.5}$, is not only a key indicator of air quality, but also an important contributor to air pollution induced health effects. For this reason, we established integrated technology of component screening, function detection, omics screening and pathway analysis, found new targets, defined the effect endpoint and health outcome, and revealed the molecular mechanism for diseases phenotype. Firstly, we determined the metal contents of $PM_{2.5}$ samples collected from a typical coal-burning city and then investigated the metabolic distributions of six metals (Zn, Pb, Mn, As, Cu, and Cd) following $PM_{2.5}$ inhalation in mice in different developmental windows, and found that $PM_{2.5}$ mainly deposited in the lung,

but $PM_{2.5}$-bound metals could reach and gather in secondary off-target tissues (the lung, liver, heart and brain) with a developmental window-dependent property. Based on this, (1) $PM_{2.5}$ aspiration caused histone modification associated lung dysfunction and inflammation, and the action restored after exposure ending and 2-week recovery. (2) $PM_{2.5}$ exposure reversibly elevated heart rate and blood pressure, induced cardiac systolic dysfunction of older mice, and reversibly induced fibrosis in juvenile and older mice. The mechanism by which $PM_{2.5}$ exposure resulted in cardiac lesions might involve oxidative stress, NADPH oxidase, TGFβ1, and Smad-dependent pathways. (3) $PM_{2.5}$ aspiration caused neuroinflammation and deteriorated synaptic function integrity and spatial learning and memory, and the effects were associated with the induction of BACE1. The action was mediated by NF-κB p65-regulated downregulation of miR-574-5p, which targets BACE1. (4) Gestational exposure to $PM_{2.5}$ leads to histopathological changes and vascularization injuries of the placenta, and caused developmental toxicity and functional damages in offspring. These findings provide new evidence for exposure evaluation and protective treatment for local population.

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Establish the Safety Threshold for Fluridone on Rotation Maize and Develop Rice Husk Biochar Regulation Strategy

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Abstract

The residual of fluridone (FLU) in field soil poses a significant threat to crop growth in rotation systems. Therefore, it is imperative to investigate the safety threshold of FLU on rotation crops and explore solutions to mitigate the damage caused by FLU residues. In this study, the uptake kinetics of FLU in rotation crops (maize) were first evaluated by hydroponic experiments. FLU is rapidly taken up by plant roots within 72 h and translocated to the leaves, resulting in leaf bleaching. Hydroponic experiments then were conducted to simulate the absorption of FLU by maize seedlings from soil pore water (SPW), and determined no-significant-effect-concentration (NSEC) of FLU on maize seedlings is 4-6 μg/L by Concentration-response (C-R) curves. Subsequently, adsorption experiments were performed to elucidate the ability of rice husk biochar (RH500) in regulating FLU levels in SPW. The presence of RH500 significantly reduced FLU concentrations in SPW by up to 98.1%. Furthermore, isothermal adsorption experiments investigated how RH500 influenced the distribution of FLU across different soil environments. A reliable mathematical model was developed for predicting FLU concentrations in SPW when RH500 was added. Validation results demonstrated that the predicted values closely aligned with experimental data (slope = 1.18), with an R^2 value exceeding 0.9, indicating reasonable prediction

accuracy within an acceptable range. In conclusion, this study has developed an effective approach to establish a safety threshold for the detrimental effects of residual herbicides on rotational crops and proposes a RH500-based solution to mitigate crop damage caused by the residual herbicide FLU in soil.

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Deciphering carcinogenesis of PFOA in gastric cancer through network toxicology, molecular docking, and cellular experiments

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Abstract

Perfluorooctanoic acid (PFOA) is predominantly ingested by human beings through drinking water and food, with the stomach being the first long-exposure organ. However, there is still a gap in the carcinogenesis of PFOA in the stomach. In our in vitro experiment, higher concentrations of PFOA resulted in cell elongation and disrupted cell proliferation in human gastric mucosal epithelial cells (GES-1). To reveal the mechanism of PFOA toxicity, 32 potential common targets of gastric cancer genes and PFOA were identified using network toxicology. Based on the Kyoto Encyclopedia of Genes and Genomes pathway as well as the Gene Ontology, we found these targets involved in metabolic processes and the PPAR signaling pathway. Meanwhile, 5 core targets were highlighted: PPARA, PPARD, FABP3, FABP4, and FABP5. Their interaction energies with PFOA are −6.56 - −8.32 kcal·mol^{-1}, 5-7 fold lower binding energy than the threshold of −1.2 kcal mol−1 for spontaneous bonding. PPAR inhibitor (GW9662, 10 μM) and ferroptosis inhibitor (Ferrostatin-1, 2 μM) prevent GES-1 cells from ferroptosis induced by PFOA (200 ng·L^{-1}), which indicated PFOA-induced gastric cancer through PPAR-ferroptosis pathway. This study provided a new modeling approach for studying the carcinogenicity of emerging pollutants.

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Advances in Bioaccumulation and Precision Ecotoxicology for Contaminants of Emerging Concern

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Abstract

Translation of ecotoxicology to the practice of ecological risk assessment and natural resource management aims to protect biodiversity and ecosystem services, yet our future ability to do so

relies on the development of a precision ecotoxicology approach wherein we leverage the genetics and informatics of species to better understand and manage the aquatic risks of global pollution. This effort is needed because biodiversity declines are pronounced, and the importance of developing new approaches for chemicals, waste and pollution prevention are receiving unprecedented attention around the world. For example, empirical safety information is unavailable for the majority of the >350,000 chemicals and chemical mixtures listed for global commerce, and the flows of rivers and base flows to bays and estuaries can be dominated by or dependent on sewage or reclaimed wastewater, which includes diverse contaminants of historic and emerging concern. Herein, persistence cut-off values, which are routinely used during chemical assessment and management, are challenged by site-specific changes in effective exposure duration. Recent efforts to understand bioaccumulation and ecotoxicology of human pharmaceuticals in the environment is affording opportunities to develop an understanding of bioaccumulation for ionizable chemicals and other organic contaminants, including per- and polyfluoroalkyl substances, that fall outside of the applicability domain of historic models for nonionizable compounds. Coupling developments in bioaccumulation science and precision ecotoxicology with sustainable molecular design and other elements of green and sustainable chemistry and engineering promises to advance the science and the practice, to stimulate innovation in chemicals development, and to reduce chemical risks in urbanizing aquatic systems.

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Prioritizing Known and Unknown Identification in Complex Env/Bio Samples

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Abstract

Identification of environmental pollutants with harmful effects is commonly conducted by non-targeted analysis (NTA) using liquid chromatography coupled with high resolution mass spectrometry (LC-HRMS). It primarily relies on matching experimental MS spectra with library or *in silico* spectra and further confirmation by standards. Prioritization of possible candidates is important yet challenging because of the large number of candidates from MS acquisitions. We aim to prioritize candidates to the exposure potential of organic chemicals by their toxicities of multiple endpoints in the matrix. We have developed an R package application, "NTAprioritization", for fast prioritization of suspect lists in NTA approaches. This package automates screening and prioritization of suspect lists according to the fragmentation spectra (MS/MS) matching score by library searching with a combination of retention time prediction (RT-MS/MS ranking: RT-MS/MS Level 1 – 4), and the toxicity (Toxicity ranking: Tox Level 1 – 3). The package allows users to select 7 toxicities, including toxicities at 6 endpoints and the

EPA ToxPi score from ToxCast database. For validation, we used this workflow to identify pollutants in a sludge water sample spiked with 28 environmental pollutants with different toxicity potential. The workflow reduced the candidate list of over 6,982 candidates to a final list of 2,779 compounds. Finally, 21 of 28 spiked standard candidates were prioritized in 5 tiers (Tier 1 to 5) by combining both RT-MS/MS Level and Tox Level. Overall, this study shows the added value of an automated prioritization R package for the fast screening of environmental pollutants based on the NTA method. The package is available online (https://github.com/FangLabNTU/NTAprioritization.git).

1104

Theoretical Study on the Iodine Oxoacids-driven Nucleation

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Abstract

Iodine oxoacids (HIO_3 and HIO_2)-driven nucleation is suggested to efficiently contribute to new particle formation in marine atmosphere. However, the knowledge of which atmospheric vapors can enhance iodine oxoacids-driven nucleation remains limited, hindering understanding of their contribution to particle formation in the marine atmospheres. In this work, we propose the following research ideas: revealing iodine oxoacids-driven nucleation mechanism ® constructing a high-throughput model for predicting the enhancing potential (EP) of precursors ® identifying the highest EP precursor, solving the current problem of difficulty in identifying nucleation precursors.

We first investigated the formation mechanism and kinetics of the HIO_3-HIO_2 system using theoretical methods. The results showed that HIO_2 has strong halogen bond (XBs) forming ability and exhibits base behavior when interacting with HIO_3, resulting in a high nucleation rate of the HIO_3-HIO_2 system. Based on the understanding of this mechanism, we inferred that various compounds, such as organic acids, amines, etc. could interact with iodine oxoacids, enhancing their nucleation via hydrogen bonds (HBs), XBs and acid-base reactions. Therefore, we calculated the formation free energy (ΔG) values of the dimer clusters for selected compounds with HIO_3 or HIO_2. Combined the calculated ΔG values and atmospheric concentrations of the considered precursors, the EP of precursors were evaluated and two quantitative structure-activity relationship (QSAR) model were constructed. It was found that sulfur oxoacids {(methanesulfonic acid (MSA) and sulfuric acid (SA)} have the highest EP for HIO_3-HIO_2-driven nucleation. In addition, while atmospheric bases like diethylamine (DEA) have high potential to enhance HIO_3-driven nucleation, their role in HIO_2-driven nucleation is negligible. By further investigation of larger SA/MSA-HIO_3-HIO_2 clusters, it was found that

sulfur oxoacids can participate in and enhance HIO_3-HIO_2 driven nucleation in the realistic marine atmosphere. Moreover, HIO_3-HIO_2 is an efficient enhancer for sulfur oxoacids-driven nucleation in the marine atmosphere.

16. Atmospheric Toxicology

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The Effect of Anthropogenic Activities on Chlorinated Paraffins in the Atmosphere Using Polyurethane Foam Passive Air Sampling (PUF-PAS) in Ghana

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Abstract

There are large knowledge gaps concerning environmental levels and fates of many organic pollutants, particularly for chemicals of emerging concern in tropical regions of the Global South. In this study, we investigated the levels of chlorinated paraffins (CPs), its potential sources and, human health risks in the air from e-waste sites, urban areas, commercial areas and control/background areas of Ghana. In passive air samples, medium-chain CPs (MCCPs) dominated with a total concentration of 1560 ng/m^3 and an average concentration of 26.0 ng/m^3. Short-chain CPs (SCCPs) had a total concentration of 209 ng/m^3 and an average estimated concentration of 3.48 ng/m^3 whiles, C9-CPs had a total concentration of 32.6 ng/m^3 and an estimated average concentration of 0.544 ng/m^3. MCCPs were higher by a factor of 7.5 times to SCCPs and a factor of 48 times to C9-CPs. $C_{14}Cl_8$ was the dominant congener in MCCPs and $C_{10}Cl_7$ was the dominant congener in SCCPs. The main sources of C9-CPs and SCCPs were from the e-waste sites whiles, MCCPs were from urban areas. C9-CPs, SCCPs, and MCCPs had cancer risks ranging from 4.55×10^{-8} to 1.07×10^{-6}, 2.50×10^{-8} to 7.60×10^{-6}, and 8.90×10^{-7} to 1.20×10^{-4}, respectively in that order. For non-cancer risks, we assessed the margin of exposure (MOEs), hazard quotient (HQ) and estimated daily intake (EDIs). The cancer and non-cancer risks associated with CPs were found to be within the acceptable range, suggesting that brief exposure has no significant health effect; however, extended exposure may have deadly consequences. To the best of our knowledge, this is the first study on CPs in Ghana's atmosphere, and e-waste was the country's main source of CPs. The results of this study will help regulatory bodies create policies and procedures to control the use, and disposal of chlorinated paraffins.

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Co-exposure of ozone and polystyrene nanoplastics synergistically induced airway inflammation: Evidence and mechanisms at multiomics levels

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Abstract

OBJECTIVE: As the common air pollutants, ozone (O_3) could be absorbed on nanoplastics (NPs), which generate O_3 in the photodegradation process, suggesting O_3 and NPs could be co-exposed in air. However, there is no report on health effect of co-exposure of O_3 and NPs. In this study, we investigated the effect and mechanisms of O_3 combined-exposed with polystyrene nanoplastics (PS-NPs), the most important representative of NPs, on airway inflammation.

METHODS: C57BL/6J mice (SPF degree, 6–8 week) were assigned to 9 groups, and O_3 (0.60 and 1.00 ppm) and PS (1.82×10^{11} and 3.64×10^{11}) were exposed individually or in combination for 14 days (4h/d). Lung function, lung pathology, proteins (IL-6, IL-1β, CC16) of lung tissues were determined by whole body plethysmography, HE, PAS and MASSON staining, and ELISA, respectively. The mechanism of airway inflammation was further analyzed by transcriptomics and metabolomics. The interaction between combined exposure factors was calculated by factorial design analysis of variance and interaction types were analyzed using exponential addition.

RESULTS: Combined exposure of O_3 and PS exacerbated airway inflammation. The 1.00ppm O_3 + $1.82\times10^{\wedge11}$ PS group demonstrated a synergistic effect on Penh, Tr, Tv, PAU, the number of white blood cells, IL-6 and CC16. The differential genes and metabolites caused by O_3 and PS expoure were mainly involved in circadian rhythm and ABC transporter. Moreover, Per2, Per3 and hypoxanthine were positively correlated with IL-6 and IL-1β, and negatively correlated with CC16 by Pearson correlation analysis. Linoleic acid metabolism and ABC transporter pathway are common pathways of transcriptomics and metabolomics, in addition, Per2 and Per3 were positively correlated with prostaglandin F2b and 20-HETE, and negatively correlated with pyridoxal phosphate.

CONCLUSION: Co-exposure of O_3 and PS-NPs could synergistically induce airway inflammation in mice, which may be by affecting the linoleic acid metabolism and the ABC

transporter. To our knowledge, this study is the first study to discover the synergistically effect and mechanism of O_3 and PS-NPs on respiratory system, which may provide the targets for preventing airway inflammation induced by air pollutants co-exposure.

KEYWORDS: Ozone, Polystyrene nanopla stics, Airway inflammtion, Transcriptomics, Non-target metabolomics

This study was supported by the National Natural Science Foundation of China (No. 42377433)

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The Neurotoxicity Effect and Molecular Mechanism in Response to Atmospheric $PM_{2.5}$ Inhalation

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Abstract

The limited but growing emerging evidence suggests that $PM_{2.5}$ exposure can affect the nervous system, causing neuroinflammation, synaptic dysfunction and cognitive deterioration. Our findings showed $PM_{2.5}$ was mainly deposited in the cytoplasm of alveolar epithelial cells in the lungs of mice, while the $PM_{2.5}$ bound metals could reach and gather in secondary off-target tissues (lung, liver, heart and brain) with a developmental window-dependent property following $PM_{2.5}$ inhalation. $PM_{2.5}$ exposure selectively changed the levels of total triglycerides and total cholesterol, which may have an important impact on the neurodegenerative diseases and cognitive impairment. Further studies confirmed that $PM_{2.5}$ was mainly deposited in the lungs after exposure, which induced systemic inflammatory response, resulting in changes in synaptic structure and function in mouse hippocampus, and disrupting spatial learning and memory. In addition, our study further revealed that $PM_{2.5}$ stimulates neuronal inflammatory cytokines to activate NF-κB, and the binding of NF-κB to the miR-574-5p promoter region is an important regulatory step in the initiation of the BACE1 signaling pathway through miR-574-5p, which ultimately leads to neurodegenerative changes and functional impairment.

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Assessing the Quantitative Contribution of Microbial Components and Their Sources to *in vitro* Bioactivities of Airborne Fine Particulate Matter

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Abstract

Air pollution stands as the leading environmental health risk globally. Exposure to ambient fine particulate matter ($PM_{2.5}$) has been statistically linked with the development of respiratory diseases using a range of methods from *in vitro* cell assays to *in vivo* exposure tests and epidemiological investigations. Nevertheless, pinpointing the specific components and sources of $PM_{2.5}$ that can be causally linked to respiratory illnesses remained a major challenge. The toxic effects and health impacts of chemical constituents from human-made sources have been extensively investigated. However, the extent to which microbial components and their sources contribute to the bioactivities of $PM_{2.5}$ has yet to be quantitatively explored.

A quantitative framework was established to assess the role of endotoxin from gram-negative bacteria in the *in vitro* induction of interleukin-8 (IL-8) by $PM_{2.5}$ from contrasting ambient environments. Endotoxin was found to contribute more to IL-8 induction by $PM_{2.5}$ from a coastal site (0.6-10%) than from an urban site (0.2-3%), which is three to five orders of magnitude higher than its negligible fraction of $PM_{2.5}$ mass (<0.0001%). The discrepancy observed for endotoxin whose toxicity contribution to $PM_{2.5}$-induced effects disproportionately surpassed actual mass fraction may exist for other immunologically active microbial constituents (*e.g.*, exotoxins, fungal allergens).

The sources of gram-negative bacteria shifted from natural dominance (>50%) at the coastal site to anthropogenic dominance (>70%) at the urban site. These anthropogenic sources, such as the built environment, sewage treatment works, and humans, fall outside the source categories currently regulated and/or controlled. Additionally, gram-negative pathogens were elevated in the urban site. As global efforts focus on further reducing anthropogenic emissions, it will become increasingly important to consider the unconventional anthropogenic and natural sources of microbially-shared $PM_{2.5}$ toxicity.

This work underscores the need to reveal the impact of microbial constituents and their distinctive sources on $PM_{2.5}$ toxicity across geographical gradients in climate zones and urbanization levels and suggests a shift towards incorporating biological factors in air quality management.

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Risk assessment of the lipid metabolism-disrupting effects of nitro-PAHs

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Abstract

Nitro-polycyclic aromatic hydrocarbons (NPAHs) are of increasing global concern due to their ubiquitous occurrence and long-range transport in the environment. However, their potential metabolism-disrupting effects, especially nuclear receptor-related lipid disorders, are still poorly understood. Targeting estrogen receptor α(ERα), this study for the first time evaluated the lipid metabolic effects of NPAHs using in vitro and in vivo models. The results indicated that four of the five NPAHs tested exhibited significant ERα agonistic activities, and induced increased secretion of 17β-estradiol (E2) in HepG2 cells. Furthermore, lipidomic analysis showed that exposure to the candidate NPAH (3-nitrofluoranthene, 3-NFA) led to elevated epatic levels of triacylglycerols and cholesteryl esters. Importantly, the lipid overload induced by 3-NFA was verified in the livers of zebrafish larvae using Oil Red O staining. Additionally, significant increases in E2 production and the expression levels of associated genes further supported the involvement of the ERα signaling pathway in the lipid metabolic perturbation induced by 3-NFA. These results provide novel insight into the lipid metabolism-disrupting effects induced by NPAHs and may offer a better understanding of the environmental risks of NPAHs.

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Application prospects of stem cells in atmospheric toxicology

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Abstract

Frequent exposure to air pollutants during pregnancy has been linked to a series of detrimental consequences on fetal development, such as interfering with embryo implantation, fetal development, neonatal nervous system development and even stillbirth, according to epidemiological studies. As a result, the environmental health effects of air pollutants, especially the developmental toxicological effects, deserve further attention. ESCs are derived from the inner cell mass of the embryonic blastocyst stage, and their biological characteristics of infinite proliferation and multi-directional differentiation make them an incomparable advantage in predicting developmental toxicology. Currently, models based on ESCs and SSCs, their precursor cells (such as myocardial breast precursor cells), and some specialized somatic cells (such as neurons and adipose cells) have demonstrated that these cells are highly sensitive to air pollutant exposure, holding the promise that the developmental toxic effects of pollutants on the neural development, skeleton formation, immune cell differentiation, and developmental programming of cardiovascular would be studied further.

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Screening of pro-inflammatory components based on $PM_{2.5}$ exposomics methods

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Abstract

More than 35% of Chinese adults are in a state of glucose metabolism disorder characterized by insulin resistance (IR). Population with glucose metabolism disorder will intensify human oxidative stress after exposure to fine particulate matter ($PM_{2.5}$), which will lead to type II diabetes. $PM_{2.5}$ has a high content and complex composition of organic components, with traditional measurements of PAHs (usually 16 PAHs prioritized by the US EPA) accounting for only about 1.5% of the mass of organic components in $PM_{2.5}$. Therefore, it is necessary to systematically evaluate the role of organic components in exacerbating oxidative damage exposed to $PM_{2.5}$, in order to take targeted protective measures for susceptible populations.

This study is based on the SCOPE elderly population panel study at Peking University (108 individuals, 2013/8-2015/2). We developed an ultra-high sensitivity injection method with ultra-low sample size, coupled with gas chromatography-high-resolution time-of-flight mass spectrometry (GC-ToF-MS) technology to analyze 1327 components of individual exposomics in organic components of 424 follow-up visits. Based on the association with exhaled nitric oxide (eNO)/interleukin-6 or serum IL-1 β/IL-6, a comprehensive multivariate and univariate mixed effect model was used to screen and discover that over 400 polycyclic aromatics emitted from outdoor combustion emission play an important role in exacerbating respiratory oxidative stress and inflammation, while indoor sources of monocyclic aromatics can exacerbate systemic inflammation. Using an explanatory random forest method combined environmental variables and source biomarkers, primary combustion aromatic species with high unsaturation, high octanol water partition coefficient (logKow), and low volatility were responsible for the exacerbation of IR and the increase in eNO levels; The aromatic compounds with multiple carbonyl and oxygen atoms, low logKow generated through atmospheric secondary oxidation are related to the exacerbation of urinary malondialdehyde (MDA) by IR.

This study shows for the first time that IR can aggravate oxidative stress after exposure to specific PM2.5 components, which may be a key factor in accelerating the course of diabetes.

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Crystalline Silica Particles Lead to Pulmonary Fibrosis Through Interleukin-11-Mediated Fibroblast Metabolic Reprogramming

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Abstract

Background: Environmental exposure to crystalline silica (CS) particles occurs during natural, industrial, and agricultural activities. Prolonged inhalation of CS particles can cause silicosis, a serious pulmonary interstitial fibrosis disease worldwide. Interleukin-11 (IL-11) has been confirmed as a pro-fibrotic effector during fibrosis, but its specific mechanisms underlying silicosis are still unknown.

Methods: We established the mouse silicosis model by using CS particles (1-2 μm) and IL-11 intervention model by using AAV6-IL-11 shRNA or IL-11 neutralizing antibody to investigate the effect of IL-11 on glycolysis reprogramming during silicosis. To further uncover the underlying mechanisms, fibroblast activation models, as well as IL-11 and its downstream pathway inhibition model *in vitro* were constructed.

Results: We observed that CS exposure induced lung fibrosis in mice and activated fibroblasts, accompanied by increased IL-11 expression and metabolic reprogramming switched from mitochondrial respiration to glycolysis. Besides, we observed that CS exposure increased the expression of transforming growth factor-β1, which in turn led to the elevated level of IL-11 in fibroblasts, and the latter promoted the glycolysis process, thereby facilitating the fibroblast-myofibroblast transition (FMT). Mechanistically, IL-11 could activate the extracellular signal-regulated kinase (ERK) pathway and subsequently increase the expression of hypoxia inducible factor-1α (HIF-1α) by enhancing the protein translation and delaying the degradation. Elevated HIF-1α promoted the expression of glycolytic enzymes (e.g., hexokinase 2, phosphofructokinase 1, pyruvate kinase M2, and lactate dehydrogenase A), thereby driving fibroblasts towards a fibrotic phenotype, and ultimately contributing to the formation of silicosis. Additionally, targeting IL-11 effectively diminished fibroblast activation and glycolysis augmentation, and attenuated CS-induced lung myofibroblast generation and fibrosis.

Conclusions: Our findings demonstrated that the profibrotic effect of IL-11 during silicosis relied on glycolysis reprogramming, which not only helps understand the toxic effect and mechanisms of environmental CS particles on pulmonary health more comprehensively and deeply but also provides novel insights into the potential therapeutic targets of silicosis.

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Role of Microglia Polarization Induced by Glucose Metabolism Disorder in the Cognitive Impairment of Mice from $PM_{2.5}$ Exposure

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Abstract

Studies have found that $PM_{2.5}$ can damage the brain, accelerate cognitive impairment, and increase the risk of developing a variety of neurodegenerative diseases. However, the potential molecular mechanisms by which $PM_{2.5}$ causes learning and memory problems are yet to be explored. In this study, we evaluated the neurotoxic effects in mice from 12 weeks of $PM_{2.5}$ exposure, and found that this exposure resulted in learning and memory disorders, pathological brain damage, and M1 phenotype polarization on microglia, especially in the hippocampus. Proteomic analysis, as well as validation results, suggested that $PM_{2.5}$ exposure led to abnormal glucose metabolism in the mouse brain, which is mainly characterized by significant expression of hexokinase, phosphofructokinase, and lactate dehydrogenase. We therefore administered the glycolysis inhibitor 2-deoxy-D-glucose (2-DG) to the mice exposed to $PM_{2.5}$, and showed that inhibition of glycolysis by 2-DG significantly alleviated $PM_{2.5}$-induced hippocampal microglia M1 phenotype polarization, and reduced the release of inflammatory factors, improved synaptic structure and related protein expression, which alleviated the cognitive impairment induced by $PM_{2.5}$ exposure. In summary, our study found that abnormal glucose metabolism-mediated inflammatory polarization of microglia played a role in learning and memory disorders in mice exposed to $PM_{2.5}$. This study provides new insights into the neurotoxicity caused by $PM_{2.5}$ exposure, and provides some theoretical references for the prevention and control of cognitive impairment induced by $PM_{2.5}$ exposure.

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Could the association between ozone and arterial stiffness be modified by fish oil supplementation

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Abstract

Background: Arterial stiffness (AS) is an important predicting factor for cardiovascular disease. However, no epidemiological studies have ever explored the mediating role of biomarkers in the association between ozone and AS, nor weather fish oil modified such association.

Methods: Study participants were drawn from the UK biobank, and a total of 95,699 middle-aged and older adults were included in this study. Ozone was obtained from Community Multiscale Air Quality (CMAQ) model matched to residential addresses, fish oil from self-reported intake, and arterial stiffness was based on device measurements. First, we applied a double robust approach to explore the association between ozone or fish oil intake and arterial stiffness, adjusting for potential confounders at the individual and regional levels. Then, how triglycerides, apolipoprotein B (Apo B)/apolipoprotein A (ApoA) and non-high-density lipoprotein cholesterol (Non-HDL-C) mediate the relationship between ozone and AS. Last, the modifying role of fish oil was further explored by stratified analysis.

Results: The mean age of participants was 55 years; annual average ozone exposure was associated with ASI (beta:0.189 [95%CI: 0.146 to 0.233], P < 0.001), and compared to participants who did not consume fish oil, fish oil users had a lower ASI (beta: 0.061 [95%CI: -0.111 to -0.010], P = 0.016). The relationship between ozone exposure and AS was mediated by triglycerides, ApoB/ApoA, and Non-HDL-C with mediation proportions ranging from 10.90% to 18.30%. Stratified analysis showed lower estimates on the ozone-AS relationship in fish oil users (P = 0.011).

Conclusion: Ozone exposure was associated with higher levels of arterial stiffness, in contrast to fish oil con-sumption, which showed a protective association. The association between ozone exposure and arterial stiffness was partially mediated by some biomarkers. In the general population, fish oil consumption might provide protection against ozone-related AS.

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Ambient Levels, Sources, and Source-specific Health Risks of $PM_{2.5}$-bound Organophosphate tri-esters and di-esters in Shenzhen Atmosphere

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Abstract

Concerns about the adverse health impacts of organophosphate esters (OPEs) – widely used as flame retardants and plasticizers – are growing, yet the understanding of the high-risk sources OPEs in fine particulate matter ($PM_{2.5}$) remains insufficient. This study employed atmospheric pressure gas chromatography mass spectrometry and liquid chromatography-tandem mass spectrometry to investigate twenty OP-triesters, including thirteen conventional and seven novel OPEs, as well as ten OP-diesters in $PM_{2.5}$ samples collected in Shenzhen during a 1-yr period. The median concentrations detected were 6399 pg m^{-3} for OP-triesters (with a range of 3509–13082 pg m^{-3}) and 1196 pg m^{-3} for OP-diesters (ranging from 83 to 5983 pg m^{-3}). We observed substantially higher levels of OP-triesters during wet seasons compared to dry seasons, while

OP-diesters showed minimal seasonal fluctuation. Using a positive matrix factorization model, we identified six emission sources for OP-triesters, with waste incineration contributing most significantly to both traditional (62.3%) and novel (76.3%) OPE levels, particularly during wet seasons. OP-diesters were found to originate from primary emissions and secondary degradation. The inhalation risk assessment for co-exposure to both compound classes in $PM_{2.5}$ suggested a low overall risk, but with heightened concerns for OP-triesters from waste incineration processes. A targeted risk-based prioritization revealed that certain novel OPEs, specifically resorcinol bis(diphenyl)phosphate, isodecyl diphenyl phosphate, and bis(2,4-di-tert-butylphenyl) phosphate, may pose more severe health risks through mechanisms affecting the estrogen and aromatic hydrocarbon receptors, as well as oxidative stress, compared to traditional OPEs. These findings highlight the need for increased scrutiny on novel OPEs and their emission sources to better protect public health.

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Effects of prenatal $PM_{2.5}$ exposure on synaptic development of male offspring and its molecular mechanism

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Abstract

Backgroud: Exposure to the air pollutant $PM_{2.5}$ during pregnancy may impact the neurodevelopment and cognitive function of male offspring. Synapses, as the structural basis of information transmission between neurons, play a crucial role in neurodevelopment. However, the effect of $PM_{2.5}$ on synaptic development remains unclear.

Objective: This study aims to investigate whether maternal exposure to $PM_{2.5}$ influences the synaptic structure and function of male offspring and to elucidate the molecular mechanisms underlying synaptic deficits.

Methods: Pregnant mice were treated with either saline or a $PM_{2.5}$ suspension solution at a dose of 3 mg/kg body weight via oropharyngeal aspiration, three times per week. Synaptic morphology, number, and thickness of cortical tissues in male offspring were assessed using transmission electron microscopy on postnatal days 1, 7, and 21 (PND1, 7, and 21). Immunofluorescence staining was employed to label various postsynaptic components and observe structural changes in different types of synapses. RNA-seq analysis was performed on PND 21. Additionally, qRT-PCR was utilized to measure the expression of hub genes associated with key biological processes.

Results: Male mice exposed to $PM_{2.5}$ during pregnancy did not exhibit significant changes in synaptic density at PND 1, 7, and 21. However, exposure to $PM_{2.5}$ led to a significant reduction in synaptic length and an increase in synaptic thickness at PND 7 and 21. Moreover, there was an increase in inhibitory postsynaptic density expression. Differentially expressed genes in the exposed group were notably

enriched in Wnt-related pathways, with key genes Fzd5, Fzd10, Lrp6, and Wnt3 showing significant upregulation at different developmental time points.

Conclusion: Prenatal $PM_{2.5}$ exposure upregulated the Wnt signaling pathway in the cerebral cortex of male mice, leading to alterations in synaptic structure, particularly an increase in inhibitory postsynaptic density, which subsequently contributes to neurodevelopmental disorders.

Key words : Prenatal $PM_{2.5}$ exposure ; Synaptic development; Wnt signaling pathway; Neurodevelopmental disorder

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Airborne Nanoplastics Exposure Inducing Irreversible Glucose Increase and Complete Hepatic Insulin Resistance

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Abstract

As an emerging type of pollutant, microplastics have become a global environmental problem. Approximately, a fifth of the global burden of type 2 diabetes can be attributed to air particulate pollution. However, scientific knowledge remains limited about the effects of airborne nanoplastics (NPs) exposure on metabolic diseases. In this experiment, a whole-body exposure system was used to simulate the real atmospheric environment, and three exposure concentrations combined with the actual environmental concentration were selected to explore the effects of airborne NPs on metabolic diseases. Based on histological analyses, metabolic studies, gene expression, metabolites, and molecular signaling analyses, mice exposed to airborne NPs were observed to show a phenotype of systemic inflammation and complete insulin resistance featuring excessive drinking and eating, weight loss, elevated blood glucose, and decreased triglyceride levels. After airborne NPs exposure, mice were intolerant to glucose and tolerant to insulin. In addition, airborne NPs exposure could result in long-term irreversible hyperglycemia. Together, the research findings provide a strong basis for understanding the hazards of airborne nanopollution on metabolic disorders.

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Analysis of the correlation between air pollution and birth defects: based on a distribution-lag nonlinear model

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Abstract

Background

The ongoing decline in global fertility rates has heightened the urgency of investigating the causes of BDs (BDs). Airborne pollutants, as exogenous toxins capable of crossing the placental barrier, have garnered significant attention.

Methods

The data of BDs were obtained from five hospitals in Changzhi city from 2019 to 2021, and the air quality data were obtained from the hourly observation data of five monitoring stations in Changzhi city, and the weekly average value was calculated. The distributed lag non-linear model (DLNM) was used to obtain the exposure-lag-effect non-linear relationship to assess the lag effect of weekly air pollution on the risk of fetal BDs.

Results

During the study period, totally 83350 cases of perinatal infants were recruited, and the incidence of BDs was 19.95‰. Our analysis indicated that in early and mid-pregnancy, air pollutants increased the risk of BDs.

For different types of BDs, each 10 μg/m^3 increase in SO_2 (weeks 12-24), NO_2 (weeks 6-11 and 23-26), PM_{10} (weeks 18-24), $PM_{2.5}$ (weeks 11-21), O_3 (weeks 6-14 and 36-38) and CO (weeks 39-40) increased the risk of CHDs, with the highest risk observed at week 17 (SO_2, RR=1.045, 95% CI: 1.018-1.072), week 23 (NO_2, RR=1.024, 95% CI: 1.001-1.047), week 21 (PM_{10}, RR=1.006, 95% CI: 1.001-1.012), week 16 ($PM_{2.5}$, RR=1.013, 95% CI: 1.005-1.021), week 8 (O_3, RR=1.027, 95% CI: 1.005-1.049) and week 40 (CO, RR=1.194, 95% CI: 1.006-1.418). An increase of 10 μg/m^3 in $PM_{2.5}$ (weeks 16-20 and 32-34) and CO (weeks 15-24) increases the risk of external ear malformations, with the highest risk observed at week 18 ($PM_{2.5}$, RR=1.039, 95% CI: 1.004-1.075) and week 19 (CO, RR=1.495, 95% CI: 1.092-2.049). Each 10 μg/m^3 increase in NO_2 (weeks 3-12), NO_X (weeks 3-5), NO (weeks 3-4) and PM_{10} (weeks 3-8) significantly increases the risk of cleft lip and/or palate, with the highest risks observed at week 3 (NO_2, RR=1.010, 95% CI: 1.003-1.209; NO_X, RR=1.051, 95% CI: 1.002-1.103; NO, RR=1.150, 95% CI: 1.006-1.316; PM_{10}, RR=1.030, 95% CI: 1.003-1.058).

Conclusion

Air pollutants exposure could increase the risk of BDs, and the most crucial susceptibility windows for the exposure were mainly in the first and second trimesters. The association between different pollutants and the classification of BDs also varies. Our work makes an initial contribution to targeted prevention and control measures for various types of BDs.

Keywords: Air pollution; BDs; Distribution lag nonlinear model

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Fine particulate matter ($PM_{2.5}$) exposure affects the health of mice with a sex-dependent property

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Abstract

As the prime air pollutant affecting human health, fine particulate matter ($PM_{2.5}$) is nearly related to various diseases. Most toxicological studies are devoted to a particular organ or system, and tend to favour males as subject, however this preference is unscientific. It has been found that experimental animals of different sexes differ markedly in their susceptibility to certain drugs and do not respond consistently to various stimuli. In this study, we focused on the effects that $PM_{2.5}$ exposure via intratracheal instillation posed to the basic physiological index (BPI) of adult mice of different sexes. The results demonstrated that $PM_{2.5}$ led to decreased red blood cells (RBC) and haemoglobin (HGB) in males, but the white blood cells (WBC) increased signally without sex differences. In addition, there were no significant changes in the heart rate (HR) and systolic blood pressure (SBP) of the mice, while the diastolic blood pressure (DBP) and mean blood pressure (MBP) showing a clear trend of increasing in the males, not the females. Furthermore, we detected the fasting blood glucose (FBG) and the serological indicators of liver function and found that $PM_{2.5}$ markedly elevated the FBG of the females compared with the males, but the male mice exhibited more obvious abnormity in liver function. Specifically speaking, the levels of alanine aminotransferase (ALT), aspartate aminotransferase (AST) and total bile acids (TBA) were significantly higher in the males' serum following $PM_{2.5}$ exposure, rather than the females. In a nutshell, our study indicated that male mice were susceptible to $PM_{2.5}$ exposure than females, which provided experimental evidences for the propensity to select male animals and underscored the importance of reducing the sources of $PM_{2.5}$.

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Neuronal and astrocytic lipid metabolic coupling mediate ozone-induced learning and memory impairment

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Abstract

Surface ozone (O_3) causes a state of chronic oxidative stress and lipotoxicity in brain, increasing the risk of neurodegenerative diseases. Metabolic coordination between neurons and astrocytes is critical for the health of the brain. However, neuron-astrocyte coupling of lipid metabolism, particularly in response to O_3-induced lipotoxicity, remains largely uncharacterized. We established murine models with whole-body O_3 inhalation in female C57BL/6J mice (0.5/1.5 ppm, 4 h/day, for 28 days) to investigate the effects of O_3 exposure on mouse neurobehaviors and disturbances in lipid production and transport between neurons and astrocytes. Mice exposed to O_3 were then treated with N-acetylcysteine (NAC) or citicoline sodium (CDP) to directly assess the role of ROS or lipids on ozone-induced neurotoxicity.The results showed that O_3 led to impairment in learning and memory, accompanied by neuronal loss, glial cell activation and neuroinflammation and lipid peroxidation. We also found that a key consequence of ROS in response to O_3 exposure is the accumulation of lipid droplets (LDs) in brain. And in particular, O_3 exposure triggered c-jun-N-terminal kinase (JNK) and sterol regulatory element binding protein (SREBP) activity to induce lipid formation in neurons. In astrocytes, O_3 activated the liver X receptor (LXR) and but interfered with the upregulation of downstream target genes, ABCA1 and ApoE, which may lead to a decrease in lipid transport efficiency from neurons to astrocytes and an increase in the outcome of lipid peroxidation, exacerbating neuronal damage. In addition, the disruption of mitochondrial oxidative phosphorylation-related genes suggested that ozone exposure simultaneously interfered with lipid degradation. Our study mechanistically revealed that the disturbances in lipid synthesis, transport and metabolism induced by ozone exposure promote neurodegeneration, shedding light on neuron-astrocyte lipid metabolic coupling mediating O_3-induced neurotoxicity. And the NAC/CDP supplementation effectively attenuated O_3-induced lipid metabolism disorder and learning and memory impairment, providing the potential approach for improving the pathology of O_3 pollution-induced neurodegenerative disease.

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Emission characteristics of sulfate from industrial sources and their impacts on aerosol toxic effect

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Abstract

The significance of acidity in the toxicity of atmospheric particulate matter (PM) has been acknowledged since the London Fog in 1952. However, there is limited knowledge about the effects of acidity on particle toxicity. This manuscript presents a trend of toxic potency enhancement with acidity increasing. The oxidative stress and cytotoxicity potencies of acidified PM at pH of 1-2 were up to 2.8-5.2 and 2.1-13.2 times higher than those at pH of 8-11, respectively. The toxic potencies of PM collected from real-world smoke plumes at the pH of 2.3 were observed to be 9.1-18.2 times higher than those at the pH of 5.6. In addition, the solubility of insoluble metals (such as Fe) dramatically increased by 2-3 orders of magnitude during the acidification process. Our study reveals that the toxic potencies of PM can be mediated by acidity via dissolving insoluble metals bonded in PM. The new findings elucidate the epidemiological association between sulfate and adverse health outcomes, highlighting acidic sulfates enhance PM toxicity by promoting metal dissolution.

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Sex- and age-specific association between ethylene oxide exposure and serum sex steroid hormones: Evidence from NHANES 2013–2016

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Abstract

Abstract

Background: Although previous studies suggested a potential link between exposure to Ethylene oxide (EO) and reproductive complications, the precise impact of EO on serum sex steroid hormones—crucial regulators of reproductive health, remains uncertain.

Objective: Using data from the National Health and Nutrition Examination Survey (NHANES) to explore the age- and sex-specific relationship between EO exposure and serum sex steroid hormones.

Methods: This cross-sectional study analyzed NHANES data from 2013 to 2016, examining 3750 participants. Children, adolescents, younger adults, and older male adults who had available data on hemoglobin adduct of EO (HbEO), serum sex steroid hormones, including testosterone (TT), estradiol (E_2), sex hormone-binding globulin (SHBG), the ratio of TT to E_2 (TT/E_2), and the free androgen index (FAI), and covariates were selected. The relationships between ln-transformed blood HbEO concentration and ln-transformed sex hormone indicators by age and sex group were investigated using a statistical model based on survey linear regression.

Results: Linear regression analysis revealed a significant positive association between ln-transformed HbEO concentration and ln-transformed serum TT and SHBG levels in the general population, excluding

E_2, TT/E_2, and FAI levels. The observed association exhibited distinct sex- and age-dependent patterns, with younger adult males experiencing increases in ln-transformed TT, SHBG, and the TT/E_2 ratio, while younger adult females displayed elevated ln-transformed SHBG levels in response to higher ln-transformed HbEO levels. Additionally, a higher ln-transformed TT/E_2 ratio concurrent with elevated ln-transformed HbEO concentration was observed in older adult males (*p* trend: 0.02). Notably, no substantial associations were detected in children or adolescents, regardless of sex.

Conclusions: This study underscores the substantial effects of EO exposure on serum sex steroid hormones, with notable differences observed between age groups and sexes. It highlights the importance of continuous EO monitoring, given its potential to disturb hormonal homeostasis, particularly in younger male adults.

Key words: EO exposure; Sex steroid hormones; NHANES; Sex differences; Age differences

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Long-term ambient ozone exposure with incident atherosclerotic cardiovascular disease and the potential role of ferroptosis

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Abstract

Objective:

The available literature on the incident risk of atherosclerotic cardiovascular disease (ASCVD) with long-term ozone pollution is still limited and the mechanisms need to be explored. Ferroptosis is considered to play an important role in the progress of atherosclerosis. Nevertheless, whether ambient ozone exposure influence AS progression through affecting ferroptosis is unknown.

Materials and Methods:

This study included 353,402 participants without ASCVD who were recruited into the UK Biobank cohort during baseline years 2006-2010. The annual ozone concentrations in the warm season at 0.1° × 0.1° resolution were estimated by combining ozone ground measurements and chemical transport model

estimates. Adjusted covariates including age, sex, ethnicity, assessment centre, Townsend deprivation score, smoking, alcohol consumption, education level, economic status, family history of cardiovascular disease, other air pollutants ($PM_{2.5}$) as well as road traffic noise. Cox proportional hazards regression analysis was employed to quantify the risks of ozone exposure on incident ASCVD. $ApoE^{-/-}$ mice were assigned to ambient ozone or filtered air for 3 months via a whole-body exposure system. Biomarkers of ferroptosis were examined by immunohistochemistry staining, blood iron and lipid indicators were measured by ELISA assay.

Results:

During a median 12.4 years of follow-up, 31,635 participants with ASCVD were ascertained. For per IQR (3.6 ppb) increase in ozone, the hazard ratio (HR) of developing ASCVD was 1.04 (95%CI: 1.01, 1.07). Animal experimental study indicated $ApoE^{-/-}$ mice exposure to ozone exhibited significant higher iron concentration in the blood and iron deposition in the aorta than the control mice. Furthermore, key proteins of anti-ferroptosis including GPX4 and SLC7A11 showed a significant reduction trend. Total cholesterol and triglycerides in the serum were significantly increased.

Conclusion:

The longitudinal evidence suggested that long-term ambient ozone exposure is associated with higher incident risk of ASCVD, and further animal experiments demonstrated that ferroptosis would be an important mechanism in the adverse influence of ambient ozone exposure on ASCVD.

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Spatial regulation of NMN supplementation on brain lipid metabolism upon subacute and sub-chronic PM exposure in C57BL/6 mice

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Abstract

Background Atmospheric particulate matter (PM) exposure-induced neuroinflammation is critical in mediating impairment in nervous system. Nevertheless, a successful intervention has not yet been established.

Results In this study, we investigate the effect of b-nicotinamide mononucleotide (NMN) supplementation on the nervous system damage upon PM exposure and the mechanism of spatial regulation in lipid metabolism. 120 C57BL/6 male mice were subjected to 11-day (subacute) or 16-week (sub-chronic) real ambient PM exposure. Supplementation of NMN boosted the level of nicotinamide adenine dinucleotide (NAD^+) in the mouse brain by 2.04 times. This augmentation effectively reduced neuroinflammation, as evidenced by a notable decrease in activated microglia levels across various brain regions, ranging from 29.8% to 39.9%. Whole brain lipidomics analysis revealed that NMN intervention led to an increased content of ceramide (Cer) and lysophospholipid in brain following subacute PM exposure, and a decreased triglyceride (TG) and glycerophospholipids (GP) following sub-chronic PM exposure, which conferred mice with anti-neuroinflammation response, enhanced immune function, and enhanced membrane stability. In addition, we revealed that the hippocampus and hypothalamus could be the most sensitive brain regions in response to PM exposure and NMN supplementation. Particularly, the alteration of TG (60:10, 56:2, 60:7), diacylglycerol (DG, 42:6), and lysophosphatidylcholine (LPC, 18:3) are the most profound, which was correlated with the changes in functional annotation and pathway perturbation including oxidative stress, inflammation, and membrane instability unveiled by spatial transcriptomic analysis.

Conclusions This study demonstrates that NMN intervention effectively reduces neuroinflammation in the hippocampus and hypothalamus after exposure to PM by modulating spatial lipid metabolism. Strategies targeting lipid homeostasis enhancement can offer significant protection against brain injuries associated with air pollutant exposure.

17. Aquatic Toxicology

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The Differential Effects of Triphenyl Phosphate (TPHP) and Cresyl Diphenyl Phosphate (CDP) on the Visual System of Zebrafish Larvae

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Abstract

Vision is a critical sensory that allows perceiving environment and guiding behavior for living organisms, which has been progressively recognized as a sensitive target for environmental pollutants. Since brominated flame retardants are banned globally, organophosphate flame retardants (OPFRs) as their ideal substitutes have caused extensive concerns. The toxicity of OPFRs on human and wild animals also lead to the appearance of emerging OPFRs (eOPFRs)

with more stable properties. In this study, we focused on the visual toxicity of triphenyl phosphate (TPHP) and one kind of eOPFR, cresyl diphenyl phosphate (CDP), on zebrafish larvae at environmentally relevant concentrations (3, 30 nM). After 5 days of exposure, both CDP and TPHP significantly affected the vision-guided behavior of zebrafish larvae, with elevated apoptosis and structural changes in the retina. The expression of key enzyme genes in phototransduction was altered, accompanied by a decrease in cGMP concentration. It was observed that a collective upregulation of opsin genes involving the formation of color vision and a more sensitive response to color perception were induced by TPHP, contrary to the consequences of CDP exposure. A transcription factor, *tbx2a*, was discovered to be possibly responsible for the differentiated effects on photoreceptor patterning. Given that TPHP and CDP differ in structures by only one methyl group, we suspected that the presence of methyl group caused the significant variation between two OPFRs. These findings provided new clues for the toxicological mechanisms of OPFRs, and revisited the question regarding the safe substitutes for those emerging contaminants.

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Assessing the Ecotoxicity and Risk of Four Pesticides Commonly Detected in Waterways Discharging to the Great Barrier Reef Lagoon, Australia

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Abstract

Pesticides are widely used in agricultural and urban environments and can subsequently contaminate surface waters. Globally, pesticide runoff has been identified as one of the main contributors to poor water quality, this is also the case in Queensland, Australia, where discharge from catchments can carry pesticides to the Great Barrier Reef (GBR) lagoon. The ability to assess the hazard and risk posed by pesticide active ingredients (PAIs) to aquatic ecosystems relies on the availability of water quality guidelines, which can be compared against concentrations detected in the environment through monitoring programs. Over 70 PAIs and break-down products are frequently detected in GBR catchment waterways. However, many do not have water quality guidelines in the Australian and New Zealand Guidelines for Fresh and Marine Water Quality. As a result, the potential risk to aquatic organisms is unknown, hindering the assessment of the water quality condition of GBR ecosystems. The current study proposes default guideline values (DGVs) for two fungicides (carbendazim and the chlorothalonil

degradate, 4-hydroxychlorothalonil) and two insecticides (dimethoate and methoxyfenozide) that are commonly detected in GBR catchment waterways. The proposed DGVs are then compared to monitoring data from the Great Barrier Reef Catchment Loads Monitoring Program to assess the hazard and risk to aquatic ecosystems. The proposed DGVs have been derived using the Australian and New Zealand nationally endorsed method which recommends the use of a species sensitivity distribution approach. Exceedances of the concentrations protecting 95% of aquatic species (i.e., PC95) were observed for three of the four toxicants and exceedances of the PC99 were observed for all four toxicants. Using the hazard quotient method, six high hazard sites were identified, where the risk to aquatic species reached a maximum of 53, 20 and 27% of species potentially affected for 4-hydroxychlorothalonil, carbendazim and methoxyfenozide, respectively. The results highlight a potentially serious threat to aquatic ecosystems at the identified sites. The proposed DGVs can be applied to national and international waterways outside of the GBR region, subject to the availability of pesticide monitoring data. This allows the potential hazard and risk to aquatic ecosystems to be evaluated and thus enables a more accurate assessment of ecosystem condition and increased protection of aquatic ecosystems.

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Effects of Emerging Pollutant Mixtures: Assessing the Impact of Caffeine and Ionic Liquid Combinations on Cyanobacteria and Diatom Species

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Abstract

The ubiquitous occurrence of emerging contaminants poses a significant risk to aquatic ecosystems, potentially leading to their degradation. Presently, risk and hazard assessments primarily focus on analyzing the impacts of individual chemicals. However, ecosystems face exposure to complex mixtures of pollutants. The interactions among these pollutants, coupled with their persistent presence in aquatic environments, heighten the overall risk to organisms and may lead to unforeseen adverse consequences.

The aim of the presentation is to offer a comprehensive overview of the challenges and potential hazards associated with the presence of mixtures of micropollutants in aquatic environments, with a focus on the effects of ionic liquids and other organic micropollutants.

Ionic liquids (ILs) have garnered significant interest in various industrial sectors due to their distinctive characteristics. However, their persistence and unusual physicochemical properties pose a considerable risk to aquatic ecosystems. Therefore the study aimed to identify the types of interactions between target emerging pollutants mixtures composing of ILs representative IM1-8C$(CN)_3$ and caffeine considered an indicator of anthropogenic contamination, reflecting inputs from urban, industrial, and agricultural sources. Caffeine, a well-known stimulant has garnered

attention as an emerging and pseudo persistent pollutant in aquatic environments including marine water systems.

The findings presented include an examination of the chronic exposure of microorganisms found in brackish coastal waters and the open Baltic Sea basin, such as the cyanobacteria *Microcystis aeruginosa*, and the diatom *Phaeodactylum tricornutum*, to contaminants mixtures. Measurements of pigment concentrations were complemented by the assessment of photosynthetic parameters. Variations in chlorophyll fluorescence kinetics, which define the redox states of photosystem I/II and are directly linked to electron transfer efficiency, were quantified.

Photosynthesis processes, and pigment ratios were affected in all targeted microorganisms. Through the application of mathematical models such as concentration addition (CA) and independent action (IA), followed by Model Deviation Ratio (MDR) evaluation, primarily synergistic interactions were identified in the studied mixtures. The study results offer valuable insights into the effects of ionic liquids and other organic micropollutants on photosynthetic microorganisms.

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Mapping the risk of ciprofloxacin in European waterbodies: incorporating bioavailability

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Abstract

The fluoroquinolone ciprofloxacin (CIP) is a widely prescribed antibiotic applied in human and veterinary health care. With its production and application, the compound has been detected in surface waters worldwide, which may lead to unwanted ecotoxicological consequences such as the development of antimicrobial resistance (AMR). On the other hand, recent studies have shown that the ecotoxicity and bioavailability of CIP is affected by water chemistry factors, namely, environmental pH and the dissolved organic carbon (DOC). Therefore, a comprehensive environmental risk assessment (ERA) for CIP needs to encompass the interplay between CIP and environmental conditions.

This study incorporated bioavailability into the ERA of CIP. With a CIP bioavailability model, the sensitivity of European water bodies to CIP, expressed by an environmental prediction no-effect concentration ($PNEC_{ECO}$), was estimated under four simulation scenarios. They are (1) the conventional scenario (no bioavailability incorporated), (2) the worst-case scenario (pH affects bioavailability, but DOC has no effect), (3) the average scenario (both pH and DOC affect bioavailability, weak CIP-DOC interaction), and (4) the best-case scenario (both pH and DOC affects bioavailability, strong CIP-DOC interaction). Probabilistic risk assessments were performed based on Monte Carlo simulation using CIP occurrence data and $PNEC_{ECO}$ obtained in different scenarios. Probability of risk (P_{risk}), uncertain risk ($P_{uncertain\ risk}$), and safe (P_{safe}) were assessed for Europe as a whole and for ten nations specifically.

Results indicate that the $PNEC_{ECO}$ had a high regional variability. Western Austria, northern and central Italy, southern Greece, and Norway appeared to be more susceptible to CIP. On the European scale, P_{risk} was between 9.8% (best-case) and 21.7% (conventional) across different scenarios, showing a clear influence caused by DOC. The country specific P_{risk} also presented high variations. The P_{risk} estimated for Spain and the Netherlands was below 10% in all scenarios, and that for France was 13-21%. The influences of pH and DOC were greater on the P_{risk} estimated for Germany and Portugal, which ranged from 32-67% and from 4-99%, respectively. Austria, Croatia, Czech, Hungary, and Slovakia observed probability of uncertain risk between 21% and 50%, while the incorporation of bioavailability could reduce uncertainties. Overall, the inclusion of water chemistry factors enables a more accurate ERA.

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TransPharm: a comparative study of the environmental risk of ciprofloxacin and its environmentally degradable alternative ciprofloxacin-hemi: from human to river

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Abstract

The fluoroquinolone antibiotic ciprofloxacin (CIP) is a pseudopersistent contaminant detected in water bodies across the globe. It is a human and veterinary medicine that is commonly prescribed to treat various bacterial infections. The compound works by interfering with the DNA replication process of bacteria, which ultimately inhibits the growth of bacteria. However, as CIP is insensitive to biodegradation, it is prone to remain the environments and thereby contribute to antimicrobial resistance (AMR) crisis.

Since 2022, the European Union (EU) project 'Transforming into a sustainable European pharmaceutical sector' (TransPharm), has been devoted to developing alternative compounds for fluoroquinolone antibiotics that are lower in environmental impacts in their entire life circle. Within the project, a greener alternantive for ciprofloxacin, CIP-Hemi, has been developed. The new fluoroquinolone CIP-Hemi has a higher degradability than its parent compound CIP, while possessing a lower ecotoxicity.

This current study conducted a comparative environmental risk assessment (ERA) of CIP and CIP-Hemi to compare their environmental impact. From application, to wastewater treatment, to residues in aquatic ecosystems, the fate of CIP and CIP-Hemi were compared.

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Development of the Imidacloprid Temporal Response Surface and Ramifications for Aquatic Ecosystems in the Great Barrier Reef Catchment Area

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Abstract

The neonicotinoid imidacloprid is detected in an average of 54%, but up to 100%, of all samples collected by the Great Barrier Reef (GBR) Catchment Loads Monitoring Program. In some monitoring locations, imidacloprid concentrations remain elevated for up to five months, often above the relevant ecosystem protection guidelines. A growing body of literature highlights the potential for neonicotinoid insecticide toxicity to increase over time due to irreversible binding to target receptors within the body of aquatic organisms. Toxic effects may accumulate within organisms and ecosystems that are exposed to a single extended exposure or repeated pulses of neonicotinoids. Therefore, the impact on aquatic ecosystems in the GBR catchment area may be greater than previously estimated using water quality thresholds that are derived using relatively short-term toxicity test data. To address this issue, the temporal response surface (TRS) was developed as a novel and practical method to estimate the cumulative ecosystem impact of repeated or prolonged imidacloprid exposure. This innovative approach incorporates exposure duration as a third axis in the traditional species sensitivity distribution (SSD) method. The TRS was then applied to a real-world data set generated by the GBR Catchment Loads Monitoring Program, in which imidacloprid data from 28 monitoring sites (representing 22 unique river basins that drain to the GBR lagoon) across seven sampling years were used to provide a revised estimate of the risk that incorporates exposure duration. A framework was developed to calculate exposure duration and recovery windows for the time series data, which dictated where on the temporal response surface the risk (as percent affected fraction of the ecosystem) would be calculated.

Although initially applied to imidacloprid in the GBR catchment area, our developed methodology can be adapted for any toxicant (pesticide or otherwise) with delayed or time-cumulative toxicity characteristics, thereby addressing a critical global gap in risk assessments. The TRS method will be published in two papers (a method paper and a case study paper) and an open source CRAN R package, facilitating global accessibility and adaptation for diverse risk assessment needs. This presentation will introduce the TRS method and will briefly cover the case study results, providing a holistic estimate of the risk posed by imidacloprid in the GBR catchment area.

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Size Matters Less? Exploring the Intricacies of Polystyrene Nanoplastic Toxicity in Zebrafish

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Abstract

Abstract:

Nanoplastics (NPs) have been studied extensively in recent years due to their potential toxicity, often finding that smaller particles exhibit higher toxicity due to increased surface area and uptake. We hypothesize that nanoparticle toxicity is more influenced by chemical and environmental conditions than size alone. We investigated the embryonic and neurobehavioral effects of polystyrene nanoplastics (PS-NPs) of different sizes (50 nm, 200 nm, and 1000 nm) on zebrafish larvae. Embryos were exposed to a wide concentration range of PS-NPs (0.1 to 10 ppm) from 6 to 120 hours post-fertilization (hpf). Quantitative endpoints included mortality, hatching, deformities, locomotor activities, and biochemical and transcriptomic responses. Contrary to previous studies, PS-NP exposure had no significant effect on survival, hatching, deformities, or locomotor activities, likely due to thorough dialysis removing toxic plastic chemical leachates. NPs were found in the yolk and digestive tract, dominantly in the intestine, which was supported by super-resolution fluorescence bio-imaging. RNA sequencing revealed the highest number of differentially expressed genes after exposure to 1000 nm PS-NPs. KEGG enrichment identified the circadian rhythm pathway as significantly affected, and GO enrichment highlighted neurobehavioral terms such as circadian regulation of gene expression and phototransduction. Biomarkers such as AChE and caspase 3 were significantly altered after exposure to 1000 nm PS-NPs. These findings suggest that nanoplastic toxicodynamics is complex and influenced by factors beyond size, challenging the notion that smaller nanoparticles are inherently more toxic.

Keywords: *Danio rerio*; embryotoxic; larval behavior; neurotoxicity; transcriptomics

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Membrane Receptor-Mediated Thyroid Hormone Disrupting Effects and Their Mechanism of Action by Organophosphate Esters

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Abstract

Organophosphate esters (OPEs) are experiencing a dramatic increase in production, usage, and environmental exposure, raising significant concerns about their toxicity, particularly their thyroid hormone-disrupting effects. However, their toxic mechanism of thyroid hormone-disrupting effects remains unclear. Preliminary studies suggest that the membrane thyroid hormone receptor $\alpha_v\beta_3$ may play a vital role in mediating the thyroid hormone-disrupting effects of OPEs. Therefore, this study employed an integrated *in silico*, *in vitro*, and *in vivo* testing strategy to investigate the membrane receptor $\alpha_v\beta_3$-mediated thyroid hormone-disrupting effects and the mechanism of action (MoA) of OPEs.

The affinity of OPEs with the membrane receptor $\alpha_v\beta_3$ was detected using an *in vitro* radioligand binding assay. The binding activities of 18 OPEs to $\alpha_v\beta_3$ were identified, with RIC_{20} values (the 20% relative inhibitory concentration) ranging from 2.22×10^{-6} to 6.64×10^{3} nmol/L. Akyl-OPEs and halogenated-OPEs showed stronger binding activity than aryl-OPEs. The binding mechanism was further elucidated by molecular docking, pharmacophore, and quantitative structure-activity relationship models. OPEs were found to bind to $\alpha_v\beta_3$ by hydrogen bonding, with the -P=O structure of OPEs, the key amino acid residues, and the appropriate cavity volume of $\alpha_v\beta_3$ identified as the molecular, biological and spatial bases for hydrogen bond formation.

Tris(1,3-dichloro-2-propyl) phosphate (TDCPP) was selected as a representative OPE. Zebrafish exposure experiments revealed that TDCPP at concentrations of 400 and 600 μg/L significantly changed the growth and development, altered the thyroid hormone levels, and affected the motor behavior of zebrafish larvae. Besides, TDCPP significantly inhibited motor neuron development in zebrafish larval even at an environmentally relevant concentration of 50 μg/L. Based on transcriptomic and proteomic analyses, the MoA of TDCPP was proposed. The interaction of TDCPP with $\alpha_v\beta_3$ was identified as the pivotal molecular initiating event, with the activation of mitogen-activated protein kinase signaling and calcium signaling pathways being key toxicological events, ultimately leading to neurodevelopmental abnormalities in zebrafish. This mechanism was further validated through competitive inhibition and specific blocking experiments. This study provides a scientific basis for the toxicological evaluation and environmental safety management of OPEs.

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A Review on the Occurrence and Ecotoxicity of Biodegradable Microplastics in Aquatic Environments: New Cause for Concern

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Abstract

Biodegradable plastics (BPs) have been widely advocated as a sustainable alternative to petroleum-derived polymers, aiming to mitigate the burgeoning crisis of microplastic pollution. However,

incomplete biodegradation of BPs can generate more and smaller particles, such as microplastics, which may persist in environments. Knowledge of the fate and effects of biodegradable plastics, especially BPs, in the aquatic environment remains limited. We investigate the concentrations, detection methods, and adverse effects of BPs on aquatic organisms in various aquatic environments. BPs, such as poly (lactic acid), polyhydroxyalkanoates, poly (butylene adipate-co-terephthalate), and poly (butylene succinate), are found in wastewater, reservoirs, and marine environments at concentrations between 0.054 and 180 μg/L. Their environmental levels are negatively correlated with their degradation capacity in water. BPs adversely affect aquatic microbial communities, plant adaptability, and animal physiology, with their toxicity increasing upon degradation. This review advocates for a critical reassessment of the use, disposal, and management strategies surrounding BPs.

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Environmental concentrations *S*-6PPD-quinone caused more serious hepatotoxicity than *R*-enantiomer and racemate in *Oncorhynchus mykiss*

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Abstract

6PPD-quinone (6PPD-Q) is chiral with two enantiomers. In this study, the toxic mechanism of 6PPD-Q to *O. mykiss* liver was investigated after 96 h exposure at the environmental concentrations (0.1 and 1 μg/L) from the enantiomeric level. Effects on biochemical, pathological and ultrastructural changes were assessed, and metabolomic was conducted to address the potential mechanism of 6PPD-Q-induced hepatotoxicity. The levels of catalase (CAT), glutathione-S-transferase (GST), glutathione (GSH) and malondialdehyde (MDA) had a significant decline. Histopathological analysis showed the hepatocyte space became smaller, nuclear morphology changed, and nucleolysis occurred. Simultaneously, mitochondria malformation and vesicle-like structure dilation of the endoplasmic reticulum (ER) were observed in hepatocytes, which was the most serious after *S*-6PPD-Q exposure. Metabolomic data revealed that some amino acid metabolism, folate biosynthesis, taurine and hypotaurine metabolism and purine metabolism were mainly disturbed, which were consistent with the mitochondria dysfunction and ER stress. The number of differential metabolites and the affected pathways was in the order of *S*-6PPD-Q (216, 31) > *rac*-6PPD-Q (88, 28) > *R*-6PPD-Q (56, 19). Thus, 6PPD-Q-induced hepatic mitochondria dysfunction and ER stress, causing metabolic disturbance and oxidative stress might be the toxic mechanism of 6PPD-Q to *O. mykiss* liver, and the *S*-6PPD-Q effects were the most serious.

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The effect of water hardness on the toxicity of zebrafish embryo during exposure to pesticides transformation products: a case study with 3-phenoxybenzoic acid

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Abstract

There is limited research on the aquatic toxicity of transformation products (TPs) of pesticides, as well as the impact of environmental factors. 3-phenoxybenzoic acid (3-PBA), a common TP of multiple synthetic pyrethroids (SPs), is found in surface waters due to the widespread use and fast degradation or metabolism of SPs. However, the toxicity of 3-PBA may be influenced by environmental factors such as water hardness, which affects the newly formed active group (-COO–) in its structure. To investigate the effects of water hardness on the aquatic toxicity of 3-PBA to zebrafish embryos, a two-factor experiment was conducted with 3-PBA in three different water hardness levels (50, 125, and 250 mg/L $CaCO_3$). Our results demonstrated that increased water hardness decreased the acute toxicity of 3-PBA, as evidenced by increased LC_{50} values from 7.86 mg/L to 28.74 mg/L. Co-exposure to 3-PBA and different hardness increased hatching rates, with medium hardness showed the strongest effect. Furthermore, elevated water hardness also reduced malformation rates at the highest concentration of 3-PBA (700 μg/L). A dose-dependent relationship was found between 3-PBA concentration and the locomotor activity of larvae in the medium-high water hardness exposure group. For exposure groups with the same 3-PBA concentration, the rank order for triiodothyronine (T3) levels of larvae in different water hardness groups was 125 mg/L > 50 mg/L > 250 mg/L. On the other hand, as the concentration of 3-PBA increased, the levels of T3 also showed a concentration-dependent increase in each water hardness group. Differently, levels of T4 in low-medium water hardness group showed a significant decrease in each 3-PBA exposure group. In the combined exposure of 3-PBA and water hardness, the mRNA expression levels of most genes were up-regulated, especially in the middle water hardness exposure group.

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3,3',5,5'-tetrabromobiphenyl (BB-80) and its hydroxylation product (OH-BB-80) mediate immunotoxicity and inhibit embryonic development in zebrafish (*Danio rerio*) via the TLR4/NF-κB signaling pathway

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Abstract

Abstract: Polybrominated biphenyls (PBBs) are metabolically transformed into monohydroxylated PBBs (OH-PBBs) in the environment and living organisms. Although OH-PBBs pose a significant health threat to organisms, little is known about the immunotoxicity of OH-PBBs. Therefore, the objectives of

this study was to validate BB-80 and OH-BB-80 induced immunotoxicity and to explore the associated pathway mechanisms. Early development of zebrafish (*Danio rerio*) larvae was inhibited by 10 μg/L BB-80 and OH-BB-80, as indicated by negative changes in developmental indices. BB-80 and OH-BB-80 induced oxidative stress, significantly up-regulated reactive oxygen species (ROS) and reactive nitrogen species (RNS), and activated the antioxidant enzyme system at 10 μg/L. The mRNA expression levels of inflammatory cytokines and inflammatory chemokines were up-regulated, indicative of the onset of inflammation in zebrafish after BB-80 and OH-BB-80 exposure. In addition, downregulation of toll-like receptor 4 (TLR4), MyD88, and NF-κB pathway-related genes was observed, suggesting that BB-80 and OH-BB-80 target the TLR/NF-κB signalling pathway. Molecular docking data showed that BB-80 and OH-BB-80 bound stably to TLR4. Taken together, BB-80 and OH-BB-80 mediate immunotoxicity and early developmental suppression associated with the TLR4/NF-κB signaling pathway. Our results further the understanding of BB-80- and OH-BB-80-induced immunotoxicity, highlighting the need for toxicological studies to examine the toxic effects of the transformation products of PBBs.

Keywords: Immunotoxicity; Inflammation; Oxidative stress; TLR4/NF-κB; Zebrafish

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Responses and molecular mechanisms of nuclear receptor HR96 to DSP toxins in the mussel *Perna viridis*

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Abstract

Diarrheal shellfish poisoning (DSP) toxins are one of the most prevalent marine biotoxins with the highest incidence of poisoning in the world. When humans accidentally consume shellfish contaminated with DSP toxins, they can experience diarrhea and put themselves at risk of tumors in the digestive system. Compared with human susceptibility to DSP toxins, shellfish show some tolerance to DSP toxins, and the toxicity of DSP toxins to shellfish tends to decrease with the duration of exposure or the accumulation of toxins, which may be related to the complex metabolic process in shellfish, but the mechanisms are currently still unclear. Xenobiotic nuclear receptors play an important regulatory role in the metabolic detoxification of xenobiotic contaminants in animals, but their role in the tolerance mechanism of DSP toxins in bivalves is rarely reported. In this study, we investigated the potential role and mechanisms of HR96 in DSP toxin tolerance in the mussel *Perna viridis*. We found that after exposure to DSP toxin, HR96 was significantly upregulated and positively correlated with the overexpression of genes related to metabolic detoxification in the digestive glands of *P. viridis*. Knockdown of HR96 could reverse the DSP toxins-induced overexpression of metabolic detoxification-related genes and increase DSP toxins accumulation in the digestive gland, ultimately aggravating tissue damage, whereas activation of HR96 could significantly reduce DSP toxins content in tissues, alleviate tissue damage and improving individual physiological status. Transcriptome analysis on the digestive glands of *P. viridis* with HR96 knockdown showed that HR96 can reduce the toxicity of DSP toxins

to mussels by regulating the expression of metabolic detoxification-related genes, such as CYP3A4, GST-like, and ABCC10, thereby enhancing the function of the metabolic detoxification system. Our findings suggest that DSP toxins can activate the nuclear receptor HR96 in a ligand-dependent manner and induce the overexpression of CYP450, GST, and ABC transporter proteins, which contribute the tolerance of *P. viridis* to DSP toxins.

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Effects of carbamazepine on the central nervous system of zebrafish at human therapeutic plasma levels

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Abstract

The fish plasma model (FPM) facilitated the environmental risk assessment of human drugs by using existing data on human therapeutic plasma concentrations (HTPCs) and predicted fish plasma concentrations(FPCs). However, studies on carbamazepine (CMZ) with both the mode of action (MOA) based biological effects at molecular level (such as neurotransmitter and gene level) and measured FPCs are lacking. Bioconcentration of CMZ in adult zebrafish demonstrated that the FPM underestimated the bioconcentration factors (BCFs) in plasma at environmental CMZ exposure concentrations (1–100 mg/L). CMZ significantly increased glutamic acid (Glu) and gamma-aminobutyric acid (GABA) , decreased acetylcholine (ACh)
and acetylcholinesterase (AChE) as well as inhibited the transcription levels of gabra1, grin1b, grin2b, gad1b, and abat when the actual FPCs were in the ranges of 1/1000 HTPC to HTPC. It is the first read-across study of CMZ integrating MOA-based biological effects at molecular level and FPCs. This study facilitates model performance against a range of different drug classes.

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An integrated multi-omics approach demonstrates environmentally relevant concentration of octocrylene inhibits the growth of *Tetradesmus obliquus* via affecting photosynthesis and metabolism

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Abstract

Octocrylene (OC) is a widely used organic UV absorber and a common ingredient in coral-friendly sunscreen at present. However, recent studies have revealed its impacts on aquatic organisms, such as causing mitochondrial dysfunction, inhibiting cell growth, etc. In the present study, we investigated stress response and the related molecular mechanisms of green algae *Tetradesmus obliquus* exposed to OC at four concentrations (1, 10, 100, and 500 μg/L) during a 7-day exposure period. Results revealed a concentration-dependent growth inhibition of *Tetradesmus obliquus* exposed to OC, with an approximately 24% growth inhibition being observed in the 500 μg/L treatment group by the end of exposure. Meanwhile, after 7 days, chlorophyll a (Chl a), Chl b, and carotenoid (CAR) contents were 20%-40% lower in the 500 μg/L treatment group compared to the control group. The maximum photochemical quantum yield (Fv/Fm) showed a significant negative correlation with OC concentration on day 1 to day 7. Furthermore, the levels of reactive oxygen species (ROS), malondialdehyde (MDA), and glutathione (GSH) in the 500 μg/L treatment group were significantly higher first but then were significantly lower than in the DMSO group, with differences ranging from 33% to 97%. In contrast, the activities of superoxide dismutase (SOD), catalase (CAT) and ribulose-1,5-bisphosphate carboxylase/oxygenase (Rubisco) showed opposite patterns in the 500 μg/L treatment group versus the control group, with differences ranging from 22% to 349%. Results from transcriptomic and metabolomic analyses suggest that OC inhibited lipid metabolism, amino acid metabolism, purine metabolism, and pyrimidine metabolism in *Tetradesmus obliquus*. This study will help us gain a better understanding of the impact of OC on aquatic environments.

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The endocrine disrupting effects of parabens on zebrafish (*Danio rerio*)

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Abstract

As a group of prevalent synthetic preservatives, parabens were widely added in foodstuffs, cosmetics and pharmaceuticals. The extensive use of parabens inevitably induced the considerable release into environment, which have been ubiquitous detected in global aquatic system. The potential endocrine disrupting effects of parabens on fish were still unclear. Hence, the endocrine disrupting effects of four commonly-used parabens, including methyl paraben (MeP), ethyl paraben (EtP), propyl paraben (PrP) and butyl pararben (BuP), were investigated on zebrafish in the early stage. The results showed that paraben exposure significantly altered the zebrafish development, causing decreased hatching rate, body length and heart rate, as well as increased malformation rate. The disruption of chemicals on thyroid, reproductive, and adrenal endocrine systems were subsequently determined. It was observed that four parabens exposure obviously alter the corresponding hormones involved in endocrine systems, as well as the genes

transcriptional levels related to hypothalamic−pituitary−thyroid (HPT), hypothalamic−pituitary−gonad (HPG), and hypothalamic−pituitary−adrenal (HPA) axes respectively. Further *in vitro* and *in silico* studies demonstrated that parabens displayed binding and transactivation activity with key receptors involved in endocrine systems. This study provided fundamental data on the safety evaluation of parabens and expanded knowledge of their toxicity on aquatic organisms.

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Neurotoxicity of β-citronellol Induced by KYN to 3-HK Metabolic Activation

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Abstract

Citronellol is a volatile fragrance chemical with a floral scent that is widely used in various consumer products such as cosmetics, perfumes and household products. Citronellol is known to have positive effects, such as relaxing and calming, and is considered a relatively safe chemical. However, there is a lack of comprehensive research on the health effects and underlying mechanisms of citronellol. Therefore, we performed experiments in which zebrafish larvae were exposed to citronellol after early neurogenesis to elucidate its neurological effects. Our results showed that citronellol exposure induced behavioral abnormalities, increased reactive oxygen species (ROS) and inflammatory responses in zebrafish larvae, particularly through activation of the 3-hydroxykynurenine (3-HK) pathway and subsequent neurosteroid activation. These metabolic changes, including 3-HK, were confirmed not only in zebrafish but also in mouse models following oral administration and in brain organoids. Furthermore, using animal and brain chip models, we confirmed that citronellol crosses the blood-brain barrier (BBB) and accumulates in the brain. Our results demonstrated the induction of 3-HK-mediated ROS production and neuroinflammatory cascades in the brain following citronellol exposure, underscoring the potential necessity for regulatory restrictions on its use.

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Molecular Toxicity Identification and Evaluation (mTIE) applied in diagnosing the developmental toxicity of organic micropollutants in the Qiantang River

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Abstract

The Qiantang River contains a significant amount of organic micropollutants, which pose potential developmental toxicity to organisms, threatening the ecological environment and human health. In the presence of complex organic micropollutants in the Qiantang River, relying solely on a single toxic pathway for biological effect evaluation may not encompass all developmental toxic pathways adequately. Moreover, pinpointing the key developmental toxic substances through chemical analysis can be challenging. Therefore, the mTIE strategy was introduced in this study. It combined dose-dependent transcriptomics with non-targeted chemical screening to evaluate and diagnose the potential developmental toxicity of Qiantang River surface water.

In this study, model biological zebrafish embryos were selected as research objects to evaluate the developmental toxicity of organic micropollutants extracted from the surface water of the Qiantang River. The results showed that the LC50 of zebrafish embryo toxicity ranged from 139.4 REF to 325.8 REF. Cardiac pericardial edema, hepatic lipid vacuolation and lipid accumulation, as well as curvature of the notochord were observed at 100 REF. Liver toxicity-related pathways such as metabolism of xenobiotics by cytochrome P450, Drug metabolism-Cytochrome P450, etc., were identified through dose-dependent transcriptomics screening. The Regulation of actin cytoskeleton and the MAPK signaling pathway are related to cardiotoxicity. After that, 135 and 289 chemical substances were screened from environmental samples in summer and winter, respectively, using non-targeted GC-MS. The peak area, acute developmental toxicity, biological pathway correlation, and active structure obtained by mTIE were then scored. Dibutyl phthalate(DiBP) was identified as the key developmental toxic substance at the Jiuxi site in summer. The contribution rate of acute toxicity was 26.07%. This research can offer technical support for ensuring the drinking water safety of residents living in the lower reaches of the Qiantang River.

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Triclocarban (TCC) and Triclosan (TCS) induced lipid metabolism in *Rana nigromaculata*

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Abstract

Triclocarban (TCC) and Triclosan (TCS) are broad-spectrum antimicrobial agents widely distributed in aquatic environments, posing significant risks to aquatic organisms. However, their potential impacts on amphibian health remain poorly understood. In this study, adult black-spotted frogs were exposed to TCC and TCS at concentrations of 0, 1, 10, and 100 μg/L for 21 days to investigate their effects on hepatic lipid metabolism. Our findings reveal that TCC and TCS induced disruptions in hepatic lipid metabolism, leading to elevated serum lipid levels by downregulating fatty acid uptake and transport while upregulating fatty acid catabolism. Consequently, there was a marked decrease in hepatic total cholesterol and triglyceride levels alongside a significant increase in serum total cholesterol and triglyceride concentrations. Lipidomic analysis demonstrated substantial alterations in liver lipid profiles following exposure, particularly affecting glycerophospholipids (GP), suggesting a targeted impact on glycerophospholipid metabolic pathways. PPARs (peroxisome proliferator-activated receptors) play a pivotal role in hepatic lipid metabolism. Molecular docking results indicated that TCC and TCS exhibit strong binding affinity towards PPARα and PPARγ, crucial regulators of lipid metabolism. Specifically, the binding energies were -7.7 and -7.8 kcal/mol for TCC and -6.8 and -6.9 kcal/mol for TCS with PPARα and PPARγ, respectively. In conclusion, our study highlights that exposure to TCC and TCS disrupts hepatic lipid metabolism in black-spotted frogs, revealing previously unrecognized hazards of these antimicrobials to amphibians. These findings contribute novel insights into the potential ecological risks posed by TCC and TCS in aquatic environments.

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Can Changes in Plasma Proteins Across Ontogeny and Species Mediate Patterns of Per- and Polyfluorinated alkyl substance (PFAS) Bioaccumulation and Toxicity? A Case Study with Amphibian Models

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Abstract

A central theme of available bioaccumulation and toxicity studies for wildlife exposed to PFAS is that species tend to vary substantially, both for bioaccumulation potential and for thresholds for adverse effects. PFAS are known to interact strongly with proteins and research suggests that circulating protein concentrations can mediate bioaccumulation potential. Amphibians have become an important model in PFAS ecotoxicology, but bioaccumulation rates and toxicity can vary dramatically across studies, for reasons that remain unclear. Understanding the relations between protein levels across species, age and developmental stages might explain differences in observed bioaccumulation rates and, in turn, differences in toxicity thresholds across available studies. Interestingly, amphibian species can differ strongly in plasma protein concentrations both across taxa and development; species that remain aquatic

as adults (e.g., Pipids, like *Xenopus laevis, Silurana tropicalis*) tend to maintain lower plasma protein concentrations, whereas species that become terrestrial after metamorphosis, (e.g., Ranids, like *Rana pipiens, Rana nigromaculata*) experience sharp increases in plasma proteins during and after metamorphosis. These differences provide an opportunity to explore the role of proteins, yet, no systematic studies have examined how differences in protein concentrations across species, life stages, or age for this group might mediate bioaccumulation or toxicity of PFAS. **We tested the hypotheses that, in amphibians, 1) plasma protein concentrations change across age and stage in ways concordant with life history, 2) that these changes correlate with observed PFAS bioaccumulation rates, and finally, 3) that differences in thresholds of toxicity are correlated with protein-mediated differences in uptake.** To test these, we are using a combination of existing data and unpublished data from our lab that compares protein levels across development for *Xenopus* and *Rana* species, their correlations with differences in bioaccumulation, and ultimately, differences in patterns of toxicity. Our data will enable better synthesis of how PFAS accumulate in and affect amphibians and will provide a way to understand why studies across species and life stages come to such variable conclusions in these important models. This work is part of a continuing line of evidence emphasizing the importance of protein concentrations as mediators of PFAS bioaccumulation and toxicity.

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Sustained Exposure to Triclosan and Triclocarban Disrupts Homeostasis of the Enterohepatic Axis in the Black-spotted Frog (*Pelophylax nigromaculata)*

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Abstract

Triclosan (TCS) and triclocarban (TCC) are widely used broad-spectrum biocides that are common contaminants of water and soil and have high environmental persistence. However, the safety of TCS and TCC for amphibians remains largely unknown. Here, we used a model of the black-spotted frog (*Pelophylax nigromaculata*) to assess the potential ecological risks of continuous exposure to TCS and TCC at environmental concentrations. TCS and TCC are absorbed and circulate in the bloodstream, with the vast majority going to the gut for metabolic processing with the liver. The results of the gut microbiome showed that TCS and TCC significantly increased the abundance of Proteobacteria, which led to the elevation of the bacterial-derived endotoxin lipopolysaccharide (LPS) in the plasma, and LPS entered the liver along with the blood circulation, and the levels of the pro-inflammatory cytokines IL-6, IL-1β, and TNF-α were also dysregulated, and the markers of damage in the liver, ALT, and AST, had a significant elevation. Subsequently, a significant increase in catalase and glutathione peroxidase activities as well as glutathione and malondialdehyde levels was detected in TCS- and TCC-exposed frogs, suggesting that oxidative stress damages the liver and induces up- and down-regulation of inflammation-related genes in the NF-κB pathway. These findings suggest that TCS and TCC may exert hepatotoxic effects on *P. nigromaculata* by disrupting the enterohepatic axis, which in turn induces hepatic inflammation and oxidative stress.

517

Peek-A-Boo Test: A Simple Test for Assessing the Effect of Chemical Pollutants on Medaka Fish Behavior

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Abstract

The behavior of organisms is essential for their survival, and recent studies have highlighted concerns about "ecological death," where non-lethal chemical exposure can lead to behavioral changes that result in population declines (Scott and Sloman, 2004). We believe that a simple yet effective behavioral test is necessary to evaluate the actual impact of pollutants on aquatic organisms. In 2024, we developed a simple behavioral test, named the *Peek-A-Boo* test, to assess the effect of anxiolytics on the behavior of a model fish (medaka, Oryzias latipes). This test involved examining the response of medaka to an image of a predator fish (donko fish, *Odontobutis obscura*). To determine the efficacy of the *Peek-A-Boo* test for assessing fish behavior, we conducted exposure tests with diazepam (a benzodiazepine) and chlorpyrifos (an organophosphate pesticide). The diazepam exposure test showed that medaka exposed to diazepam approached the image 0.22 to 0.65 times faster and spent 1.8 to 2.7 times longer near the image compared to the solvent control group across all diazepam exposure levels (0.8, 4, 20, or 100 µg/L) ($P < 0.05$). Conversely, the chlorpyrifos exposure test indicated that medaka exposed to chlorpyrifos (5 µg/L) took longer to approach the image than the solvent control group. Quantifying swimming trajectories using Shannon's information entropy one minute after image presentation revealed a trend of decreased information entropy (more monotonous trajectories) in the exposure groups (1.25, 5, 20 µg/L) (P value, 0.101–0.158), suggesting that exposed fish continued to exhibit wary behavior towards the image longer than the solvent control group. Hence, we confirmed that the *Peek-A-Boo* test can be used to assess the toxicity of pollutants on medaka behavior, particularly in evaluating anti-predator behavior.

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Exploring the Developmental Proteome and Life-stage Specific Sensitivities of Larval Zebrafish to a Model Toxicant

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Abstract

Toxicological safety data for environmental contaminants is necessary to characterize hazards and risks to both human and ecological health, yet is deficient for most existing chemicals. These deficiencies, coupled with the significant time and monetary costs of traditional toxicity testing, have prompted a shift towards methods that reduce the number of animals. Due to their high fecundity, rapid development, and sensitivity, current in vivo screening measures commonly utilize embryonic fish as toxicity models such as the fish embryo toxicity (FET) test. Previous research from our lab identified that larval zebrafish exposed to the antihistamine diphenhydramine (DPH) demonstrate increased mortality, uptake, and behavioral toxicity when compared to the embryonic stage. However, whether molecular initiation events influenced such age-specific differences was not investigated.

We examined this research gap by analyzing changes in protein expression and behavior of zebrafish exposed to DPH at sublethal concentrations across embryonic and early larval stages. Analysis of photolocomotor behavior confirmed previously observed dose-dependent responses to DPH, and age-specific responses differed following DPH exposure. Proteomic analysis identified >6300 proteins (at 5 % false discovery rate), resulting in differential expression of proteins implicated in morphogenesis, angiogenesis, and neural development. By contrasting changes in behavior and whole-body protein expression across different developmental and exposure conditions, this study provides a basis to further examine how age-specific sensitivities affect early life-stage response to toxicants.

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Triclosan exposure induces immunotoxic impacts by disrupting the immunometabolism, detoxification, and cellular homeostasis in blood clam (Tegillarca granosa)

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Abstract

Omnipresent presence of triclosan (TCS) in aqueous environment puts a potential threat to organisms. However, it's poorly understood about its immunometabolic impacts of marine invertebrates. In present study, we use a representative bivalve blood clam (Tegillarca granosa) as a model, investigating the effects of TCS exposure at 20 and 200 μg/L for 28 days on immunometabolism, detoxification, and cellular homeostasis to explore feasible toxicity mechanisms. Results demonstrated that the clams exposed to TCS resulting in evident immunotoxic impacts on both cellular and humoral immune responses, through shifting metabolic pathways and substances, as well as suppressing the expressions of genes from the immune– and metabolism–related pathways. In addition, significant alterations in contents

(or activity) of detoxification enzymes and the expression of key detoxification genes were detected in TCS-exposed clams. Moreover, exposure to TCS also disrupted cellular homeostasis of clams through increasing MDA contents and caspase activities, and promoting activation of the apoptosis–related genes. These findings suggested that TCS might induce immunotoxic impacts by disrupting the immunometabolism, detoxification, and cellular homeostasis.

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Effects of polystyrene nanoplastics on apoptosis, digestive enzymes, and intestinal histological structure and flora of swamp eel (*Monopterus albus*)

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Abstract

Nanoplastics (NPs) in the environment have attracted attention worldwide as a new class of pollutant. However, their impacts on aquatic organisms are only beginning to be unraveled. The current study investigated the toxic effects and mechanisms of action of polystyrene NPs (PS-NPs, 100nm) on liver apoptosis and the intestinal histological structure and flora of the economically important eel *Monopterus albus* after exposure to 0, 0.5, 1, 5, or 10 mg/L PS-NPs for 28 days. The results showed that intestinal trypsin and amylase of *M. albus* treated with 10 mg/L PS-NPs were significantly different from the control group ($p < 0.05$), and that the intestinal structure was slightly damaged. 16S rRNA sequencing showed that *Lactococcus garvieae* and *Bifidobacterium longum* were the dominant flora in the intestinal tract of *M. albus* treated with 10 mg/L PS-NPs. For genes expressions, *TGF-β*, *Hsp70*, *Caspase-9*, and *Bax* were significantly elevated in the liver of *M. albus* in the groups treated with PS-NPs compared with the control group, suggesting that PS-NPs triggered an immune response and apoptosis in liver tissue. In conclusion, the exposure to high concentrations of PS-NPs can produce apoptosis in the liver of *M. albus* and affect the immune response and intestinal bacterial community structure, leading to intestinal flora dysbiosis. The results of this study provide a scientific basis for understanding the toxic effects of PS-NPs on *M. albus* and potential ecological risk assessment strategies.

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Changes in life-history traits, antioxidant defense, energy metabolism and molecular outcomes in the cladoceran Daphnia pulex after exposure to polystyrene microplastics

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Abstract

Ubiquitous plastic pollution is a threat to the organisms' survival and ecosystem functions, especially in aquatic environments. Although there is increasing concern about the toxicity of microplastics, knowledge about the effects of microplastics of diverse sizes and adverse impacts on freshwater organisms is still limited. In the present study, the alteration in life-history traits, antioxidant defense and energy metabolism of the model freshwater zooplankton Daphnia pulex were assessed after chronic exposure to gradient concentrations (0.5, 1, 2 and 4 mg/L) of 500-nm polystyrene microplastics (PS-MPs). Changes in protein abundance were analyzed using proteomics after exposure to 1 mg/L of PS-MPs for 14 days. The results showed that ingested PS-MPs accumulated in the digestive tract of D. pulex. 2 and 4 mg/L of PS-MPs inhibited the survival function and 4 mg/L of PSMPs reduced the body length of D. pulex after 14 or 21 days of exposure. The exposure did not decrease the fecundity of D. pulex. After 14 days of exposure, PS-MPs changed the antioxidant capacity in a dose-dependent way and all concentrations of PS-MPs induced lipid oxidative damage. Exposure to 500-nm PS-MPs for 14 days decreased glucose and fructose contents and disturbed the lipid transport and utilization in D. pulex. Meanwhile, PS-MPs activated DNA repair and transcription regulation but inhibited lipid metabolism and response to unfolded or misfolded proteins. These results indicated that chronic exposure to 500-nm PS-MPs negatively affected D. pulex and showed similar toxic mechanisms to smaller nano-sized microplastics. Exposure to 500-nm PS-MPs resulted in restricted resources such as inhibited antioxidant capacity or energy metabolisms and D. pulex showed a potential trade-off among life-history traits to maintain fecundity at the cost of self-maintenance. The present study offers perspectives for understanding the differences in ecological effects caused by microplastics of different sizes.

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Toxicity of antimony to Daphnia magna: Influence of environmental factors, development of biotic ligand approach and biochemical response at environmental relevant concentrations

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Abstract

Acute toxicity of antimony pentavalent to neonatal Daphnia magna and the influence of water quality parameters were investigated, and enzymatic activities of organisms at environmentally relevant levels of antimony were determined. EC50 values of antimony to neonatal D. magna were 90.3 and 63.8 mg/L at 24 and 48 h of exposure, respectively. Dissolved organic matter (FA and HA) and cation (Ca2+, Mg2+ or Na+) had significant protective effects on D. magna against antimony toxicity. With increasing pH in the

range from 7.4 to 8.5, increase of EC50 were observed due to the competition of OH- on biotic ligands. Based on the biotic ligand model (BLM) concept, stability constants for the binding of Sb(OH)-6 and OH- to the biotic ligand were estimated, and the LogKXSb(OH)6 and LogKXOH- were 3.137 and 2.859, respectively. Moreover, antimony exposure in low concentrations significantly increased MDA levels and maybe exert oxidative stress to the organisms. Antimony can also induce toxicity in D. magna by affecting oxidative stress and neurotransmitter systems. The relatively comprehensive toxicological data can contribute to the toxicity prediction and ecological risk assessments of antimony.

711

Microcystin-LR induces estrogenic effects at Environmentally relevant concentration in black-spotted pond frogs (*Pelophylax nigromaculatus*): *in situ, in vivo, in vitro,* and *in silico* investigations

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Abstract

Harmful cyanobacterial blooms are frequent and intense worldwide, creating hazards for aquatic biodiversity. The potential estrogen-like effect of Microcystin-LR (MC-LR) is a growing concern. In this study, we assessed estrogenic potency of MC-LR in black-spotted frogs through combined field and laboratory approaches. In thirteen bloom areas of Zhejiang province, China, the MC-LR concentrations in water ranged from 0.87 to 8.77 μg/L and were correlated with sex hormone profiles in frogs, suggesting possible estrogenic activity of MC-LR. Tadpoles exposed to 1 μg/L, an environmentally relevant concentration, displayed a female-biased sex ratio relative to controls. Transcriptomic results revealed that MC-LR induces numerous and complex effects on gene expression across multiple endocrine axes. In addition, exposure of male adults significantly increased the estradiol (E2)/ testosterone (T) ratio by 3.5-fold relative to controls. Downregulation of genes related to male reproductive endocrine function were also identified. We also showed how MC-LR enhances expression of specific estrogen receptor (ER) proteins, which induce estrogenic effects by activating the ER pathway and HPG axis. In aggregate, our results reveal multiple lines of evidence demonstrating that, for amphibians, MC-LR is an estrogenic endocrine disruptor at environmentally relevant concentrations.

Because MC-LR affects large areas of aquatic systems worldwide, the ecological consequences of MC-LR may be much more dramatic than previously assumed, especially if MC-LR is indeed an estrogenic endocrine disruptor. This study presented here support the need for a shift in MC-LR risk assessment, provides multiple lines of evidence across levels of biological organization showing that environmentally relevant levels of MC-LR cause estrogenic endocrine disruption. Experimental findings were also consistent with observed patterns of feminization in the field. Studies linking estrogenic effects like those observed here with population-level consequences are badly needed to understand whether MC-LR is a hazard for other species persistence.

746

Determination of the Optimal Sample Size for Medaka Fish Behavioral Assessment by the Bootstrap Method

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Abstract

Even without causing immediate death, environmental pollutants can lead to "ecological death" by altering behavior and reducing individual or population numbers (Scott and Sloman, 2004). Recently, the use of behavioral tests with aquatic organisms, particularly fish, has become more prominent in evaluating waterborne pollutants. However, the reproducibility of these tests is often questioned due to individual behavioral variations. Although previous studies, including ours, have increased the number of observed individuals to address this issue, the statistically optimal sample size remains undetermined. Our study aimed to determine the optimal sample size for behavioral tests in medaka (Oryzias latipes), accounting for individual behavioral diversity. We tested 121 medaka fish (68 males, 53 females) using the Open Field Test, Peek-A-Boo Test (Takai et al., 2023), Sociability Test (Takai et al., 2022), and Color Preference Test in a glass tank (19 cm × 19 cm × 19 cm). In the Peek-A-Boo test, the median time for fish to approach the predator picture was 102 seconds (mean 100.5 ± 59.7 seconds, relative standard deviation 59.4%). The bootstrap analysis showed that observing 22 or more fish resulted in a mean and median change rate within 10%, with a relative standard deviation around 60%, indicating that observing 22 or more individuals yields reproducible results that reflect individual behavioral characteristics. This study concludes that while 22 or more test fish can produce reproducible results in behavioral tests like the Peek-A-Boo test, this number is not optimal for animal welfare. Future behavioral tests should aim to develop methods that accurately assess behavioral effects with fewer organisms, balancing the need for reliable behavioral indicators in toxicity evaluation with animal welfare concerns.

750

6PPD and its quinone metabolite 6PPD-Q at environmental concentrations induce lipid metabolism disorder in the liver of frog

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Abstract

6PPD and its oxidation product 6PPD-Q has been widely detected in aquatic environments. Recently 6PPD-Q has been shown to be lethally toxic to salmonid silverfish. However, its toxicity is species-

different, more researches should be carried out on more organisms, such as frogs. Here, male black-spotted frogs (Pelophylax nigromaculatus) were exposed to environmentally relevant concentrations (0, 1, and 10 μg/L) of 6PPD or 6PPD-Q for 21 days; biochemical analyzes, metabolomics, molecular docking, and gene expression assays followed. 6PPD and 6PPD-Q bioaccumulated in the liver in a dose-dependent manner. Furthermore, exposure to 10 μg/L 6PPD and 6PPD-Q led to reduction in liver body ratios. Furthermore, metabolomics analyzes revealed that 6PPD and 6PPD-Q induced differential expression of metabolites in pathways mainly enriched in unsaturated fatty acid biosynthesis, arachidonic acid metabolism, and linoleic acid metabolism. Exposure to 10 μg/L 6PPD and 6PPD-Q led to a rise in LDL-C levels by 4.49 and 4.88 times, TC levels by 2.22 and 4.35 times, and TG levels by 1.90 and 2.25 times. In addition, 6PPD-Q can affect lipid metabolism by inhibiting the transcription of lipolysis-related genes and promoting intrahepatic lipid accumulation. Finally, we modelled the binding of the key proteins PPARα and PPARγ to 6PPD and 6PPD-Q and showed binding energies of -7.6 kcal/mol and -8.0 kcal/mol, -7.6 kcal/mol and -7.6 kcal/mol, respectively. In conclusion, our study reveals 6PPD and its quinone metabolite 6PPD-Q at environmental concentrations induce lipid metabolism disorder in the liver of frog. The toxic effects of 6PPD and 6PPD-Q exposure on the liver of the black spotted frog, and improves our understanding of the health risks of 6PPD and 6PPD-Q in amphibians.

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Hexafluoropropylene oxide trimer acid (HFPO-TA) disrupts sex differentiation of zebrafish (*Danio rerio*) via an epigenetic mechanism of DNA methylation

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Abstract

Hexafluoropropylene oxide trimer acid (HFPO-TA), a novel alternative to perfluorooctanoic acid, has been proved to have estrogenic effects. However, it is not known whether it could disrupt the sex differentiation of fish during the gonadal development. Therefore, in this study, zebrafish were exposed to HFPO-TA from 2 hours post fertilization (hpf) to 60 days post fertilization (dpf) in order to investigate its effects on the sex differentiation. The results indicated that HFPO-TA exposure disrupted steroid hormone homeostasis, delayed gonadal development in both females and males, and resulted in a female-skewed sex ratio in zebrafish. The HFPO-TA exposure up-regulated the gene expressions of *cyp19a1a*, *esr1*, *vtg1* and *foxl2*, while down-regulated those of *amh*, *sox9a* and *dmrt1*. These suggested that HFPO-TA dysregulated the expressions of key genes related to the sex differentiation of zebrafish, promoted the production and activation of estrogens, and further induced the feminization. Furthermore, it is interesting to find the promoter hypomethylation of *cyp19a1a* and promoter hypermethylation of *amh* in male zebrafish, which were proved to be negatively correlated with their gene expressions. These indicated that HFPO-TA dysregulated the expressions of these key genes via the DNA methylation in their promoters. Therefore, the HFPO-TA exposure disrupted the sex differentiation of zebrafish via an epigenetic mechanism of DNA methylation, and ultimately resulted in the female-skewed sex ratio. Overall, this

study proved adverse effects of HFPO-TA on the sex differentiation of fish, and provided novel insights into the underlying epigenetic mechanism.

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Assessment of hepatopancreas toxicities in the white shrimp, *Litopenaeus vannamei*, after exposure to sulfamethoxazole (SMX) and tire microplastics (TMPs), alone or in combination

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Abstract

The hepatopancreas, as the metabolic center of crustacean invertebrates, plays crucial roles in metabolic detoxification and nutrient storage. Although the impacts of the two ubiquitous pollutants, sulfamethoxazole (SMX) and tire microplastics (TMPs), on environmental pollution and aquatic organisms have increasingly attracted attention, little is known about their toxicities on the hepatopancreas, especially lipid metabolism, of crustaceans. In this study, we exposed a commercially important crustacean species (*Litopenaeus vannamei*) to SMX and TMPs, alone or in combination, for 14-days. Then, the effects of SMX and TMPs exposure were evaluated by histological observation as well as quantification of hepatopancreatic lesion- and lipid metabolism-related parameters. In addition, to reveal potential mechanisms underlying the hepatoxicity observed, the accumulation of SMX in the shrimp and the comparative transcriptomic were also investigated. Our results showed that with exposure of the whiteleg shrimp to the pollutants tested, (1) the hepatopancreas was evidently histological injured and the hepatopancreatic lesion markers (alcohol dehydrogenase, aspartate aminotransferase and alanine aminotransferase) marked elevated; (2) the number of lipid droplets increased in the hepatopancreas and the fatty acid composition changed; (3) the activities of fatty acid synthetase, ATP-citrate lyase, acetyl-CoA carboxylase and the content of triglyceride and total cholesterol tended to increase and activity of lipase decreased; (4) the fatty acid synthesis-related pathways up-regulated, fatty acid decomposition-related pathways down-regulated, and oxidative stress- and detoxification-related pathways obviously disordered; (5) a significant amount of SMX accumulated in shrimp treated with SMX-containing seawater. Overall, the data illustrated that SMX-TMPs co-exposure was more toxic than single exposure to these pollutants. Meanwhile, these results also demonstrated that SMX and TMPs may exert hepatotoxic impacts on *L. vannamei* by accumulating *in vivo* and inducing physiological disorders of lipid metabolism and detoxification, which could carry out a severe threat to the wellness of this important crustacean species.

854

Ecotoxicological effects of nonylphenol and cadmium exposure individually and combined on zebrafish (Danio rerio)

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Abstract

Endocrine disrupting chemicals (EDCs) have widespread environmental distributions, yet study of the combined ecotoxicology of phenolic and heavy metal endocrine disruptors on organisms is limited. In this study, different concentrations of nonylphenol (NP) and cadmium (Cd) were used for 28 days in single and combined exposure experiments of zebrafish and the histological changes in the liver, antioxidant capacity and transcriptional responses were evaluated. The results indicated that NP and Cd both induced severe liver tissue damage in a concentration-dependent manner. Combined long-term exposure to high concentrations of NP and Cd significantly increased the total antioxidant capacity of liver tissue. The significant effects of NP exposure were mainly on the endocrine system, lipids, carbohydrate and amino acid metabolic pathways. The differential expression of genes increased significantly with combined exposure to NP and Cd, and more genes were down-regulated than up-regulated, resulting in more repressive genes that affect DNA damage repair. This study contributes to the understanding of the health risks to aquatic organisms from the co-existence of phenols and heavy metal endocrine disruptors.

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Toxicity Prediction and Risk Assessment of Per- and polyfluoroalkyl substances (PFASs) for Threatened and Endangered (T&E) Fishes

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Abstract

The number of Threatened and Endangered (T&E) species in the IUCN Red List has reached nearly 45,000, with about 25% being freshwater fish. Per- and polyfluoroalkyl substances (PFAS) are compounds in which one or more hydrogen atoms on the carbon chain are partially or fully replaced by fluorine atoms. Numerous studies have shown that PFAS are seriously polluting aquatic environments and causing harm to aquatic organisms. Due to the inability to directly conduct toxicity experiments on T&E species, there is a lack of toxicity data on PFAS for these species, making risk assessment

challenging. In recent years, the development of computational toxicology has provided new tools and methods to address this issue.

This study, using growth, development, and morphological toxicity as examples, established predictive models for the toxicity of PFOA, PFOS, PFBA, PFHxA, PFHxS, PFNA, and PFDA to T&E fishes in the Yangtze River using machine learning models (Random Forest (RF), Artificial Neural Network (ANN), XGBoost) and QSAR-ICE models. It then calculated the predicted no effect concentration (PNEC) for each PFAS, assessing the ecological risk of PFAS in the habitats of T&E fishes in the Yangtze River.

The results showed:

1. RF exhibited the best fit among the three machine learning models, with R^2 values of 0.95 and 0.64 for the training set and validation set, respectively, and reliable results in 10-fold cross-validation (Q^2 = 0.70) and external data set validation (Q^2_{ext} = 0.80).

2. The species-family level QSAR-ICE model had good indicators, with R^2 (0.71-0.90), MSE (0.19-0.62), and a cross-validation success rate (67%-88%), reliably predicting the toxicity data at the family level for T&E fishes.

3. Both models' predictions showed that the genus *Acipenser* exhibited high sensitivity to multiple PFAS, consistently falling below the 5th percentile in species sensitivity distribution curves for several PFAS.

4. Risk quotient (RQ) assessment of the habitats of T&E fishes in Yibin, Yichang, Poyang Lake, and Shanghai indicated that PFHxA had the highest risk in Yibin. However, PFAS pollution in the habitats of T&E fishes in the Yangtze River is still within a controllable range, with little impact on their growth and development.

This study provides a new method for obtaining chronic toxicity data and conducting risk assessments for T&E fishes in aquatic environments.

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The effects of exogenous nucleobases on the growth and microcystins production of *Microcystis aeruginosa*

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Abstract

Nucleobases, as structural components of DNA and RNA, play an essential role in dissolved organic nitrogen (DON) in natural waterbodies. The effects of nucleobases on the growth and microcystins (MCs) production of *Microcystis aeruginosa* were investigated with guanine (G), adenine (A), uracil (U), thymine (T) and cytosine (C) as sole nitrogen sources. The algal cell density, pH, Chl-*a*, phycobiliproteins, soluble protein, extracellular nitrogen concentration and five MCs generation quotas were measured, along with comprehensive transcriptomic and metabolomic profiling. The results showed that *Microcystis aeruginosa* utilized 8.0 mg/L of G, 8.0 mg/L of A, 1.59 mg/L of U, 0.95 mg/L of T, and 1.98 mg/L of C after 6 days of incubation. There was no significant difference in the intracellular content of G and A in algae cells supplied with G and A as nitrogen sources; However, the intracellular content of U, T, and C was significantly higher in algae cells supplied with U, T, and C as nitrogen sources. Further research showed that G and A were converted into other forms in the medium before entering the cells, with ammonia and urea collectively accounted for over 50%. When U, T, and C served as the sole nitrogen source, the cellular C/N ratio is markedly elevated compared to the control group with nitrate as the sole nitrogen. Compared to the control groups, algal cell density, pH, Chl-*a*, soluble protein, phycocyanin (PC) and allophycocyanin (APC) were not substantially different in G and A, but they were significantly lower in U, T, and C. Furthermore, MCs quotas in G and A were marginally lower than those in the control group, whereas MCs quotas in U, T, and C were significantly lower. Among these, MC-RR, the congener with the highest nitrogen content, experienced the greatest reduction in production. Transcriptomic and metabolomic integrative analysis revealed that most genes related to nitrogen metabolism, amino acid biosynthesis and metabolism, ABC transporters, MCs biosynthesis were upregulated in U, T, and C to maintain normal biological activity, while most genes related to photosynthesis, energy metabolism and carbon fixation were downregulated to save energy. In addition, regulated pathways are associated with purine and pyrimidine metabolism, amino sugar and nucleotide sugar metabolism, and aminoacyl-tRNA biosynthesis. The results may help explore the physiological and molecular regulatory roles of nitrogen in the formation of HABs and MCs production.

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Evidence of strobilurin fungicides and their metabolites in Dongjiang River ecosystem, southern China: Bioaccumulation and ecological risks

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Abstract

Despite the widespread application of strobilurin fungicides (SFs) in agriculture, little is known about their distribution and bioaccumulation in aquatic ecosystems. In this study, the concentrations of 12 SFs and two of their metabolites were determined in abiotic (water and sediment; n = 83) and biotic (plant, algae, zooplankton, and fish; n = 123) samples collected from a subtropical freshwater ecosystem, namely, Dongjiang River wetland, in southern

China. Among the 12 SFs measured, azoxystrobin (AZ) was the major fungicide found in surface water (median: 2.20 ng/L) and sediment (0.064 ng/g dry wt.). Azoxystrobin acid (AZ-acid), a metabolite of AZ, was the major analyte in the plant samples and had a median concentration at 0.36 ng/g dry wt. In algae and zooplankton, (Z)-metominostrobin was the predominant fungicide and had median concentrations of 3.52 and 5.55 ng/g dry wt., respectively. In fish muscle, dimoxystrobin (DIMO) was the major SF and had a median concentration of 0.47 ng/g dry wt. The bioconcentration factor (BCF) values of AZ-acid, trifloxystrobin (TFS), and pyraclostrobin (PYR) in algae and zooplankton and AZ-acid, PYR, TFS, TFS-acid, picoxystrobin, and DIMO fish muscle exceeded 1000 L/kg (algae, zooplankton, and fish concentrations were expressed on a dry basis), suggesting that these fungicides can accumulate in biota. A positive association between log BCFs of SFs fish and logKow of SFs and a negative correlation between log BCFs and the log solubility index were observed. Additionally, the risk quotient (RQ) was calculated to evaluate the potential ecotoxicological risk of SFs to different aquatic organisms (algae, zooplankton, and fish). The PYR and DIMO concentrations at 19 sampling sites had RQ values $>$0.1, indicating moderate ecotoxicological risks to aquatic organisms. This study is the first to document the widespread occurrence of SFs and their metabolites in aquatic ecosystems and to elucidate the bioaccumulation potential of SFs in aquatic organisms.

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Chronic Neurotoxic Effects of Environmental Concentration of Fluoxetine Exposure on Zebrafish: From Adult to Offspring

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Abstract

The COVID-19 pandemic has increased environmental contamination of antidepressant pharmaceuticals, posing a threat to the survival and development of non-target aquatic organisms as well as the stability of aquatic ecosystems. However, literature is scarce on the chronic and eco-toxic effects of antidepressants, highlighting an urgent need for relevant studies. In light of this, we aim to investigate the neurotoxic effects and molecular mechanisms associated with chronic exposure to low-dose of fluoxetine (FLX) in zebrafish through the "gut-brain axis" and elucidate its intergenerational toxic impacts. Following a 28-day exposure to FLX at a concentration of 50ng/L, adult female zebrafish underwent behavioral observation post-exposure before being mated with normal males to produce F1 larvae. HE staining and Illumina technology were used to determine histopathological damage and transcriptome sequencing of the intestinal tissues, and 16s rRNA sequencing was performed on the intestinal contents. Analysis revealed a significant reduction in condition factors as well as intestinal villous epithelial goblet cell count within the treatment group when compared to controls. Transcriptome analysis identified 409 differential expressed genes (DEGs), with KEGG enrichment revealing eight significantly enriched pathways associated with these DEGs. In addition, 16s rRNA data indicated a reduced relative abundance of *Proteobacteria* and *Actinobacteriota* alongside an increased presence of *Fusobacteriota* and *Bacteroidota* within the treatment group. Notably elevated mortality rates along with decreased hatching rates and body length were observed among F1 offspring from treated groups; changes in oxidative stress indexes further suggest potential intergenerational effects. The findings offer empirical backing for enhancing the assessment of environmental health risks associated with emerging drug contaminants. Correspondence: panchenyuan@shu.edu.cn (C. Pan) & mingyang@shu.edu.cn (M. Yang)

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Effects of eutrophication on the production and bioavailability of methylmercury in the surface water of reservoirs on a subtropical plateau

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Abstract

Eutrophication of aquatic ecosystems is a serious problem that can lead to changes in the bioavailability of mercury (Hg) and methylmercury (MeHg); however, few studies have generated quantitative estimates of the effects of eutrophication on the bioavailability Hg and MeHg, but has not been clear yet. Here, we determined the concentrations of total mercury (THg) and methylmercury (TMeHg) in samples of both surface water and phytoplankton collected from five reservoirs on the Yunnan–Guizhou Plateau, Southwest China with contrasting trophic states. The concentrations of THg and TMeHg in surface water ranged from 2.1 to 23 ng/l and from 0.02 to 0.65 ng/l, respectively. Large-scale variation in phytoplankton was also observed in these reservoirs, with THg ranging from 29 to 290 ng/g and TMeHg ranging from 0.56 to 11 ng/g. THg in surface water was highest in November and low in April and August. By contrast, TMeHg in surface water was highest in April, followed by November, and lowest in August. Both chlorophyll *a* and the trophic level index (TLI) were strongly positively correlated with MeHg and the methylation efficiency (estimated as the percentage of THg as TMeHg, %TMeHg) in surface water (coefficients of determination of 0.89 and 0.78, respectively). However, a negative correlation between TLI and %TMeHg in phytoplankton was observed. These findings indicate that an increase in nutrient concentrations could increase the %TMeHg of water but decrease the %TMeHg of phytoplankton in eutrophic reservoirs. Generally, our results show that eutrophication has a complex effect on the fate of MeHg in reservoirs on a subtropical plateau.

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Key components inducing hormetic effects in eight-components of skin care product mixtures to *Vibrio qinghaiensis* sp.-Q67

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Abstract

Previous studies have found that the active components in skin care products (SCPs) can induce the hormesis to *Vibrio qinghaiensis* sp.-Q67 (Q67). However, the relationship between the hormesis of various components and mixtures in SCPs have not been studied. In this study, time-dependent microplate toxicity analysis was used to test the luminescence inhibition toxicity of Q67 under five exposure time (0.25, 3, 6, 9 and 12 h). The results showed that two components (1,1′-Oxydi-2-propanol, Polyethylene glycol 400) showed monotone S-shaped concentration-response curve (CRCs), six components (D-Mannitol, EDTA disodium salt, Ethanol, Glycerol, Phenoxyethanol, and Tranexamic acid) showed J-shaped CRCs with stimulatory effect, and six ternary mixtures composed of any J-shaped and two S-shaped showed different hormesis phenomena. The mixture containing full-time hormesis components produced hormesis at all times, while the maximum stimulatory effect were lower than that of a single component. In the ternary mixture, the synergistic toxicity interaction plays a leading role. Through contribution effect and synergism-antagonism heatmap analysis, D-mannitol, EDTA disodium salt and Tranexamic acid were identified as the key components affecting the stimulating effect of eight-membered mixtures. This study can provide a reference for the analysis and screening of key components of hormesis.

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Exposure to Thimerosal Induces Behavioral Abnormality in The Early Life Stages of Zebrafish *via* Altering Amino Acid Homeostasis

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Abstract

Thimerosal (THI), a widely used mercury-based preservative, has become an important source of organic mercury pollutants in aquatic ecosystems. However, information about its adverse effects on fish is extremely scarce. In this study, we exposed zebrafish embryos to THI at 0 (control), 5.0, and 50 ng/L from 0 to 5 days post fertilization (dpf), and examined variations in their survival, development, behavior, free amino acid contents, and monoamine neurotransmitter levels. The result showed that THI did not significantly alter the survival, heart rate, and hatching time in zebrafish embryos. However, exposure to THI significantly elevated the average swimming velocity in the dark periods (136-154% of control) and duration of thigmotaxis in the light period (141-142% of control) in zebrafish larvae (at 5 dpf). Besides, THI also significantly altered the amino acid contents (51-209% of control) and monoamine levels (70-154% of control) in zebrafish larvae, depending on the exposure concentrations. Furthermore, correlation analysis detected several significant correlations between behavioral traits and the contents of neurotransmission-related amino acids and monoamine neurotransmitters. Our results suggested that THI, even at environmentally relevant concentrations, could disrupt the behavior of zebrafish larvae by altering their amino acid and related neurotransmitter homeostasis. Those findings would help better understand the toxicity of THI to fish and provide theoretical foundations for assessing its ecological risks to aquatic ecosystems.

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Marine Ecotoxicology and Climate Change: Understanding the Influence of Multiple Stressors on Chemical Effect Thresholds

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Abstract

Over the past two decades, my research has focused on developing environmental quality benchmarks, such as water and sediment quality guidelines, to regulate and manage chemical contaminants in Europe and China. The primary goal is to determine the effect threshold of a chemical (referred to as the trigger value) and ensure that its environmental concentration remains below this threshold, thereby safeguarding the aquatic ecosystem and its inhabitants. However, as I delved deeper into this field, I discovered numerous unresolved challenges associated with establishing effect thresholds for chemicals. In this presentation, I will specifically address and emphasize some of the significant obstacles encountered in determining trigger values for protecting aquatic ecosystems from chemical pollution, considering environmental factors such as pH, salinity, and temperature (termed multiple stressors) that are inherently influenced by climate change. Finally, I will propose potential solutions and advocate for increased research efforts to enhance the ecological realism in establishing trigger values, ultimately leading to more effective environmental protection measures.

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Local thermal adaption mediates the sensitivity of Daphnia magna to nanoplastics under global warming scenarios

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Abstract

The toxicity of nanoplastics at environmentally relevant concentrations has received widespread attention in the context of global warming. Despite numerous studies on the impact of mean temperature (MT), the effects of daily temperature fluctuations (DTFs) on the ecotoxicity of nanoplastics remains largely unexplored. Moreover, the role of evolutionary adaptation in assessing long-term ecological risks is

unclear. Here, we investigated the effects of polystyrene nanoplastics (5 μg L-1) on Daphnia magna under varying MT (20 ◦C and 24 ◦C) and DTFs (0 ◦C, 5 ◦C, and 10 ◦C). Capitalizing on a space-for-time substitution approach, we further assessed how local thermal adaptation affect the sensitivity of Daphnia to nanoplastics under global warming. Our results indicated that nanoplastics exposure in general reduced heartbeat rate, thoracic limb activity and feeding rate, and increased CytP450, ETS activity and Hgb concentrations. Higher MT and DTFs enhanced these effects. Notably, clones originating from their respective sites performed better under their native temperature conditions, indi- cating local thermal adaptation. Warm-adapted low-latitude D. magna showed stronger nanoplastics-induced increases in CytP450, ETS activity and Hgb concentrations under local MT 24 ◦C, while cold-adapted high- latitude D. magna showed stronger nanoplastics-induced decreases in heartbeat rate, thoracic limb activity and feeding rate under high MT than under low MT.

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Integrate transcriptomic and metabolomic analysis reveals the underlying mechanisms of behavioral disorders in zebrafish (*Danio rerio)* induced by imidacloprid

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Abstract

Imidacloprid, a widely used neonicotinoid insecticide, poses a significant threat to aquatic ecosystems. Behavior is a functional indicator of the net sensory, motor, and integrative processes of the nervous system and is presumed to be more sensitive in detecting toxicity. In the present study, we investigated the behavioral effects of imidacloprid at the level of environmental concentrations (1, 10 and 100 μg/L) for a constant exposure to zebrafish adults, and performed the integrated transcriptomic and metabolomic analysis to analyze the molecular mechanism underlying behavioral effects of imidacloprid. Our results show that imidacloprid exposure significantly induce behavioral disruptions characterized by anxiety, depression, and reduced physiological function including exploratory, decision, social interaction and locomotor activity. Integrated transcriptomic and metabolomic analysis indicate that the disruption of circadian rhythm, metabolic imbalance of arginine and proline, and neurotransmitter disorder are the underlying molecular mechanisms of behavioral impairment induced by imidacloprid. The “gene-metabolite-disease” network consisted by 11 metabolites and 15 genes is associated human disease Alzheimer’s disease (AD) and schizophrenia. Our results confirm the behavioral impairment induced by imidacloprid at environmental concentrations for constant exposure. The identified genes and metabolites can be used not only to illustrate the underlying mechanisms, but also can be developed as biomarkers in determining the ecological risk of imidacloprid to aquatic organisms even *Homo sapiens*.

18. Marine Pollution and Ecotoxicology

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Species-Dependent Malformation and Mechanical Weakening in Algal Cell Walls Reveal Microplastic Disturbance at the Nanoscale

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Abstract

Microplastics (MPs) are increasingly prevalent in coastal waters where algal communities thrive. Despite numerous recent studies highlighting MP toxicity to algae from physiological and molecular dimensions, it is still unclear how MPs may affect algal cell walls by causing physical disruptions down to the nanoscale. Here, we specifically target the morphological and mechanical changes in four distinct algae exposed to MPs of varying sizes. With high-resolution imaging, we elucidated the diverse MP–algae interaction patterns mediated by cellular appearance. Quantitative analysis via image processing further confirmed that smaller MPs are associated with greater height fluctuation and nanostructural irregularity in the cell surface. Moreover, on non-porous cell walls, we detected abnormal creases and pit-like depressions that are mechanically fragile, as evidenced by their low modulus and unconstant adhesion compared to adjacent intact areas. The magnitude of these malformations and mechanical weakening in cell surfaces showed significant interspecies variability and correlations with MP size. This work provides visual and nanometric evidence on how individual algal cells suffer from MPs at the physical level, unveiling a species-specific susceptibility to MPs among marine phytoplankton with distinct surface characteristics.

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Statistical approaches for estimating no-effect toxicity concentrations in ecotoxicology

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Abstract

The primary concern of most environmental regulatory risk assessments is whether there is a level of toxicity that poses a risk to the survival of a population. Generally, in a protective-risk management framework, the goal is to determine the concentration at which there can be considered no adverse effects on the ecosystem.

A range of new statistical approaches is being developed and/or adopted in ecotoxicology that, when combined, can greatly improve the estimation of no-effect toxicity values from concentration–response (CR) experimental data. In particular, we compare the existing no-effect-concentration (NEC) threshold-based toxicity metric with an alternative no-significant-effect-concentration (NSEC) metric suitable for when CR data do not show evidence of a threshold effect. Using a model- averaging approach, these metrics can be combined to yield estimates of N(S)EC and of their uncertainty within a single analysis framework. The outcome is a framework for CR analysis that is robust to uncertainty in the model formulation, and for which resulting estimates can be confidently integrated into risk assessment frameworks, such as the species sensitivity distribution (SSD).

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bayesnec: An R Package for CR Modelling and Estimation of toxicity metrics

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Abstract

The bayesnec package has been developed for R to fit concentration(dose) - response curves (CR) to toxicity data for the purpose of deriving no-effect-concentration (NEC), nosignificant- effect-concentration (NSEC), and effect-concentration (of specified percentage ‘x’, ECx) thresholds from non-linear models fitted using Bayesian Hamiltonian Monte Carlo (HMC) via brms (Bürkner 2017, 2018) and rstan (Stan Development Team 2021a) or cmdstanr (Gabry and Češnovar 2022). In bayesnec it is possible to fit a single model, custom models-set, specific model-set or all of the available models. When multiple models are specified, the bnec function returns a model weighted average estimate of predicted posterior values. A range of support functions and methods is also included to work with the returned single, or multi-model objects that allow extraction of raw, or model averaged predicted, NEC, NSEC and ECx values and to interrogate the fitted model or model-set. By combining Bayesian methods with model averaging, bayesnec provides a single estimate of toxicity and associated uncertainty that can be directly integrated into risk assessment frameworks.

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The Progress and Prospects of the Global Estuaries Monitoring Programme

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Abstract

Currently, more than 100,000 chemical substances are used in our daily lives and industries. Among them, 4,000 pharmaceuticals are used for preventing and treating human and animal diseases. Many of these chemicals eventually find their way into estuaries through various pathways, such as rivers, surface runoff, and partially treated wastewater discharged from treatment plants. There is a lack of information at a global level regarding the occurrence and environmental risks of different chemical contaminants in urbanized estuaries, particularly in Africa, South America, Southeast Asia, and Oceania coastal areas.

To address this issue, the Global Estuaries Monitoring (GEM) Programme aims to develop standardized methods for sampling, extracting, detecting, and quantifying priority chemical contaminants in water samples collected from major urbanized estuaries worldwide. These methods will enable a scientifically sound comparison of contamination profiles across various estuaries.

The GEM Programme is one of the first Ocean Decade Programmes endorsed by the United Nations Decade of Ocean Science for Sustainable Development (2021-2030) on June 8, 2021. The study focuses on six key aspects, including capacity building, standardization of research methods, promotion of best practices in pollution monitoring and control, data sharing, co-designing research strategies, and revealing the estuary health status.

Over the past two years, we have been fully committed to method development and establishing connections with global collaborators. GEM has already developed and verified a robust analytical method to quantify 65 pharmaceuticals in river, estuary, and marine water samples for the GEM Programme, using only a small sample volume. This allows for economical transportation of collected samples to State Key Laboratory of Marine Pollution in Hong Kong for chemical analysis. We have also received contributions from more than 160 estuaries across 54 countries. Currently, samples are being collected from these major urbanized estuaries globally.

The GEM Programme aims to contribute to unveiling the global pollution situation and promoting best practices to combat pollution problems, thus achieving cleaner estuaries for a better and greener future. We warmly welcome everyone to share and contribute to the GEM programme.

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Assessment of the status of Emerging Contaminants in New Zealand

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Abstract

Emerging contaminants (ECs) are newly identified synthetic or naturally occurring chemicals detected in the environment and potentially hazardous to humans and ecosystems. This multidisciplinary research addressed concerns raised about the risk ECs pose in New Zealand.

We had 3 objectives:

1) confirm the presence of ECs and their risks,

2) develop a National Strategy to Manage Emerging Contaminants in New Zealand, and

3) engaged across multiple sectors to raise awareness and discuss solutions.

We used an effect-based monitoring (EBM) method to investigate ECs in water and sediment. Passive sampling devices (PSDs) were used to capture contaminants at low concentrations in water. The sample extracts were tested with a battery of in vitro bioassays covering main mechanisms of toxicity including genotoxicity, endocrine disruption, and bactericidal and herbicidal activities, as per the EBM protocol. The risk quotient results indicate high risk related to estrogenicity, dioxin-like and herbicidal activities particularly at sites downstream from municipal wastewater treatment plant discharges and landfills. Both estrogenic and herbicidal activities were elevated in the agricultural areas. The results are evidence that chemical contaminants persist in the New Zealand environment at levels that pose a risk to exposed biota.

A Strategy to Manage ECs in New Zealand was developed over 7 years and is now available. The Strategy elevated the need for the regional sector's science and technology strategy to acknowledge ECs, the need for clear leadership and the coordination and appropriate communication channels required to enable effective dissemination and uptake across a range of agencies and communities.

We focused on two catchments representing main land uses: an estuary in Southland in a mainly agricultural zone, and the highly urbanised Whau River in Auckland where we have long-lasting relationships with Māori, community and council. The programme included a National Advisory Panel with members from governments, industry and Māori to help guide implementing the outcomes. This cross sectoral network provided key mechanisms to communicate the outcomes generated through conferences, workshops, hui, research articles and reports.

The next step is to use Non-Targeted and Targeted Analyses to identify the ECs causing the biological effects. Once the ECs are known, the sources will be identified and solutions developed to reduce the risk to human and ecosystems.

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Contaminants of Emerging Concern in the Coastal Ecosystem of the Northern South China Sea

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Abstract

Rapid economic expansion, urbanization, and industrialization in the Greater Bay Area (GBA) of China contribute to a substantial release of various environmental pollutants, including contaminants of emerging concern (CECs) as a research hotspot, into the Pearl River Estuary and adjacent northern South China Sea (NSCS). Indo-Pacific humpback dolphin (*Sousa chinensis*) and finless porpoise (*Neophocaena phocaenoides*) are two resident marine cetacean species in the NSCS. As apex predators, cetaceans are susceptible to exposure to high amounts of pollutants, especially persistent ones, making them ideal biomonitors for tracing environmental pollutants on a large time scale. Here, we introduced two prominent groups of pollutants with persistence potential, per- and polyfluoroalkyl substances (PFASs) and halogenated flame retardants (HFRs), both comprising legacy substances as globally banned/restricted chemicals and manufactured replacements/alternatives as CECs. Target analysis and nontarget/suspect screening were applied to investigate PFASs and HFRs in Indo-Pacific humpback dolphins and finless porpoises stranded in Hong Kong waters over the past decade.

We found that: (1) significant increasing temporal trends were observed in the concentrations of two emerging PFASs, perfluoroethylcyclohexane sulfonate and 2,3,3,3-tetrafluoro-2-propanoate, indicating increasing pollution by these substances; (2) forty-four PFASs from nine classes were additionally identified via nontarget screening, among which fifteen compounds were reported for the first time in marine mammals; (3) significant decreasing temporal trends were observed in the concentrations of tetra-/penta-/hexa-bromodiphenyl ethers (tetra-/penta-/hexa-BDEs), probably because of their phasing out in China; and (4) eight brominated compounds were additionally identified via suspect screening, where a positive correlation was found between the concentrations of tetra-BDE and methyl-methoxy-tetra-BDE (Me-MeO-tetra-BDE), indicating the metabolism of tetra-BDE as a potential source of Me-MeO-tetra-BDE in marine mammals. Our results reveal the recent pollution status of PFASs and HFRs in the GBA of China, highlighting replacements/alternatives to be CECs and providing evidence for evaluating the effectiveness of various control measures on banned/restricted chemicals.

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An Overview of the Occurrence and Ecotoxicological Risk of Environmental Liquid Crystal Monomers in the Pearl River Estuary

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Abstract

The widespread use, recycling and disposal of electronic devices (e-devices) result in the release of numerous hazardous substances into the environment. Liquid crystal monomers (LCMs), which are key materials in the manufacture of liquid crystal display (LCD) panels, have recently raised significant concerns as a class of emerging contaminants related to e-waste. LCMs have been detected in sediment samples collected near e-waste recycling facilities. However, LCMs can be emitted at various stages throughout the lifecycle of e-device, including production, routine use, recycling, and disposal, leading to a significant input of environmental LCMs into aquatic environments. Using Hong Kong and the Pearl River Estuary as examples, we have demonstrated that LCMs emitted from household e-devices can enter the municipal sewage system and be discharged through the effluent from wastewater treatment plants, leading to the widespread occurrence of these harmful e-waste pollutants in coastal environments. Further investigation is urgently needed to assess the ecological impact of environmental LCMs on marine ecosystems and to develop active treatment and control measures for LCMs in sewage systems.

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Rapid Number-Mass Concentration Conversion and Environmental Transport Behavior of Marine Microplastics

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Abstract

Researchers have recognized land-originated microplastics as the primary sources of microplastics in the oceans, and the movement of atmospheric and riverine microplastics towards the sea is a global concern. However, there is a significant difference in how field occurrence investigations convey microplastic concentration (as number concentration) versus mass flux (as mass concentration). An immediate challenge is to develop effective conversion models that can establish a correlation between these two significant paradigms. Ultimately, we created a set of precise models for the conversion of microplastic mass, which we then applied to real environmental samples. Further, we present a comprehensive analysis of microplastics in the marine boundary layer along a cruise route spanning from the mid-Northern Hemisphere to Antarctica. We present data on both the number concentrations and the converted mass concentrations of microplastics in the Southern Ocean and Antarctica's inland environment. Our findings indicate that microplastics in the shape of fibers are transported more effectively than microplastics in the shape of fragments along the transect. Furthermore, the transport dynamics of microplastics are generally

comparable to those of non-plastic particles. Our research reveals that morphology is the primary factor that influences the transport of microplastics to distant regions in the marine environment.

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Entanglement of Daphnia magna by Fibrous Microplastics through “Hook and Loop” Action

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Abstract

Entanglement, often associated with the interaction of large marine plastics and larger animals, has not yet been reported in the context of microplastics (MPs) and small organisms. The primary objective of this study is to investigate if the entanglement is a relevant pathway of interaction between MPs and small zooplankton species, such as *Daphnia magna*, as well as to decipher the potential effects on the daphnid behavior and the underlying mechanisms. Hence, *D. magna* was exposed to fibrous MPs at concentrations ranging from 1 to 1000 items/mL for 7 days. Results revealed that the tail claws of *D. magna* exhibited entanglement with numerous fibers, prominently visible in the 100 items/mL treatment. Additionally, the swimming speed and projected area of swimming trajectories of daphnids significantly decreased in the 100 items/mL group compared with the control. On the first day of exposure, the swimming trajectories of daphnids in the control group covered approximately 33% of the observation dish, whereas those in the 100 items/mL group swam primarily in small areas near the walls, accounting for only about 3% of the dish area. However, the occurrence of entanglement and slow swimming was less pronounced in the 1000 items/mL group due to the aggregation of fibrous MPs. Scanning electron microscopy revealed that *D. magna* possessed a rich spine structure on the surface of their bodies, particularly on their antennae and tails. The entanglement interaction between spines and fibrous MPs bears a striking resemblance to the manufactured “hook and loop” structures of Velcro, which are widely utilized in shoes, bags, and clothing. Overall, the results of this research revealed that entanglement is observed in small animals exposed to fibrous MPs, highlighting the direct biological effects of MPs beyond ingestion. The entanglement can be likened to the “hook and loop” action due to the abundance of spine structures, a feature commonly found in various small animals. This warrants further investigation to understand if this non-ingestive interaction mechanism will be observed in other aquatic small organisms. The entanglement led to changes in the swimming behavior of daphnids, potentially affecting their ability to forage for food and increasing their vulnerability to predators. The extent to which entanglement and “hook and loop” action contribute to overall impact of MPs exposure is still open and merits further investigations.

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The Alteration of Toxicity in Marine Organisms by Micro and Nanoplastics, Co-Existing With Organic Chemicals at Environmentally Relevant Concentrations

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Abstract

Micro and nanoplastics (MNPs) as emerging contaminants have become a global environmental issue due to their small size and high bioavailability. However, there are still knowledge gaps regarding effects of co-existing pollutants on their toxicity to marine organisms at their respective environmentally relevant concentrations. Herein we investigated developmental toxicity, histopathological alterations caused by co-exposure of polystyrene nanoplastics (PS-NPs) and bisphenol A (BPA) to marine medaka, *Oryzias melastigma* and potential molecular mechanisms were explored. Embryos at 6 hours post-fertilization were exposed to 50-nm PS-NPs (55 μg/L) or BPA (100 μg/L) or co-exposed to a combination of both. Results showed that PS-NPs exhibited decreased embryonic heart rate, larval body length, and embryonic survival as well as larval deformities such as hemorrhaging and craniofacial abnormality. When co-exposed, BPA mitigated all the adverse developmental effects caused by PS-NPs. PS-NPs also led to an increase in histopathological condition index of liver with early inflammatory responses, while co-exposure of BPA with PS-NPs did not. Our data suggest that the toxicity reduction of PS-NPs in the presence of BPA might result from the decreased bioaccumulation of PS-NPs caused by the interaction between BPA and PS-NPs. We also investigated the accumulation and toxicity of benzo[a]pyrene (B[a]P, 0.4 nM), in the marine mussel *Mytilus galloprovincialis* over a 4-day of exposure with or without the presence of 10 μm polystyrene microplastics (PS-MPs) (10 particles/mL). The presence of PS-MPs significantly decreased B[a]P accumulation in soft tissues of *M. galloprovincialis* by approximately 6.7%. Single exposure of PS MPs or B[a]P decreased the mean epithelial thickness of digestive tubules and enhanced reactive oxygen species levels in haemolymph, while upon co-exposure the adverse impacts were alleviated. Real-time q-PCR results showed that most selected genes involved in stress response (*FKBP*, *HSP90*), immune (*MyD88a*, *NF-κB*) and detoxification (*CYP4Y1*) were induced for both single exposure and co-exposure. The co-presence of PS-MPs down-regulated the mRNA expression of *NF-κB* in gills compared with of B[a]P alone. Adverse outcomes for the co-existence of marine emerging pollutants under long-term conditions remain to be further validated.

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Enantioselective Toxicokinetics of Metoprolol and Venlafaxine in Marine Medaka

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Abstract

The increasing usage of pharmaceuticals worldwide and their incomplete removal by wastewater treatment has led to the widespread release of pharmaceutical residues into the aquatic environment. Metoprolol (MTP) is one of the most widely used *β*-blockers, and venlafaxine (VLF) is one of the most prescribed serotonin and norepinephrine reuptake inhibitors. Research have shown that both MTP and VLF exhibit considerable toxicity to aquatic organisms. More than 50% of currently marketed pharmaceuticals are chiral (such as MTP and VLF), and they often exhibit enantioselectivity in environmental distribution, fate, and ecotoxicity. However, there is still limited research on the uptake and depuration of chiral pharmaceuticals in marine organisms. Accordingly, the aims of the present study were to (a) provide first-hand data on the toxicokinetics of two chiral pharmaceuticals among different tissues of a model fish species marine medaka (*Oryzias* melastigma); (b) investigate the bioconcentration characteristics of chiral pharmaceuticals (MTP and VLF) from an enantiomeric perspective; and (c) identify possible pharmaceutical metabolites using a suspect screening analytical approach. The enantiospecific toxicokinetics of MTP and VLF, including uptake and depuration rate constants, depuration half-life ($t_{1/2}$), and bioconcentration factor (BCF), were reported for the first time, and the highest tissue-specific BCFs of the four enantiomers were all found in the eyes. The results of whole fish demonstrated *S*-VLF had a higher BCF than *R*-VLF, while no significant difference was observed in BCFs between *S*- and *R*-MTP. Different enantiomers showed different metabolic tendencies that *O*-desmethyl-MTP (ODM) and *α*-hydroxy-MTP (AHM) were the main MTP metabolites identified via suspect screening, and the ratios of ODM to AHM were 3.08 and 1.35 for *S*- and *R*-MTP, respectively. *N*,*O*-didesmethyl-VLF (NODDV) and *N*-desmethyl-VLF (NDV) were the main VLF metabolites, and the ratios of NODDV to NDV were 1.55 and 0.73 for *S*- and *R*-VLF, respectively.

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Analysis for Vertical Profiles of Polycyclic Aromatic Hydrocarbons in the Sea of Japan and Arctic Ocean during 2020-2023

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Abstract

Polycyclic aromatic hydrocarbons (PAHs), which originate from incomplete combustion of organic matter and leakage of petroleum products, are hazardous pollutants with potential adverse carcinogenic. In recent years, global atmospheric PAHs emissions have been decreasing, whereas atmospheric PAHs in the Arctic region have remained at low levels. PAHs in the ocean are transported vertically under a variety of influences, the main controlling factors of which are unknown by the ocean region. In the Japan Sea, which is affected by East Asian countries, and in the Arctic Sea, where PAHs loading due to global warming is a concern, information on PAHs vertical transport is essential for assessing their effects on marine organisms. This study aimed to characterize the vertical distribution of PAHs and analyze the vertical transport process in the Japan Sea and Arctic Ocean.

From 2020 to 2023, 10−15 L of seawater was collected from the surface to a depth of 45-350 m, from the East China Sea to the Japan Sea, and from the northern North Pacific to Chukchi Sea. The seawater samples were particle-separated with a GFF (pore size: 0.5 μm) and then concentrated for dissolved organic matter with a solid-phase extraction C18 disk. The collected particulate and dissolved PAHs were extracted with CH_2Cl_2, separated, and measured by HPLC (fluorescence detector) for 14 PAHs.

PAHs in the Japan Sea in 2020−2023 ranged from 0.4−4.1 ng L^{-1} (total dissolved PAHs: $\Sigma_{14}PAH_{diss}$) and 0.01−0.72 ng L^{-1} (total particulate PAHs: $\Sigma_{14}PAH_{part}$), while Arctic Ocean ranged from 0.15−2.07 ng L^{-1} ($\Sigma_{14}PAH_{diss}$) and 0.01−0.18 ng L^{-1} ($\Sigma_{14}PAH_{part}$). There was a positive correlation ($R^2 = 0.69$) between the $\Sigma_{14}PAH_{part}$ inventory / $\Sigma_{14}PAH_{diss}$ inventory ratio and chlorophyll *a* inventory at 0-100 m depth at five sites in the East China Sea and Japan Sea in 2022. The same was found the Yamato Basin during 2021−2023 ($R^2 = 0.70$). $\Sigma_{14}PAH_{diss}$ inventories at depths of 0−45 m at four sites in the Bering and Chukchi Seas in 2023 ranged from 27.7−82.1 μg m^{-2} and were basically higher in the north. $\Sigma_{14}PAH_{part}$ inventories ranged from 0.7−6.8 μg m^{-2} and tended to be higher in the south. There was a positive correlation ($R^2 = 0.8$) between the $\Sigma_{14}PAH_{part}$ inventory / $\Sigma_{14}PAH_{diss}$ inventory ratio and chlorophyll *a* inventory at four sites. These results suggest that adsorption by biogenic particles is the main factor controlling the vertical distribution of PAHs in the Japan Sea (0−100 m depth) and Arctic Ocean (0−45 m depth).

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Impacts of Pentachlorophenol (PCP) on Coral Reefs: Disruption of Coral-Symbiodiniaceae Symbiosis and Induction of Coral Bleaching in *Porites lutea* and *Montipora digitata*

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Abstract

Stress from chemical pollutants is among the key issues that adversely impact coral reefs. Pentachlorophenol (PCP) is widely found in coastal environments with a variety of adverse effects, and its potential impact on coral reef ecosystems is of concern. The scleractinian corals *Porites lutea* and *Montipora digitata* were used for the PCP exposure experiments in this study. Phenotype, physiological indicators, high-throughput sequencing, and RNA sequencing were used to investigate the response mechanisms of corals to PCP exposure. *P. lutea* and *M. digitata* showed bleaching after 96 hours of acute exposure at 1000 μg/L PCP, with a decrease in Symbiodiniaceae density, Fv/Fm, and chlorophyll a content.They also showed bleaching after long-term exposure to 0.1 μg/L PCP, and Fv/Fm decreased significantly to 0.481 and 0.461, respectively. Microbial community analysis revealed an increase in pathogenic bacteria such as *Citrobacter* and *Vibrio* during acute exposure, and the emergence of *Delftia* in *M. digitata* during long-term exposure. Transcriptomic analyses indicated abnormal carbohydrate and amino acid metabolism in zooxanthellae, disrupting the symbiotic relationship and triggering immune responses in the host. The toxic responses of PCP on both zooxanthellae and their host were further confirmed by the upregulation of differential metabolites and differential proteomes in *P. lutea*. These results indicate that PCP exposure might affect the balance of coral-zooxanthellae symbiosis in stony corals, impairing coral health and leading to coral bleaching.

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Variation Factor of Polycyclic Aromatic Hydrocarbons in Surface Seawater in the Arctic Ocean During 2019–2022

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Abstract

Polycyclic aromatic hydrocarbons (PAHs), a class of toxic organics, are released into the environment by incomplete combustion of biomass and fossil fuels and by oil and coal spills. In the Chukchi and Beaufort Seas facing Alaska and northern Canada, PAHs are supplied by the Mackenzie River inflow, sea ice melting, oil spills from the Prudhoe Bay Oil Field, and erosion of coal deposits, in addition to PAHs via the atmosphere mainly from forest and peat fires. In the Arctic Ocean, despite the risk of further increases in PAH loads associated with global warming and inhibition of marine organism growth owing to the co-toxicity of PAHs and other toxic organic matter, the causes of variations in PAHs in seawater remain unclear. This study aimed to elucidate the environmental behavior of dissolved PAHs in the Arctic Ocean during 2019–2022 by analyzing the 1) surface PAH distribution, 2) PAH source, 3) air-sea PAH exchange, and 4) water mass structure traced by the nuclear fuel reprocessing plant-derived ^{129}I ($T_{1/2}$: 15.7 million years). Surface seawater samples (10–15 L) were collected at 44 sites in the western subarctic North

Pacific, Bering Sea, and Arctic Ocean (Chukchi and Beaufort Seas) from August to October 2019 to 2022. Dissolved phase PAHs were concentrated into C18 disks from in-line filtered (0.5 µm glass fiber filter) seawater. PAHs were extracted from the C18 disk using dichloromethane and measured using an HPLC system with a fluorescence detector. In the Arctic Ocean, total dissolved 14 PAHs ($\Sigma_{14}PAH_{diss}$) ranged between 1.03 and 3.37 ng L^{-1} during 2019–2022, with means of 2.09±0.39 ng L^{-1} in 2019, 2.27±0.56 ng L^{-1} in 2021, and 1.41±0.23 ng L^{-1} in 2022. PAH concentrations in the Arctic Ocean decreased by -40% from 2021 to 2022. Estimated PAHs' atmospheric deposition fluxes show similar mean values of 14.9 ng day^{-1} m^{-2} in 2021 and 16.3 ng day^{-1} m^{-2} in 2022, which are 1 order of magnitude lower than the atmospheric PAHs deposition fluxes in the Sea of Japan. A negative correlation was found between salinity and $\Sigma_{14}PAH_{diss}$ and ^{129}I, in the Arctic Ocean, with a positive correlation between $\Sigma_{14}PAH_{diss}$ and ^{129}I in 2019. Thus, it is suggested that the main controlling factor of PAHs in the Arctic Ocean surface layer might be the water mass mixing of the Beaufort Gyre water (low salinity, high PAHs, high ^{129}I) influenced by sea ice melting and river water in the Beaufort Sea and the Alaska Coastal Water (high salinity, low PAHs, low ^{129}I) in the Chukchi Sea.

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Spatiotemporal Distribution of Polycyclic Aromatic Hydrocarbons Around the Kuroshio Current Area

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Abstract

The Kuroshio Current is the western boundary current of the North Pacific Ocean that transports heat, salt, chemical materials, and organisms. The waters surrounding it in the southern part of Honshu are important spawning grounds and breeding grounds for pelagic fish resources and as a distribution area for skipjack tuna. However, owing to the population and energy structure of East Asia, large amounts of harmful polycyclic aromatic hydrocarbons (PAHs), are discharged into the sea along rivers and monsoons. The seawater PAHs concentration in the East China Sea are relatively high and can be transported by ocean currents to surrounding fishing grounds. Therefore, the investigation for the distribution and transport process of PAHs in Kuroshio Current area is a valuable task.

Previous investigations in our laboratory have shown that PAHs concentrations are high in the Kuroshio Current axis surface water and low in coastal water. To grasp this phenomenon accurately, in April and August 2023, we collaborated with the Japan Fisheries Research and Education Agency to collect more than 100 samples (10–15L) in the Western Pacific. Particulate PAHs ($\Sigma_{14}PAH_{part}$) and dissolved PAHs ($\Sigma_{14}PAH_{diss}$) were separated by 0.5 µm pre-combusted glass-fiber filters and dissolved PAHs were concentrated using C18 disk. $\Sigma_{14}PAH_{part}$ and $\Sigma_{14}PAH_{diss}$ were extracted with dichloromethane and measured by a HPLC-fluorescence system.

In April 2023, PAH levels in the Kuroshio Current area were in range 1.76–5.10 ngL^{-1} for $\Sigma_{14}PAH_{diss}$, and 0.12–0.61 ngL^{-1} for $\Sigma_{14}PAH_{part}$. The concentration of $\Sigma_{14}PAH_{diss}$ in coastal surface seawater is relatively low, while it is the highest at the axis. Vertical PAHs sampling data from 0-300 m also shows similar characteristics. The inventory of ΣPAH_{diss} in seawater at depths of 0–300 m are 957 μgm^{-2} at the coast, 1119 μgm^{-2} at the

Kuroshio axis, and 988 μgm^{-2} at the offshore. The highest level of PAHs in the Kuroshio axis reflects the PAHs transport effect by Kuroshio Current. In contrast, the inventory of $\Sigma_{14}PAH_{part}$ shows the opposite characteristics (coast: 69.4 $\mu g\ m^{-1}$, axis: 62.6 $\mu g\ m^{-2}$, offshore: 69.0 $\mu g\ m^{-2}$). Among the three locations, the chlorophyll-a concentration is highest at SCM (Subsurface Chlorophyll Maximum) on the coast, where the K_d (particle-water distribution coefficient) value here is also the highest (10.4 ngL^{-1}). Therefore, particle adsorption of dissolved PAHs occurred in the coastal side of the Kuroshio Current.

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Temporal Trends of $C_{6–36}$ Chlorinated Paraffins in Sediment Cores from the Pearl River Estuary, South China

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Abstract

Chlorinated paraffins (CPs) are chemical mixtures of polychlorinated *n*-alkanes with potentially persistent, bioaccumulative, and toxic characteristics, and they are readily deposited in sediments when entering estuaries and adjacent seas; thus, concerns over their long-term discharge into the marine environment keep growing. Time-series surveys are essential for monitoring the long-term release of CPs. The present work used high-resolution mass spectrometry (HRMS) to investigate the temporal trend and congener profile of short-, medium-, and long-chain CPs (SCCPs, MCCPs, and LCCPs) in sediment cores from Hong Kong waters and Lingdingyang of the Pearl River Estuary, South China. The early production and use record of CPs dating from the 1920s to the 2010s were reconstructed in the investigated region. While SCCP levels remained stable since the 1980s, increasing trends of MCCPs and LCCPs were observed, indicating a market shift towards longer-chain homologs. The levels of very long-chain CPs (vLCCPs) semi-quantified via HRMS were positively correlated with those of other CP categories, suggesting their synchronized release in the studied area. Notably, the higher levels of vLCCPs than LCCPs suggest a potential underestimation of their historical production and use in China. These findings contribute to understanding the historical pollution patterns of CPs in the Greater Bay Area and emphasize the need for a comprehensive environmental assessment of CPs, including vLCCPs.

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Emerging Per- and Polyfluoroalkyl Substances (PFAS) Cause Intestinal Barrier Dysfunction in Marine Medaka (*Oryzias melastigma*)

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Abstract

Perfluoroethylcyclohexane sulphonate (PFECHS) and 6:2 chlorinated polyfluoroalkyl ether sulfonate (6:2 Cl-PFESA) are emerging per- and polyfluoroalkyl substances (PFAS) increasingly found in environmental and biological samples. Given their similarities in structure and physicochemical properties to legacy PFAS, it is hypothesized that PFECHS and 6:2 Cl-PFESA may induce comparable toxic effects on the digestive system *in vivo*. The present study investigated the potential digestive damage of PFECHS and 6:2 Cl-PFESA using marine medaka (*Oryzias melastigma*) as a model animal. The newly fertilized medaka were exposed to environmentally relevant concentrations (nominal: 0.1, 0.3, and 1.0 μg/L) of PFECHS and 6:2 Cl-PFESA for 90 days. Liver and intestinal samples were collected after exposure to assess PFAS bioconcentration and digestive damage potential. Results showed higher bioconcentration potential for 6:2 Cl-PFESA than PFECHS, and both emerging PFAS preferred deposition in liver over intestines. Significant alterations in intestinal digestive enzyme activity were observed in PFECHS-exposed medaka, with increased activities of disaccharidase, alkaline protease, and neutral protease. PFECHS caused the reshaping of the intestinal microbial community in medaka. The PFECHS-treated group showed a lower relative abundance of probiotics (e.g., *Bacteroides* and *Pseudomonas*) than the 6:2 Cl-PFESA-treated and control groups. In comparison, *Alkalimarinus* and pathogenic bacteria *Vibrio* exhibited higher abundance in the PFECHS-treated group. Co-occurrence network analysis revealed less complex and cooperative species interactions in medaka exposed to PFECHS than 6:2 Cl-PFESA. Correlation analysis demonstrated a close association between gut microbes and the digestive system. These findings contribute to evaluating the adverse effects of emerging PFAS and understanding the mechanisms underlying intestinal barrier function in fish exposed to new pollutants.

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How Do Microplastics and Nanoplastics Threaten Marine Protected Areas?

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Abstract

Despite extensive research on microplastic occurrence in marine environments, their status and ecological impacts in global Marine Protected Areas (MPAs) remain poorly understood. Due to their ubiquitous presence, increasing volume, and ecotoxicological effects, microplastics may pose significant threats to marine ecosystems. Our three studies provide a comprehensive overview of microplastic occurrence, abundance, distribution, and characteristics within MPAs and their buffer zones, utilizing data from over one thousand peer-reviewed articles analyzed via GIS. Additionally, nanoplastic toxicity and mechanisms were examined by analyzing 37 omics studies. Microplastics were detected in 52 MPAs, increasing to 68 MPAs when buffer zones were included. Fragments and fibers were the most common shapes, with polyethylene and polypropylene as the predominant polymers. Two-thirds of the data indicated seawater microplastic levels exceeding 12,429 items/km², highlighting that MPAs alone cannot prevent microplastic pollution. Moreover, microplastic contamination was found in sediment and biota samples from 186 MPAs, reaching 9,187.5 items/kg in sediment and 17,461.9 items/kg in organisms. High concentrations observed in multiple-use and no-take MPAs likely affected benthic species more than pelagic ones, with microplastics detected in two threatened species listed on the IUCN Red List, questioning the effectiveness of MPAs in conservation efforts. Furthermore, nanoplastics, recognized as emerging hazards, exhibit complex molecular impacts on aquatic organisms. Omics data across various taxonomic groups suggested both common and distinct toxic effects, underscoring the need for integrated omics tools to enhance predictions of ecotoxicity. These findings emphasize the urgent need for effective policies and innovative solutions to mitigate plastic pollution, improve MPA management, and safeguard marine biodiversity.

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Automated Analysis of Histological Lesions in Whole Slide Images of Fish Liver

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Abstract

Tissue changes in aquatic organisms are important to consider during environmental monitoring programs to understand individual health, and possibly ecosystem health. However, the traditional estimation by a trained histopathologist is often costly, time consuming, and prone to operator bias. Digital pathology consists in computer-based analyses with artificial intelligence and high-throughput methodologies. These approaches, which have already been adopted in biomedical applications, have not been implemented in environmental studies yet.

In this proof-of-concept research, fish liver samples, collected during an environmental monitoring study in the North Sea, were analysed. A selection of histological lesions (steatosis, melanomacrophage aggregates, haemocytes infiltration, and granulocytoma) was estimated by a trained histopathologist (traditional approach) and using a neural network model for image recognition implemented in the open-source software, QuPath (automated approach) in whole slide image (WSI) scans. A subset of WSI was used to train a pixel classifier (random forest), which was then used to automatically detect and quantify the lesions. Lesion coverage data were compared to traditional manual scoring results using various statistical tools. Obtained results were compared to manually assigned severity scores. Assuming the traditional estimation by a trained histopathologist as reference, the classifier model correctly identified 91% for steatosis, 95% for melanomacrophage aggregates, 79% for haemocytes infiltration, and 95% for granulocytoma. To improve the model prediction, data driven decision boundary between classes are also proposed. No differences between species were observed while applying the automated approach, confirming the possibilities to utilise the same lesion classifier in various fish species. These results provide the first successful base for automated lesion detection and quantification methodologies for use in aquatic organisms.

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Joint regional activities for an improved assessment of chemical pollution in the marine environment using biological effects approach - Baltic Sea case study

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Abstract

Chemical pollution is one of the top global anthropogenic pressures, impacting the health of marine biota, accelerating biodiversity loss, and influencing key functions of marine ecosystems. The current environmental monitoring and assessment approach is focused on chemical and ecological measurements. It is currently well acknowledged that the monitoring of chemical concentrations alone is not sufficient, since considering only a tiny number of substances while lots of others are left unnoticed. Moreover, the hazards related to contaminant mixtures remain undetected. To protect the ecosystem, understanding the cumulative toxicity potential of the substances present in the environment is crucial, as well as the linking of the observed effects with cost-effective management options. Examining biological effects provides an understanding of the impact of the multiple mixed effects of

contaminants on marine biota. The importance of addressing mixture toxicity and the subsequent necessity to implement effect-based methods (EBM) is indicated by numerous regulatory bodies.

Recently, efforts in supporting the implementation of EBM in the integrated chemical-biological monitoring and assessment frameworks for the Baltic Sea region resulted in developing a regional platform for EBM using support for several joint projects: “Application of biological effects methods in monitoring and assessment of contaminants in the Baltic Sea” (BEACON - Interreg Baltic Sea Region), “New approaches in determining the impacts of chemical pollution to protect the biodiversity of the Baltic Sea” (Detect2Protect – Biodiversa +), “HELCOM Biological Effects of Contaminants” (H-BEC). To complement this thematic cluster, a new Study Group named SGEFF was established with the target of harmonising EBM and guidelines jointly in the Baltic Sea and North-East Atlantic regional sea areas. National expert teams' involvement in the core group allows the activities to be run in a coordinated, effective manner on a regional scale. Through direct contact with different stakeholders, this cluster has significant potential to increase understanding of the importance of EBM in current monitoring programmes. The undertaken activities presented in this study are the basis for recommendations on harmonized procedures to be implemented at the national or regional level with the aim to establish the basis for a long-term, practical approach addressing the pollution impact on the Baltic Sea ecosystem.

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A microcosm study：Mineral sunscreens have hidden dangers to corals

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Abstract

Mineral sunscreens have emerged as a substitute for chemical sunscreens in the attempt to protect key ecosystems such as coral reefs. However, our in-depth microcosm study and field investigations into mineral sunscreens reveal irreversible damages to corals and potential pollution for the coral reef environment. Notably, the vulnerability of coral fluorescent proteins to mineral sunscreen exposure was identified, suggesting a novel mechanism for coral bleaching involving the inhibition of protein expression by metal ions and UV-filter particles released from these sunscreens. Our findings further confirmed the increased metal levels for wild corals in touristic areas, calling for thoughtful discussions among managers, producers, and consumers. This study unveils a novel threat to coral reefs, underscoring the imperative for a well-rounded approach to future sunscreen use and sustainable coral conservation.

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Toxic effects of microplastics on marine crustaceans *Artemia franciscana* and *Penaeus vannamei*

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Abstract

Plastic debris released from terrestrial sources continuously moves to the marine environment, and the ingestion of micro-sized plastics (MPs) by living organisms is a global concern. To understand and evaluate the impacts of MPs on marine organisms, we used two marine crustaceans (*Artemia franciscana* and *Penaeus vannamei*) to assess the shape-dependent toxicity of MPs. Each test species was exposed to polyethylene terephthalate-based MPs in two different shapes (fragment and fiber), and biological impacts from individual to molecular levels were observed. The PET MPs used in this study clearly induced detrimental effects, including mortality, growth inhibition, and abnormal movement in *A. franciscana*. PET MPs also caused alterations in molting patterns, organ damage, and molecular responses in transcriptomes and metabolites in *P. vannamei*. These results highlight the impacts and underlying toxicity mechanisms of environmental MPs on marine crustaceans, suggesting that MPs pose ecological risks in the ocean. *Acknowledgement-This research was supported by "Risk assessment to prepare standards for protecting marine ecosystem" of Korea institute of Marine Science & Technology Promotion (KIMST) funded by the Ministry of Oceans and Fisheries (KIMST-20220383).*

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Occurrence characteristics and endocrine disrupting effects of per- and polyfluoroalkyl pollutants in amphibians in Chaohu Lake

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Abstract

Perfluoroalkyl and polyfluoroalkyl substances (PFAS) are pervasive environmental pollutants threatening the environment and public health. However, the occurrence and ecological risks of PFAS in amphibians, which have been experiencing severe global population declines, remain unclear. This study investigates the accumulation patterns of PFAS in the Chinese toad (*Bufo gargarizans*) from Chaohu Lake and their relationship with endocrine hormones, as well as

assesses the exposure risk of perfluorobutane sulfonic acid (PFBS), the most prevalent alternative compound in the region, on *Lithobates catesbeiana* tadpoles. In the waters surrounding the lake's inlet, 39 PFAS compounds were identified, including 19 perfluoroalkyl acids (PFAAs), 8 novel PFAS, and 12 PFAS precursors. The spatial distribution of PFAS at the inlet indicates that non-point agricultural sources are significant contributors to PFAS pollution. Within the Chinese toads, the highest concentrations of PFAS were found in the liver, followed by the gonads. Male toads had significantly higher levels of PFAS in their gonads than females. Younger toads exhibited higher PFAS concentrations than older individuals. Some new PFAS alternatives, such as ADONA and 6:2 Cl-PFESA, displayed higher bioaccumulation factors (BAF) than traditional PFAS like PFOA and PFOS. For the first time, two emerging PFAS, HFPO-DA and 6:2H-PFESA, were reported in amphibians. HFPO-DA exhibited a higher relative body burden (RBB) value than PFOS, indicating its greater bioaccumulative potential compared to traditional C8 compounds. Elevated levels of estradiol in gonads correlated with increased concentrations of certain PFAS, suggesting a potential estrogenic effect, particularly in male toads. Additionally, exposure to environmentally relevant concentrations of PFBS was shown to impair the reproductive endocrine system and disrupt the metamorphosis process in *L. catesbeiana* tadpoles through the hypothalamic-pituitary-thyroid axis. These findings provide critical insights into the ecological risks posed by PFAS in Chaohu Lake to local amphibian populations.

Key words: PFAS; Chaohu Lake; Amphibians; Endocrine disorders; Reproductive system; Metamorphosis

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Nitrate and herbicides can render corals more sensitive to heat stress

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Abstract

Coral reefs around the world face the threat of ocean warming, and studies have found that environmental concentrations of herbicides and nitrate nitrogen pollution may exacerbate the degree of heat-induced coral bleaching. However, the molecular mechanisms of how corals respond to multiple environmental stresses are unclear. Through physiological, biochemical and multi-omics methods, we studied the response mechanism of corals to nitrate nitrogen or photosystem II (PSII) herbicide pollution under the background of high temperature, and found that nitrate nitrogen and PSII herbicide would exacerbate the decrease of coral photosynthetic efficiency and the breakdown of the symbiotic relationship between corals and Symbiodiniaceae. The research highlights the urgent need for more stringent seawater management strategies to effectively protect coral reefs.

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Poly- and Perfluoroalkyl Substances Induce Immunotoxicity in Fish and Interfere with BiodiversityKEYWORDS: PFASs, immunotoxicity, zebrafish, auto-toxic, biodiversity

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Abstract

Previous studies have reported the immunotoxicity of per- and polyfluoroalkyl substances (PFASs), but the mechanisms of immunotoxicity of different PFASs remains unclear. Our findings provide comprehensive evidence that widely used PFAS compounds, PFBA, PFOA, and PFNA, induce immunomodulatory effects in zebrafish and the immunotoxicity of PFASs is closely associated with the carbon chain lengths of PFASs. In addition, our results indicated that the immunotoxicity of PFASs, such as PFOSA, is attributed to itself, rather than its metabolite, further highlights the need to consider the auto-toxicity of PFOSA. Moreover, the bioaccumulation of PFASs in aquatic organisms may contribute to population declines by impairing reproductive and survival rates, thereby threatening biological diversity. Thus, the potential negative health effects and developmental outcomes to marine biota following PFASs exposure are of great concern considering the widespread exposure risk coupled with its known toxicity.

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Tire Additives in Water: Leaching, Transformation, and Environmental Risk Assessment

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Abstract

Tire wear particles (TWPs) released during vehicle driving can enter water bodies, leading to the leaching of tire additives (TAs) in the aquatic environment. However, the transformation behavior and related ecological impacts of TAs and their transformation products (TPs) remain unclear. In this study, lab-based simulation experiments and field investigations were conducted to explore the transformation mechanisms and ecological risks of TAs. After being placed in river water for 24 h, about 7%–95% (mean: 59%) of TAs were leached from TWPs. Forty-eight TPs from eight TAs were tentatively identified along with different transformation pathways via suspect screening by high-resolution mass

spectrometry (HRMS). Semiquantitative results indicated that TPs derived from N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylene-diamine (6PPD) were predominant in leachates, while aryl hydrolysis and quinone pathways were the main transformation pathways. Field investigations on urban surface water samples from 16 sites in Hong Kong revealed the occurrence of 17 TAs and one TP, with concentrations ranging from 13 to 1925 ng/L (mean and SD: 339 ± 465 ng/L). Sixteen TPs from six TAs were additionally identified via suspect screening. It is estimated that 6PPD-quinone and seven other TAs could pose medium to high ecological risk, while N-(1,3-dimethylbutyl)-N'-phenyl-p-quinonediimine, a frequently detected TP, was identified as a persistent-bioaccumulative-toxic substance.

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Integrated Full-Length Transcriptome and RNA-Seq Analysis Reveals the Underlying Molecular Mechanisms of Adaptive Response to Nutrient Loading in *Duncanopsammia peltate*

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Abstract

The coral reefs, often referred to as the "tropical rainforests of the ocean", serve as crucial habitats for a multitude of marine organisms. The reef-building corals, acting as the primary structures of these reefs, play an indispensable role in supporting and sustaining marine ecosystems; however, they are facing increasing threats from climate change and anthropogenic activities. *Duncanopsammia peltata* is a dominant coral species with important ecological significance in the waters of Dongshan Island, which can serve as a model species for understanding the mechanisms underlying coral adaptation to changing environmental conditions. To decipher the genetic basis of *D. peltata*'s in response to nutritional stress, we conducted full-length transcriptome profiling using PacBio Sequel II technology combined with RNA-Seq analysis and identified differentially expressed genes (DEGs) in *D. peltata* respectively collected from a protected area (PA), a non-protected area (NPA), and laboratory cultures (LC), and further enriched the signaling pathways associated with these DEGs. After clustering, polishing, and redundancy removing, we identified 40,936 unigenes with mean length of 2,814.3 bp and N50 length of 2,977 bp. There are 38,247 (93.43%) unigenes at least one annotated in the Nr, SwissProt, KOG, or KEGG databases. Additionally, we predicted 38,753 coding sequences, 1,361 transcription factors, 1,988 long non-coding RNAs and 5,160 simple sequence repeats. Compared with the coral in PA, the corals in NPA and LC exhibited a significant enrichment of 5,256 and 13,559 DEGs, respectively. And these DEGs are involved in signal transduction, metabolism, protein processing, and cell structure maintenance in coral from LC, but are associated wtih energy metabolism, amino acid metabolism, lipid metabolism, and intracellular waste management in NPA coral. This work sheds light on the valuable gene expression profile of coral and provides grounds for further molecular biological research to support ecological

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Understanding transport, fate, and risk of antibiotics in Singapore Coastal Waters through an integrated monitoring and modelling framework

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Abstract

Rapid urbanization, industrial development, and extensive maritime activities have introduced various contaminants into the Singapore Coastal Waters (SCWs). Emerging contaminants, such as antibiotics, are of particular concern due to their persistence and potential adverse effects on marine ecosystems, as well as their role in promoting antimicrobial resistance (AMR). In this study, we implemented an integrated sampling and modelling framework to understand the transport, fate, and ecological risk of antibiotics in the SCWs. Initially, a monthly sampling campaign was conducted at 12 sites across the SCWs from January 2022 to January 2023 to assess the prevalence and sources of antibiotics. Among the 22 targeted antibiotics, seven were frequently detected, with substantial concentrations noted for Erythromycin-H_2O (ERY-H_2O), Azidothymidine, and Clarithromycin. Subsequently, we applied a process-based hydrodynamic environmental model using the Delft3D suite, which considers the biogeochemical processes affecting ERY-H_2O, to simulate its transport and fate under the complex hydrodynamic conditions of the SCWs. The calibrated and validated model results provided reasonable predictions, with all modeled targets showing R^2 values above 0.6 and Nash-Sutcliffe Efficiency (NSE) greater than 0.5. Model results revealed that the highest concentration of ERY-H_2O occurred during the southwest monsoon, while the lowest concentration was observed during the northeast monsoon, influenced by meteorological and sea circulation patterns. Finally, the sampling and model results were integrated with a risk assessment module to evaluate the development of antimicrobial resistance (AMR) and the ecological toxicity in the aquatic environment, revealing a spatiotemporal risk hotspot with levels ranging from low to high risk. This comprehensive approach offers a proactive strategy to address the urgent challenge of antibiotic contamination in coastal ecosystems. It facilitates the development of an improved risk management framework for antibiotics in the marine environment, ultimately contributing to the preservation of both environmental and public health.

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Bacterial Diversity in Soil of Yuncheng Salt Lake Wetland and Its Response to Heavy Metals

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Abstract

Located at the southern foothills of Zhongtiao Mountain, Yuncheng Salt Lake, renowned as the "Dead Sea of China" due to its high salinity, is one of the world's famous inland salt lakes dominated by sodium sulfate. With a history of over 4600 years, salt production used to be the primary industry in the area. However, with the comprehensive cessation of salt production activities, the local government actively initiated the ecological restoration program of "reducing salt and returning the lake." In 2023, this study sampled surface soil in the research area and analyzed the bacterial diversity as well as the concentrations of eight heavy metals, including arsenic (As), cadmium (Cd), zinc (Zn), lead (Pb), chromium (Cr), copper (Cu), nickel (Ni), and mercury (Hg), aiming to provide scientific basis for local environmental management and ecological restoration. The results showed that: (1) Microorganisms in the salt lake wetland soil were mainly distributed across 58 phyla, 185 classes, 466 orders, 812 families, and 1831 genera. *Proteobacteria, Actinobacteria, Chloroflexi,* and *Acidobacteria* were the predominant taxa, collectively accounting for over 60% of the total abundance. (2) The average concentrations of the eight heavy metals in the soil of the research area, from highest to lowest, were: Zn > Cr > Pb > Cu > Ni > As > Hg > Cd. Potential ecological risk assessment indicated that Hg posed the highest risk, followed by Cd, while the other heavy metal elements exhibited lower risks. (3) Variations in heavy metal concentrations among different sampling points in the region influenced the structure of microbial communities. Redundancy analysis (RDA) revealed that the primary environmental variables affecting microbial community structure were Hg, Pb, and Cu. Heatmap analysis showed significant responses of *Acidobacteria, Chloroflexi,* and *Proteobacteria* to heavy metal concentrations, with *Vicinamibacterales* within *Acidobacteria* and *Geminicoccaceae* within *Proteobacteria* identified as the main species responding to heavy metals in the soil.

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The environmental behavior and ecological effects of typical contaminants in the coastal zone

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Abstract

The applicant has been devoted to studying the environmental behavior and ecological effects of typical contaminants in the coastal zone, achieving the following accomplishments.

1. The occurrence and fate of pharmaceuticals and personal care products (PPCPs) in wastewater treatment plant, rivers and coastal zones have been clarified. Particularly, our study on the distribution and behavior of PPCPs in Bohai sea provides novel insights into the multi-media distribution of diverse PPCPs in the marine environment and demonstrates that log Dow is a better bioaccumulation and biomagnification indicator.

2. The distribution patterns, risks and fate of persistent organic pollutants in Chinese intertidal zones have been investigated. Particularly, our study on polycyclic aromatic hydrocarbon distribution in intertidal zones provides continental-scale evidence that human activities have key and differential effects on the distribution and deposition of polycyclic aromatic hydrocarbons in intertidal sediments, and shows that pollution status and profile of polycyclic aromatic hydrocarbons can be used to index regional industrialization and urbanization status.

3. The toxic effects and associated toxicity mechanisms of MPs on soils, coastal sediment and biota have been explored. Particularly, we demonstrate the dominant role leachate-induced effects play in MP toxicity to soil fauna due to the limited ingestion of MPs and brand-specific toxicity help identify determinants of MP toxicity. By discerning the particulate- and leachate-induced effects of TWPs, we for the first time demonstrate that both particulate- and leachate-induced toxicity of TWPs to marine algae is increased after aging processes.

The research results have enriched the theoretical and technical system of environmental behavior processes, risks and bioremediation of emerging contaminants, and contributed to the sustainable development of coastal zones. Over 40 peer-reviewed scientific articles on related achievements have been published in SCI journals such as Nature Sustainability and Environmental Science & Technology.

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Are Harmful Algal Blooms Becoming the Greatest Water Quality Threat to Public Health and Ecosystems across the Freshwater to Marine Continuum? A Case Study in One Health

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Abstract

Harmful Algal Blooms (HAB) appear to be increasing within inland waters at the global scale, and represent a classic One Health challenge. When HAB events require restrictions on fisheries, aquaculture, recreation and drinking water uses of inland water bodies significant economic consequences result. Unfortunately, the magnitude, frequency and duration of HABs across the freshwater to marine continuum are poorly understood across spatiotemporal scales, and are

differentially engaged among and within countries. Beyond site-specific water quality degradation caused directly by HABs, the presence of HAB toxins can influence routine surface water quality monitoring, assessment and management practices. HABs present significant challenges for achieving water quality protection and restoration goals when these toxins confound interpretation of monitoring results and environmental quality standards implementation efforts for other chemicals and stressors. Further, cyanobacteria, prymnesiophytes and other HAB forming species differentially produce toxins across environmental gradients, which present spatiotemporal risks to aquatic and terrestrial wildlife and human health. Whether HABs presently represent the greatest threat to water quality is debatable, though HABs can cause more severe acute impacts to environmental quality than conventional chemical contamination events. In this presentation, I introduce some of our work on the subject, which is a textbook example of the One Health approach, and identify several timely research needs to engage the complexities of HAB assessment and management, to address the forcing factors for HAB formation, and to reduce the threats posed to surface water quality, particularly in the face of climate change.

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Gut microbiota-gut interaction interfere with intestinal health after microcystin-LR exposure in *Lithobates catesbeianus* tadpoles

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Abstract

There remains uncertainty regarding the influence of microcystin (MC)-LR on amphibian intestinal health, specifically how MC-LR interferes with intestinal microbiota following exposure to environmental concentrations. In this study, *Lithobates catesbeianus* tadpoles were exposed to varying MC-LR concentrations (0, 0.5, and 2 μg/L) over a 30-day period. The aim was to investigate how altered interactions between tadpole intestinal microbiota and the intestinal barrier influence intestinal health following MC-LR exposure. Following exposure to the MC-LR at low ambient concentrations, tadpole intestinal tissue was damaged. It had increased permeability, reduced pathogen inhibition capacity, and impaired digestive function. Additionally, there was a significant increase in lipopolysaccharide content and upregulation of downstream response genes, including *TLR4*, *MyD88*, and *NF-κB*, within the intestinal tissue. Therefore, the count of eosinophils and the expression of pro-inflammatory cytokines both increased. In addition, MC-LR exposure induced oxidative stress and mitochondrial structural damage by increasing the levels of reactive oxygen species in intestinal tissue. There were also significant increases in *CytoC* and *Bax* transcription and caspase 9 and caspase 3 activities. *Bcl-2* transcription was significantly downregulated, which led to the promotion of apoptosis in tadpole intestinal cells. MC-LR

exposure led to disruptions in the intestinal microbiota and metabolism of tadpoles. Correlation analysis revealed a marked correlation between the intestinal microbiota and intestinal oxidative stress, inflammation, immunity, and tissue damage. Conclusively, this study demonstrates for the first time that MC-LR significantly affects amphibian intestinal microbiota, highlighting tadpoles' susceptibility to MC-LR-induced environmental risks. Moreover, it provides a theoretical foundation for developing MC-LR detoxifying drugs in aquatic environments.

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Interactions and Effects of Microplastics with Heavy Metals in the Marine Environment.

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Abstract

As the carrier, microplastics (MPs) can adsorpt heavy metals in the marine environment and exhibit diverse interactive effects. This study investigated the adsorption capacity of Cu and Zn in the marine environment and the effects of microplastic particle size, material, pH and nutrients on the metal adsorption were conducted in the laboratory. The results showed PVC adsorption is more than PS; smaller particle sizes (50-74 um) adsorption is more than larger particle sizes (74-178)um. Langmuir could better describe the adsorption process of Cu2+and Zn2+ on the pristine MPs, which indicated that there existed a homogeneous monolayer adsorption on the surface of the pristine MPs. Increasing pH increased the adsorption of metals on MPs. when Cu^{2+} and Zn^{2+} coexist, competitive adsorption is formed, and MPs showed preferential adsorption to Zn^{2+}. The presence of PO43- promoted the adsorption behavior of metals on microplastics, and the higher the concentration, the more pronounced the promotion effect is. The effect of NO3- on the adsorption of metals on microplastics was to promote and then inhibit the adsorption of metals first, which presents an inverted "U" shape. The main influencing mechanism of primitive PS adsorption of metals is electrostatic force, while the main influencing mechanism of primitive PVC adsorption of metals is electrostatic gravitational force and complexation.

The mechanisms of biofilms adsorpt Cu and Zn and the differences metal exposure on the microbial speciese were also analyzed. the Freundlich model showed that there was inhomogeneous multilayer adsorption on the surface of plastic interstitial MPs, and their capacity to adsorb Cu and Zn increased after the coverage of the biofilm, and the chemical adsorption was the main influencing mechanism. The complexation of oxygen-containing functional groups within the biofilm contributed to the increase in metal adsorption. The abundance of microbial species in the metal-exposed interplastic samples was significantly higher than that in the non-metal-exposed interplastic samples, suggesting that bacteria can coexist with metals on the interplastic surface, and the presence of metals promotes the enrichment of microorganisms related to metal metabolism on the surface of the interplastic.

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Evaluating eDNA and eRNA Metabarcoding for Aquatic Biodiversity Assessment: From Bacteria to Vertebrates

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Abstract

Monitoring and management of the aquatic environments relies on precisive data on the integrity of ecological communities. Metabarcoding analyses of environmental nucleic acids (hereafter eNAs, including eDNA and eRNA) have generated considerable research interest owing to their cost-effective and non-invasive biomonitoring capabilities. However, the accuracy of biodiversity estimates obtained through eNAs may vary across different organismal groups. Here, we evaluated the performance of eDNA and eRNA metabarcoding across nine organismal groups, spanning from bacteria to terrestrial vertebrates, in three cross-sections of the Yangtze River. The results revealed a robust complementarity between eDNA and eRNA data. The relative detectability of eNAs was notably influenced by major taxonomic groups and the organismal sizes, with eDNA exhibiting more robust signals for larger organisms. Both eDNA and eRNA exhibited similar cross-sectional and longitudinal patterns. However, the detectability of larger organisms declined in eRNA metabarcoding, possibly associated to differential RNA-release and decay by small versus large organisms or across different organismal groups. While our work underscored the potential of eDNA and eRNA in the biomonitoring of large rivers, we pinpoint towards a differential interpretation of eDNA versus eRNA data.

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Chronic Paternal/Maternal Exposure to Environmental Concentrations of Imidacloprid and Thiamethoxam Cause Intergenerational Toxicity in Zebrafish Offspring

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Abstract

Imidacloprid (IMI) and thiamethoxam (THM) are ubiquitous in aquatic ecosystems. Their negative effects on parental fish are investigated, while intergenerational effects at environmentally relevant concentrations remain unclear. In this study, F0 zebrafish exposed to IMI and THM (0, 50 and 500 ng L^{-1}) for 144 days post fertilization (dpf) was allowed to spawn with two modes (internal-mating and cross-mating), resulting in four types of F1 generations to investigate the intergenerational effects. IMI and THM affected F0 zebrafish fecundity, gonadal development, sex hormones and VTG levels, with accumulations found in F0 muscles and ovaries. In F1 generation, paternal or maternal exposure to IMI and THM also influenced sex hormones levels, and elevated heart rate and spontaneous movement rate. LncRNA-mRNA network analysis revealed that cell cycle and oocyte meiosis related pathways in IMI groups, and steroid biosynthesis related pathways in THM groups were significantly enriched in F1 offspring. Similar transcriptional alterations of *dmrt1*, *insl3*, *cdc20*, *ccnb1*, *dnd1*, *ddx4*, *cox4i1l* and *cox5b2* were observed in gonads of F0 and F1 generations. The findings indicated that prolonged paternal or maternal exposure to IMI and THM could severely cause intergenerational toxicity, resulting in developmental toxicity and endocrine disrupting effects in zebrafish offspring.

19. Environmental Epigenetics and Omics

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Kinetics Studies of Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) Systems for Sensitive RNA Detection

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Abstract

The discovery and characterization of Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) systems with *trans*-cleavage activity led to the rise of CRISPR-based diagnostics. CRISPR-Cas13a is very useful for RNA manipulation and detection due to its function of RNA targeting and cleavage. The performance of CRISPR-based assays depends on the reaction kinetics of the CRISPR-associated (Cas) enzymes. Previous kinetics studies of CRISPR-Cas13a systems focused on understanding the kinetics of the *trans*-cleavage process, a process of non-specific cleavage of multiple fluorescence reporters after Cas13a binding to target RNA. However, the binding and activation kinetics are not clear. Both the binding between Cas13a and CRISPR RNA (crRNA) to form ribonucleoprotein and the binding of ribonucleoprotein to the target RNA are important in shaping the activity of Cas13a. We developed a sensitive technique and unraveled the kinetics of activation and *trans*-cleavage of the CRISPR-Cas system. The core of our method is the measurement of the dynamic concentration of active Cas-crRNA-activator ternary complex during its formation by monitoring the real-time *trans*-cleavage activity of Cas ternary complexes. Therefore, we overcame the sensitivity challenge in the determination of the ternary complex (active enzyme) in kinetics studies. We reported the rate constants (kon and koff) and dissociation constant (Kd) for the binding between Cas13a and its activator. We further discovered that once activated, the Cas13a system operates at a wide range of temperatures (7–37 °C) with fast *trans*-

cleavage kinetics. Our kinetics model and method also apply to other CRISPR-Cas systems with *trans*-cleavage, such as CRISPR-Cas12a. Understanding the kinetics also enabled the development of sensitive RNA detection techniques for microRNA and SARS-CoV-2 RNA.

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Metabolomics Approach Reveals the Health Risks Associated with Chlorinated Antibacterial Agent Exposure

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Abstract

Triclosan and triclocarban are common antimicrobial ingredients extensively employed in consumer and personal care products. Their frequent exposure has resulted in the wide detection in human body fluids. With the revelation of their toxic effects in recent years, exploring the human health risks of these antibacterial agents has become increasingly important. Herein, mass spectrometry-based omics approaches were applied to unveil metabolic responses induced by triclosan and triclocarban using in vivo and in vitro models. The endogenous metabolite biomarkers and biotransformation products were identified and analyzed for toxicity assessment. The roles of gut microbiota were also involved to determine the biological significance. The results showed that triclosan and triclocarban exposure can lead to the perturbation of metabolome profile in human hepatocytes. Oxidative stress-related damage is considered as one crucial factor for their hepatotoxicity. The potential effects of triclosan on human hepatocellular carcinoma development include the fast detoxication through phase II metabolism, energy metabolism enhancement and antioxidant defense system elevation. In vivo and in vitro studies also found that gut microbiota can mediate colonic metabolism of antibacterial agents, and contribute to the gut-specific toxicity. Our finding provides valuable scientific basis for human health risk assessments about chlorinated antibacterial agent exposure.

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Fucoidan mitigates the abnormal changes of club cells in mouse lung cancer induced by Benzo(a)pyrene

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Abstract

Purpose: Club cells have been identified as potential precursors of lung cancer, but their specific alterations in Benzo(a)pyrene (B(a)P)-induced lung cancer remain unclear. This study aimed to elucidate the abnormal changes of club cells in B(a)P-induced lung cancer and investigate the intervention role of Fucoidan (FCD), known for its anticancer properties.

Methods: C57BL/6 wild-type mice received intratracheal instillations of Benzo(a)pyrene [B(a)P] (1 mg/mouse) weekly for 4 consecutive weeks. FCD interventions were administered ad libitum via drinking water (low dose FCD (LFCD): 1.55g/L; high dose FCD (HFCD): 3.1g/L). Mice were sacrificed at 26 and 34 weeks to assess lung cancer occurrence, as well as the differentiation, proliferation, gene damage, and mutation of club cells.

Results: Tumors were observed at 34 weeks in three groups: B(a)P group (33.33%), LFCD + B(a)P group (25.00%), and HFCD + B(a)P group (21.42%). Cell differentiation trajectory analysis revealed that B(a)P initially inhibited club cells differentiation into ciliated cells at week 26 but promoted it by week 34. FCD intervention promoted club cells differentiation into ciliated cells at both 26 and 34 weeks. Correspondingly, B(a)P inhibited the expression of the ciliated cell marker Foxj1 gene in club cells at 26 weeks and promoted its expression at 34 weeks; HFCD promoted Foxj1 gene and protein expression in club cells at both time points. At 26 weeks, HFCD also promoted club cells to express the goblet cell marker Clca1 gene and protein. Additionally, B(a)P increased the expression of the proliferation marker ki67 gene and protein, and the gene damage protein γ-H2AX in club cells at both 26 and 34 weeks; FCD intervention inhibited these effects. Furthermore, B(a)P induced an increase in the number of mutated genes in club cells at 34 weeks, which FCD intervention could inhibit. Mutations in tumor suppressor genes such as NF1, Kmt2c, and Suz12 were detected only in club cells of the B(a)P group.

Conclusions: In the B(a)P-induced lung cancer model in mice, club cell differentiation initially decreased and then increased, proliferation accelerated, and gene damage and mutations occurred. FCD intervention reduced the incidence of B(a)P-induced lung cancer, inhibited excessive proliferation of club cells, promoted their differentiation, and alleviated gene damage and mutations.

Key words: Benzo(a)pyrene, Lung cancer, Fucoidan, Club cells

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N6-methyladenosine demethylase FTO regulates neuronal oxidative stress via YTHDC1-ATF3 axis in arsenic-induced cognitive dysfunction

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Abstract

Excessive exposure to metals in daily life has been proposed as an environmental risk factor for neurological disorders. Oxidative stress is an inevitable stage involved in the neurotoxic effects induced by metals, nevertheless, the underlying mechanisms are still unclear. In this study, we used arsenic as a representative environmental heavy metal to induce neuronal oxidative stress and demonstrated that both *in vitro* and *in vivo* exposure to arsenic significantly increased the level of N6-methyladenosine (m6A) by down-regulating its demethylase FTO. Importantly, the results obtained from FTO transgenic mice and FTO overexpressed/knockout cells indicated that FTO likely regulated neuronal oxidative stress by modulating the target gene activating transcription factor 3 (ATF3) in a m^6A-dependent manner. We also identified the specific m6A reader protein, YTHDC1, which interacted with ATF3 and thereby affecting its regulatory effects on oxidative stress. To further explore potential intervention strategies, cerebral metabolomics was conducted. Through this, we newly identified myo-inositol as a metabolite that exhibited potential in protecting neurons against oxidative stress and neurobehavioral impairments induced by arsenic. Overall, these findings provide new insights into the importance of the FTO-ATF3 signaling axis in neuronal oxidative stress from an m^6A perspective, and highlight a beneficial metabolite that can counteract the oxidative stress induced by arsenic.

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Multi-Omics Analysis of Harmful Effects of $PM_{2.5}$ on Energy Metabolism

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Abstract

Air pollution, particularly fine particulate matter ($PM_{2.5}$), presents a significant environmental health risk, linked to around seven million annual deaths globally. Composition variations in $PM_{2.5}$ contribute to diverse toxicological impacts across regions. Utilizing multi-omics approaches, we have investigated the effects of $PM_{2.5}$ on energy metabolism in various organs, selecting Taiyuan, a heavily industrialized city in Northern China, as a typical case. Our research demonstrated that $PM_{2.5}$ exposure intensifies the adverse effects of unhealthy diets on cardiovascular health and disrupts metabolism in multiple organs, including changes in branched-chain amino acid metabolism in the spleen and alterations in lipoprotein metabolism in the liver. Comprehensive year-round sampling of $PM_{2.5}$ from Taiyuan and Guangzhou (a Southern Chinese city) was analyzed, to reveal significant metabolic shifts in lung cells linked to regional $PM_{2.5}$ components. Through mass spectrometry-based metabolomics, we identified phosphocholine as a key metabolite with potential therapeutic benefits against $PM_{2.5}$-induced disruptions, enhancing cellular energy balance and viability by shifting energy reliance to fatty acid oxidation. This underscores the utility of omics approaches to decipher the toxicological effect of regional $PM_{2.5}$ exposures and identify promising interventions for countering its health effects, offering new paths for tailored public health strategies.

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Whole Transcriptome Sequencing Reveals LncRNA/circRNA-miRNA-mRNA Networks in Bisphenol AF Induced Cardiac Inflammatory Response in Zebrafish

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Abstract

Bisphenol AF (BPAF) is a fluorinated derivative of bisphenol A and widely used as BPA alternative in industry currently. Among all bisphenol analogues, BPAF ranks one of the most detected ones in various environmental media. Previous studies have shown cardiovascular toxicity of bishphenos, however, there are still many unknowns about how epigenetic regulation play roles in bisphenol-induced cardiotoxicity. In the present study, we first found the acute BPAF exposure exerts dose-dependent toxic effects on cardiac development, morphology, and function in zebrafish embryos and larvae during their early developmental stages. And then, following a 28-day exposure of adult zebrafish to an environmentally relevant concentration of BPAF, we observed the long-term BPAF exposure induces cardiac inflammation in both male and female zebrafish, and paternal exposure has a more significant impact on the cardiac function of F1 generation. The BPAF exposed zebrafish adult hearts were further subjected to high-throughput RNA sequencing, obtaining a comprehensive transcriptome database of the hearts from both sexes. These results reveals significant changes in the expression patterns of mRNA, miRNA, lncRNA, and circRNA in the hearts of both sexes upon the long-term of BPAF exposure.Utilizing bioinformatics and RNA molecular regulatory network analysis, we investigated the biological processes and signaling pathways involved in target genes regulated by non-coding RNAs. It was showed that the mRNAs in the lncRNA/circRNA-miRNA-mRNA regulatory networks are significantly enriched in various metabolic processes, myocardial contraction, ion transmembrane transport, cell contraction and multiple hydrolase activities. The above findings should help to better understand the toxicity and action mechanisms of bisphenols, and also provide scientific data for screening specific biomarkers further applied for assessing pollutant-induced cardiac toxicity. Correspondence: mingyang@shu.edu.cn (M. Yang) & zhongchen7498@hotmail.com (Z. Chen)

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Magnetic fraction of iron-doped diesel exhaust (MIDE)-induced pulmonary fibrosis: Results from RNA-seq

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Abstract

Background: Diesel doping could improve burning efficacy and decrease emission, in which iron-containing chemicals, such as ferrocene had been widely used, resulting in magnetic particles in the generated diesel exhaust. Since magnetic particles had been reported to be quite toxic, preliminary studies in our lab revealed magnetic fraction of iron-doped diesel exhaust (MIDE) could induce pulmonary fibrosis. To further elucidate underlying mechanism, RNA-seq technique was utilized to analyze potential biomarkers and molecular targets of MIDE.

Methods: Standard China VI diesel was supplemented with 820 mg/ml ferrocene, and burned in a diesel power generator. Diesel exhaust particles were collected and subjected to magnetic purification with Neodymium magnets. Collected MIDE was then exposed to hatchling chickens via intratracheal instillation. After one month, lungs were collected and subjected to RNA-seq. Differentially expressed genes (DEGs) were analyzed and qPCR tests were performed to verify RNA-seq results. Lentivirus-mediated in ovo silencing method was used to further confirm the roles of DEGs.

Results: RNA-seq identified 1972 DEGs between control and MIDE-exposed lung tissue samples (1014 up-regulated and 958 down-regulated). Among the DEGs, Spermine N1-Acetyltransferase 1 (SAT1) was selected as the potential target gene, since it had been associated with well-known pulmonary fibrosis-related pathways. qPCR verification confirmed MIDE-mediated upregulation of SAT1. Lentivirus-mediated *in ovo* silencing of SAT1 effectively abolished MIDE-induced pulmonary fibrosis.

Conclusions: MIDE-induced pulmonary fibrosis in hatchling chicken is associated with SAT1, according to the results of RNA-seq, which is further confirmed via qPCR and lentivirus-mediated in ovo silencing.

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SUMOylation Modification of FTO Facilitates Oxidative Damage Response of Arsenic by IGF2BP3 in an m6A-dependent Manner

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Abstract

N6-methyladenosine (m6A) is the most common form of internal post-transcriptional methylation observed in eukaryotic mRNAs. The abnormally increased level of m6A within the cells can be catalyzed by specific demethylase fat mass and obesity-associated protein (FTO) and stay in a dynamic and reversible state. However, whether and how FTO regulates oxidative damage via m6A modification remain largely unclear. Herein, by using both in vitro and in vivo models of oxidative damage induced by arsenic, we demonstrated for the first time that exposure to arsenic caused a significant increase in

SUMOylation of FTO protein, and FTO SUMOylation at lysine (K)-216 site promoted the down-regulation of FTO expression in arsenic target organ lung, and therefore, remarkably elevating the oxidative damage via an m6A-dependent pathway by its specific m6A reader insulin-like growth factor-2 mRNA-binding protein-3 (IGF2BP3). Consequently, these findings not only reveal a novel mechanism underlying FTO-mediated oxidative damage from the perspective of m6A, but also imply that regulation of FTO SUMOylation may serve as potential approach for treatment of oxidative damage.

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DNA methylation mediated transgenerational teratogenic effect of azoxystrobin on zebrafish (Danio rerio)

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Abstract

Numerous studies have shown that chronic exposure to environmental pollutants not only affects directly exposed individuals, but may also cause abnormalities in offspring not directly exposed through epigenetic transgenerational inheritance. Our study on azoxystrobin exposure (1, 10, and 100 μg/L, 4 days) in zebrafish found no harm to F0 embryos, yet revealed developmental malformations and impaired cardiac functionin in subsequent unexposed generations (F1, F2), confirming azoxystrobin has transgenerational teratogenic effects on zebrafish embryos. Cross-testing experiment proved that transgenerational effects induced by azoxystrobin are independent of specific gender. Further research found that the protein content of the three DNA methyltransferases (DNMTs) were significantly decreased, as well significant alterations in DNA methylation were found in both F1 and F2 embryos, indicating DNA methylation might be involved in the transgenerational effects. Integrated analysis of genome-wide DNA methylation and transcriptome reveal a total of 7 genes showed simultaneous changes in differential gene expression and methylation levels, and only the *ryr1b* gene had exactly the same differentially DNA methylation sites in F1 and F2 embryos, suggesting that the DNA methylation modification of *ryr1b* can be inherited stably. STRING analysis linked *ryr1b* to genes regulating cellular calcium homeostasis, underscoring the mechanism behind azoxystrobin's transgenerational impacts. Overall, we proposed the DNA sequence of *ryr1b* would be hypermethylated after exposure to azoxystrobin and lead to a decrease of gene expression, than resulting in regulating the expression of downstream genes and inducing calcium homeostasis imbalance, and ultimately affect the development and cardiac function of zebrafish embryos. The transgenerational inheritance of the DNA methylation of *ryr1b* incuced by azoxystrobin mediated the transgenerational inheritance of teratogenic effects, which could provide novel information to understand the underlying mechanism of multigenerational toxicity induced by environmental pollutants.

20．Role of Biotransformation in Ecotoxicology

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Use of CRISPR-cas9 Methods to Evaluate the Contribution of Flavin Monooxygenases in Pesticide Biotransformation in Zebrafish

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Abstract

Flavin-containing Monooxygenases (FMOs) are a family of enzymes that are co-localized with cytochrome P450s (CYPs) in the endoplasmic reticulum of multiple cell-types, organs, and organisms. FMOs are also similar to CYPs in that they require NADPH and oxygen. However, the substrate specificities and catalytic reaction mechanism is significantly different in that soft-nucleophilic substrates attack peroxyl-flavins located in the active site of the enzyme. Numerous studies have shown an association with expression and functionality of FMOs in animals residing in saltwater or undergoing saltwater acclimation. Isolation and sequencing of salmonid FMO1 possessed Osmoregulatory response Elements (OsREs) in the promoter region of the gene, and expression of FMO mRNA was increased following NaCl treatment in isolated hepatocytes of rainbow trout. To determine the relevance of the enzyme in osmoregulation and xenobiotic metabolism, we targeted the *D.rerio fmo5* for functional disruption using direct microinjection of CRISPR-Cas9 Ribonucleoprotein (RNP) complexes into two-cell stage embryos.. We evaluated several small guide RNAs (sgRNAs) to the *fmo5* gene for editing efficiency and identified an sgRNA targeting the region encoding the functionally essential FAD binding site which resulted in high embryo editing efficiency and no embryo-lethality. We evaluated RNP and mock microinjected embryos at 7 days postfertilization, for sensitivity to NaCl, the organophosphate insecticide, phorate, nicotine, and thiourea. Genomic DNA was prepared from each embryo and editing efficiency was evaluated by direct PCR of the targeted region, sanger sequencing, and Inference of CRISPR edits (ICE) analyses. Importantly, all FAD targeted larvae were predicted to have 95% composite loss of function in all injected animals No significant differences were observed in thiourea ,nicotine, or NaCl treatments between mock injected and larvae confirmed to have predicted functional disruption. In contrast, while 100% mortality was observed in mock injected animals treated with phorate at all concentrations, only 42% mortality at the highest concentrations was noted in the larvae with *fmo5* disruption.

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Nontarget discovery of novel metabolites for organophosphate esters in lettuce (Lactuca sativa L.): Distribution and toxicity effects

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Abstract

The absorption, translocation, and biotransformation behaviors of organophosphate esters (OPEs) and diesters (OPdEs) in a hydroponic system were investigated. The lateral root was found as the main accumulation and transformation places of OPEs and OPdEs in lettuce (*Lactuca sativa* L.). The non-target analysis using high-resolution mass spectrometry revealed five hydroxylated metabolites and five conjugating metabolites in OPE exposure group, among which methylation, acetylation, and palmitoyl conjugating OPEs were reported as metabolites for the first time. Particularly, methylation on phosphate can be a significant process for plant metabolism and diphenyl methyl phosphate (MDPP) with a higher predicted toxicity accounted for the greatest part of metabolites. Furthermore, the structure-dependent uptake, distribution, biotransformation, and potential toxicity effects of alkyl OPEs in hydroponic lettuce. Trimethyl, triethyl, and tripropyl phosphates were readily absorbed and acropetally translocated while tributyl, tripentyl, and trihexyl phosphates accumulated mainly in lateral roots. The acropetal translocation potential was negatively associated with log K_{ow} values. Trimethyl and triethyl phosphates are less prone to biotransformation, while a total of 14 novel hydrolysis, hydroxylated and conjugated metabolites were identified for other OPEs using nontarget analysis. The extent of hydroxylation decreases from tripropyl phosphate to trihexyl phosphate, but multiple hydroxylations occurred more frequently on longer-chain OPEs. Further comparative toxicity test revealed that hydrolyzed and hydroxylated metabolites have stronger toxic effects on Ca^{2+}-dependent protein kinases (CDPK) than their parent OPEs. Dibutyl 3-hydroxybutyl phosphate particularly induce the upregulation of CDPK, probably associated with adenine reduction that may play an important role in the self-defense and detoxification processes of lettuce. The results contribute to understanding the uptake and transformation behaviors of OPEs as well as their associations with toxic effect on lettuce.

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Metabolites of pesticides: a blind spot of risk assessment on pesticides

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Abstract

Risk assessment of pesticides is one of the most important parts in the risk assessment of environmental contaminations. Previous studies have showed that pesticides would pose acute toxicity, chronic toxicity, reproductive toxicity, endocrine disrupting effects, and the carcinogenic effect to organisms. However, not so much attention has been paid to the risk assessment of the metabolites of pesticides. Thus, metabolites of pesticides have become a blind spot of risk assessment about pesticides.

Our studies have showed that bifenthrin would metabolize into the estrogenic metabolite, 4-hydroxybifenthrin (4-OH-BF), in zebrafish embryos, and the formation was higher in animals after liver development (>48 hpf). Treatments with β-glucuronidase indicated that 4-OH-BF underwent conjugation in embryos. Formation was reduced by cotreatment of the cytochrome P450 (CYP450)

inhibitor, ketoconazole. Formation of 4-OH-BF was greater when treated with 1R-cis-BF compared to the S-enantiomer. However, metabolites were not observed in medaka embryos. We also combined multi-models (*in vivo*, *in vitro*, and *in silico* models) to evaluated the toxicity and endocrine disrupting effects of 5 pesticides and their 22 metabolites. And the results showed that over 50 % of the metabolites exhibited more potent toxicity and endocrine disrupting effects comparing to their parent compounds.

So, it's obvious that the lackness of risk assessment about metabolites of pesticides would result in greater environmental and health risk to human beings. And our work here can help to remind the importance of risk assessment about metabolites of pesticides and provide some instruction to the future work.

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Synthetic Antioxidants and Transformation Products as New Pollutants: From Environmental Occurrence to Human Exposure

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Abstract

Synthetic antioxidants, including synthetic phenolic antioxidants (SPAs) and organophosphite antioxidants (OPAs), are largely produced and widely used to retard oxidative reactions and lengthen shelf life of products. Limited information can be found on environmental pollution caused by these chemicals and their related transformation products. In this study, we collected environmental and human biological samples to investigate the occurrence and human exposure of these new pollutants. SPAs were widely identified in sludge and indoor dust collected from China and Canada. 2,6-Di-tert-butyl-4-methylphenol (BHT) was the primary congener in the environmental samples. The high detection of SPAs in the environment suggested their unavoidable human exposure. Indeed, human internal exposure to SPAs was confirmed by their occurrence in human serum. In agreement with environmental samples, BHT was the primary congener in human serum. In contrast to human serum, BHT was observed at very low concentrations in human urine, while 3,5-di-tert-butyl-4-hydroxybenzoic acid (BHT-COOH) was detected at high concentrations, suggesting the biotransformation from BHT to BHT-COOH in human before urinary excretion. As for OPAs, they can not be detected in most environmental samples. However, the oxidation products of OPAs can be detected at high concentrations in indoor dust. The oxidation products of OPAs, such as tris(2,4-di-tert-butylphenyl) phosphate, can be detected in SRM2585 (prepared in 1993-1994), suggesting OPAs have been used in North America more than two decades. Besides, abundance of tris(2,4-di-tert-butylphenyl) phosphate increased significantly in Artic air since 1994. This comprehensive study provides new knowledge on environmental occurrence and human exposure of synthetic antioxidants and their transformation products.

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Biotransformation and Ecotoxicology of Alternative Perfluoroalkyl Substances in Plant

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Abstract

Legacy per- and polyfluoroalkyl substances (PFASs) were regulated increasingly due to their environmental risk. Novel PFAS alternatives have emerged and replaced legacy PFASs, resulting in their ubiquitous presence in environmental media and living organisms.Fluorotelomer carboxylic acids (FTCAs) and fluorotelomer sulfonic acids (FTSAs) are commonly used as PFOA and PFOS alternatives, respectively. They have been routinely detected in environment. But their behaviors and ecotoxicology in plants are not sufficiently known. The regular and multi-omics analyses were used to comprehensively investigate the bioaccumulation, biotransformation, and toxicity of FTCAs and FTSAs in plants. Our results demonstrated that FTCAs and FTSAs could be taken up by plant roots and acropetally translocated to above-ground part of plants. Biotransformation of FTCAs and FTSAs to several intermediates and different carbon chain perfluorocarboxylic acid (PFCA) metabolites via α-and β-oxidation catalyzed by enzymes in plants was observed. Plant-associated rhizosphere bacteria and endophytic bacteria also contributed to FTCAs degradation through β-oxidation. Significant increases in Chl contents were shown in plants, indicating that they stimulated the synthesis of plant photosynthetic pigments. However, the reductions of antioxidant and metabolic enzyme activities reflected the antioxidant defense system and detoxification system of plants were both damaged, which were further confirmed by the down-regulating associated genes encoding phenylpropanoid biosynthesis, endoplasmic reticulum-related proteins, ascorbate-glutathione cycle and ABC transporters. Transcriptomic analysis indicated that differentially expressed genes (DEGs) were related to transformation and transport processes. Metabolomic analysis showed that the accumulation of these non-enzymatic antioxidants in plants could defend against oxidative stress caused by 8:2 FTSA. Integrative transcriptomic and metabolomic analysis revealed that DEGs and differentially expressed metabolites (DEMs) in plants exposed in 8:2 FTSA were predominantly enriched in the carbohydrate metabolism, amino acid metabolism, and lipid metabolism pathways, resulting in greater energy consumption, generation of more nonenzymatic antioxidants, alteration of the cellular membrane composition, and inhibition of plant development. These results are helpful to understand the environmental behaviors and ecotoxicity of FTCAs and FTSAs in plants.

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Revealing Androgen Receptor (AR) Disruptors in Sewage Sludge

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Abstract

The global practice of reusing sewage sludge in agriculture and its landfill disposal reintroduces environmental contaminants, posing risks to human and ecological health. This study screened sewage sludge from 30 Chinese cities for androgen receptor (AR) disruptors, utilizing a disruptor list from the Toxicology in the 21st Century program (Tox21), and identified 25 agonists and 33 antagonists across diverse use categories. Predominantly, natural products 5α-dihydrotestosterone and thymidine emerged as agonists, whereas the industrial intermediate caprolactam was the principal antagonist. In-house bioassays for identified disruptors displayed good alignment with Tox21 potency data, validating employing Tox21 toxicity data for theoretical toxicity estimations. Potency calculations revealed 5α-dihydrotestosterone and two pharmaceuticals (17β-trenbolone and testosterone isocaproate) as the most potent AR agonists and three dyes (rhodamine 6G, Victoria blue BO, and gentian violet) as antagonists. Theoretical effect contribution evaluations prioritized 5α-dihydrotestosterone and testosterone isocaproate as high-risk AR agonists and caprolactam, rhodamine 6G, and 8-hydroxyquinoline (as a biocide and a preservative) as key antagonists. Notably, 16 agonists and 20 antagonists were newly reported in the sludge, many exhibiting significant detection frequencies, concentrations, and/or toxicities, demanding future scrutiny. Our study presents an efficient strategy for estimating environmental sample toxicity and identifying key toxicants, thereby supporting the development of appropriate sludge management strategies.

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In-Sewer Stability of 20 Pharmaceuticals Under Nano Zero Valent Iron Dosing

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Abstract

The assessment of in-sewer stability of pharmaceuticals is one of crucial steps when applying wastewater-based epidemiology (WBE) for estimating pharmaceutical consumption at the population level. The fate

and distribution of pharmaceuticals in sewer networks are complicated, which are associated with many interactive processes. From discharging points to wastewater treatment plants (WWTPs), these chemicals may undergo a series of interactions with sewer biofilms, leading to biotransformation, hydrolysis, and adsorption processes. Lab-scale sewer reactors are useful tools to understand transformation kinetics and rates for pharmaceuticals in sewer networks, which contributes to the more accurate assessments for WBE.

In addition to natural sewer processes, chemical dosing is a common and important strategy for sewer odour control and corrosion inhibition. As an emerging synthetic material, nano zero valent iron (NZVI) has been tested for reducing the production of hydrogen sulfide through biological and/or chemical processes. Concurrently, NZVI will interact with pharmaceuticals and thereby affect their behaviours and distribution between solid and liquid phases. However, little is known about the impact of NZVI on the fate of pharmaceuticals in sewers.

This study aims to investigate and model the fate and distribution of pharmaceuticals under NZVI dosage in sewers. The results showed that the transformations were strengthened with dosing duration for most pharmaceuticals, except for paracetamol, 2-ethylidene-1,5-dimethyl-3,3-diphenylpyrolidine (EDDP), and methadone. By comparing results between batch tests applied with different NZVI dosing concentrations, it is found that adsorption was not significant responsible for the change on pharmaceuticals' stability, while biotransformation played an important role after the biofilms underwent long-term exposure to NZVI. These findings reveal impacts of NZVI on in-sewer stability and biological communities and provide insight into environmental fate and WBE application.

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Biotransformation changes toxicity and ecological risk of systemic insecticides to aquatic invertebrates

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Abstract

Biotransformation often alters chemical toxicity, yet it is a challenge to assess the impact of biotransformation process on aquatic risk of chemicals that are readily metabolizable. One reason is that it is difficult to quantify internal exposure-based thresholds for these chemicals that experience biotransformation during toxicity tests. Based on toxicokinetic models established previously, we integrated toxic unit and toxicokinetics to quantitatively assess toxicity contributions and potential risk of both parent compound and transformation products (TPs) to aquatic organisms, using systemic insecticides (fipronil and neonicotinoids) as representative toxicants. In aquatic invertebrates Chironomus dilutus and Hyalella azteca, approximately 90% of fipronil was transformed to fipronil sulfone. Fipronil and fipronil sulfone exhibited similar intrinsic toxicity to these organisms, which was contrary to conventional perception that fipronil sulfone was more toxic than its parent compound. However, biotransformation was still important in risk assessment because the TP had 10-fold

slower depuration rate than the parent compound. The amphipod H. azteca was found to be as sensitive to FIPs as the insect C. dilutus, which was previously considered ten times more sensitive based on external thresholds. This discrepancy has led to overlooking the toxicity of fipronil to H. azteca in regional risk assessments. Using the developed internal exposure-based thresholds, we evaluated lethal risk of fipronil and its metabolites to H. azteca in global surface water, showing the urgency of considering TPs in water quality assessments, especially for sensitive species that are at risk in the environment.

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Metabolic Activities in Rainbow Trout (Oncorhynchus mykiss) S9 Fractions from Liver andExtrahepatic Organs as an Alternative in vitro Ecotoxicity Assessment Approach

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Abstract

Whole body biotransformation rate constants can be calculated using an appropriate in vitro to in vivo extrapolation (IVIVE) model. These models use $CL_{IN\ VITRO,\ INT}$ rates derived with OECD Test Guideline 319B or 319A to estimate liver clearance rates, which are then extrapolated to a whole-body (in vivo) biotransformation rate constant. However, beside the liver, extrahepatic organs may also display Phase I and Phase II biotransformation activities and thereby play a role in metabolic clearance and bioaccumulation of compounds.

To adress these questions, we have maintained rainbow trout (Oncorhynchus mykiss) under controlled housing conditions according to OECD 319A/B. Specimens of eight sexually immature animals were harvested and pooled, including liver, gill, intestine, brain, heart and spleen. S9 fractions were prepared to determine the Phase I and Phase II enzyme activities by Liquid Chromatography-Mass Spectometry analysis. Cytochrome P450 activities, glucuronidation and sulfation activities were analyzed.

The liver displayed the highest Cytochrome P450 activities of all organs tested. Chorzoxazone Hydroxylase activity was only detectable in liver, 1-OH-Midazolam Hydroxylase activity was mainly restricted to liver, minor activities could be detected in intestine. However, Phenacetin-O-Deethylation was also detectable in other organs, with intestine, gill and spleen contributing 34, 18 and 11% of the total enzyme activity. Diclofenac-hydroxylase activity was present in all organs, as well as Bupropion-4-Hydroxylase activity, which was more or less evenly distributed among all

organs. Phase II activities were detected in the liver, gill, intestine and heart, but not in spleen or brain.

In summary, the liver is the major organ for detoxification of compounds. However, extrahepatic organs, mainly intestine and gill, but also the brain, heart and spleen exhibit certain cytochrome P450 activities. Phase II enzyme activities were also detected in the intestine and gill. Our results suggest that extrahepatic organs, mainly intestine and gill, should also be taken into account when bioaccumulation and in vitro clearance rates are determined for IVIVE modeling in rainbow trout.

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Microbiota-mediated biotransformation of triclosan induces colitis

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Abstract

Triclosan (TCS) is an antimicrobial agent and a major environmental pollutant widely used in consumer products. Under normal circumstances, TCS will be rapidly metabolized into non-biologically active metabolites such as "TCS-glucuronide" (TCS-G), which are easily excreted from the body. However, we have found that certain gut microbes can reactivate TCS-G and form to TCS in the gut, resulting in colitis. The new toxicological mechanism of TCS may also be applicable to toxicity studies of other environmental contaminants, and the role of gut microbiota should be considered when assessing the toxicity of environmental pollutants.

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Plant Mediated Transformations of Emerging Contaminants

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Abstract

Many emerging contaminants have reactive functional groups and may readily undergo biotransformations, such as methylation/demethylation, halogenation/dehalogenation, and conjugation/deconjugation. These transformations have been reported to occur in various biological systems. Plants come into contact with emerging contaminants in managed (e.g., constructed wetlands, agricultural fields) or natural systems (e.g., natural wetlands, estuaries) through point and non-point source pollution. Plants have a cascade of enzymes capable of mediating various biotransformations, and some of the transformation products may acquire different ecological risk potentials. Studies have shown that many emerging contaminants can directly conjugate with various endogenous biomolecules in plants to form conjugates, undergo methylation/demethylation reactions, or form halogenated derivatives. The formation of bioactive transformation products effectively prolongs the environmental cycling of emerging contaminants, and the changes in physicochemical properties also lead to differences in bioaccumulation potential and ecotoxicity. This presentation will provide an overview of knowledge on plant mediated transformations of different emerging contaminants and discuss the environmental implications as well as opportunities for fundamental and applied research to address environmental concerns surrounding emerging contaminants.

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New Insights on Free and Conjugated Forms Neonicotinoid Insecticides in Human Serum and Their Association with Oxidative Stress

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Abstract

Following exposure, neonicotinoid insecticides (NEOs) can be metabolized by both Phase I and Phase II reactions catalyzed by human cytochrome P450 enzymes. However, toxicities of parent NEOs and their metabolites are still unclear and little is known about biotransformation rates and pathways of NEOs in humans. In this study, 98 serum samples collected in China were analyzed for free, conjugated and total forms of six parent NEOs (i.e., acetamiprid (ACE), imidacloprid (IMI), clothianidin (CLO), thiacloprid (THD), thiamethoxam (THM) and dinotefuran (DIN)), and four metabolites (i.e., *N*-desmethyl-acetamiprid (*N*-dm-ACE), 1-methyl-3-(tetrahydro-3-furylmethyl) (DIN-U), 5-hydroxy-imidacloprid (5-OH-IMI), olefin-imidacloprid (Of-IMI)). NEOs and their metabolites were detected in all serum samples, and the total median concentrations of free, conjugated, and total forms of 10 NEOs were 2.04, 2.01, and 5.12 ng/mL, respectively. Conjugated forms of NEOs accounted for only half (53%) of the total forms of NEOs. Based on the profiles of Phase I and Phase II metabolites of NEOs in serum, it was found that age is a determinant in Phase I metabolism of DIN and Phase II metabolism of IMI. The Phase II metabolites of NEOs are associated with oxidative DNA damage, and the conjugated forms of IMI, DIN and 5-OH-IMI in serum were significantly positively correlated with oxidative stress. Overall, the amount of NEOs

present in conjugated forms in human serum was determined to document the existence of considerable proportion of free forms of these insecticides.

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Construction of highly effective sulfamethoxazole degrading consortium for bioaugmentation of constructed wetlands

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Abstract

Sulfonamides (SAs) are widely used in different field and residual SAs in the environment may increase the abundance of resistance genes through processes such as gene transfer, which attracts wide attention. Constructed wetland is an environmentally friendly and efficient treatment technology, in which microorganisms play an important role in SAs degradation. Bioaugmentation can enhance the pollutant removal capacity by introducing degraders. Correlative researches were usually conducted in other matrices instead of sediment and the inoculation was often a single strain rather than interacting microbial consortia. This study aimed to (1) screen and construct the efficient degradation microbial consortium of sulfamethoxazole (SMX); (2) achieve efficient and complete removal of SMX for bioaugmentation of constructed wetlands.

In this study, isotope tracer technique (benzene ring labeled ^{14}C-SMX) was used to measure mineralization efficiency and identify metabolites. Acute toxicity test of SMX and metabolites was done using luminescent bacteria. SMX could be completely removed in enrichment I generation II in 18 d and the degradation efficiency increased respiking SMX. The mineralization efficiency was only about 5% in 40 d. The main metabolite with weaker polarity than SMX was identified as hydroxyl substitution product (4-OH-SMX). It accumulated in enrichment I and its toxicity was higher than SMX. Although the degradation efficient was not bad, enrichment I was not suitable for application considering the incomplete degradation and the toxicity of the metabolite. Interestingly, degradation efficiency of generation I was not parallel in the batch experiment. Potential degraders were found through analyzing community structure. To achieve the harmless and thorough degradation of SMX, a second screening was done from another batch of sediment. A degrader was isolated and identified as *Microbacterium aureliae* (similarity was 99.93%). It could mineralize the benzene ring of SMX while 3-amino-5-methyl isoxazole (3A5MI) was accumulated in the culture. *Nocardioides* sp. N27 as degrader of 3A5MI was inoculated into the culture to establish the consortium. Two strains could cooperate and completely degrade 30 mg/L SMX in 4 h. This study offered a method for screening SMX-degraders and constructed a highly effective SMX degrading consortium, which provided effective materials for enhancement of constructed wetlands by bioaugmentation.

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Oligomer Release from the Biotransformation of PLA Bioplastics byGut Enzymes and Its Acute Inflammatory Effect

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Abstract

Although the health risks of exposure of humans to environmental microplastics are being increasingly studied, little is known about the behavior of “eco-friendly” bioplastics, particularly their effects on the gastrointestinal tract. Here we demonstrate that enzymatic hydrolysis of polylactic acid (PLA) microplastics rapidly generated excess nanoplastic particles by competing for triglyceride-degrading lipase during gastrointestinal processes. Nanoparticle oligomers were formed by hydrophobic-driven self-aggregation, and upon exposure, the oligomers and their associated nanoparticles bioaccumulated in *in vitro* as well as *in vivo* in organs including the liver, intestine, and brain. Severe intestinal damage and inflammation were mainly caused by hydrolyzed oligomers. Furthermore, screening for potential protein targets using a large-scale pharmacophore model revealed that oligomers interacted with matrix metallopeptidase 12 (MMP12), which was further validated using a protein binding assay. Moreover, a detailed mechanistic study revealed high-affinity binding of oligomers to the catalytic zinc-ion finger domain, leading to MMP12 inactivation, which mediated the adverse bowel inflammatory effects after exposure to PLA oligomers. Biodegradable plastics are considered an important solution to address global environmental plastic pollution. Thus, understanding the gastrointestinal fates and toxicities of bioplastics will provide ground-breaking data on bioplastics that pose a substantial risk to human health.

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Sediment-seawater partitioning, bioaccumulation, and biomagnification ofperfluorobutane sulfonamide in marine environment

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Abstract

Environmental occurrence of perfluorobutane sulfonamide (PFBSA) has only been recently discovered. The current knowledge regarding the occurrence and environmental behaviors of PFBSA in the marine

environment is still relatively limited. In this study, PFBSA and other 37 poly- and perfluoroalkyl substances were analyzed in seawater (n = 43), sediment (n = 43), and marine fish (n = 176) samples collected from East China Sea and Antarctic Ocean. PFBSA was detected in > 90% of seawater from East China Sea and Antarctic Ocean, with the concentrations of 1.0 − 19 ng/L and < LOD−228 pg/L, respectively. The field-based mean log-transformed sediment-seawater partitioning coefficients of PFBSA were 1.6 ± 0.19 L/kg dw and 1.1 ± 0.19 L/kg dw in East China Sea and Antarctic Ocean, respectively, which are lower than that of perfluorooctanoate and perfluorooctane sulfonate. This indicates its long-range transport potential in global oceans with ocean currents. The mean log-transformed bioaccumulation factor values of PFBSA determined in the multiple species of whole-body marine fishes from East China Sea and Antarctic Ocean were 2.3 L/kg ww and 2.4 L/kg ww, respectively, which are comparable to that of perfluoroheptanoate (2.3 L/kg ww) in marine fishes from East China Sea. We did not observe an obvious biomagnification or biodilution of PFBSA along the marine food chain in East China Sea or Antarctic Ocean. This study provides the first data on the environmental behaviors of PFBSA in the marine environment.

21. Agricultural Environment, Food and Human Health

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The environmental behavior of typical artificial sweeteners in agricultural soil and wheat: accumulation, translocation and biotransformation

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Abstract

Artificial sweeteners (ASs) are sugar substitutes that are mainly used in food, beverages, and animal feeds due to their high sweetening intensity and negligible energy intake. ASs have gained significant attention as contaminants of emerging concern due to their presence and high concentrations in various environmental matrices. Sewage irrigation, as well as the application of sludge and manure as fertilizer are the primary sources of ASs in agricultural soil. The exposure of contaminated crops through the food chain could potentially pose risks to human health. However, our current understanding of the behavior and the fate of ASs in agricultural soil-plant systems remains limited, impeding a comprehensive understanding of their environmental behavior and risks of human exposure. For this purpose, an investigation was conducted by determining seven ASs in pig feed, manure, agricultural soil, and vegetables from 16 pig farms. The mechanisms on the uptake, translocation and transformation of typical ASs by wheat was also conducted through pot experiment.

Saccharin (SAC) was predominant in feed and manure samples. The annual emission of ASs to the agricultural soil via manure was estimated. Moreover, the levels of ASs in different layers of soil and vegetables in neighboring farmland that received manure fertilizers and wastewater were consecutively monitored for 60–80 days. SAC, cyclamate (CYC) and acesulfame (ACE) were widely determined in soil and vegetables. In greenhouse soils, CYC, SAC, ACE, and sucralose were degraded quickly, with half-lives of 4.3–5.9 d, 2.7–4.2 d, 8.4–12.3 d, and 7.3–10.8 d, respectively. Lower levels of

ASs were found in deeper soil layer (20–30 cm). The ASs were considerably absorbed by plants when the ASs' concentrations were high in soil. Further investigation indicated that root uptake of ASs is an energy-consuming process, with both aquaporins and anion channels contributing to this mechanism. 21 Transportation products were identified in the hydroponic plant system and close attention should be paid to these metabolites, as some may exhibit even greater toxicity than their parent compounds. The findings of this study contribute significantly to enhancing our understanding of the fate of ASs in the agricultural soil and plant, which furthers our understanding of the potential environmental exposures of these chemicals.

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The degradation mechanism of imidacloprid in bio-electrochemical system enhanced by iron-carbon composite material

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Abstract

The problem of water pollution caused by pesticide residues has seriously threatened the safety of aquatic animals and human health. As one of the neonicotinoid pesticides, imidacloprid (IMI) has a very stable molecular structure and is difficult to decompose naturally in the environment. Soil infiltration system is widely used in rural domestic sewage treatment scenarios because of its advantages of simple management, low operating cost, good nitrogen and phosphorus removal effect and stable treatment effect. However, rural sewage is often low in C/N ratio, which leads to a lack of carbon source for heterotrophic microorganisms in the anaerobic section of soil infiltration systems, hindering their growth and causing the inability to provide electrons for the degradation process of IMI. Based on the above problems, this study used ternary micro-electrolysis ceramsite as a medium to construct a bio-electrochemical system (BES) enhanced by micro-electrolysis to study the removal effect of IMI by the system. In this study, the feasibility of IMI degradation by ternary micro-electrolysis-enhanced BES was investigated using laboratory batch experiments; the response relationship between the IMI removal effect in the system and the physicochemical factors, such as influent C/N, ceramic granule dosage and current density, was investigated; and the law and pathway of IMI removal by ternary micro-electrolysis-enhanced BES was revealed, so as to provide a new way for bioremediation of rural farmland wastewater.

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Can urease inhibitor NBPT be transferred from pasture to milk?

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Abstract

NBPT (N-(n-butyl) thiophosphoric triamide) is the only commercial urease inhibitor to date. To improve fertiliser using efficiency and mitigate fertiliser negative effects, NPBT-coated urea and other controlled-release fertilisers could be potential solutions. When the NPBT-coated urea is applied to pasture lands, we need to evaluate the absorption of NBPT by grass and further transfer to milk in the dairy system.

A field plant uptake trial of NBPT-coated urea was conducted in a pasture farm of Victoria, Australia by using 3 NBPT-level treatments and 7 replications. The grass was harvested three times at the end of weeks 4, 7, and 10 and used for NBPT determination. Moreover, a 7-day cow feeding trial with NBPT-coated urea was conducted at a dairy farm by using 2 treatments and 10 replications.

A set of NBPT extraction and quantification methods was developed by using LCMS-QQQ method. The method was robust, reproducible, accurate and stable.

The quantitative analytical results showed that there was no observed NBPT absorption by grass and nil NBPT was detected in the milk samples. There is minimal ecological and healthy risk in utilizing NBPT-coated urea in the dairy pasture.

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Exposure Assessment and Health Risk Characterization of Typical Nonionic Surfactants in Agro-products and Agricultural Soils

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Abstract

Nonionic surfactants (NSs) are widely used in global agricultural production. Since the toxicological risks of some typical NSs have been revealed, NSs or their metabolites have become potential risk factors in the chain of "agricultural environment, food and human". However, the knowledge gaps and challenges in the exposure assessment and health risk characterization of NSs need to be addressed by the following studies:

(1) Exposure levels of typical NSs in agro-products and agricultural soils

We have developed the quantitative analysis methods of NSs, including nonylphenol ethoxylates, tristyrylphenol ethoxylates, polyoxyethylene tallow amine, and trisiloxane ethoxylates. The residue levels and congener profiles of these NSs in agro-products and agricultural soils have been investigated. Nevertheless, further investigation at a larger spatiotemporal scale will be required to ascertain the exposure levels.

(2) Fate and exposure routes of typical NSs in crops and agricultural soils

We have explored the dissipation patterns and dietary risks of typical NSs in crops and soils. Representative outcomes are as follows: (a) The dissipation rate of these polymers was related to the carrier medium, the degree of polymerization, and the dose applied; (b) Oligomers with long ethylene oxide chains tended to dissipate into short-chain oligomers; (c) Dietary risks of these NSs were at a lower level under field trials.

Furthermore, the exposure routes of NSs in agro-products and agricultural soils still need to be explicated. Therefore, the migration and transformation mechanism of congeners with different polymerization degrees in soil-crop systems and their tissue-specific distribution and bioaccumulation in crop will be further studied.

(3) Toxicity effects and health risk characterization of typical NSs

We will conduct *in vivo*/*in vitro* toxicology trials to refine data. Additional attention will be paid to the toxic effects of individual oligomers, and the synergistic toxic effects of typical NSs with pesticides at environmental concentration levels. Moreover, a comprehensive risk assessment model should be established to characterize the health risk of NSs to humans.

The above studies can establish a research paradigm for the risk of human exposure to NSs through the agricultural environment and food. This will be conductive to explore the potential associations of NSs among the agricultural environment, food, and human health.

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The environmental health burden of pesticides: A National Perspective from the United States.

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Abstract

Some agricultural pesticides can elicit adverse health impacts in humans. Occupational exposure to agricultural pesticides, for example, has been found to be correlated with a variety of adverse health outcomes, including Parkinson's disease, Alzheimer's disease, and non-Hodgkin Lymphoma. In contrast, the influence of incidental (non-occupational) pesticide exposure and adverse human health impacts has

not been thoroughly studied and remains poorly understood. One major challenge is that pesticide exposure pathways for non-occupational community members is difficult to ascertain, particularly at large geographic scales (i.e., state-wide, regional, or national). Fortunately, the USGS populates and maintains a website (https://water.usgs.gov/nawqa/pnsp/usage/maps/) that provides usage information for over 500 pesticides for every county in the United States from 1992 until 2017 on an annual basis. These data shed considerable light on geographic variation in pesticide use on the state, regional, and national levels. For example, the pesticide profile among the 11 states found in the western United States is divided into three distinct groups: the herbicide dominated states (CO, MT, NM, UT, WY), the fumigant dominated states (CA, ID, NV, OR, WA), and AZ, which uses the two pesticide groups at more or less the same amount. These differences in state and county pesticide profiles were correlated with total cancer and pediatric cancer incidence on both a state and county scale. Within Idaho, a principal component analysis found that pesticide usage, principally, but not exclusively, of fumigants was significantly correlated with pediatric cancer incidence. The research conducted for the 11 western states was so promising that we have begun to develop a national assessment of pesticide use on a state-by-state basis. It is interesting to note that across the United States, those states that specialize in the growth of animal feed (corn and soybeans) tend to have glyphosate as the single most heavily used pesticide within the state. States that grow produce for human consumption, tend to have a more diverse pesticide profile. Assessing the pesticide load that US residents are exposed to is a challenging and nuanced process. The USGS database provides invaluable information that can be used to develop a national assessment of pesticides and the environmental health burden that they may pose.

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Mitigation effects and microbial mechanism of two ecological earthworms on the uptake of chlortetracycline and antibiotic resistance genes in lettuce

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Abstract

The contamination of greenhouse vegetable soils with antibiotics and antibiotic resistance genes (ARGs), caused by the application of livestock and poultry manure, is a prominent environmental problem. In this study, the effects of two ecological earthworms (endogeic *Metaphire guillelmi* and epigeic *Eisenia fetida*) on the accumulation and transfer of chlortetracycline (CTC) and ARGs in a soil–lettuce system were studied via pot experiments. The results revealed that earthworm application accelerated the removal of the CTC from the soil and lettuce roots and leaves, with the CTC content reducing by 11.7-22.8%, 15.7-36.1%, and 8.93-19.6% compared with that of the control, respectively. Both earthworms significantly reduced the CTC uptake by lettuce roots from the soil ($P < 0.05$) but did not change the CTC transfer efficiency from the roots to leaves. The high-throughput quantitative PCR results showed that the relative

abundance of ARGs in the soil and lettuce roots and leaves decreased by 22.4-27.0%, 25.1-44.1%, and 24.4-25.4%, respectively, with the application of earthworms. Earthworm addition decreased the interspecific bacterial interactions and the relative abundance of mobile genetic elements (MGEs), which helped reduce the dissemination of ARGs. Furthermore, some indigenous soil antibiotic degraders (*Pseudomonas*, *Flavobacterium*, *Sphingobium*, and *Microbacterium*) were stimulated by the earthworms. The results of redundancy analysis indicated that the bacterial community composition, CTC residues, and MGEs were the main parameters affecting the distribution of ARGs, accounting for 91.1% of the total distribution. In addition, the bacterial function prediction results showed that the addition of earthworms reduced the abundance of some pathogenic bacteria in the system. Overall, our findings imply that earthworm application can substantially reduce the accumulation and transmission risk of antibiotics and ARGs in soil–lettuce systems, providing a cost-effective soil bioremediation practice for addressing antibiotic and ARGs contamination to guarantee the safety of vegetables and human health.

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New Evidence of p-Phenylenediamines (PPDs) and its Derived Quinones (PPDQs) in Marine Fish

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Abstract

Widespread detection of p-phenylenediamines (PPDs), the effective antioxidants used in tire rubber products, and their derived quinones (PPDQs) have been identified in various environmental compartments, such as runoff water, soil, dust, and sediment. However, limited data available regarding the occurrence of PPDs and PPDQs in the marine fish species. Herein, we aimed to determine the levels and profiles of seven PPDs and five PPDQs in the most common marine fish species from 7 coast waters alongside the Pearl River Delta (PRD), as well as to explore the potential sources of these pollutants. Ubiquitous occurrence of PPDs and PPDQs was observed in the 172 marine fish samples. The mean levels of total PPDs were observed as follows: *Sparus latus* (1440.49 pg/g, wet weight [ww]), *Harpodon nehereus* (395.73 pg/g, ww), *Sillago sihama* (876.42 pg/g, ww), *Nemipterus virgatus* (555.28 pg/g, ww), and *Larimichthys polyactis* (474.77 pg/g, ww). A similar trend was found for total PPDQs: *Sillago sihama* (405.70 pg/g, ww) >, *Nemipterus virgatus* (393.98 pg/g, ww) >, *Sparus latus* (387.12 pg/g, ww) >, *Larimichthys polyactis* (377.98 pg/g, ww) >, and *Harpodon nehereus* (83.56 pg/g, ww). Unlike the main components reported in environment compartments, N, N'-bis(1,4-dimethylpentyl)-p-phenylenediamine (77PD) and N-phenyl-N'-cyclohexyl-p-phenylenediamine (CPPD) were the primary PPDs in marine fish, accounting for 52.49 % and 24.40 % respectively.

Meanwhile, N-isopropyl-N'-phenyl-p-phenylenediamine quinone (IPPDQ) was the principal PPDQs with a percentage of 62.72 %. The principal component analysis of the 12 target compounds revealed that the sources could be categorized into three types, including tire rubber, wire and cable rubber coating, and other unidentified sources. This study underscores the significance of monitoring contaminants in marine products, particularly emerging pollutants such as PPDs and PPDQs, which may pose potential health risks to humans through food consumption.

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Infantile Internal and External Exposure to Neonicotinoid Insecticides: A Comparison of Levels Across Various Sources

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Abstract

Little is known about exposure of infants to neonicotinoid insecticides (NEOs). In this study, concentrations of six parent NEOs (p-NEOs) and *N*-desmethyl-acetamiprid (*N*-dm-ACE) were measured in urine and whole blood samples from infants, in addition to breast milk, infant formula and tap water collected in South China. The p-NEOs with the highest median concentration in urine (0.25 ng/mL) and blood (1.30) samples was dinotefuran (DIN), while imidacloprid (IMI) was abundant in breast milk (median: 0.27 ng/mL), infant formula (0.22) and tap water (0.028). The older infants (181-360 days) might face higher NEOs and *N*-dm-ACE exposure than younger infants (0-180 days). Blood samples contained significantly ($p < 0.01$) higher median concentration of $\sum_6$p-NEOs (2.03 ng/mL) than that of urine samples (0.41), similar to acetamiprid (ACE), IMI, thiacloprid (THD), DIN and *N*-dm-ACE, suggesting that NEOs readily partition into blood. Furthermore, breast-fed infants tend to have higher exposure levels than formula-fed infants. Infant formula prepared with tap water augmented the daily intake (DI) of ∑NEOs. The external sources contributed 80% of the total dose to IMI and clothianidin (CLO) exposure, while other unknown sources contributed to ACE, THD and DIN exposure, in infants. To the best of our knowledge, this is the first study to assess levels and sources of infantile exposure to NEOs through internal and external exposure assessment.

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Effects of Pyrethroid Insecticides on Gestational Diabetes Mellitus and Glucose Homeostasis

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Abstract

Pyrethroids, a class of extensively used insecticides, may pose health risks to humans. Whether pyrethroid exposure contributes to the development of gestational diabetes mellitus (GDM) in pregnant women remains unknown. The potential association of urinary concentrations of pyrethroid metabolites [3-phenoxybenzoic acid (3-PBA) and 4-fluoro-3-phenoxybenzoic acid] with the risk of GDM was assessed using a nested case-control study of 220 GDM cases and 440 controls from a prospective cohort. The mediation roles of oxidative stress biomarkers [advanced glycation end products (AGEs) and malondialdehyde (MDA)] in the associations were investigated. Urinary concentrations of 3-PBA in these cases were significantly higher than those of the controls. Urinary 3-PBA was positively associated with the risk of GDM. The adjusted odds of GDM significantly increased by 32% in each unit increment of the ln-transformed concentration of urinary 3-PBA. The significant dose-response relationships of GDM with serum AGEs (Ptrend = 0.03) and MDA (Ptrend < 0.001) were observed. There were no significant correlations between 3-PBA and AGEs or MDA, nor was there a significant mediation effect of AGEs or MDA on the association of 3-PBA with GDM. We provide the first evidence that early gestational exposure to pyrethroids is an environmental risk factor for GDM.

We further investigated the diabetogenic effects and mechanisms of action of exposure to environmentally relevant doses of cypermethrin (CP), one of the most commonly used pyrethroids, in animal models. Consumption of a high calorie diet (HCD) significantly enhanced the bioaccumulation of CP in the liver of adult mice. CP exposure at the lowest dose in the range of human daily intake exacerbated HCD-induced insulin resistance. In HCD-fed mice, CP treatment significantly decreased hepatic glucose uptake by impairing the translocation of glucose transporter GLUT2. CP exposure regulated hepatic AKT2/GSK3β/GYS2 pathway, thereby reducing glycogenesis and stimulating gluconeogenesis in the livers of HCD-fed mice. Hepatic transcriptome data showed that CP exposure of HCD-fed mice increased hepatic expression of thioredoxin-interacting protein (Txnip) and vanin-1 (VnnI) genes, which were involved in regulating GLUT2 translocation and AKT2/GSK3β/GYS2 pathway activity, respectively. CP treatment significantly decreased hepatic glucose uptake in HCD-fed mice by impairing the translocation of glucose transporter GLUT2, which was modulated by upregulation of TXNIP. CP exposure regulated hepatic AKT2/GSK3β/GYS2 pathway through upregulation of VNNI, thereby reducing glycogenesis and stimulating gluconeogenesis in the livers of HCD-fed mice. This is the first study to show that an enrichment of lipophilic CP in the liver significantly disrupted glucose homeostasis and caused prediabetic phenotype.

In conclusion, exposure to pyrethroids is an environmental risk factor for GDM and impaired glucose homeostasis.

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Cadmium Redistribution in Edible Tissues of Steamed Swimming Crab (*Portunus Trituberculatus*) and Its Human Health Risk Assessment

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Abstract

Cadmium is one of the heavy metal elements specifically enriched in swimming crabs (*Portunus trituberculatus*) and is also one of the harmful heavy metal elements that have attracted worldwide attention. At the same time, swimming crabs is a kind of seawater crab that is deeply loved by consumers. Cadmium enters the human body along with the process of consuming *Portunus trituberculatus*, causing harm to human health. At present, many reports have studied the accumulation of cadmium in crabs in different areas around the world, and carried out relevant health risk assessment studies. However, it is noteworthy that the redistribution and risk assessment of cadmium in swimming crabs, which are mainly processed by steaming, have not yet received attention. In daily life, people usually consume steamed crabs, and only focusing on cadmium accumulation in fresh crabs is not enough to fully evaluate the potential health risk to humans, which is why the redistribution characteristics of cadmium and the health risk assessment of steamed crabs need to be investigated and revealed. In order to reveal the characteristics of cadmium redistribution and the risk assessment of consumption of *Portunus trituberculatus* after steaming, we designed three experiments， and the results revealed that cadmium will transfer from brown meat (hepatopancreas and gonads) to leg muscle during steaming, and the level was nearly tenfold higher than that of raw leg muscle. The reasons of steaming practices on the cadmium redistribution in edible tissues of the swimming crabs were discussed, and for the first time, variation in cadmium speciation by steaming is proposed as a potential factor leading to the redistribution of cadmium. Moreover, while the consumption of white meat does not pose a health risk to consumers based on the target hazard quotient (THQ) and target cancer risk (TCR), attention and evaluation are warranted for the consumption risk of cadmium in brown meat from steamed swimming crabs sourced from Shanghai. our results strongly suggest the consideration of the effects of steaming process when assessing human health risk of consuming the edible crab tissues regarding cadmium. This study provided guidance for the local residents on consuming swimming crabs by steaming. Besides, it provides a theoretical background for studying the change of cadmium morphology and the transformation mechanism of cadmium during steaming.

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The Response of Rice Rhizosphere Bacterial Community to Cadmium-Contamination

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Abstract

Rice rhizosphere microbial community could be affected by the concentration of heavy metal in paddy, which in turn affects rice growth. In the present study, the rhizosphere bacterial community of rice from three cadmium (Cd)-contaminated sites, which located in Yunnan (Y), Hunan (H) and Guizhou (G) province, were studied through culture-independent method. The results showed that *Bradyrhizobium*, *Mycolicibacterium* and *Priestia* were the dominant bacteria of rice rhizosphere bacterial community, and their abundance increased with Cd concentration increasing. Contrary to this, the richness of rice rhizosphere bacterial community significantly decreased with Cd concentration increasing. In addition, it was found that the diversity of rice rhizosphere bacterial community significantly reduced in site H, where paddy soils had higher Cd concentration and the lowest pH. Notably, the dominant rhizosphere bacteria *Mycolicibacterium* and *Priestia* showed a significant correlation with Cd and Zinc concentration, therefore, the role of them worth further study in the future. Meanwhile, beta nearest taxon index (βNTI) was calculated using the null model (999 randomizations) to evaluate the relative importance of determinism and stochasticity in bacterial community assembly processes. The result indicated that deterministic processes were the critical process driving rice rhizosphere bacterial community assembly in three sites. However, the stochastic processes of bacterial community contributed more to paddies with higher Cd concentration, meaning the rice rhizosphere bacterial community in higher Cd-contaminated site has more variable assemblage. The present study not only throw lights on microbiome of Cd-contaminated paddy, but also provide growth promoting bacteria for rice safe and efficiency production.

Keywords: rice; cadmium contamination; rhizosphere; microbial community; assembly processes

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Agricultural input, mass load and their associated risk of neonicotinoid insecticides to the Yangtze River, China: An exploration as ecological protection threshold

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Abstract

Neonicotinoid insecticides (NNIs) have attracted global concern due to its extensive use in agricultural activities and their potential risks to the animal and human health. Extensive studies were conducted within the midsection of the Yangtze River to explore the environmental and health impacts. Eleven NNIs were analyzed in 108 river water and sediment samples from three seasons (normal, dry and wet season), from which we detected a minimum of seven NNIs in the water and four NNIs in the sediment, with total concentrations ranging from 12.33 to 100.5 ng/L and 0.08 - 5.68 ng/g, respectively. This was consistent with the results in the whole Yangtze River, with the total concentration for NNIs in sediments of <LOD–1.18 ng/g (mean: 0.19 ng/g). The vertical distribution was top (0.28 ng/g) > bottom (0.20 ng/g), and the horizontal distribution was upstream (0.46 ng/g) > midstream (0.28 ng/g) > downstream (0.09 ng/g). The levels of NNIs in both river water and sediment within the midsection of Yangtze River were primarily influenced by the extent of agricultural activities. The estimated annual load of NNIs in the midsection of Yangtze River totaled 40.27 tons, and April was a critical contamination period. Relative potency factor (RPF) analysis of the human exposure risk revealed that infants faced the greatest exposure risk, with an estimated daily intake of 11.27 $ng \cdot kg^{-1} \cdot bw \cdot d^{-1}$. The acute and chronic thresholds were established for aquatic organisms by employing the Species Sensitive Distribution (SSD) method (acute: 384.1 ng/L; chronic: 168.9 ng/L). Based on the findings from midsection of Yangtze River, 33% of the river water samples exceeded the chronic ecological risks thresholds. This is close to the entire Yangtze River, which the results of risk quotients (RQ) method showed that over 30% of the sediment samples reached the “moderate risk”. Therefore, there is an urgent need for intervention programs to guarantee the safety of the river for aquatic life in the Yangtze River Basin.

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Mitigation of Copper Oxide Nanoparticles (CuO NPs) Toxicity in Lettuce (Lactuca sativa L.) Through Fertilization

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Abstract

The widespread production and use of Copper Oxide Nanoparticles (CuO NPs) have resulted in their release into various environmental media, including soil and water. CuO NPs can be absorbed by plant tissues through their roots, potentially affecting their growth and development. This study aims to investigate the effects of CuO NPs on lettuce at different levels, including phenotypic, physiological, biochemical, and metabonomic, and to determine whether fertilization can alleviate these effects. Our findings demonstrate that CuO NPs have significant impacts on the phenotypic and biochemical characteristics of lettuce. Exposure to 20 mg/kg CuO NPs resulted in a 25% reduction in fresh weight and a 26.9% decrease in plant height. Additionally, both 20 mg/kg and 100 mg/kg CuO NPs led to a 31.0% and 41.4% increase in chlorophyll content, respectively, while significantly elevating the Cu content in lettuce tissues. Furthermore, CuO NPs exposure heightened the levels of oxidative stress products such as malondialdehyde and hydrogen peroxide in lettuce leaves, and altered the metabolic pathways of ascorbic acid and glutathione, thereby affecting the lettuce's antioxidant system. Remarkably, the application of fertilizer enhanced the anti-oxidative stress capacity of lettuce by activating the synthesis of Glutathione

and related pathways. This activation reduced the impact of CuO NPs on oxidative stress and antioxidant enzyme systems, thereby mitigating their effects on lettuce fresh weight and height. In conclusion, our study highlights the adverse effects of CuO NPs on lettuce and the potential of fertilization to alleviate these effects, which implicate for the safe use and disposal of CuO NPs in agriculture and the environment.

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Rhizosphere fungal community of rice from various cadmium-contaminated paddies

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Abstract

Rhizosphere microbial community served a crucial function in modulating host plants' growth in heavy metal-contaminated fields. To understand the rhizosphere fungal community and its role on rice growth under variable cadmium (Cd)-contaminated environments (lightly contaminated, LC; moderately contaminated, MC; heavily contaminated, HC), rice rhizosphere fungal community were investigated in the present study through Illumina HiSeq method. The result indicated that Cd contamination reduced the diversity and species richness of rice rhizosphere fungal community. In addition, the dominant genera of rice rhizosphere fungal community from the three sites were different. In LC area, they were *Pseudeurotium*, *unclassified Sordariales*, *Linnemannia*, and *Neurospora*, while, in MC area, they were *Talaromyces*, *Westerdykella*, *unclassified Hypocreales*, and *Penicillium*. In HC area, they were *Saitozyma*, *Mortierella*, *Fusarium*, and *Talaromyces*, among which *Talaromyces* is the common genus of MC area and HC area. Correlation Heatmap analysis indicated that *Unclassified Sordariales, unclassified Hypocreales, unclassified Ascomycota*, and *Linnemannia* exhibited a significant negative correlation with Cd concentration ($P \leq 0.001$), whereas *Fusarium* and *Saitozyma* showed a positive correlation with Cd concentration ($P \leq 0.001$). The role of these isolates on rice growth and Cd tolerance needs further study. Concurrently, the genera with a significant correlation with zinc contamination were consistent with Cd contamination, but the correlation was reversed. Redundancy analysis further elucidated that organic matter and total nitrogen constitute pivotal determinants influencing the changes of rhizosphere fungal community structure in LC area. This suggests that the deleterious impacts of Cd on LC paddy ecosystems can be mitigated through the supplementation of exogenous nutrients.

Keyword: rice rhizosphere soil; cadmium contamination; fungal community; diversity;

Acknowledgments

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22. Exposure and Health Risks of Toxic Pollutants

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In Vivo Fate of Aryl Phosphorus Flame Retardants and A Novel Toxicological Perspective via Gut-Liver Axis in Mice

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Abstract

Aryl phosphorus flame retardants (aryl-PFRs), such as triphenyl phosphate (TPHP) and diphenyl phosphate (DPHP), are widely used and commonly present in the environment as emerging pollutants. To accurately assess the toxicity of aryl-PFRs *in vivo* and predict the risk they may pose to environmental and human health, it is essential to first determine the fate of these compounds within a biological organism. The sub-acute, chronic and recovery experiments were integrated to provide a new perspective regarding the biotransformation, bioaccumulation and bioelimination of emerging pollutants in C57BL/6J male mice. TPHP was almost completely metabolized by mice, with DPHP being the major metabolite formed. Compared to TPHP, the rates of degradation and elimination of DPHP were slower and its bioaccumulation potential was higher. Furtherly, to mimic a realistic exposure scenario, TPHP/DPHP were exposed at an estimated daily intake dose and a health reference dose, via their diet. Hazard for mice chronic exposed to TPHP is associated with increased liver total cholesterol levels that are correlated with fatty acids accumulation and gut microbiota alterations. One potential toxic threat of DPHP is related to reduction of the brain neurotransmitters involved in serotonergic and glutamatergic synapse, which may be attributed to the disrupted liver tryptophan and nucleotide metabolism. Alteration of the gut microbiota by aryl-PFRs and their association with metabolic syndromes mediated via gut−liver axis could constitute a significant risk factor associated with the presence of these chemicals in the environment. Different toxicities of TPHP and DPHP emphasize the urgent need for more careful consideration of environmental transformation products during the safety assessments of commercial chemicals.

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Chemical exposome, ultrafine particles, and Glioblastoma: A new perspective

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Abstract

Glioblastomas (GBM) are the most common primary brain tumours in adults whose causes are yet to be established. Although environmental exposures are suspected, available data is limited, mainly due to analytical constraints and the challenges associated with obtaining brain samples for cohort studies. In this regard, the association between chemical exposure and GBM remains an uncharted frontier. This study seeks to investigate the chemical exposome in GBM and explore a potentially underexplored source of exposure: Ultrafine particles (UFPs), the smallest component of air particulate matter. This idea is substantiated by the ability of UFPs to penetrate the brain and transport hazardous substances. Furthermore, previous epidemiological research has hinted at a plausible correlation between UFPs in ambient air and disease incidence.

Our study relied on a unique retrospective cohort comprising 500 patients, featuring high-quality histopathology brain tumor samples. The dataset, known as the Bellvitge Glioma Cohort (BGC) HUB-IDIBELL, spans from 2005 to the present. Additionally, non-tumor brain tissue samples from autopsies were included. In this proof-of-concept study, we examined 33 GBM samples and 20 non-tumoral samples, employing a comprehensive approach that combined HRMS-based wide-scope target and nontarget strategies. Furthermore, we analyzed 20 samples of PM2.5 and UFPs from the metropolitan area of Barcelona, the origin of the cohort patients.

We identified 49 exogenous chemicals, encompassing a diverse range of industrial compounds. While the chemical profiles in glioblastoma (GBM) sometimes differ significantly from those in healthy brain tissue obtained from autopsies, these findings do not establish a direct link to disease onset. Nevertheless, the results highlight the necessity for comprehensive assessments of the potential effects on GBM onset. Notably, the identification of various air pollutants, primarily associated with road traffic, such as tire additives, supports the hypothesis that numerous hazardous chemicals (many still unidentified) may access the brain via the olfactory pathway. To support this hypothesis, we analyzed 24 UFP samples collected in the Barcelona area, where the majority of Bellvitge Glioma Cohort (BGC) patients resided. Our approach resulted in the detection of over 20,000 features, representing potential hazardous chemicals, including some previously identified in the brain (e.g., tire additives).

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Increase of the indoor concentration of volatile organic compounds after the use of incense and scented candle in studio apartments determined using passive sampling

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Abstract

Burning incenses and scented candles may provide harmful chemicals. Although many studies have evaluated volatile organic chemicals emitted by their use and related health risks, extension of our understanding for guiding appropriate use under various use conditions is necessary. In this study, emission characteristics of commercial incenses and scented candles were evaluated in a laboratory chamber using real-time measurement and the time-weighted average exposure concentrations of monoaromatic compounds and monoterpenes were assessed using passive samplers while volunteers living in a studio apartment use them. After burning incense, the average levels of benzene increased from 1.4 to 100 μg m3. The presence of a wood core in commercial incense products was the main cause of high benzene emission by burning them although the increase in benzene was also influenced by factors such as the brand of the products, the number of incense sticks burned, the duration of each burning session, and ventilation period. Electrical warming of scented candles increased the levels of monoterpenes by factors of 16–30 on average. Considering the emission characteristics found in this study, exposure to benzene and monoterpenes could be mitigated by cautious use of those products in residential areas.

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Effects of household fragrant plants on indoor VOCs in residential environments

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Abstract

Prior to this study, only the positive effects of indoor plants, particularly their ability to remove volatile organic compounds (VOCs), have been the focus of research. The present study aimed to investigate the potential adverse effect of indoor plants on indoor terpene levels. The exposure levels of selected VOCs, including terpenes (limonene and a-pinene) emitted by fragrant plants in home, were assessed using a passive sampling method. A previously developed passive sampler composed of an expanded polytetrafluoroethylene membrane and adsorbent (ePTFE PS) was used to measure indoor VOCs. Thirty volunteers were recruited and asked to wear the ePTFE PS while deploying potted fragrant plants inside their own home for 3 h. Because many consumers prefer hydroculture, removing pot to avoid bugs,

volunteers were asked to wear the ePTFE PS while deploying fragrant plants, transferred from pot to water, inside their own home for 3 h. The indoor concentrations of terpenes in apartments were elevated by deploying fragrant plants, especially for hydroculture. The average concentration of limonene after deploying fragrant plants on water was 89 μg m^{-3}, which was greater than that before use by a factor of 2.3. This may lead to an increase in wheezing, asthma, exhaled nitric oxide, and unwanted byproducts that adversely affect human health. Therefore, cautious usage of fragrant plants indoors, is needed to reduce exposure to terpenes.

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Placental transfer and subsequent toxicity of aromatic amine antioxidants (AAs) and *p*-phenylenediamine quinone (PPD-Qs)

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Abstract

Aromatic amine antioxidants (AAs), as rubber additives, and their ozone photochemical oxidation products of *p*-phenylenediamine quinone (PPD-Qs), have attracted great attention recently due to their wide environmental occurrences and toxicity. However, there's no research on the gestational exposure, trans-placental transfer mechanisms, and subsequent toxicity of AAs and PPD-Qs. Herein, we developed an evaluation system that integrates human biomonitoring, uterine perfusion in pregnant rats, and a placental cell line to 1) investigate the potential presence of twenty AAs and six PPD-Qs in the paired maternal urine and amniotic fluid samples from parturient women (n = 53 pairs) by liquid chromatography-mass spectrometry; 2) explore the transplacental transportation patterns and mechanisms of AAs and PPD-Qs by conducting uterine perfusion in pregnant rats and performing molecular docking analysis; and 3) assess AAs and PPD-Qs' cytotoxicity toward placental cells by performing cell viability experiments and transcriptomics analysis.

1. A direct evidence of the intrauterine exposure of AAs and PPD-Qs were observed that ΣAAs (median: 8.57 and 15.4 ng/mL) and ΣPPD-Qs (0.236 and 2.29 ng/mL) were detected in the human maternal urine and amniotic fluid samples.
2. What's more, nine analytes with higher detection frequencies or detection levels in human maternal urine and amniotic fluid samples were selected to evaluate their trans-placental transfer mechanisms. The result of self-established rat uterine perfusion model and molecular docking analysis suggested that passive diffusion and active transport patterns were involved in the trans-placental transfer.
3. Cell viability experiments showed different acute toxicity patterns across different PPDs and PPD-Qs. The mixture of PPDs or PPD-Qs were found as the potential agonist to Wnt (wingless) signaling pathway (A pathway commonly involved in embryonic development) by transcriptomics analysis.

In conclusion, AAs and PPD-Qs can transfer across the placental barrier via passive diffusion and active transport and have adverse effect on the placental cells during pregnancy. This study will help raise

concerns regarding intrauterine exposure, trans-placental transfer mechanisms and subsequent toxicity to the placental cells of AAs and PPD-Qs during pregnancy.

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Exposure to melamine and its derivatives in northeast Australia population: Diversity in gender and age

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Abstract

Melamine, which is notorious as its illegal addition in food scandals, is a versatile compound with various industrial applications, including flame retardants and raw materials of plastic products, generating their widespread environmental occurrence. The aim of this study was to provide the first assessment of exposure to melamine and its derivatives in the general Australian population. De-identified urine specimens stratified by age and sex were obtained from a community-based pathology laboratory and pooled (n=48, pools of 100) in 2012-2013 and 2022-2023. Melamine, cyanuric acid, and ammelide are widely exposed in Australian residents, with a geometric mean of 3.65, 24.4, and 3.85 ng/mL, respectively. No difference is observed in melamine and its derivative concentrations between 2012-2013 and 2022-2023, which explains that melamine and its derivatives have been used before 2012. Melamine and cyanuric acid have higher concentrations in females (4.22 and 40.9 ng/mL) compared with those in males (3.15 and 14.8 ng/mL) ($p<0.05$), indicating that females have much more serious risk of melamine and its derivative exposures. The concentrations of melamine and cyanuric acid are higher in 0-14 years old group (5.10 and 86.3 ng/mL) than 15-45 and >45 years old groups (2.93 and 2.98 ng/mL, $p<0.05$; 11.5 and 10.4 ng/mL, $p<0.01$), showing children and youth are melamine and its derivative exposure high-risk group. However, higher concentration of ammelide has been shown in >45 years old group (5.10 ng/mL) compared with 0-14 and 15-45 years old groups

(3.03 ng/mL, p<0.05; 4.61 ng/mL, p<0.01). To the best of our knowledge, this is the first study to document the ubiquitous occurrence and gender and age variations of human exposure to melamine and its derivatives in Australia. There is a need for special attention to melamine and derivative exposures concerning females and children.

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Investigation of the effect of perfluorooctanoic acid (PFOA) on nitrosative stress in MCF-7 cell based on scanning electrochemical microscopy (SECM) technique

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Abstract

As a vital factor in cell metabolism, nitric oxide (NO) is associated with nitrosative stress and subsequent inflammations and diseases. In organisms, L-arginine produces high levels of NO in a short period of time. low localized concentrations of NO can have positive effects (as neuroprotectants, etc.), however, pathological mechanisms can be triggered when NO reaches high levels. the reaction of NO with O2- to produce ONOO- has a high toxicity, followed by a rapid conversion to NO2- and -OH under acidic conditions. These reactive species are key signaling substances involved in cellular stress, injury. In situ real-time monitoring of NO is challenging due to its relatively trace concentration and fast diffusion in cell. Here, we used a modified scanning electrochemical microscopy (SECM) technique to real time monitor NO release from single MCF-7 cell stimulated by perfluorooctanoic acid (PFOA). It has been proposed that PFOA is strongly associated with cellular stress. The results showed that the oxidative response of NO continued to increase with the gradual increase of PFOA concentration at the beginning, suggesting that the stimulated MCF-7 cell produced excessive amounts of NO at this time, leading to nitrosative stress. As the concentration of PFOA exposure was further increased, the NO release showed a decreasing trend. This was attributed to the oxidative damage produced by the cell at high concentrations, leading to mitochondrial dysfunction, which reduced NO release. In addition, the cell viability assay also confirmed this result. This study explores the production level of RNS in organisms, the transformation mechanism, and the dynamic changes in response to external stimuli, and provides new ideas for toxicity assessment of environmental pollutants, health diagnosis and disease treatment.

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Effects of different forms of lithium on reproductive toxicity in mice

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Abstract

With the implementation of the dual-carbon policy, there has been a significant surge in the need for lithium-ion batteries (LIBs), resulting in the widespread utilization of lithium cobaltate (LCO) as the cathode material in LIBs. The utilization of these materials has made lithium-ion and LCO emerging environmental pollutants. Given that the particles are of a size that can be breathed in by humans, this presents a potential risk to both the ecosystem and human health, necessitating scrutiny of their potential toxicity and health impacts. At present, there are few studies on the toxicity of different forms of lithium (lithium-ion and LCO) to male reproduction. The mechanism of lithium-induced testicular injury is not well understood. Therefore, in this paper, a mouse exposure model was established to investigate the effects of different forms of lithium on the male reproductive system to simulate human environmental exposure. After five weeks of exposure, enzyme-linked immunosorbent assay (ELISA) on mice serum, and oxidative stress markers on mice epididymis and testicular tissue were conducted. The results are as follows: 1) HE staining on the testis showed that compared with the control group and the low-concentration lithium group, the high-concentration lithium group and LCO group exhibited obvious atrophy of interstitial cells and vacuolation of spermatogenic cells and interstitial cells. Exposure to high concentrations of lithium and LCO is associated with reduced diameter and area of spermatogenic tubules. 2) Exposure to high concentrations of lithium and LCO significantly inhibited serum testosterone content in mice. 3) High concentrations of lithium and LCO can increase the production of large amounts of reactive oxygen species (ROS) and malondialdehyde (MDA) in mice, inducing oxidative stress in testis. In addition, RNA sequencing of testes separately revealed 883 and 1312 genes that were differentially expressed in Li500 group and LCO500 group compared to control group. The Venn diagram showed that 552 genes were differentially expressed simultaneously in Li500-vs-control and LCO500-vs-control, indicating that other molecular mechanisms may be involved in LCO-induced testicular reproductive toxicity. The findings of this study may provide new perspectives for understanding the reproductive toxicity of different forms of lithium in mammals.

Keywords: toxicity; lithium ion; lithium cobaltate; reproductive toxicity

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Lead pollution and children lead exposure in China: disparity, challenge, and policy

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Abstract

Lead (Pb) is a neurotoxic metal, and no level of lead exposure is safe for children. China has still experienced problems on child lead poisoning even though the Chinese government has phased out leaded gasoline since 2000. The underlying problem affecting the lead pollution-related health of children in China remains to be comprehensively investigated. It is found that although the significant decline of BLLs, as the Geometric Mean (GM), from 91.40 μg/LGM in 2001 to 37.52 μg/LGM in 2018 is observed, the average BLLs of children are still above 50 μg/L or more [average 59.70 (60.50-65.02, 95%CI) μg/LGM] after phasing out leaded gasoline since 2000 in China. Lead exposure causes 29.67 MID per 1,000 children with a loss of 98.23 (59.40-146.21, 95%CI) DALYs per 1000 in China, which is greater than the levels reported from the Western Pacific Region and other low- and middle-income countries. Although the disparities in BLLs in China are strongly influenced by unequal distributions of potential multi-lead related sources (soil lead, PM2.5 lead, dust lead), unbalance development of local industrialization and economies, as well as incorrect health care for younger children, the notable emissions from coal combustion (CC) and non-ferrous metals (NMS) exploitation dominate the crucial sources of low-level lead exposure to children after phasing out leaded gasoline in China currently. Faced with the unequal and disparate distribution of BLLs in China, the big bottleneck is to decrease the BLLs exertions of 36-45 μg/L in the next few decades. The Chinese government needs to make more efforts on developing more strict guidelines, implementing more policy strategies on prevention and management of blood Pb poisoning, and monitoring the nationwide changes in children's BLLs continuously

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6PPD-Q Induces Liver Lesion in Human Through Immune and Metabolic Dysregulation: New Evidence from Traffic Policemen

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Abstract

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Traffic patrol police exposure to pollutants from traffic sources such as $PM_{2.5}$, car wear and tear particles can lead to various diseases, especially liver diseases. Recently, the antioxidant *N*-(1,3-dimethylbutyl)-*N′*-phenyl-p-phenylenediamine (6PPD) and its quinone product 6PPD-quinone (6PPD-Q) in rubber have attracted attention due to their ecological risk. Although the hepatotoxicity of 6PPD and 6PPD-Q on mice are documented, the extent of their prevalence and implications for human health remain inadequately elucidated. In the current study, traffic policemen were recruited to analyze the distribution of 6PPD and 6PPD-Q in human serum and urine. Simultaneously, their physiological characteristics were conducted by five types of functions, including 24 biochemical parameters to assess immune function, liver function,

renal function, blood glucose levels, and lipid profile. For the first time, we found that the concentrations of 6PPD (1.03 ng/ml) and 6PPD-Q (2.22 ng/ml) in traffic patrol policemen serum were significantly higher than in office-based policemen serum ($p < 0.001$), with the detection frequency of 85–100%. Quantile G-Computation（Qgcomp） analysis exhibited that with each quartile increase in the concentrations of 6PPD and 6PPD-Q in serum and urine, immune cells increased ranging from 90% to 120%, and the triglycerides increased by 60%. In contrast, the fasting glucose decreased by 31%. Among them, the weight attributed to 6PPD-Q ranged from 44% to 63%. The results of the Weighted Quantile Sum (WQS) revealed that with each decile increase of 6PPD and 6PPD-Q in serum, total bilirubin and indirect bilirubin increased by 16% and 18%, respectively. Among them, the weight of 6PPD-Q consistently exceeded 50%. Bayesian Kernel Machine Regression (BKMR) analysis also exhibited similar trends. Therefore, the concentrations of 6PPD-Q in serum exert a more pronounced effect on glucose and lipid metabolism, dysregulation of immune cells, which may lead to human liver lesion. Furthermore, the logistic regression revealed that for one unit increase of 6PPD-Q in serum, the risk of human liver lesion increased by 2.31 times. Our study highlights the potential health risks associated with high exposure to 6PPD and 6PPD-Q.

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Chemical Analysis Complements Mosquito Bioassays to Assess Risk and Benefit of Indoor Residual Spray Pesticide Application for Mosquito Control

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Abstract

Indoor residual spraying (IRS), where long-lasting pesticide is applied on surfaces that mosquitoes may rest, is widely recommended by World Health Organization (WHO) for mosquito control to prevent diseases such as dengue and malaria. However, if misapplied, pesticides potentially pose public health and environmental risks. This study evaluated the suitability of an IRS product to control dengue mosquitoes in a minor construction site within an urban residential area in Singapore. Chemical analysis and bioassays were used to investigate quality of application and bioefficacy, to evaluate benefits, risks, and suitability for larger-scale deployment.

Following IRS treatment of various substrates (cement, metal board, ceramic tile) by a pest control operator, surfaces were systematically swabbed and the samples chemically extracted and analyzed by GCMS to quantify the active ingredient (AI). Large variations in application rate was observed, at up to 4x the recommended application rate at some locations. Over 8-week follow-up post-application, AI concentrations on cement and metal board decreased significantly but remained relatively constant on ceramic tile. Bioefficacy was assayed using WHO cone bioassay where lab-reared local mosquitoes were exposed to treated surfaces and mosquito mortality evaluated 24h post-exposure was compared against WHO's efficacy threshold of 80% mortality. Results correlated with measured AI concentrations: mortality declined rapidly from 88% to 42% after 2 weeks for cement but persisted on ceramic tiles (>99%

mortality) till 8 weeks post-application, indicating that substrate properties influence treatment outcome, with porous surfaces showing faster loss of AI concentration and bioefficacy. The durability of efficacy was significantly shorter than the "up to one year" long-lasting performance stated on product information. This can lead to sub-lethal exposure of *Aedes* mosquitoes resulting in insecticide resistance.

Our study demonstrates the complementary use of chemical analysis and bioassays to determine the quality and efficacy of IRS, highlighting the risk of over-application of IRS and potential environmental contamination or unintended dermal/inhalation exposure to humans, suggesting that environmental and public health risks outweigh the benefits of IRS. It highlights the importance of the evaluation in the local context to safeguard environmental and human health and strengthen mosquito control strategies.

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Exposure Experiments and Machine Learning Revealed That Personal Care Products Can Increase the Skin Exposure of Semivolatile Organic Compounds

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Abstract

Personal care products (PCPs) are widely used in people's daily lives. The potential risks of semi-volatile organic compounds (SVOCs) due to their adsorption by PCPs from the environments have not received enough attention. We investigated the effects of PCPs on human dermal exposure to 5 kinds of SVOCs through experiments from volunteers, explored the impact mechanism of PCP ingredients on dermal exposure using polydimethylsiloxane (PDMS) to simulate real skin surface, and predicted SVOC concentrations in human serum (C_{serum}) based on machine learning algorithms. After applying 4 different PCPs: lotion, baby oil, sunscreen, and blemish balm, the dermal adsorption of SVOCs via hand or forehead significantly increased by 1.63±0.62, 1.97±0.73, 1.91±0.48, and 2.03±0.59 times respectively, which may be due to the absorption effects of the PCP ingredients. Some PCP ingredients, can significantly increase the dermal adsorption of SVOCs and the permeation of SVOCs. Transdermal exposure risks of SVOCs were calculated under the scenarios of applying PCPs or not. PCPs can either increase or decrease the transdermal exposure risks of SVOCs depending on the properties of their ingredients. The oily baby oil caused the maximum hazard quotient for the SVOC congeners, and those caused by the PCPs were even higher for infants than adults. We predicted the C_{serum} based on the SVOC concentrations on the forehead using QSAR models and machine learning. Extra Trees was the best algorithm for predicting C_{serum}, and the predicted C_{serum} was comparable to those measured C_{serum}. This study for the first time elucidated that the application of PCPs can cause significantly higher dermal concentrations and exposures of SVOCs from the environments, subsequently resulting in potentially higher health risks.

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Climate Change and Health

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Abstract

Climate change is the most pressing global environmental issue of our time. With the continued advancement of global industrialization and accelerated economic growth, it has given rise to a series of complex ecological and health crises. The frequent occurrence of extreme temperature events and drastic temperature fluctuations have become the new normal in today's climate patterns. Simultaneously, the interaction effects between climate change and air pollution have become more significant. For example, the restricted dispersion and accumulation of pollutants under low-temperature conditions indicate that new types of complex environmental events are spreading globally, posing unprecedented challenges to human production activities.

Climate change not only exacerbates the frequency and intensity of heatwaves and cold spells but also profoundly affects the distribution and concentration of atmospheric pollutants, thereby altering the pollution exposure of human living environments. Numerous studies have shown that climate change and air pollution significantly aggravate the burden of cardiovascular diseases, respiratory diseases, and various acute and chronic health issues, even expanding the spread of infectious diseases. Long-term exposure to high concentrations of air pollution leads to rising incidence rates of diseases such as asthma and lung cancer, posing a direct threat to public health.

However, the inequity in global development further exacerbates the regional differentiation of environmental issues, with low- and middle-income countries and impoverished areas bearing heavier health and economic burdens. In the global sustainable development agenda, the position of vulnerable groups is increasingly prominent. Children, women, and other marginalized social groups are becoming the focal points of environmental health risk research, with their vulnerability being particularly significant in the face of environmental pollution. In the face of a series of complex challenges, future environmental health research needs to place greater emphasis on equity and sustainable development to develop adaptive strategies to mitigate the impacts of climate change.

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Developing dietary strategies to reduce bioavailability and toxicity of arsenic following oral exposure: Mechanisms and health implications

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Abstract

Arsenic (As) exposure has been related to many diseases including cancers. Using dietary strategies to lower As oral bioavailability can protect against As toxicity. When As is ingested, stepwise As transformation occurs in the gastrointestinal (GI) tract, with inorganic arsenate (iAs^{V}) and arsenite (iAs^{III}) being more toxic and more readily absorbed than monomethylarsenate (MMA^{V}) and dimethylarsenate (DMA^{V}). iAs^{V} is absorbed in the small intestine via phosphate (P) transporters in the apical membrane of enterocytes, while iAs^{III} is by aquaglyceroporins. Given this, it is hypothesized that strategies that can improve As biotransformation to low-bioavailability DMA^{V} in the intestine lumen, down-regulate the transporter expression of P transporters in intestinal epithelial cells, and enhance As biotransformation to MMA^{V} and DMA^{V} in the tissue can help to reduce bioavailability and toxicity of As.

To test the above hypothesis, a mouse bioassay was conducted to assess As relative bioavailability (RBA) in 3 indoor dust samples, which were amended into mouse chow without and with addition of $CaHPO_4$, $CaCO_3$, Ca gluconate, Ca lactate, Ca aspartate, and Ca citrate at 200, 1000, or 5000 mg Ca g^{-1}. We found that organic Ca minerals particularly Ca aspartate reduced As oral bioavailability most effectively by 41-72% at 5000 mg Ca g^{-1}, due to its side effect of decreasing duodenal expression of P transporters while not increasing As solubility in the intestine.

We further investigated the role of dietary prebiotic supplementation in stimulating gut microbiota to enhance As biotransformation and thereby lower early-life As exposure. We found that GOS supplementation at 5% (w/w) caused a significant proliferation of *Akkermansia* and *Psychrobacter*, reduced percentage of inorganic arsenite (iAs^{III}) and iAs^{V} by 47.4% and 65.4% in the intestine of mice, and 43.7–74.1% reduction in As concentrations in mouse blood, liver, and kidney and As urinary excretion factor (UEF).

We also investigated effects of polyphenols that have antioxidant and anti-inflammatory properties on As bioavailability, biotransformation, and toxicity, showing that although As bioavailability was elevated with some polyphenols, the cancer risk was greatly reduced due to higher DMA^{V} (52.1–67.6% vs 31.4%) and lower iAs^{V} contribution (4.95–10.7% vs 27.9%) in liver of mice treated with polyphenols.

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Foliar uptake, translocation, and trophic transfer risks of deuterium labeled nanoplastics

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Abstract

Nanoplastics (NPs) are widely detected in the atmosphere and are likely to be deposited on plant leaves. However, our understanding of their foliar uptake, translocation, and trophic transfer profiles is limited due to a lack of quantitative analytical tools to effectively probe mechanisms of action. Here, using self-synthesized deuterium (^{2}H) stable isotope labeled polystyrene nanoplastics (^{2}H-PSNPs), the foliar accumulation and translocation of NPs in lettuce, as well as the dynamics of NP transfer along a lettuce-snail terrestrial food chain, were investigated. Raman imaging and scanning electron microscopy demonstrated that foliar applied NPs aggregated on the leaf surface, entered mesophyll tissue via the stomatal pathway, and were eventually translocated to root tissues. Quantitative analysis showed that increasing levels of foliar exposure to ^{2}H-PSNPs (0.1, 1, and 5 mg/L in spray solutions, equivalent to receiving 0.15, 1.5, and 7.5 μg/d of NPs per plant) enhanced NPs accumulation in leaves, with concentrations ranging from 0.73 to 15.6 μg/g (dw), but only limited translocation (< 5%) to roots. After feeding on 5 mg/L ^{2}H-PSNPs-contaminated lettuce leaves for 14 days, snails accumulated NPs at 0.33 to 10.7 μg/kg (dw), with an overall kinetic trophic transfer factor of 0.45, demonstrating trophic dilution in this food chain. The reduced ingestion rate of 3.18 mg/g/d in exposed snails compared to 6.43 mg/g/d in control snails can be attributed to the accumulation of ^{2}H-PSNPs and elevated levels of chemical defense metabolites in the lettuce leaves, which decrease the palatability for snails and disrupted their digestive function and bile secretion. This study provides critical quantitative information on the characteristics of airborne NPs bioaccumulation and the associated risks to terrestrial food chains.

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Percutaneous Penetration and Dermal Exposure Risk Assessment of Quaternary Ammonium Compounds (QACs) in Textiles

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Abstract

Quaternary Ammonium Compounds (QACs), distinguished by a central ammonium core complexed with alkyl and aromatic substituents, are known to perturb the integrity of bacterial membranes. This disruption is attributed to the covalent interaction of QACs with the membrane's phospholipids and proteins, thereby impairing permeability. Consequently, QACs are extensively incorporated into textile products as antimicrobial agents, potentially representing a significant route of dermal exposure to these compounds.

However, the bioavailability and underlying mechanisms associated with the dermal absorption and penetration of QACs have yet to be elucidated. In this context, to quantitatively assess the transdermal

permeation of QACs, an in vitro model employing EpiKutis 3D-Human Skin Equivalents (3D-HSE) was utilized to investigate the percutaneous penetration mechanism of QACs. Following a 48-hour exposure period, it was observed that approximately 32.3% of Benzalkonium chloride (BAC), 32.1% of Alkyltrimethylammonium chloride (ATMAC), and 18.4% of Didecyldimethylammonium chloride (DDAC) permeated through the skin model to reach the receptor fluid. Notably, a positive correlation was identified between the octanol/water partition coefficient (log Kow) and the molecular weight (MW) of the QACs, with higher values correlating to diminished skin permeability.

Furthermore, the molecular mechanisms governing the transport of QACs across the dermal barrier are not fully understood. The present study is poised to delve deeper into this area, aiming to provide a comprehensive elucidation of the processes involved in the transdermal migration of QACs.

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Particle morphology and soil properties affect the retention of copper oxide nanoparticles in agricultural soils

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Abstract

The interaction between nanoscale copper oxides (nano-CuOs) and soil matrix significantly affects their fate and transport in soils. This study investigates the retention of nano-CuOs and Cu^{2+} ions in ten typical agricultural soils by employing the Freundlich adsorption model. Retention of nano-CuOs and Cu^{2+} in soils was well fitted by the Freundlich model. The retention parameters (K_D, K_F, and N) followed an order of CuO NTs > CuO NPs > Cu^{2+}, highlighting significant impact of nano-CuOs morphology. The K_F and N values of CuO NPs/Cu^{2+} were positively correlated with soil pH and electrical conductivity (EC), but exhibited a weaker correlation for CuO NTs. Soil pH and/or EC could be used to predict K_F and N values of CuO NPs or CuO NTs, with additional clay content should be included for Cu^{2+}.The different relationship between retention parameters and soil properties may suggest that CuO NTs retention mainly caused by agglomeration, whereas adsorption and agglomeration were of equal importance to CuO NPs. The amendment of Ca^{2+} at low and medium concentration promoted retention of nano-CuOs in alkaline soils, but reduced at high concentration. These findings provided critical insights into the fate of nano-CuOs in soil environments, with significant implications for environmental risk assessment and soil remediation strategies.

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Protein and fat influence on arsenic and lead relative bioavailability in contaminated soils: Mechanisms and health implications

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Abstract

The process of oral exposure to contaminated soil is often accompanied by food intake. However, it remains unclear the effect of food composition on the relative bioavailability (RBA) of arsenic (As) and lead (Pb) in soils. With the high protein and high fat diet in recent years, it is necessary to clarify the effects of protein and fat on As- and Pb-RBA in soil. In this sudy, the effects of high-protein and high-fat diet on As- and Pb-RBA in three soils were investigated using an in vivo mice model. The results showed that the Pb-RBA in the high-protein and high-fat diet groups were 1.5-2.64 and 3.15-6.04 times higher than that in the normal diet group, respectively. The As-RBA in the high-fat group increased by 1.33-1.38 times, while no significant change was observed in the high-protein diet group. In vitro gastrointestinal simulated solution extraction showed that protein and fat were hydrolyzed into small molecular products in digestive juice, which were combined with As and Pb to promote their dissolution The results of AB-PAS and TUNEL staining of mouse intestinal sections showed that high protein and high fat intake damaged the intestinal mucus layer, thinned the matrix, and increased the number of intestinal villus cells and the apoptosis rate of intestinal epithelial cells. Gut microbiology results complemented the explanation of changes in intestinal permeability, with high fat intake causing a significant decrease in microbial abundance and promoting intestinal inflammation.In conclusion, the intake of high protein and high fat diet promoted the dissolution and transmembrane absorption of As and Pb in the digestive tract, thereby improving the As- and Pb-bioavailability in soils.

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Incident cardiovascular disease caused by high level of selenium exposure: a population-based study

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Abstract

Selenium (Se), an essential trace element, plays a critical role in maintaining human health. However, increasing evidence suggests that high Se exposure may be associated with adverse health effects. In this

study, we evaluated both linear and nonlinear dose-response relationships between urinary Se levels and incident cardiovascular disease (CVD) events in the Strong Heart Study. The median (interquartile range) of urinary Se was 49.0 (36.7–67.4) μg/g creatinine. The multivariable adjusted hazard ratios (95% confidence interval) of incident CVD, coronary heart disease, and stroke comparing the 75th versus 25th percentile of urinary Se distributions were 1.11 (1.01–1.22), 1.05 (0.94–1.17), and 1.08 (0.88–1.33), respectively. In flexible dose–response models, an increased risk for CVD incidence was observed when urinary Se level exceeded 60 μg/g creatinine. For CVD mortality, an insignificant U-shaped relationship was found across urinary Se levels. Moreover, there was no evidence of effect modification by other urinary metal/metalloid levels. Our findings suggest that elevated Se exposure is a potential risk factor for CVD, especially in Se-replete populations.

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Ca Minerals and Oral Bioavailability of Pb, Cd, and As from Indoor Dust in Mice:Mechanisms and Health Implications

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Abstract

BACKGROUND: Elevating dietary calcium (Ca) intake can reduce metal(loid)oral bioavailability. However, the ability of a range of Ca minerals toreduce oral bioavailability of lead (Pb), cadmium (Cd), and arsenic (As) from indoor dust remains unclear.

OBJECTIVES : This study evaluated the ability of Ca minerals to reduce Pb, Cd, and As oral bioavailability from indoor dust and associated mechanisms.

METHODS : A mouse bioassay was conducted to assess Pb, Cd, and As relative bioavailability (RBA) in three indoor dust samples, which were amended into mouse chow without and with addition of $CaHPO_4$, $CaCO_3$, Ca gluconate, Ca lactate, Ca aspartate, and Ca citrate at 200-5,000 μg/g Ca. The mRNA expression of Ca and phosphate (P) transporters involved in transcellular Pb, Cd and As transport in the duodenum of mice was quantified using real-time polymerase chain reaction. Metal(loid) speciation in the feces of mice was characterized using X-ray absorption near-edge structure (XANES) spectroscopy.

RESULTS: In general, mice exposed to each of the Ca minerals exhibited lower Pb-, Cd-, and As-RBA for three dusts. However, RBAs with the different Ca minerals varied. Among minerals, mice fed dietary $CaHPO_4$ did not exhibit lower duodenal mRNA expression of Ca transporters but did have the lowest Pb and Cd oral bioavailability at the highest Ca concentration (5,000 μg/g Ca; 51%-95% and 52%-74% lower in comparison with the control). Lead phosphate precipitates (e.g., chloropyromorphite) were observed in feces of mice fed dietary $CaHPO_4$. In comparison, mice fed organic Caminerals (Ca gluconate, Ca lactate, Ca aspartate, and Ca citrate) had lower duodenal mRNA expression of Ca transporters, but Pb and Cd oral bioavailability was higher than in mice fed $CaHPO_4$. In terms of As, mice fed Ca aspartate exhibited the lowest As oral bioavailability at the highest Ca concentration (5,000 μg/g

Ca; 41%-72% lower) and the lowest duodenal expression of P transporter (88% lower). The presence of aspartate was not associated with higher As solubility in the intestine.

DISCUSSION: Our study used a mouse model of exposure to household dust with various concentrations and species of Ca to determine whether different Ca minerals can reduce bioavailability of Pb, Cd, and As in mice and elucidate the mechanism(s) involved. This study can contribute to the practical application of optimal Ca minerals to protect humans from Pb, Cd, and As coexposure in the environment

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Exposure to organophosphorus flame retardants and plasticizers in children: Thyroid nodule and mediation role of oxidative stress

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Abstract

Organophosphorus flame retardants and plasticizers (OPFRs) are widely used in consumer and industrial products and have been implicated in adverse health outcomes. Human exposure to OPFRs raises concerns due to their endocrine disruptive potentials. Clinical detectable thyroid nodules are less common in children than adults. However, they are associated with an increased risk of malignancy which is much higher than adults. The effects of OPFRs on children thyroid nodules and the mediating role of oxidative stress in children have not been studied so far. In this study, concentrations of 7 OPFRs, levels of three oxidative stress biomarkers (8-oxo-7,8-dihydro-2'-deoxyguanosine (8-OHdG), malondialdehyde (MDA) and dityrosine (diY) were determined in 521 children urine samples collected from a coastal urbanized region and moderate socioeconomic status. The median creatinine-adjusted level of urinary 7 OPFRs concentrations ranged from 0.02 to 0.64 μg/g. Diphenyl phosphate (DPHP) and isopropyl phenyl phenyl phosphate (ip-PPP) are extensively detected with a median creatinine-adjusted level of 0.46 μg/g and 0.64 μg/g, respectively. Triphenyl phosphine oxide (TPPO) is a novel OPFRs detected in children, which has positively association with thyroid nodule in children. In addition, the multiple linear regression model revealed that most OPFRs were significantly positively correlated with three oxidative stress markers (β range from 0.085 to 0.367). Mixture effect regression showed that TPPO were the strongest contributors to increasing of MDA. Furthermore, 8-OHdG and diY, the biomarker of DNA and proteins damage, was found to be the mediator (>25%) for the association between thyroid nodule and OPFRs, suggesting that DNA and protein damage are involved in the onset of children thyroid nodules. Our findings suggest potential thyroid risks of OPFRs exposure on children and the potential influence mediated by oxidative stresses of DNA damage and protein peroxidation.

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Dihalogenated Nitrophenols in Drinking Water: Prevalence, Resistance to Household Treatment, and Cardiotoxic Impact on Zebrafish Embryo

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Abstract

Dihalogenated nitrophenols (2,6-DHNPs) are a group of emerging aromatic disinfection byproducts (DBPs) detected in drinking water, but limited information is available regarding their persistency and toxicological risks. In the present study, we found that 2,6-DHNPs are resistant to treatment in major drinking water (sedimentation and filtration) and households (boiling, filtration, microwave irradiation, and ultrasonic cleaning) treatment processes. To further assess their health risks, we conducted a series of toxicology studies using zebrafish embryos as the model organism. Our findings reveal these emerging 2,6-DHNPs showed 248 times greater lethal toxicity than the regulated DBP, dichloroacetic acid. Specifically, at sublethal concentrations, exposure to 2,6-DHNPs generated reactive oxygen species (ROS), caused apoptosis, inhibited cardiac looping, and induced cardiac failure in zebrafish. Remarkably, the use of a ROS scavenger, N-acetyl-L-cysteine, considerably mitigated these adverse effects, emphasizing ROS's essential role in 2,6-DHNP-induced cardiotoxicity. Our findings draw attention to the cardiotoxic potential of 2,6-DHNPs in drinking water even at low concentrations of 19 μg/L and the beneficial effect of N-acetyl-L-cysteine in alleviating 2,6-DHNP-induced cardiotoxicity. This study underscores the urgent need for heightened scrutiny of these emerging compounds in public health discussions.

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Emerging disinfection byproducts 3-bromine carbazole induces cardiac developmental toxicity via aryl hydrocarbon receptor activation in zebrafish

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Abstract

3-bromine carbazole (3-BCZ) represents a group of emerging aromatic disinfection byproducts (DBP) detected in drinking water; however, limited information is available regarding its potential cardiotoxicity. To assess its impacts, zebrafish embryos were exposed to 0, 0.06, 0.14, 0.29, 0.58, 1.44 or 2.88 mg/L of 3-BCZ for 120 hours post fertilization (hpf). Our results revealed that ≥1.44 mg/L 3-BCZ exposure induced a higher incidence of heart malformation and an elevated pericardial area in zebrafish larvae; it also decreased the number of cardiac muscle cells and thins the walls of the ventricle and atrium while increasing cardiac output and impeding cardiac looping. Furthermore, 3-BCZ exposure also exhibited significant effects on the transcriptional levels of genes related to both cardiac development (*nkx2.5*, *vmhc*, *gata4*, *tbx5*, *tbx2b*, *bmp4*, *bmp10*, and *bmp2b*) and cardiac function (*cacna1ab*, *cacna1da*, *atp2a1l*, *atp1b2b*, *atp1a3b*, and *tnnc1a*). Notably, N-acetyl-L-cysteine, a reactive oxygen species scavenger, may alleviate the failure of cardiac looping induced by 3-BCZ but not the associated cardiac dysfunction or malformation; conversely, the aryl hydrocarbon receptor agonist CH131229 can completely eliminate the cardiotoxicity caused by 3-BCZ. This study provides new evidence for potential risks associated with ingesting 3-BCZ as well as revealing underlying mechanisms responsible for its cardiotoxic effects on zebrafish embryos.

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Quantitative Screening of Environmental Liquid Crystal Monomers (LCMs) in Human Plasma and Their Neurotoxic Effects in Cultured Neurons

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Abstract

Liquid crystal monomers (LCMs) is a major component used to manufacture liquid crystal display (LCD) of electronic devices, which generally consisting of 10-20 different LCMs per panel. These LCMs leak into the environment as organic pollutants (e.g. indoor dusts), and are absorbed into human body via ingestion, inhalation and dermal contact. With an increasing production and disposal of LCD devices, human exposure to environmental LCMs has become a global health concern. Currently at least 89 LCMs are classified as highly persistent and bioaccumulative. However, whether they induce neurotoxicity to impact neuronal health remain unclear.

To assess human exposure, 80 target LCMs in plasma collected from a cohort of local elderly residents (40-90 years old) in Hong Kong were quantified by GC-MS/MS. We developed a real-time, bioluminescence-based assay using differentiated human SH-SY5Y neuronal cells to screen for cytotoxicity of 10 most abundant LCMs identified in the Pearl River Estuary (PRE) region near Hong Kong. Bioaccumulation and metabolism of selected toxic LCMs in blood were assessed in young C57/BL6 mice after single oral gavage of LCMs.

Our GC-MS/MS measurements showed at least 24 different LCMs in the plasma of our local elderly cohort. Among the 10 most abundant LCMs in PRE, 3VbcH (CAS No. 116020-44-1; LCM-2), MeP3bcH

(CAS No. 84656-75-7; LCM-13) and 3cH2B (CAS No. 84540-37-4; LCM-16) caused significant neuronal cell death at their environmentally relevant concentrations (ranging from 0.5 to 20 ng/ml) after 72-hr exposure in SH-SY5Y cells. Strikingly, the plasma detection rates of LCM-2 and LCM-13 were both over 90%. Treatment with LCM-2, LCM-13, and LCM-16 impaired cell proliferation and neuronal differentiation (neurite growth) in SH-SY5Y cells. Single oral administration of LCM-2 and LCM-16 in mice resulted in a marked elevation of blood LCM levels at 1 and 6 hr post-treatment.

This study revealed bioaccumulation of 24 different LCMs in human plasma. In particular, 3VbcH (LCM-2), MeP3bcH (LCM-13) and 3cH2B (LCM-16) demonstrated significant neurotoxic effects to cell proliferation and neuronal differentiation. Our findings provide insights into the contamination and potential health risks of LCMs in the context of their exposure, bioaccumulation, and neurotoxicity to human brains.

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Study on Hydrophobicity Quantification Method and Sorption Prediction Model of Dissolved Organic Matter Based on Aqueous Two-Phase System

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Abstract

Organic matter plays an important role in the environment as a good sorbent and carrier of organic pollutants, and the equilibrium partitioning between organic matter and pollutants is an important environmental process.

In the field of the sorption behavior of organic matter, the partition theory is the basic theory for the adsorption of hydrophobic organic pollutants by organic matter. The organic carbon-normalized partition coefficient, K_{OC}, is an important parameter for evaluating the sorption capacity of organic matter, as well as an important parameter and indicator for environmental model construction and environmental risk assessment. However, in practice, it is important to develop a reliable and accurate prediction model because of hard obtaining. Currently, the model commonly used for K_{OC} prediction is mainly the linear free energy model, but the linear free energy model does not solve the problem of heterogeneity of organic matter well, and the nature of the organic matter will also determine the size of K_{OC}, which affects the accuracy of the model prediction, of which hydrophobicity is one of the important properties of organic matter.

We propose a new method to quantify the hydrophobicity of organic matter using a two-phase aqueous system. It is found that the partition coefficients (K_{ATPS}) of organic matter in the two-phase system correlate well with the elemental, structural, and thermodynamic parameters commonly used to characterize its hydrophobicity. Therefore, the K_{ATPS} can be used to quantify the hydrophobicity of organic matter, and the simplicity, rapidity, low cost, environmental friendliness, almost no pre-treatment, and small sample size of the two-phase system also contribute to the efficient and routine characterization of the interfacial properties of organic matter. Based on the parameters characterizing the hydrophobicity of organic matter (K_{ATPS}) and the nature of organic pollutants (K_{OW}), a new adsorption prediction model,

the two-phase system model, was obtained by theoretical derivation, which can simultaneously consider the nature of organic matter and organic pollutants. The accuracy of the model is significantly improved, which provides a reliable modeling basis for the risk assessment and pollution control of new organic pollutants.

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Widening the Lens on Human Exposure to the "Chemical Cocktail" in Tianjin

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Abstract

Despite the global distribution of emerging pollutants and there is a lack of biomonitoring data and health impact studies in Tianjin, China. In this study, we constructed a cross-sectional study and collected urine from 240 participants, completed urine biomonitoring for 98 exposures and 4 oxidative stress biomarkers by liquid chromatography-tandem mass spectrometry. The models were applied for exposure characterization and regression analysis of the 26 high-frequency exposures. Our findings indicate that increased levels of oxidative stress were associated with increased exposure to environmental chemical mixtures. Through the application of WQSR, BKMR, qgcomp models, including OH-NAP, OH-PHEN, and OH-PYR; DEP, DMP, DMTP, and TCPY; BPMA, CMEMA, HPMMA, and MHA; BPS and BP3, thirteen key emerging environmental pollutants exhibited significant dose-response relationships with oxidative stress levels In summary, this study not only provided biomonitoring data for population of Tianjin but also explored the relationship between emerging pollutants and oxidative stress. To provide scientific basis for formulating public health intervention measures for new pollutant exposure in Tianjin, and to provide theoretical basis for in-depth causal research between environmental exposure and human health in the future.

826

Understanding the importance of legacy and emerging contaminant bioavailability for human health exposure assessment

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Abstract

When considering exposure to environmental contaminants, chemical daily intake may be quantified by considering exposure magnitude, frequency and duration. Exposure magnitude will be influenced by the concentration of the contaminant in various matrices but also by its bioavailability (i.e. the proportion of the total contaminant concentration that is absorbed into the systemic circulation following ingestion, inhalation or dermal contact). Contaminant bioavailability may be influenced by a number of physiological parameters in addition to physico-chemical properties of the contaminant and its matrix. In the absence of site-specific data, the default bioavailability value for a number of contaminants of concern is 100%. It is assumed that contaminant bioavailability is equivalent to that in the exposure medium used to derive the toxicity reference value. Acknowledging that default values may not reflect all variables that influence contaminant bioavailability, site-specific assessment may be performed where such assessments are deemed feasible and valuable for improving the characterisation of risk at a given site. This presentation will detail toxicokinetic and bioavailability approaches for refining legacy (arsenic) and emerging contaminant (PFAS) exposure via the oral ingestion pathway. In addition, complementary analyses will be highlighted that provide a lines-of-evidence approach for elucidating factors influencing bioavailability outcomes.

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Photofate of a Next Generation Breast Cancer Drug

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Abstract

Endoxifen is an effective metabolite of tamoxifen, a commonly used chemotherapy drug, and has been detected in the final effluent of a municipal wastewater treatment plant (WWTP). Endoxifen has emerged as a potential breast cancer drug based on a recently completed clinical trial. Endoxifen in the water environment could bring negative effects to aquatic lives as demonstrated by its toxicity to *Daphnia pulex*. Our research group has investigated ways to degrade endoxifen and found that it is biorecalcitrant but very photodegradable. Endoxifen in water was degraded by at least 99.1% after 35 seconds of ultraviolet (254 nm) irradiation. Photodegradation of endoxifen in treated wastewater at ultraviolet (UV) doses used for disinfection in WWTPs resulted in reduction of endoxifen by 30 to 71%. Endoxifen in treated wastewater was photodegraded by sunlight at 83%, whereas in receiving surface water it was photodegraded at 61% after 150 min of irradiation. Multiple photodegradation by-products (PBPs) were identified for both the cases of UV and sunlight radiation and almost all of them are potentially more toxic than endoxifen itself. The adoption of endoxifen as a breast cancer drug should proceed with extreme caution as highly toxic PBPs are potentially generated if endoxifen is present in treated wastewater disinfected by UV radiation and in receiving surface water exposed to sunlight.

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Metabolism of the Orally Ingested Arsenic by Human Gut Microbiota and Health Risks

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Abstract

The importance of arsenic (As) metabolism by human gut microbiota has been evidenced by in vitro methods (e.g., Simulator of Human Intestinal Microbial Ecosystem) and an in vivo mouse model. Some main findings included that (i) a significant increase in colon As bioaccessibility contributed from the dissolution of As associated with amorphous and crystalline Fe/Al (hydr)oxides. Based on sequential extraction, it inferred that the priority sequence in As transformation by human gut microbiota was dissolved As(V), As(V) sorbed to mineral surfaces, crystalline As(V)-bearing minerals and As sulfides. Arsenic bioaccessibility was predominantly contributed by Fe(III) dissolution for jarosite, and microbial reduction of Fe(III) and As(V) for goethite. (ii) Elevated As methylation was presented with increasing soil organic matter and decreasing soil pore size, as well as microbial Fe(III) reduction. Higher As bioaccessibility of colon phase was mainly contributed from reductive dissolution of As(V)-bearing Fe(III) (oxy)hydroxides. Arsenic mobility and biotransformation by human gut microbiota (carrying *arrA* and *arsC* genes) are strongly controlled by microbial Fe(III) reduction coupled with soil particle size. (iii) The cefoperazone treatment (especially under high arsenic exposure) reduced arsenic accumulation in blood and organs such as liver, spleen and ileum. A total of 17 ABGs were detected in the mouse gut, and their abundances (e.g., *arsC*, *arsH* and *arsB* genes) were markedly reduced in the antibiotic-treated mice exposed to arsenic. The ABGs were remarkably correlated with specific gut bacteria and metabolic profiles, exemplified by *Prevotellaceae* carrying *arsC* gene involved in amino acid metabolism, and *Erysipelotrichaceae* as *aoxA* gene carrier alleviating histamine accumulation. Understanding the role of gut microbiota in metabolism of the orally ingested As in human gastrointestinal tract could be important for arsenic induced toxicity, bioavailability and disease risk.

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Characteristics and human health risk assessment of organochlorine pesticides pollution by using bioaccessibility analysis in soils of typical chemical plant site in China

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Abstract

In this study, ten soil samples from a typical organochlorine pesticide contaminated site in Yangtze river delta region in China were collected. Dichlorodiphenyltrichloroethane (DDT), dichlorodiphenyldichloroethylene (DDE) and dichlorodiphenyldichloroethane (DDD) concentrations were determined and Bioavailability of p,p'-DDT, p,p'-DDE and DDD in soil were measured by adsorbent material method (2,6-diphenylene-oxide porous polymer resin, Tenax). Then the health risks associated with different pollution sources were calculated.

The results showed bioaccessibility of organic chlorine pesticides in the soil ranged from 3% to 62%. The contribution rates of p,p'-DDT, p,p'-DDE and DDD to cancer risks via oral exposure pathways decreased by using bioaccessibility analysis, and further analysis of exposure pathways revealed that children generally had higher contribution rates than adults. Under the condition of meeting the maximum acceptable value of health risk, the remediation target values for p,p'-DDT, p,p'-DDE and DDD increased by 1.45, 4.37, and 1.04 times, respectively, and the volume of remediated soil decreased by approximately 33.9%-85.4%.

Therefore, incorporating the analysis of bioavailability of pollutants in development land soil into the entire process decision-making system for soil pollution investigation, risk assessment, and remediation governance can objectively and rationally quantify health risks of populations on contaminated sites. This approach allows for the scientific consideration of health risks, control of remediation costs, effective cost savings, and precise remediation implementation.

Key words: organic chlorine pesticides; risk assessments; bioaccessibility; soil

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Insights into health risks of face paint application to opera performers: The release of heavy metals and potential toxicity mechanism

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Abstract

Heavy metals (HMs) are commonly used as ingredients of colorants in cosmetics and capable of entering the human circulation system via dermal absorption. The use of face paint cosmetics can cause skin diseases in opera performers due to the presence of toxic ingredients such as HMs. However, a large knowledge gap still exists concerning HM bioaccessibility in face paints and potential health risks attributed to their usage. Here, we investigated the contents of eight HMs (As, Cd, Cr, Co, Cu, Ni, Pb, and Zn) and *in vitro* bioaccessibility (IVBA) of main HMs in face paints, as well as the consequent health risks and potential toxicity mechanisms. Among the 91 face paint products available in domestic markets based on paint usage habits of opera performers, at least four of the eight HMs were detected and the average contents of As, Cd, Co, Cr, Cu, Ni, Pb, and Zn were 1.8, 0.6, 4.4, 23.1, 610, 7.6, 16.2, and 10415 μg/g, respectively. Samples from the most frequently used paint brand contained the highest HM contents. Moreover, HM contents in the paints were color-specific, *e.g.*, significantly higher Cu contents in green

paints. IVBA of Cr, Cu, Pb, and Zn in the products was, on average, 1.1, 2.2, 1.6, and 1.2% through dermal contact, respectively. The influence of factors related to real-life conditions on HM release was examined, *e.g.*, the stage lighting, status of the sweating process, and the pH of the sweat. Stage light irradiation increased the IVBA to the average of 4.8, 34.9, 5.7, and 1.9% for Cr, Cu, Pb, and Zn, respectively. The increase was mainly due to the light-induced generation of reactive oxygen species, particularly hydroxyl free radicals. Acidic sweat and dynamic incubation also promoted the release of HMs. The vitality of 3D skin models and skin sensitization risk assessment indicated that dermal contact with face paints might induce predictable skin damage and potential skin diseases. Transcriptional response of human skin keratinocytes further demonstrated that long-term exposure to face paints could exacerbate inflammation evidenced by the up-regulation of inflammation-related genes and enrichment of inflammation-related pathways, among which TNF was the key regulator and connector. To our knowledge, this is the first in vitro study demonstrating occurrence of bioaccessible HMs in face paint cosmetics and revealing their health risks as well as potential toxicity mechanism, which call for stricter regulations in face paint safety.

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New Insights into Renal Clearance and Potentials for Oxidative Stress of Primary Aromatic Amines in Humans

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Abstract

Primary aromatic amines (PAAs) are a class of industrial and environmental pollutants with high thermal stability and carcinogenicity. However, their human exposure levels have until now remained unexplored. This study investigates the presence of 28 PAAs in 180 paired human urine and blood samples collected from Shenzhen of China. Aniline, 3,4-DAAS (3,4-diaminoanisole), *o*-TD (ortho-toluidine), *m*-TD (meta-toluidine), 4-CA (4-chloroaniline), *p*-TD (para-toludine) and *o*-anisidine (ortho-anisidine) identified as the predominant substances. PAAs demonstrated a significant preference for blood distribution, with median total concentration of 28 PAAs was 2.23 ng/mL in urine and 22.49 ng/mL in blood. Renal clearance of PAAs were all lower than those of nicotine and cotinine. Among these PAAs, *o*-anisidine, aniline and 4-CA shown lower renal clearance 0.05<1.32<1.38 mL/day/kg (median value). Smokers pay more PAAs exposure compare to non-smokers. In non-smokers (healthy populations), male and younger have significantly higher PAAs exposure. Additionally, PAAs level is significantly associated with tobacco markers nicotine and cotinine. Notably, 8-OH-dG significantly associated with concentration of PAAs, underscoring their contribution to oxidative stress. The predominate eight PAAs all could biologically significantly bind with human CYP3A4 and hemoglobin. 4,4-MBCA (4,4'-methylenebis(2-chloroaniline)) showing the strongest potential for binding to two proteins. This study represents the first comprehensive investigation into the prevalence of PAAs as a class of emerging pollutants widespread in human paired biomatrix,

underscoring their hazardous nature and adverse effects to human, necessitating heightened attention and further research in the future.

925

Association of air pollutant and non-optimal temperature exposure with placental abruption: a nested case-control study based on 0.95 million of birth registrations in Chongqing

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Abstract

Objective:

This study proposes to explore the associations between long-term and short-term exposures to six air pollutants and temperature and the risk of placental abruption (PA).

Methods:

Nested in the Chongqing Live Birth Cohort, 956,868 birth registrations were obtained, and cases of PA were identified according to ICD-10 code O45. After exclusion and case-control matching, a total of 798 cases and 3192 controls were retained for inclusion in the analysis.

Multi-source data such as ground monitoring and meteorological data were obtained and formed by multiple interpolation as grid data set, which was matched with the residential address of the subjects, and the daily average exposure of each subject during the study period were obtained.

Conditional logistic regression models were constructed to estimate OR and 95% CI corresponding to the risk of PA for each interquartile increase in exposure in five potential windows, and to calculate an overall trend P value.

Distributed lag non-linear model (DLNM) based on conditional logistic regression was fitted to estimate the association between elevated cumulative lag per IQR of 1-7 days of air pollution and PA. and estimate the association between elevated temperature and PA compared with 15 ℃.

Results:

Mean NO_2 exposure throughout pregnancy at Q3 and Q4 concentrations was associated with an elevated risk of PA to 1.76-fold (1.21-2.55) and 2.21-fold (1.35-3.60), respectively, $P<0.001$. Pre-pregnancy, first trimester, second trimester, and third trimester exposure to Q3 and Q4 levels of NO_2 was associated with an elevated risk of PA. Exposure to extreme cold temperatures during pre-pregnancy (2.25, 1.03-4.91) and third trimester (2.90, 1.35-6.21) was associated with an increased risk of PA.

There was a significant association between NO_2 and an elevated risk of developing PA within a cumulative lag of 4-7 days before onset, with an OR of 1.38 (1.11-1.73) to 1.54 (1.18-2.02) corresponding to an OR per IQR increase in NO_2, $P<0.001$. Compared with 15 °C, lower temperature was associated with an increased risk of PA with increasing cumulative lag day.

Conclusion:

The results of this study show that both long-term exposures to NO_2, and before delivery were consistently associated with an elevated risk of PA, suggesting that NO_2 may be an important risk factor for PA. Control of NO_2 emissions and personal protection may help reduce the risk of PA in pregnant women.

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Knowledge on Melamine and Its Derivatives: from Environmental Occurrence to Human Exposure Assessment

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Abstract

As a PMT/vPvM substance, melamine is widely found in different microenvironments around the world, and general population is unconsciously exposed to such substances. As a substitute for halogen and organophosphorus flame retardants, melamine-based nitrogenous flame retardants (NFRs) have been used rapidly in recent years. However, their current pollution status and human health hazards are not well understood. Herein, we introduce the assessment of NFRs from their environmental occurrence to human exposure. Our environmental monitoring work found that melamine and its three derivatives, including cyanuric acid, ammelide and ammeline, have been detected in various environmental matrices, such as natural water, surface soil, sediment, sewage sludge, and indoor dust. Nevertheless, limited information is available on human exposures, other than dietary sources, to melamine and its derivatives. Based on human biomonitoring studies and exposure assessment models, we assessed the internal exposure load and external exposure routes of different populations to NFRs. The correlations between NFRs exposure and human urinary system diseases were explored through epidemiological investigation. In short, this study is expected to provide scientific support for the evaluation of NFRs' safety in use.

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Large Geographical Scale Study on the Concentrations, Distribution, and Source Analysis of Neonicotinoid Insecticides in Surface Waters of South China

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Abstract

Neonicotinoid insecticides (NEOs) have gained widespread usage as the most prevalent class of insecticides globally and are frequently detected in the environment, posing potential risks to biodiversity and human health. This study investigated the residual levels, distribution, and source of eight parent neonicotinoid insecticides (p-NEOs) and three NEO metabolites (m-NEOs) in surface waters of river–estuary–ocean systems on a large geographical scale in South China. Imidacloprid, thiamethoxam, acetamiprid, and clothianidin were dominant NEOs in surface waters. High levels of ∑NEOs were found in the upper reaches of Guangzhou section of the Pearl River (PR_GZ), indicating multiple input sources of NEOs in PR_GZ. Specifically, wastewater discharged from wastewater treatment plants (WWTPs) have been identified as a substantial source of environmental NEOs. Additionally, the decreased influence of terrestrial input and human activities was observed along with the flow direction, where the order of ∑NEOs concentration was PR_GZ (inland river, 64.5 ng/L) > Pearl River Estuary (estuary, 33.9 ng/L) > Xisha Islands of the South China Sea (SS_XS, open sea area, 27.0 ng/L); and the level in Northwestern South China Sea (coastal sea, 49.9 ng/L) was also higher than that in open sea area. The estimated annual fluxes of NEOs released into the South China Sea totaled 34.8 ± 20.4 tons, most of which come from the Pearl River basin. To the best of our knowledge, this is the first study to assess the concentrations, distribution, and source analysis of NEOs in river–estuary–ocean systems in South China.

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Risk of Invasive Breast Cancer under Co-exposure of Genetic Burden and Exposure to Di-2-ethylhexyl phthalate: Cohort Analysis of Women in the UK Biobank

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Abstract

Abstract

Background: Breast cancer is considered to result from a combination of genetic and environmental factors, but the degree to which an exposure to phthalates may increase the risk of invasive breast cancer remains equivocal, especially for women with different genetic burden

Methods: Using Cox proportional hazards regression models, we estimated the association between di-2-ethylhexyl phthalate (DEHP) exposure by water and risk of invasive breast cancer, stratified by genetic risk group among 252,915 women from the UK Biobank (UKB). Yearly-average level of DEHP exposure were estimated for each individual by linking chemical monitoring record of European Environment Agency with home address of the participants by Kriging interpolation model. Polygenic risk score (PRS) was calculated using a Standard Set for all individuals in UKB

Results:

An above-median exposure of DEHP (> 8000.25 μg/L) was associated with 1.125 fold risk of overall invasive breast cancer (95% CI, 1.082, 1.171, $p < 0.001$). As for hormone receptor positive (HR+) breast cancer, the upper median level of DEHP was positively associated with 1.214 fold risk (95% CI, 1.01,1.339, $p < 0.001$). In the women with highest 10% PRS burden, high DEHP exposure was associated with 1.143 fold risk (95% CI, 1.050 to 1.243, $p = 0.002$), while the effect size was 1.121 for the rest women (95% CI, 1.072 to 1.173, $p < 0.001$). There was no interaction between the DEHP exposure and PRS, either for all or for HR+ breast cancer. Compared with both low PRS and low DEHP exposure, those with high DEHP exposure and high PRS had 3.055 fold risk of all invasive breast cancer (95% CI, 2.841 to 3.286, $p < 0.001$), whereas 1.122 (95% CI, 1.072 to 1.173, $p < 0.001$) and 2.672 fold risk were respectively in low-PRS/high-DEHP group and high-PRS/low-DEHP group (95% CI, 2.529 to 2.822, $p < 0.001$). Furthermore, compared with the women with both low PRS and low DEHP exposure, those with both high DEHP exposure and high PRS showed 3.945 fold risk of HR+ breast cancer (95% CI, 3.330 to 4.679, $p < 0.001$), while 1.191 (95% CI, 1.061 to 1.337, $p < 0.001$)and 3.295 fold risk were respectively found in low-PRS/high-DEHP group and high-PRS/low-DEHP group (95% CI, 2.895 to 3.752, $p < 0.001$)

Conclusion: Our findings suggest that co-exposure of DEHP and genetic burden may substantially increase the risk of invasive breast cancer, especially for HR+ breast cancer.

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Application of Manganese Oxides on Controlling the Release and Reduction of Soil Arsenic under Microbial Reducing Conditions

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Abstract

The oxidation and immobilization of arsenic (As) by manganese oxides have been shown to reduce As toxicity and bioavailability under aerobic conditions. However, under anaerobic conditions where As has higher mobility and toxicity, the effect of manganese oxides on controlling As release and reduction remains unknown. Our study constructed an anaerobic As(V)-reducing environment, and investigated the impact of different manganese oxides (δ-MnO_2, α-MnO_2, and γ-MnO_2) on the fate of aqueous and goethite-adsorbed As. Results showed that all manganese oxides exhibited the strongest As immobilization in neutral environment and the highest As oxidation ability in alkaline environment. Additionally, δ-MnO_2 showed much higher immobilization and oxidation ability for As (52.3%, 50.7%) compared to α-MnO_2 (24.6%, 35.2%) and γ-MnO_2 (38.1%, 34.3%) in both aqueous and solid phases. Therefore, δ-MnO_2 was selected to further explore its impact on the fate of As in different Fe-minerals. Without δ-MnO_2 addition, the release of As from goethite was much higher than that from ferrihydrite and hematite. The addition of 3.1 mM Mn reduced the release of As by 0.3%, 46.3%, and 6.7% for ferrihydrite, goethite, and hematite, respectively. Meanwhile, the solid-phase As(V) content increased by 9.8%, 39.4%, and 7.4%, respectively, indicating that δ-MnO_2 had the strongest oxidation and immobilization effect on goethite-adsorbed As. This was achieved because goethite particles were evenly distributed on δ-MnO_2 surface, which supported As(III) oxidation; while ferrihydrite strongly aggregated, which hindered the oxidation of As(III). In flooded soil system, δ-MnO_2 can inhibit As release in all soil types, but its effectiveness is strongly influenced by the soil physicochemical properties. Under microbial reducing conditions, As in sandy soil was more easily released than that in clay soil. The addition of δ-MnO_2 hindered the release of As by 96.4%, 90%, and 78.6% from sandy soil, sandy loam soil, and clay soil, respectively. This is because sandy soil has larger particles and better permeability, which is conducive to the interaction with δ-MnO_2, thereby promoting the oxidation and immobilization of As. Overall, the results clarified the most suitable conditions for δ-MnO_2 as a remediation agent for flooded sites. This study contributes to reducing the environmental and health risks of soil As and developing effective remediation strategies for anaerobic As-contaminated environments.

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Preliminary exploration of the correlation and mechanism between per- and polyfluoroalkyl substances and type 2 diabetes

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Abstract

- Background: Previous studies have confirmed that per- and polyfluoroalkyl substances (PFASs) affect human health, but the association between PFASs exposure and type 2 diabetes (T2DM) remains controversial.
- Objective: This study aimed to assess whether PFASs exposure is associated with T2DM and elucidate the possible molecular mechanism, and further provide a scientific basis for assessing the health risks of PFASs exposure.
- Methods: We conducted a cross-sectional study of 904 participants from the National Health and Nutrition Examination Survey (NHANES) 2017-2018, multivariable logistic regression was performed to explore the relationship between the concentration of PFASs in human serum and T2DM; the Comparative Genomics Database (CTD) was used to screen for key genes that are commonly affected by PFASs, functional and pathway enrichment was performed to explore the possible pathway mechanisms.
- Result: We observed associations of PFASs exposure with T2DM (P<0.05). In a multivariable logistic regression model adjusted for sociodemographic, behavioural, and health characteristics, log-transformed serum concentrations of PFASs was associated with T2DM [Perfluorooctanoic acid (PFOA): OR=0.172, 95% CI: 0.171-0.172, P<0.001; perfluorooctane sulfonic acid (PFOS): OR=0.448, 95% CI: 0.447-0.448, P<0.001; perfluorohexane sulfonic acid (PFHxS): OR=0.242, 95% CI: 0.241-0.242, P<0.001]. Besides, dose-response relationships were analyzed to clarify effects of PFAS exposure on T2DM risk at different exposure levels. Multivariable logistic regression models showed that compared to the lowest quartiles, elevated odds of T2DM risk were observed in the other quartiles of PFOA and PFHxS (P<0.001), but the risk of T2DM in the last two quartiles of PFOS were significantly reduced (P<0.001). CTD was identified 32 key targets of PFASs on T2DM. The Kyoto Encyclopedia of Genes and Genomes (KEGG) enrichment analysis suggested PFASs mainly works through multiple pathways in non-alcoholic fatty liver disease, adipocytokine signaling pathway, insulin resistance, etc.
- Conclusions: The study implies a potential association between long-term PFASs exposure and T2DM through multi-faceted mechanisms. It is suggested that attention be given to the possibility of T2DM in people undergoing prolonged PFASs exposure, and further verify the mechanism of T2DM caused by PFASs exposure.

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Maternal and Infant Exposure to Polycyclic Aromatic Hydrocarbons (PAHs) and Associations with Congenital Heart Disease

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Abstract

Congenital heart disease (CHD) is one of the most common types of congenital birth defects globally, characterized by high incidence, disability, and mortality rates, posing a serious threat to human health. Polycyclic aromatic hydrocarbons (PAHs) are semi-volatile organic pollutants widely present in the atmosphere. PAHs can trigger various cardiovascular diseases such as hypertension, arrhythmias, and atherosclerosis. However, the impact of PAH exposure on CHD and its association with the risk of CHD incidence remain unclear. In this study, seven hydroxylated polycyclic aromatic hydrocarbons (OH-PAHs) were determined in 132 maternal peripheral blood and 71 neonatal umbilical cord blood collected from newborn CHD children and their mothers. The results showed detectable levels of OH-PAHs in both maternal peripheral blood and newborn umbilical cord blood. 1-hydroxynaphthalene (1-OH-Nap) and 2-hydroxyfluorene (2-OH-Fluo) were the predominant OH-PAHs in peripheral blood, with geometric mean concentrations of 0.057 ng/mL and 0.102 ng/mL, respectively. 2-hydroxynaphthalene (2-OH-Nap) and 2-OH-Fluo were the main OH-PAHs in umbilical cord blood, with concentrations of 0.574 ng/mL and 0.287 ng/mL, respectively. The calculation results of placental transfer efficiency (TTE) indicated that OH-PAHs have high TTE, allowing them to cross the placental barrier and potentially impact normal fetal growth and development. The binary logistic regression analysis revealed a significant negative correlation between the concentration of 2-OH-Fluo in umbilical cord blood and the risk of CHD. Bayesian kernel machine regression (BKMR) analysis demonstrated a significant association between combined exposure to OH-PAHs in umbilical cord blood and a reduced risk of CHD in newborns. Furthermore, 2-OH-Fluo in umbilical cord blood showed an independent effect on CHD. The level of free thyroxine (FT4) in peripheral blood showed a significant negative correlation with the risk of CHD (p=0.009), while the correlations of thyroid-stimulating hormone (TSH) and free triiodothyronine (FT3) with CHD risk approached significance. 1-OH-Nap and TSH, as well as 2-OH-Fluo and FT3 in peripheral blood may exhibit antagonistic interactions regarding their effects on CHD. This suggests that assessing the impact of OH-PAHs on CHD needs to consider complex biological mechanisms. This study provides important theoretical support for exploring the underlying mechanisms of PAHs exposure and CHD risk.

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Reducing arsenic in rice by modulating the P uptake pathway

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Abstract

Arsenic (As) accumulation in rice grains poses health risk to humans. Plants including rice take up arsenate (AsV) by phosphate transporters. Previously, we found that OsPT4 played a critical role in AsV uptake and translocation in rice. Knocking out OsPT4 can decrease inorganic As accumulation in rice grains. Recently, we investigated the roles of rice phosphate transporter OsPht1;9 and OsPht1;10 in arsenate uptake and transport. On the basis of transcriptome database and quantitative real-time polymerase chain reaction (qRT-PCR), we found that the expression of OsPht1;9 was stable under As exposure. And OsPht1;10 expression levels were up-regulated 4.7 times under As exposure. In yeast mutant strain EY917 (lacking all five phosphate transporters), compared with OsPht1;4, the growth of yeast that expressed OsPht1;9 or OsPht1;10 was significantly inhibited by As(V), showing strong affinity and transport capacity for arsenate. Additionally, we constructed OsPht1;9 and OsPht1;10 double knockout rice mutants by CRISP-Cas9 technology for endogenous experiments. When cultivated in medium (+P or -P) with As(V), the tolerance of rice mutants to As(V) was enhanced compared with the wild type. The shoots arsenic accumulation in rice mutants decreased by 46% to 66% under hydroponics. Analysis of the xylem sap showed that As(V) concentrations in rice mutants were 16.5%-34.8% lower than WT controls. When grown in the pot soils with As, the As concentrations in grains and straws of rice mutants were reduced significantly, especially the grain As accumulation decreased by 24%-39%. More importantly, knocking out of OsPht1;9 and OsPht1;10 had minimal effects on phosphorus content and yield of rice. The results of this study showed that knocking out OsPht1;9 and OsPht1;10 genes could reduce rice grain As accumulation without affecting its utilization of phosphorus nutrition and growth and yield. This study shed light on engineering low-arsenic rice and improving food safety.

1052

Overlooked Contribution of Dermal Exposure of PFAS: from in Vitro and in Vivo Tests to Physiologically Based Toxicokinetic Models

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Abstract

Sunscreens are recommended for all-year-round application on exposed skin surfaces for protection against ultraviolet radiation, wherein per- and polyfluoroalkyl substances (PFAS) are commonly added either as active ingredients or impurities. Both *in vitro* and *in vivo* studies have highlighted the potential dermal permeation of PFAS, which raises specific concerns regarding human exposure risks related to the repeated, long-term application of sunscreens containing PFAS.

Understanding the body loading after the application of PFAS-containing products in humans is crucial for assessing exposure risk in realistic scenarios. However, previous studies have relied solely on organic solvents as exposure vehicles to explore the body loading after a single skin exposure, which does not accurately reflect actual human exposure conditions. Hence, our primary focus was to investigate the impact of sunscreen ingredients on the skin penetration of PFAS, followed by long-term repeated skin exposure experiments in mice, for establishing a physiologically based toxicokinetic (PBTK) models capable of predicting the temporal body

loading of PFAS. For the first time, these PBTK models were successfully validated using independent data from mice receiving commercially sunscreens purchased form the market. Based on the refined PBTK model, we underscore a significant exposure risk of PFAS associated with the application of commercial sunscreen on a wide skin area. This emphasizes the need for caution in scenarios involving sunscreen application, particularly during the summer months.

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Microplastic co-exposure elevates cadmium accumulation in mouse tissue after rice consumption: Mechanisms and health implications

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Abstract

Rice cadmium (Cd) and microplastics are prevalent contaminants, posing a co-exposure threat to humans by means of dietary intake. To assess whether co-exposure of microplastics affects the bioavailability of rice Cd, mice were exposed to Cd-contaminated rice with microplastic co-exposure. We found that polyethylene (PE), polystyrene (PS), polypropylene (PP), and polyamide (PA) microplastic co-exposure via diet consumption (2 μg g^{-1}) caused 1.17–1.38-fold higher Cd accumulation in tissue of mice fed by Cd-rice. For mice with co-exposure of PE microplastics, the higher rice-Cd bioavailability corresponded to colonization of *Lactobacillus reuteri* (38.9 % vs 17.5 %) in the gut compared to control mice, which caused higher production of gut metabolites particularly peptides, likely causing a 'side effect' of elevating Cd solubility in the intestinal lumen. In addition, abundance of sphingosine 1-phosphate in the gut of mice was reduced under PE microplastic exposure, which may reduce intracellular calcium ions (Ca^{2+}) in enterocytes and form a weaker competition in pumping of intracellular Ca^{2+} and Cd^{2+} across the basolateral membrane of enterocytes, leading to higher Cd^{2+} transport efficiency. The results suggest elevated Cd exposure risk from rice consumption with microplastic co-exposure at environmentally relevant low concentrations.

1084

Cellular absorption and cytotoxic mitigation of heavy metals in mining vegetables in southwest China: Mechanistic insights and health implications

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Abstract

The existing health risk assessment models often rely on total concentrations of contaminants, neglecting cellular absorption, leading to an overestimation of risks due to a lack of toxicological verification. In this study, the content, bioaccessibility, and health risk evaluation of Cr, Ni, Cu, and As in vegetables from mining areas in Southwest China were examined. The cytotoxicity and gastric absorption of heavy metals and underlying mechanisms as well as the toxic mitigation approach after consumption of risky vegetables were explored. Our results showed that the heavy metals in cabbage, celery, and garlic seedlings were within the safety limit, even though grown in contaminated soils. The bioaccessibility of As, Cu, Ni, and Cr in vegetables in the gastric phase is from 6.92% to 81.15%, with mint having the highest bioaccessible concentrations of Cr (32.7 μg/kg), Cu (540.1 μg/kg), and As (103.9 μg/kg). The Hazard Quotient and Hazard Index values of the bioaccessible metals suggested an unacceptable cancer risk. Besides, the vegetable extracts increased cell apoptosis and tight junction disruption. Unexpectedly, the high-risk mint extract with the greatest bioaccessibility didn't cause cytotoxicity but inhibited cell apoptosis and enhanced cellular tight junction, evidenced by the upregulation of Zonula Occludens-1, Occludin, and Claudin 3, and a decrease in cellular heavy metal uptake. Furthermore, the mint extract could alleviate garlic seedling extract-induced cytotoxicity, indicating that the special substance in mint has protective effects. Taken together, special components in vegetables, cellular uptake, and toxicity of heavy metals should be considered in the accurate assessment of health risks.

1085

Metal(loid)s in agricultural soil from main grain production regions of China: Bioaccessibility and health risks to humans

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Abstract

Unintentional ingestion of metal-contaminated soils may pose a great threat to human health. To accurately evaluate the health risks of heavy metals in soils, their bioaccessibility has been widely determined by *in vitro* assays and increasingly employed to optimize the assessment parameters. Given that, using meta-analysis, we analyzed the literature on farmland heavy metals (HMs, As, Cd, Cr, Cu, Hg, Pb, Ni, and Zn) in Chinese main grain production regions. We collected their total and bioaccessibility data to assess their human health risks accurately. Monte Carlo simulation was used to reduce the uncertainty in metal concentration, intake rate, toxicity coefficient, and body weight. We found that the mean concentration (0.47 mg/kg) and geological accumulation index (I_{geo}, 0-5.24) of Cd were the priority position of controlling metals. Moreover, children are more vulnerable to carcinogenic risks than adults. Soil mineralogy, physicochemical properties, Fe, and the types of *in vitro* assays are the influencing factors of bioaccessibility discrepancy. Furthermore, appropriate bioaccessibility determination methods can be adapted according to the differences in ecological receptors for the risk assessment, like developing a "personalized assessment" scheme for polluted farmland soil management. Collectively, bioaccessibility-based models may provide an accurate and effective approach to human health risk assessment.

1100

Polystyrene nanoplastics at predicted environmental concentrations enhance the toxicity of copper on *Caenorhabditis elegans*

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Abstract

Excessive nanoplastics not only pose a direct threat to the environment but also have the propensity to adsorb and interact with other pollutants, exacerbating their impact. The coexistence of nanoplastics and heavy metals in soils is a prevalent phenomenon. However, limited research existed about the joint effects of the two contaminants on soil organisms. In this paper, we ascertained the combined toxicity of polystyrene nanoplastics (PS-NPs) and copper (Cu^{2+}) on soil organisms (*Caenorhabditis elegans*) at quantities that were present in the environment, further exploring whether the two toxicants were synergistic or antagonistic. The outcomes manifested that single exposure to low-dose PS-NPs (1 μg/L) would not cause significant damage to nematodes. After treatment with PS-NPs and Cu^{2+}, the locomotion ability of nematode was impaired, accompanied by an elevation in reactive oxygen species (ROS) level and a biphasic response in antioxidant enzyme activity. Moreover, combined exposure to PS-NPs and Cu^{2+} induced the mRNA up-regulation of *vit-6*, *cyp-35a2*, *hsp-16.2*, *age-1*, and *cep-1*, both of which were stress-related genes. The comparative analysis between groups (with or without PS-NPs) revealed that the combined exposure group resulted in significantly greater toxic effects on nematodes compared with Cu^{2+} exposure alone. Furthermore, the addition of PS-NPs influenced the metabolic profiles of *Caenorhabditis elegans* under Cu^{2+} stress, with numerous differential metabolites associated with oxidative damage or defense mechanism. Overall, these findings manifested that PS-NPs at the expected environmental concentration elevated Cu^{2+} toxicity on nematodes.

1106

Ubiquity of Synthetic Phenolic Antioxidants in Children's Cerebrospinal Fluid from South China: First Evidence for Their Penetration across the Blood−Cerebrospinal Fluid Barrier

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Abstract

Synthetic phenolic antioxidants (SPAs) and relevant transformation products (TPs) are potentially neurotoxic pollutants to which humans are widely exposed. However, their penetration behavior across the brain barrier and associated exposure to the central nervous system (CNS) remain unknown. This study is the first to investigate a wide range of 30 SPAs and TPs, including emerging SPAs, in matched serum and cerebrospinal fluid (CSF) samples from children in Guangzhou, China. Sixty-two children of either sex aged<14 years with nonbloody CSF and complete clinical information were included. The findings demonstrated the ubiquitous occurrence of many SPAs and TPs, particularly BHT, 2,4-di-*tert*-butylphenol (DBP), AO 1010, AO 1076, BHT-Q, and BHT-quinol, not only in serum but also in the CSF. Median total concentrations of SPAs and TPs were up to 22.0 and 2.63 ng/mL in serum and 14.5 and 2.11 ng/mL in CSF, respectively. On calculating the penetration efficiencies across the blood−CSF barrier (BCSFB) ($R_{CSF/serum}$, $C_{CSF/serum}$) for selected SPAs and TPs, their $R_{CSF/serum}$ values (median 0.52−1.41) were highly related to their physicochemical properties, indicating that passive diffusion may be the potential mechanism of BCSFB penetration. In addition, the $R_{CSF/serum}$ values were positively correlated with the barrier permeability index R_{Alb} ($Albumin_{CSF}/Albumin_{serum}$), indicating that barrier integrity is an important determinant of BCSFB penetration. Overall, these results will improve our perception of human internal exposure to SPAs and lay a solid foundation for assessing the risk of CNS exposure to various SPAs.

1107

Occurrence of Multiple Classes of Emerging Synthetic Antioxidants, Including Aromatic Amine, Macromolecular Hindered Phenols, and Organophosphites, in Human Milk: Implications for Infant Exposure

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Abstract

Synthetic antioxidants (AOs) have received increasing attention in recent years due to their environmental ubiquity. However, lactational exposure to these emerging contaminants of current concern remains unknown. In this study, 21 amine antioxidants, 18 macromolecular hindered phenol antioxidants, 3 organophosphite antioxidants, and 2 p-phenylenediamine-derived quinones (PPD-Qs) were integrated into a dedicated screening in human milk from South China. Among all 42 target AOs, 19 were detected, but no PPD-Qs were detected in any of the samples. Eight AOs, including N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylenediamine (6PPD), were frequently detected in more than half of the samples. The summed concentrations of all detectable AOs in human milk ranged from 133 to 7,560 pg/mL, with a median of 713 pg/mL. Significant correlations were observed among the concentrations of amine and phenol antioxidants. The preliminary risk assessment revealed that under the high exposure scenario, the overall daily intake of all identified AOs through breastfeeding might pose a non-negligible health risk to newborns. This study is the first to attempt to comprehensively identify a wide range of emerging AOs prevalent in human milk. The findings call for urgent concern for infant exposure to these widely used but less well evaluated chemicals and a possible increased accumulative risk in the future.

1125

Chromium oral bioavailability in contaminated-soils from different sources: Cr speciation and mouse model

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Abstract

Soil contamination by chromium (Cr) has attracted public attention due to its ubiquity in the environment and toxicity to humans. Both chromate (CrVI) and chromite (CrIII) are present in soils, with CrVI being much more toxic and mobile than CrIII. Given the complexity in alteration of Cr species in the gastrointestinal tract, few studies have focused on its bioaccumulation and bioavailability using a mouse model. In this study, 16 soils contaminated from different industrial activities were chosen to determine their Cr accumulation in different tissues, and changes in Cr speciation at various stages after feeding 10-

days based on a steady state mouse model. The Cr accumulation in mouse organs after exposing to CrVI were 1.6-2.6 fold greater than those exposing to CrIII. Further, Cr relative bioavailability (RBA) was measured using a newly-developed mouse urinary-excretion bioassay. Results show that Cr via oral digestion was mainly accumulated in the kidneys, with Cr-RBA in soils varying from 5.1 to 50%, averaging 16%. Besides soil properties, variation in Cr-RBA also depended on its contamination sources. Soils impacted by electroplating had the lowest Cr-RBA at 5.9% while soils near electronic waste dismantling showed the highest Cr-RBA at 28%. In addition, soils near tanneries had not only high Cr-RBA at 24% but also the highest Cr accumulation in the tissues. Further, instead of the CrVI contents in contaminated soils, Cr-RBA was closely related to unreduced CrVI contents in the intestines, with 90% of CrVI being reduced before its absorption. This study helps to evaluate the health risks associated with Cr-contaminated soils by measuring Cr-RBA via a mouse model and its influences by Cr speciation in Cr-contaminated soils.

1126

Dermal Exposure to Chromium in Leather: Speciation, Bioaccessibility, Permeability, and Health Risk Assessment

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Abstract

Chromium (Cr) is a toxic and carcinogenic metal, which exists as chromate (CrVI) and chromite (CrIII) in soils, with CrVI being commonly used in leather production. With the increasing demand for leather products, the health risks associated with Cr in leather products from dermal contact require more scrutiny. Most studies have focused on total Cr contents in leather products, with few investigating the bioaccessible Cr and Cr permeability. In this study, we analyzed 105 industrial leather samples for total Cr, Cr speciation and bioaccessible Cr contents. Further, we selected 5 samples with the highest bioaccessible Cr contents to assess Cr permeability through the skin using Franz diffusion cells. Total Cr contents ranged from 32 to 45,800 mg kg-1, with CrVI contents being 0–64.3 mg kg-1 and averaging 14.3 mg kg-1. Notably, 82% of the samples exceeded the standard limit of 3 mg CrVI kg-1. The bioaccessible Cr contents varied with leather color, from 260 (black) to 3,990 (blue) mg kg-1 and were positively correlated with CrVI contents. Specifically, leather products with brighter colors (blue, red, purple, yellow, orange and green) had higher bioaccessible Cr and CrVI contents. Moreover, the 24-h permeation tests indicated a positive correlation between Cr permeability and CrVI concentration in simulated sweat solutions, allowing us to refine the human health risk assessment for Cr in leather products. The long-term dermal exposure to Cr in leather products poses both non-carcinogenic and carcinogenic risk for adults and children. This study suggests colored leather products may pose exposure via dermal contact, emphasizing the need for increased attention to potential Cr exposure from leather products.

23. Climate Change and Health

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The Impacts of Climate Change on Human Health in ASEAN

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Abstract

Climate change is an existential threat to humanity. The impacts on human health cannot be underestimated. This paper aims to provide an overall summary of human health impacts, and specifically on a few case studies from Singapore, Malaysia and Indonesia. Climate change can be categorized into: (a) Rising temperatures; (b) More extreme weather; (c) Increasing CO_2 levels; and (d) Rising sea levels. Each of this category has a severe health impact including: respiratory (asthma) and cardiovascular diseases; water-related infection (diarrheal); heat-related illnesses; mental health and well-being; food-related infection (*Salmonella*); vector-borne infection (malaria, dengue); and injuries and fatalities. Ten Southeast Asian countries collectively grouped under the Association of Southeast Asian Nations (ASEAN) predominantly lies in the humid tropics. As such, high rainfall and temperatures exacerbated by climate change have a significant impact health. Singapore, being a small island country, is extremely vulnerable to climate change impacts. Dengue fever is caused by infection with a dengue virus transmitted to humans through the bite of an infected *Aedes* mosquito. Because of increasing rainfall and temperature rise due to climate change, there is a significant increase in dengue fever cases. This increased trend is also found in other Southeast Asian countries such as Malaysia and Indonesia. Aggressive intervention measures are implemented in Singapore by using the Wolbachia-Aedes mosquito suppression strategy with some success. A research project - Project HeatSafe - is a collaborative, multi-disciplinary research project based at the National University of Singapore that focuses on the protection of people from rising temperatures due to climate change. The project seeks to understand the complex threat that heat exposure poses to human health, well-being, and work productivity in Singapore and other tropical countries; and to identify sustainable preventive policies and actions that reduce these impacts. Investigation the impact of rising heat levels on occupational workers, the study found that extreme heat exposure was linked to an increased risk of low sperm count and concentration. In addition, the higher the physical and mental exertion for a job role, the higher the productivity and economic losses due to heat stress. By 2035, the impact of heat stress on certain key sectors could mean a S$2.2 billion reduction in economic output in Singapore.

573

Climate Change, Ambient Pollution and Risk for Stillbirth

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Abstract

Stillbirth rate has been decreasing slowly since 2000, and it is a serious public health issue that has been neglected for a long time. Investigating the risk factors of stillbirth and precisely estimating relevant disease burden would greatly assist in the targeted formulation of preventive policies. We have been dedicated to efficiently utilizing global birth and infant databases, covering countries and regions where stillbirths are prevalent (e.g., South Asia, Africa), to conduct a series of epidemiological studies investigating the risks of stillbirth associated with climate change and ambient pollution. We designed a self-matched case-control method to compare gestational exposures and birth outcomes across different pregnancies of the same mother, and established the respective exposure-response function to calculate disease burden. Approximately 39.7% (0.83 million) of stillbirths could be attributable to fine particulate matter ($PM_{2.5}$) exposure during pregnancy exceeding the reference level of 10 $\mu g/m^3$. Due to climate change leading to frequent wildfire events and rising temperature, we further emphasize the health risk of these environmental exposure. Based on our studies, fire-sourced $PM_{2.5}$, as a key attributor to stillbirths, was more toxic than non-fire $PM_{2.5}$. Fire-related stillbirths were spatially clustered, leading to an inequality. For non-optimal temperature, we reported a U-shaped exposure–response function with the lowest risk of stillbirth corresponding to 12.8 ℃ based on a meta-analysis, and projected trends of temperature-related stillbirths under different scenarios of global warming. Across the 141 non-western countries, the number of temperature-related stillbirths in 2095 would increase by 19.3% (95% CI 3.5–36.4%), 29.7% (95% CI 11.6–43.8%), and 52.1% (95% CI 28.5–62.9%) under the slow (SSP 1-2.6), middle (SSP2-4.5), and fast (SSP5-8.5) global-warming scenarios, respectively. Fetuses and pregnancy women are vulnerable to inappropriate external environments. Prioritizing control these crucial exposures will help in safeguarding maternal and infant health.

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The modification effect of ozone pollution on the associations between heat wave and cardiovascular mortality

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Abstract

Epidemiological evidence concerning whether ozone modifies the impact of heat waves remain unexplored, especially in developing countries. To comprehensively evaluate the potential modification effect of ozone on heat wave impacts in warm seasons, we adopted a dataset (including mortality from overall cardiovascular diseases, chronic heart diseases and cerebrovascular diseases) in 250 Chinese cities from 2015 to 2019. A conditional quasi-Poisson regression model within the framework of the space-time-stratified case-crossover design was applied to obtain province-level associations, and a meta-analysis was adopted to pool province-level associations to national-average associations. Ozone concentration was categorized into low, medium and high levels using the 33rd and 66th percentiles of the location-specific levels as cutoffs, then we calculated the effect of heat waves in various ozone strata.

Further stratification analyses on sub-populations (age group, sex and occupation) and regions were carried out. Heat waves were found to be positively associated with mortality from overall cardiovascular diseases (RR=1.043, 95% CI: 1.027-1.059). Higher concentrations of ozone significantly enhanced the effects of heat waves on cerebrovascular mortality. The mortality risk of heat waves was 1.071 (95% CI: 1.036-1.108) and 1.069 (95% CI: 1.039- 1.100) at the medium and high levels, respectively (P for interaction=0.012 and 0.040, compared to the low level). A significant modification effect of ozone on the cerebrovascular mortality impact of heat waves was observed among people over 75, males and farmers, as well as in southern China and temperate climatic zones. Our findings suggest that ozone might potentially modify the mortality effect of heat waves.

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The Influence of Humid Heat on Morbidity of Megacity Shanghai in China

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Abstract

Background: Increased attention has been paid to humid-heat extremes as they are projected to increase in both frequency and intensity. However, it remains unclear how compound extremes of heat and humidity affects morbidity when the climate is projected to continue warming in the future, in particular for a megacity with a large population.

Methods: We chose the Wet-Bulb Globe Temperature (WBGT) index as the metric to characterize the humid-heat exposure. The historical associations between daily outpatient visits and daily mean WBGT was established using a Distributed Lag Non- linear Model (DLNM) during the warm season (June to September) from 2013 to 2015 in Shanghai, a prominent megacity of China. Future morbidity burden related to the combined effect of high temperature and humidity were projected under four greenhouse gases (GHGs) emission scenarios (SSP126, SSP245, SSP370 and SSP585).

Results: The humid-heat weather was significantly associated with a higher risk of outpatient visits in Shanghai than the high-temperature conditions. Relative to the baseline period (2010–2019), the morbidity burden due to humid-heat weather was projected to increase 4.4% (95% confidence interval (CI): 1.1%–10.1%) even under the strict emission control scenario (SSP126) by 2100. Under the high-GHGs emission scenario (SSP585), this burden was projected to be 25.4% (95% CI: 15.8%–38.4%), which is 10.1% (95% CI: 6.5%–15.8%) more than that due to high-temperature weather. Our results also indicate that humid-hot nights could cause large morbidity risks under high-GHGs emission scenarios particularly in heat-sensible diseases such as the respiratory and cardiovascular disease by the end of this century.

Conclusions: Humid heat exposures significantly increased the all-cause morbidity risk in the megacity Shanghai, especially in humid-hot nights. Our findings suggest that the combined effect of elevated temperature and humidity is projected to have more substantial impact on health compared to high temperature alone in a warming climate.

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Projections of Future Heat-related Physical Activities Losses Under Climate Change and Population Scenarios in China

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Abstract

Existing studies have found that rising temperatures have increased the risk of heat-related illnesses during outdoor physical activity. Foreign studies have revealed the relationship between the two, and issued guidelines for safe exercise in high temperature weather. However, most of the current domestic research in China focuses on military training, heat related sports performance research or physiological and biochemical changes. There is still a lack of relevant empirical research to explain the relationship between meteorological conditions and safe physical activity in the whole population, especially the prediction research for the future period is not perfect. To the best of our knowledge, physical activity intensity is highly correlated with the risk of heat stress, which is also widely accepted and applied in the study of labor productivity and military training. It is therefore necessary to classify physical activity into appropriate intensity levels in order to correctly and specifically assess heat-related risks and losses. This study mainly reveals the impact of increasing climate warming on the overall population's participation in physical activity in China. In terms of geographical scale, an analysis at the city level was conducted. In terms of time scale, this study for the first time evaluated the hours loss from outdoor physical activity caused by extreme hot weather under different future scenarios. The outdoor sports activities often carried out by Chinese people are classified into three kinds of intensity: high, medium and low.

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Study on indoor thermal perception, behavioral adaptation in late pregnancy and their effects on adverse birth outcomes in South China

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Abstract

In the context of global warming, researching and improving the thermal environment and thermal perception are particularly important for public health, especially for vulnerable groups such as pregnant women. The thermal perception and adaptation of pregnant women are unique and can affect the health of their offspring. However, little is known about their thermal perception and adaptation, and the relationship with birth outcomes. We conducted a prospective study involving 1,680 pregnant women admitted to the hospital for delivery during the summer months in South China. The demographic characteristics, indoor thermal perception (thermal sensation, comfort, preference, acceptability, and tolerance), and behavioral adaptations (i.e., regulation of behavior to achieve thermal comfort) for the month preceding the survey were collected. By following them up to delivery, birth outcomes were collected including gestational age and birth weight. We assessed the association between indoor environment and thermal perception, and identified acceptable temperature range (ATR). Structural equation model was employed to assess the association between thermal perception, behavioral adaptation, and adverse birth outcomes. A large proportion expressed discomfort with the environment (87.1%) and found it intolerable (30.1%). The upper limit of the ATR for the surveyed pregnant women was determined to be 24.4 ℃. Higher ambient temperature, relative humidity, maternal age, and prenatal BMI were found associated with an increased level of thermal perception ($\beta = 0.093$, $P < 0.01$; $\beta = 0.314$, $P < 0.001$; $\beta = 0.061$, $P < 0.05$; $\beta = 0.060$, $P < 0.05$, respectively). This, in turn, influenced the use of air conditioning ($\beta = 0.129$, $P < 0.001$), which were associated with reduced risk of small for gestational age ($\beta = -0.081$, $P < 0.05$). The results will guide individualized thermal adaptation and optimize thermal environment for pregnant women.

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Effect of Extreme Heat on Cardiovascular Morbidity

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Abstract

Background: This study investigates the impact of fine particulate matter ($PM_{2.5}$) and heat exposure on the incidence of cardiovascular disease (CVD) from the perspective of long-term environmental exposure.

Methods: Based on newly assessed individual exposure levels to extreme heat (annual ratio of extreme heat days (AREHD) and annual ratio of extreme heat hours (AREHH)) and high-resolution $PM_{2.5}$ exposure levels, we used an Cox proportional hazards model in a multi-region cohort study to investigate the associations between extreme heat, $PM_{2.5}$ exposure, and CVD risk. Multiple sensitivity and subgroup analyses were conducted. Additionally, we explored the nonlinear association between combined exposure to PM2.5 and extreme heat and the incidence of CVD.

Findings: Among 5,838,833 baseline participants without CVD, 414,218 developed CVD during follow-up. $PM_{2.5}$ exposure (HR: 1.364, 95% CI: 1.358-1.371, per IQR increase) and extreme heat (AREHD: HR:

1.011, 95% CI: 1.010-1.011, per 1% unit increase; AREHH: HR: 1.013, 95% CI: 1.012-1.014, per 1% unit increase) were associated with an increased risk of CVD. There is a clear non-linear interaction between $PM_{2.5}$ and extreme heat on the risk of CVD (*P*-Interaction<0.001). Participants exposed to the highest quartile of $PM_{2.5}$ and the second or third quartile of extreme heat exhibited the highest risk of CVD compared to those in the lowest quartile for both $PM_{2.5}$ and extreme heat exposure ($PM_{2.5}$-fourth quartile and AREHD-third quartile, HR: 2.245, 95% CI: 2.214-2.275; $PM_{2.5}$-fourth quartile and AREHH-second quartile, HR: 2.184, 95% CI: 2.158-2.211).

Interpretation: This study updates and expands the evidence on the risk of CVD associated with high temperature exposure and $PM_{2.5}$, emphasizing their nonlinear interaction and the potential for synergistic risk increase under combined exposure.

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Ambient temperature and humidity exposure associated with the risk of spontaneous abortion in early pregnancy

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Abstract

Abstract: The case-control study enrolled 1002 spontaneous abortion cases and 2004 normal pregnant controls living in Nanjing, China. We used distributed lag nonlinear models (DLNMs) with a logistic regression model to analyze the association between ambient temperature and humidity and spontaneous abortion (SA), and further identified critical exposure window and the effect of different ambient temperature. Finally, stratified analysis was conducted to explore the impact on pregnant women with different characteristics.

Objectives: The study aims to explore the association between ambient temperature and humidity and SA, based on short-term and long-term exposure, and to further identify critical exposure windows and the impact on pregnant women with different characteristics.

Methods: The study included SA cases (n = 1002) and normal pregnant controls (n = 2004) living in Nanjing, China. Based on short-term and long-term exposure, the association between ambient temperature and humidity with SA was analyzed using logistic regression model. Then, critical exposure window and the effect of different ambient temperature were observed through distributed lag nonlinear model (DLNM). Finally, stratified analysis was conducted to explore the impact on pregnant women with different characteristics.

Results: Based on short-term exposure, a significant correlation was found between ambient temperature (OR: 1.08, 95% CI: 1.06-1.10) and humidity (OR: 1.01, 95% CI: 1.00-1.02) with SA. A similar correlation was also found for long-term exposure, with effect values of 1.19 (95% CI: 1.15-1.22) and 1.20 (95% CI: 1.16-1.24), respectively. There was an exposure-lag-response relationship between ambient temperature and SA, and critical exposure window of ambient temperature was lag 15-28 days. Based on this conclusion, we found that high ambient temperature increased the risk of SA. Among pregnant women of different ages, gestational weeks, number of births, and pregnancy seasons, ambient temperature was associated with an increased risk of SA. Specifically, under short-term exposure, the impact of ambient temperature was more pronounced in older women, those with fewer gestational weeks, parous women, and those pregnant during the cold season.

Conclusion: There was a significant correlation between both short-term and long-term exposure to ambient temperature and humidity and SA.

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Emerging health risks from compound weather and climate extremes shaped by climate change

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Abstract

Climate change has not only altered the profile (e.g., frequency and intensity) of single weather and climate extremes, but also created new fashions of combinations. The concurrence, clustering and cascading of multiple extremes, termed as compound events, tend to cause larger impacts, but were seldomly taken into account in impact evaluation and risk assessment, especially in the human health sector. Through an impact-centric perspective, we defined several types of compound events, including compound hot extremes, flood-heatwave temporally/spatially compounding events, heat-ozone events and heat-drought-fire-flood-landslide hazard chain. We have quantitatively confirmed that some of these compound events are more damaging to human health than their occurrence in isolation. Based on state-of-the-art observations and climate simulations, we also project future risks of these low-likelihood high-impact climatic hazards with important implications on health. These results accentuate the necessity and urgency of accounting for compound events in assessing health impacts and risks in a warming climate.

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Introduction to the Application of High-Temperature Health Meteorological Public Service Products

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Abstract

The frequency, intensity, and duration of high-temperature events in China have significantly increased over the past few decades. This trend shows regional disparities, with Xinjiang and the middle and lower reaches of the Yangtze River emerging as the two major centers of summer heatwaves in China. The frequency of high temperatures at night has increased more rapidly than that during the day in recent decades. Existing research indicates that the disease burden from high-temperature events occurring sequentially day and night is the highest. Against the backdrop of global warming, the impact of high temperatures on human health is becoming increasingly severe, leading to greater demand for public meteorological services, especially in the construction of meteorological service systems dedicated to human health. There is also a growing demand for the development and application of high-temperature health meteorological service products. The high-temperature health and heatstroke meteorological forecast is a representative product of summer health meteorological services. The heatstroke forecast model incorporates the maximum daily temperature and relative humidity as forecast factors, reflecting the combined effects of temperature and humidity on human health. Based on the analysis of the impact of the duration of heat on human health, a heatstroke meteorological level has been established. This product has been serving the public through new media since 2009. The relevant meteorological industry standards were also published and implemented in 2023.

24. Metal Environmental Criteria and Health

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Evaluation of Effects-Based Methods and Cyanobacterial Bloom Indicators for Enhanced Water Quality Monitoring in Laguna Lake (Philippines)

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Abstract

Laguna Lake (Philippines), the third largest lake in Southeast Asia, experiences water pollution that impacts the environment, human health, and socio-economic development. More specifically, Laguna Lake receives inputs from point (industrial, domestic sewage) and non-point (urban and agriculture runoff)

sources and has been documented to have elevated levels of conventional pollutants (nutrients and heavy metals) and trace organic chemicals (pesticides, polycyclic aromatic hydrocarbons, endocrine disrupting compounds), as well as the regular occurrence of cyanobacterial blooms. Therefore, it is essential to implement robust monitoring methods and ensure effective communication of priorities. In this study, we combined effects-based methods (*in vitro bioassays*) with Microcystin-LR concentrations to characterize the Laguna Lake pollution across 15 stations and create a baseline assessment of organic chemicals loading, identify potential ecotoxicity concerns (cytotoxicity, mutagenicity, estrogenicity), and evaluate cyanobacterial blooms. We then compared these results with regularly monitored conventional parameters taken concurrently with the sampling campaign and assessed the utility of effects-based methods in evaluating overall water quality. A robust water quality index (WQI) was established to improve reporting on the environmental state and communication between researchers, policymakers, and the local communities. Our results indicate cytotoxicity (3.73 to 270.3 IC10-REF) and mutagenicity (0.315 to 0.683 µg/L 4-NQO eq), suggesting impacts of organic chemical loading into the lake. However, we did not detect estrogenicity despite previous studies indicating the presence of estrogens. We observed elevated levels of microcystin-LR (0.2 µg/L and ~134.66 µg/L), which highly correlated with cytotoxicity (r=0.84). Finally, the WQI indicated that northern West Bay has the poorest water quality, regardless of which parameters were included in the WQI calculation. The use of effects-based monitoring results as parameters for WQI calculation was explored. This analysis suggested that current conventional monitoring parameters may not accurately assess water quality, particularly during cyanoblooms. Overall, our results indicate a need for a long-term monitoring plan in Laguna Lake that considers cyanobloom presence and effects-based monitoring.

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Environmental Management of Copper Emissions from Impressed Current Anti-Fouling System in Marine Vessels

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Abstract

Copper is common antifoulant for marine applications and is gaining use in impressed current antifouling systems (ICAF). ICAF systems prevent marine growth, e.g., on cooling systems, by emitting ionic copper to seawater from the electrolysis of copper anodes. While effective at preventing marine growth, the cumulative impact of copper releases from ICAF systems to the marine environment may cause unintended environmental impacts.

This study reports the findings of an investigation into the environmental risk of copper emissions from the ICAF systems of 4 tugboats to a semi-enclosed tug pen in a tropical marine port. Copper releases was estimated at 1.7 kg Cu/day based on anode depletion and resulted in elevated dissolved seawater concentrations of up to 14 µg Cu/L in the pen during comprehensive routine monitoring.

A timeseries of sediment, biota, and dissolved seawater copper concentrations from routine monitoring were supplemented with targeted investigations into water quality parameters including total suspended solids concentrations and composition, dissolved organic carbon concentrations, and metal fractions including total and time-averaged labile copper concentrations measured by the diffusive gradients in thin-films (DGT) technique.

The availability of a comprehensive monitoring dataset allowed for a detailed understanding of copper exposure which was used to inform risk. The environmental risk of copper was found to be low due to its chemical speciation, the lack of accumulation in sediments, and the rapid dispersion outside of the tug pen. Measurements revealed that 36% of copper was DGT-labile and 6% particulate bound which corroborated thermodynamic modelling suggested that 77 ± 11% of copper would be bound to dissolved organic matter.

This study highlights an emerging and understudied source of copper emissions to harbours and allowed for an interesting comparison of measurement criteria and protection goals in the context of the Australian and New Zealand Water Quality Guidelines. This is timely given the proposed new default copper water quality guideline values that include a tiered approach and a dissolved organic matter correction.

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Endocrine disruption and persistency in the United Nations Globally Harmonized System: implications for metals

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Abstract

Clear and consistent information on the hazards of chemicals is critical to ensure their safe use. More than 75 countries worldwide have implemented the United Nations Globally Harmonized System (UN GHS) for the classification and labelling of chemicals. Recently, the European Union has proposed to add new concepts in the UN GHS, including endocrine disruption and persistency. However, applying these new concepts to metals requires specific guidance and expertise. This creates scientific challenges for authorities and industry.

This presentation will discuss the science needed to apply new UN GHS concepts to metals. Metals and metal compounds are different from other chemicals. They are not bioavailable in the environment, but they may become bioavailable after transformation and dissolution (OECD, 2002). This produces dissolved metal ions which may cause environmental effects. The dissolved metal ions may also, over time, be complexed and removed from aquatic systems through further environmental transformation processes. Due to these specific processes, the persistency measures used for organic substances do not apply to metals (Adams et al., 2022). The UN GHS (Annex 9.7) already considers these processes for

metals. The persistency of metals should therefore not be used as a basis for hazard classification in the UN GHS.

Metals and the endocrine system interact in complex ways (Brix et al., 2023). Some metals are essential to physiological systems, including the endocrine system, and nonessential metals can have similar physiochemical attributes. Consequently, metals may cause indirect effects on the endocrine system via multiple interlinked pathways. Metals may also elicit physiologically appropriate compensatory endocrine-mediated responses, which is termed endocrine modulation. These processes should not be confused with endocrine disruption. A framework has been developed, with examples, to allow assessors to differentiate between the different types of interactions of metals and the endocrine system (Brix et al., 2023).

References

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Chemical Speciation in Environmental Criteria and Health

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Abstract

Chemical speciation is critical to the toxicity and health risk of environmental contaminants. Among the more than 200 chemical species of arsenic, the inorganic arsenic species present in drinking water is highly toxic, whereas arsenobetaine commonly detected in seafood is not a health concern. However, current environmental criteria and standards have primarily based on the total concentrations of metals and metalloids. With only a few exceptions, most criteria and standards have ignored speciation information. This presentation will discuss current challenges, knowledge gaps, and research needs for integrating chemical speciation information into considerations of environmental criteria and standards. Using arsenic speciation as an example, this presentation will highlight recent advances in analytical

technology for chemical speciation analysis, address issues in understanding metabolism and biotransformation, and provide perspectives on the need for collaboration among laboratory and regulatory scientists of multiple disciplines.

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Seawater Quality Criteria and Ecotoxicity Risk Assessment of Zinc Oxide Nanoparticles Based on Data of Resident Marine Organisms in China

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Abstract

Water quality criteria (WQC) for zinc oxide nanoparticles (ZnO NPs) are crucial due to their extensive industrial use and potential threats to marine organisms. This study conducted toxicity tests using marine organisms in China, revealing LC_{50} or EC_{50} values for ZnO NPs ranging from 0.36 to 95.6 mg/L across seven species, among which the salinity lake crustacean zooplankton *Artemia salina* exhibited the highest resistance, while diatom *Phaeodactylum tricornutum* the most sensitive. Additionally, the EC_{10} or maximum acceptable toxicant concentration (MATC) values for ZnO NPs were determined for five species, ranging from 0.03 to 2.82 mg/L; medaka *Oryzias melastigma* demonstrated the highest tolerance, while mysis shrimp *Neomysis awatschensis* the most sensitive. Based on the species sensitivity distribution (SSD) method, the derived short-term and long-term WQC for ZnO NPs were 138 μg/L and 8.37 μg/L, respectively. These values were further validated using the sensitive species green algae *Chlorella vulgaris*, confirming effective protection. There is no environmental risk observed in Jiaozhou Bay, Yellow River Estuary and Laizhou Bay in the northern coastal seas of China. This study provides important reference data for the establishment of water quality standards for nanoparticles.

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Seawater Quality Criteria and Ecotoxicity Risk Assessment of Zinc Oxide Nanoparticles Based on Data of Resident Marine Organisms in China

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Abstract

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The toxicity and organic carbon effect of nickel on zebrafish in aquatic environment

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Abstract

Heavy metal pollution continues pose a threat to to the global environment and human health. Nickel (Ni), one of Earth's most abundant elements, is found in various environmental media such as soil and water, as well as in organisms. Studies have shown that Ni, which persists in aquatic environments for a long time, can exhibit higher toxic effects after undergoing complex processes of migration, transformation, and biological interactions. However, most of these studies only focus on a single life stage, and there is a lack of research on different life stages Additionally, our previous research found that organic carbon (OC) in water can affect the toxicity of metals to various aquatic organisms. Therefore, to better clarify the toxicity of Ni in water environment, it is essential to further investigate the impact of OC on Ni, including an in-depth exploration of Ni transformation patterns and environmental behavior, and ecotoxicity. This study focus on the toxic effects of Ni on zebrafish at different life stages and the toxic changes of Ni under the regulation of TOC reveal the toxic mechanisms of Ni on aquatic organisms.Firstly, we conducted acute toxicity tests on zebrafish at different life stages exposed to various concentrations of Ni.

The LC_{50} values for zebrafish embryos, juveniles, and adults, noting that juveniles are more sensitive to Ni. This increased sensitivity is potentially due to the generation of free radicals and resultant oxidative damage when Ni enters the body. In addition, we performed exposure experiments of total organic carbon (TOC) affecting toxicity of Ni on zebrafish at different life stages.The result showed that.TOC could alleviate the toxicity of Ni to zebrafish embryos and juveniles. Moreover, after analysising the correlation between dissolved organic carbon (DOC) or TOC and the toxicity of Ni to different fish in USEPA ECOTOX database, it found the toxic effects of nickel on zebrafish at different life stages and the toxic changes of nickel under the regulation of TOC generally. These findings provid the foundation for assessing the ecological risk of Ni to aquatic organisms at different life stages.

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Detection of Estrogenic Activities in Laguna Lake and its Tributaries

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Abstract

Laguna Lake, the third largest natural lake in Southeast Asia and the largest lake in the Philippines, supplies a large portion of local water and fish in the Greater Manila Area. However, the lake has experienced a decline in water quality due to household, agricultural, and industrial runoffs that flow from tributaries into the lake. Because of previous studies highlighting the presence of endocrine disrupting chemical (EDC) pollutants, such as bisphenol A (BPA) and per- and polyfluoroalkyl substances (PFAS), we investigated whether the lake and its tributaries are experiencing an accumulation of estrogenic contaminants. Surface water samples of Laguna Lake and its tributaries were collected last March 2020. While all sampling stations exhibited low estrogenic activities using an estrogen receptor-driven luciferase reporter assay (T47D KBLuc cell line), the level of estrogenic activities were significantly higher in tributaries compared to the Laguna Lake itself. The tributaries terminating in the East Bay have the highest estrogenic activities compared to other parts of the lake, followed by those from Northwest and Central Bay. Overall, this study provided evidence of continued estrogenic contamination coming from tributaries, posing an increased threat to local water and fish supply of Laguna Lake if left unchecked.

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Models for Predicting Toxicities and Water Quality Criteria of Microplastics to Protect Aquatic Organisms

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Abstract

Managing plastic waste and addressing the ecological and environmental risks of micro- and nanoplastics (MNPs) are challenging global health issues. The hazards of MNPs are determined by structural composition, environmental medium, and targeted aquatic taxa. However, the heterogeneity of the toxicity data results in a ~100,000-fold difference in the water quality criteria (WQC) for MNPs. In this study, three machine learning algorithms (*i.e.*, random forest (RF), k-nearest neighbour (kNN), and support vector machine (SVM)) were used separately to construct a model for predicting the ecotoxic effects and deriving WQC, in freshwater or saltwater, for five representative MNP polymer types. The RF model produced the best performance in prediction. From a feature importance analysis, particle size and density were the main influencing factors (~72%) for deriving protective WQC. Based on the reported environmental hazards, under the same environmental conditions, the five types of high-density polymers were ranked in increasing order for adverse effects potential: polyethylene < polypropylene < polyvinyl chloride < polyethylene terephthalate < polystyrene. The WQC for protecting aquatic organisms from MNPs-induced adverse effects was lower in saltwater than in freshwater. Under different site-specific environmental scenarios, high-density fibrous polystyrene (100–1,000 nm) in saltwater posed the greatest risk. This study provides a scientific model for preventing and controlling aquatic ecological risks of MNPs.

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Influence of Water Quality Variations in the Yangtze River Basin on the bioavailability of nickel and water quality criteria

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Abstract

The Yangtze River Basin is a crucial water system in China, characterized by significant geographic diversity that results in notable discrepancies in water quality factors across different regions. Nickel industries are strategically located along the Yangtze River Basin, and the detection rate of nickel in this region is relatively high. However, the current water environmental quality standards for nickel management only provide a single safety limit, without specifying corresponding standards based on different water quality conditions. Therefore, scientifically evaluating the impact of nickel on aquatic ecological health, considering bioavailability, is crucial for the economic development and refined environmental management of upstream and downstream enterprises involved with nickel.

This study aims to investigate the bioavailability responses of nickel to three native aquatic species : the cladoceran *Simocephalus vetulus*, the coelenterate *Hydra vulgaris*, and the alga *Navicula pelliculosa*. in China, based on actual water samples collected from different points in the upper, middle, and lower reaches of the Yangtze River Basin. Assessment outcomes for each species revealed substantial disparities in toxicity

thresholds. The research highlights the significant impact of water chemistry constituents, including hardness, pH, and DOC, on the nickel toxicity to native Chinese aquatic organisms. This is underscored by the varying response of bioavailability to these factors. The findings emphasize the necessity of considering bioavailability when establishing nickel water quality criteria. Nickel water quality criteria and standard should be tailored to diverse regional water environmental conditions, thereby enhancing the scientific rigor and precision of water environmental quality management.

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Iron minerals: A frontline barrier against combined toxicity of microplastic and arsenic

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Abstract

Microplastics (MPs) are emerging containments and inevitably interact with heavy metals. The coexistence of MPs and arsenic (As) in terrestrial ecosystems presents challenges to agriculture safety and human health risk. In this study, we assessed the mitigation effect of goethite, a prevalent iron mineral in soil, on the combined toxicity of MPs and As. We investigated the mitigation effect according to the migration pattern of MPs and As in terrestrial environment, that is, from the soil medium to the soil-plant interface and then to the plant body. We found that the presence of goethite could reduced the combined toxicity of MPs and As, the half-lethal concentration (LC50) of MPs and As to wheat seeds, a model crop plant, was increased from 6.56 mg/kg to 9.15 mg/kg. This was primarily attributed to the adsorption and immobilization of MPs and As on the soil medium and soil-plant interface. In our study, goethite reduced soluble As by 48.29% under the combined pollution scenarios and formed iron plaques on wheat roots, effectively obstructing the transfer of MPs and As into plants. Furthermore, in the presence of goethite, the accumulation of As and MPs in wheat seedlings was significantly reduced, and the enzymatic and non-enzymatic antioxidants in wheat seedlings was relatively upregulated. Thus, iron minerals can serve as pioneering barriers to combined toxicity of MPs and

As. Our findings contribute to the understanding of the combined toxicity and toxicity mitigation of MPs and As in crops and offer potential strategies for reducing their human health risk.

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Associations of Exposure to Fine Particulate Matter Mass and Constituents with Systemic Inflammation: A Cross-Sectional Study of Urban Older Adults in China

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Abstract

Systemic inflammation is a key mechanism in the development of cardiovascular diseases induced by exposure to fine particles (particles with aerodynamic diameter ≤2.5 μm [PM2.5]). However, little is known about the effects of chemical constituents of PM2.5 on systemic inflammation. In this cross-sectional study, filter samples of personal exposure to PM2.5 were collected from community-dwelling older adults in Tianjin, China, and the chemical constituents of PM2.5 were analyzed. Blood samples were collected immediately after the PM2.5 sample collection. Seventeen cytokines were measured as targets. A linear regression model was applied to estimate the relative effects of PM2.5 and its chemical constituents on the measured cytokines. A positive matrix factorization model was employed to distinguish the sources of PM2.5. The calculated source contributions were used to estimate their effects on cytokines. After adjusting for other covariates, higher PM2.5-bound copper was significantly associated with increased levels of interleukin (IL)1β, IL6, IL10, and IL17 levels. Source analysis showed that an increase in PM2.5 concentration that originated from tire/brake wear and cooking emissions was significantly associated with enhanced levels of IL1β, IL6, tumor necrosis factor alpha (TNFα), and IL17. In summary, personal exposure to some PM2.5 constituents and specific sources could increase systemic inflammation in older adults. These findings may explain the cardiopulmonary effects of specific particulate chemical constituents of urban air pollution.

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Environmental risk assessment of tailings ponds in China

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Abstract

In view of the complexity of the environmental risks of tailings ponds and their characteristics of climate change and prominent risks and hidden problems in recent years, it is very important to establish an index system that can reflect both the environmental risks of tailings ponds and natural disasters, so as to better assess the environmental risks of tailings ponds. Existing studies mainly consider the environmental risk of single tailings pond, lack domain scale analysis, and rarely consider the influence of tailings pond control mechanism, environmental vulnerability and natural disasters. Based on the hierarchical analysis-entropy weight method, this paper constructs a comprehensive assessment model of the environmental risk of the tailings pond, and makes a comprehensive assessment of the environmental risk of the tailings pond in China. The results show that high-risk tailings ponds account for about 9.24% of the total, mainly distributed in southern China and the Qinling Mountains. Low-risk tailings ponds account for about 10.12% of the total, mainly distributed in Inner Mongolia and Hebei. The rainstorm has a great impact on the environmental risk escalation of the tailings pond, increasing the high-risk area by 41.67%. Under the influence of the earthquake, the environmental risk distribution of tailings ponds is high in the south and low in the north. The high-risk tailings ponds account for about 2.12% of the total, mainly distributed in Yunnan and Gansu provinces.Under the influence of the earthquake, the environmental risk distribution of tailings ponds is high in the west and low in the east. The high-risk tailings ponds account for about 5.06% of the total, mainly distributed in Yunnan and Gansu provinces.

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Comparative Analysis of Dissolved Oxygen Predictions in the Yellow River Basin Using Different Environmental Predictors Based on Machine Learning

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Abstract

Dissolved oxygen (DO) serves as a crucial water quality indicator reflecting river health. Machine learning (ML) models have gained popularity for water quality prediction; however, their accuracy heavily depends on predictor variables. Predictor availability varies considerably, prompting the inquiry of whether easily accessible catchment attributes, when combined with ML—specifically a random forest (RF) model—can effectively predict river DO dynamics in the Yellow River Basin (YRB). Is there a necessity to collect additional water quality data to improve model performance? To address this, we collected ~11,500 monthly DO data from 135 monitoring sites in the YRB from 2016-2022 and categorized predictor variables into three groups: catchment attributes and meteorology (CAM), water quality parameters (WQPs), and a combination of both (CAM + WQP). The RF models achieved satisfactory performance, with Nash–Sutcliffe efficiency exceeding 0.35 at 68.38%, 61.03%, and 72.06% of sites for CAM, WQP, and CAM + WQP, respectively. CAM alone outperformed WQP alone, with marginal improvement upon including WQP. Nevertheless, all models encountered difficulties with sites

showing substantial DO fluctuations, indicating inherent model limitations in reproducing extreme values. Conversely, in heavily human-impacted regions like the Fen River Basin, the addition of WQP notably improved DO prediction accuracy, attributed to the partial reflection of anthropogenic activities through WQP. Despite this, both WQP and CAM + WQP models exhibited diminished performance in highly urbanized areas, implying that WQP inadequately captures human impacts. Further analysis revealed several factors impeding DO predictions, including unbalanced data in high-altitude watersheds, insufficient anthropogenic emission data, and a lack of water transfer information. Additionally, through feature importance and partial dependence analysis, key factors affecting DO were identified, including water and soil temperature, precipitation, and pH. Our findings underscore the need for additional DO sampling sites in the plateau region of the YRB. Moreover, recognizing the limited enhancement offered by WQP and its spatial extrapolation constraints, acquiring additional data on anthropogenic activity may prove more beneficial in enhancing DO prediction than solely monitoring WQPs.

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Interaction of Polycyclic aromatic hydrocarbons with Microplastics: Adsorption and Desorption

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Abstract

Plastic particles are widely distributed in the aquatic environment and can interact with other pollutants, becoming the carrier of pollutants, then increasing the probability of pollutants entering the human digestive tract and risk to human health. In this study, the adsorption of 15 polycyclic aromatic hydrocarbons (PAHs) on polyethylene (PE) and polymethyl methacrylate (PMMA) and the desorption behavior in the simulated digestive system were systematically studied. The adsorption experiments results indicated that the crystal structure, morphology and surface functional groups of microplastics greatly affected the adsorption capacity of PAHs on the surfaces of MPs. The adsorption efficiency of PAHs on the surfaces of PE was 1.4 - 3.8 times higher than that of PMMA. For different kinds of PAHs, the adsorption capacity increased with the increase of molecular weight of PAHs. Desorption experiments conducted in simulated gastrointestinal fluid, the results demonstrated that the type of MPs, gastrointestinal environment, and physicochemical properties of PAHs could significantly affect the desorption of PAHs from MPs. The desorption efficiency of PAHs from the surfaces of PMMA was significantly higher than that of PE, and the desorption rate was much faster. Compared with enzyme-free digestive fluid, the enzyme significantly promoted the desorption of PAHs from the surfaces of MPs. The desorption efficiency of 15 PAHs from the surfaces of PE decreased gradually with the number of PAHs rings, while it was opposite to PMMA, which attributed to the hydrophobicity of PAHs and surface polarity of MPs. Risk assessment were evaluated by comparing the daily intake with

the carcinogenic level indicated by acceptable daily intake the results indicated that PAHs pose a high risk to human health after desorption from MPs in digestive fluid.

To our knowledge, this is the first attempt at the adsorption of 15 PAHs on MPs and the desorption behavior in a simulated human digestive system, the results helpful to evaluate the human carcinogenic risk of PAHs that enter human digestive tract with MPs. In addition, this paper has been published in the Chemical Engineering Journal.

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Traditional and Emerging Organophosphate Esters in the Yangtze River Basin: Multimedia Distribution, Driving Factors, Potential Sources, and Risk Assessment

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Abstract

As alternatives to brominated flame retardants, organophosphate esters (OPEs) are widely used in industrial production and daily life. In addition to traditional OPEs (tOPEs) such as tris(2-chloroethyl) phosphate (TCEP) and triphenyl phosphate (TPHP), more and more emerging OPEs (eOPEs), such as bisphenol A bis(diphenyl phosphate) (BDP) and resorcinol bis(diphenyl phosphate) (RDP), are frequently detected in environmental and human samples. However, whether the ecological and health risks of eOPEs are higher than those of tOPEs still deserves further investigation. Therefore, in this work, surface water, sediment, and suspended particulate matter (SPM) samples near important aquatic habitats and drinking water sources in Yibin (YB), Yichang (YC), Shanghai (SH), and Poyang Lake (PY) of the Yangtze River Basin were collected. Moreover, 12 tOPEs and 7 eOPEs in these media were analyzed using high-performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS) to elucidate the contamination characteristics and potential risks. The total concentrations in surface water, sediment, and SPM in the four regions were 22.86—1397.53 ng/L, 2.39—75.96 ng/g dw, and 2.73—1588.21 ng/g dw, respectively. According to the redundancy analysis, temperature, dissolved oxygen (DO), and pH played an important role in driving the presence and distribution of OPEs in surface water. Source identification revealed that wastewater treatment plant discharges and traffic discharges were the main sources of OPEs in PY. OPEs mixtures caused low risk and above at most points in the four regions, with the total risk quotient (RQ_T) ranked by substituent: Aryl-OPEs>Cl-OPEs>Alkyl-OPEs, among which TPHP had the highest risk. Notably, although the concentrations of eOPEs were much lower than those of tOPEs, they

posed medium to high ecological risks to aquatic organisms at some sites, which were mainly caused by BDP and RDP. Based on Monte Carlo simulation analysis, it was found that the non-carcinogenic and carcinogenic risks of OPEs to human health are negligible, but the health risks to children are higher than those to adults. In addition, sensitivity analysis showed that the main factors leading to the non-carcinogenic and carcinogenic health risks were tris(1-chloro-2-propyl) phosphate (TCIPP) and TCEP, respectively. This study can provide a scientific basis for the regulation and control of environmental risks of tOPEs and eOPEs.

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Studies on Water Quality Criteria for Bioaccumulative substances

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Abstract

Over the past few decades, studies have been carried out on water quality criteria (WQC) for pollutants such as heavy metals and organic pollutants in China, and WQC for these pollutants have been obtained. However, such water-based criteria that do not consider bioavailability and bioaccumulation especially for bioaccumulative substances may lead to under-protection of aquatic organisms accordingly. Bioaccumulative and persistent contaminants can bioaccumulate through the food chain, thus causing serious harm to wildlife at higher trophic levels. Research has shown that tissue concentrations directly reflect the bioavailability of biocumulative chemicals. Herein, a tissue-based method was adopted to derive the WQC for bioaccumulative substances selenium (Se) and dieldrin. Water and fish samples were collected from Taihu Lake and Yellow River estuary to investigate Se distribution characteristics and bioaccumulation factors (BAFs) in aquatic ecosystems. Tissue-based toxicity data were collected to generate species sensitivity distribution (SSD) to determine criteria formulated as tissue concentrations that are protective of targeted species. WQCs were derived from tissue-based criteria by using BAFs. Quotient and probabilistic methods were used to assess the ecological risk. The results revealed that the average levels of Se in the water samples were 1.54 and 1.07 μg/L and that the average Se levels in the fish samples were 0.87 and 0.66 mg/kg in Taihu Lake and the Yellow River estuary, respectively. Furthermore, the calculated BAF for Se in fish was 618.69 L/kg, and the calculated WQC for Se to protect aquatic organisms was 0.29 μg/L. The high levels of ecological risk associated with Se in Taihu Lake and the Yellow River estuary indicate that the aquatic risk of Se warrants further attention. For dieldrin, the tissue-based criteria and the WQCs were calculated for protection of aquatic life and wildlife (e.g. mammalians, avians). Incorporating more exposure data, tissue-based criteria may give a new insight into environmental risk identification. Studies on WQC for biocumulative substances can provide scientific guidance for setting water quality standards to enhance protection of aquatic life, ensuring environmental management in China.

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National Reconnaissance of Antimicrobial Occurrence in Australian Wastewater and their Socioeconomic Correlates

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Abstract

The improper and excessive use of antimicrobial agents exacerbates the development and dissemination of antimicrobial resistance (AMR), which has become a global environmental challenge. A critical approach to combating AMR involves monitoring antimicrobial usage. However, despite Australia's already elevated and rising per capita antimicrobial use, research focusing on its surveillance remains scarce. The present study investigated the occurrence and use of 102 common antimicrobials and their transformation products (TPs) in wastewater influent samples collected from 50 wastewater treatment plants (WWTPs) across Australia on Census Day 2021, encompassing ~50% of the national population. This wastewater data was subsequently cross-referenced with catchment-matched Census data to identify population-level socioeconomic factors correlated with antimicrobial use. The results indicated that 41 antimicrobials and 15 TPs were detected in Australian wastewater influent, spanning various antimicrobial groups such as β-lactams, quinolones, sulfonamides, macrolides, tetracyclines, azoles, lincosamides, and aminoglycosides. Notably, 30 analytes were detected at a frequency >50%. Amoxicilloic acid and cephalexin occurred at the highest concentrations and population-normalized mass loads. Correlation analysis revealed a significant association between the consumption of certain antimicrobials, especially quinolone antibiotics, and various aspects of the population's socioeconomic status, including income, education, occupation, housing, race, health condition, and transport. For example, antimicrobial use correlated positively with higher income, education level, and occupational status, as well as crowded living conditions and frequent use of public transportation. Conversely, it negatively correlated with people having long-term health conditions. Our study offers a comprehensive insight into the patterns of antimicrobial use at the population level in Australia and highlights potential socioeconomic drivers of their use.

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Advancing Exposome Research: High-Throughput Chemical Isotope Labeling LC-MS for Comprehensive Metabolome and Exposome Analysis

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Abstract

LC-MS is widely used for chemical detection and identification. There are some limitations in conventional label-free LC-MS techniques, including limited detection sensitivity for some compounds and difficulty in performing accurate quantification without isotope standards. This presentation highlights recent advancements in chemical isotope labeling (CIL) LC-MS techniques tailored for exposome research, emphasizing their application in high-throughput analysis and precise quantification, particularly in human serum/plasma samples. After a brief introduction to the CIL LC-MS methodology, new developments in sample preparation, separation, MS and MS/MS analysis, data processing, and database creation for compound identification will be discussed. Case studies will illustrate the utility of CIL LC-MS in elucidating exposome profiles, assessing exposure-response relationships, and identifying novel biomarkers of environmental exposure.

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Identification of exhaled VOCs biomarkers for human sub-health status using a de-confounding factors coupled with machine learning method

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Abstract

Exhaled volatile organic compounds (VOCs) biomarkers had potential application in identifying disease or health status using machine learning methods. However, confounding factors such as gender, age, smoke and body mass index would lead to some spurious exhaled VOCs biomarkers associated with disease or health status. In this study, exhaled VOCs from above 1000 cohorts were measured using a proton transfer reaction time-of-flight mass spectrometry (PTR-TOF-MS). Random forest (RF) coupled with the SHapley Additive exPlanations (SHAP) machine learning

was used to identify and predict exhaled VOCs biomarkers for three sub-health indicators including transglutaminase (TG), low-density lipoprotein (LDL) and total bilirubin (TB). To further eliminate the interference of confounding factors on exhaled VOCs biomarkers, a propensity score matching was used to match the cohorts based on a Mahalanobis distance. The area under the receiver operating characteristic (AUROC) scores of the RF in three sub-health indicators were below 0.6 for the unmatching cohorts, which was significantly lower than 0.9 for the matching cohorts. The SHAP analysis revealed that $C_3H_2N_2S$, $C_9H_{14}O_6$, $C_{16}H_{22}N_2O_6$ and $C_{20}H_{23}N_3O_2$ had positively correlate with TG, indicating that four exhaled VOCs biomarkers increased with increasing in content of TG. The C_3H_4, C_2H_3N and C_2H_4O showed opposite tendencies. Furthermore, C_4H_4OS, $C_6H_4O_5$, $C_7H_{10}O_3$, $C_9H_{14}O_6$ and $C_{19}H_{38}$ exhibited the positive contributions to LDL and TB, whereas C_2H_4O was negative correlation with LDL and TB. This study highlighted that de-confounding factors using machine learning method can increase prediction accuracy of exhaled VOCs biomarkers for human sub-health status.

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Long-term (2012-2021) Trends in Exposures to Bisphenols, Parabens, Triclosan and Triclocarban in General Population of Queensland, Australia

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Abstract

Human beings are consistently exposed to a wide array of hazardous chemicals through the everyday use of consumer products. It is crucial to assess the exposure to these chemicals, as well as trends in such exposure, at the population level. This provides essential evidence for chemical management and risk mitigation. The objective of this study is to investigate temporal trends (from 2012 to 2021) in human exposures to bisphenols, parabens, triclosan, and triclocarban in the general population of Queensland, Australia.

De-identified urine samples were collected in 2012/2013, 2014/2015, 2017/2018, 2018/2019, and 2020/2021 in collaboration with a community-based pathology laboratory. Individual samples were grouped by age strata: 0–5, 5–15, 15–30, 30–45, 45–60, and >60 years, as well as by sex (male and female). One milliliter of pooled urine was thawed and extracted using a solid-phase extraction method after being spiked with internal standards and β-glucuronidase. Sample analysis was performed using a Shimadzu UHPLC system coupled with a Sciex 6500+ QTRAP mass spectrometer. Synthetic urine served as blank samples, and analytical precision and accuracy were assessed using native-fortified synthetic urine.

When combining data from all age and sex groups for each year/round, the concentrations of bisphenol A (BPA), triclosan (TCS), triclocarban (TCC), butylparaben (BuP), and isobutylparaben (iBuP) decreased significantly over the last decade, while the concentration of BPS increased significantly during the same period. The concentrations of MeP, EtP, and PrP remained relatively consistent. For the antimicrobial TCS, concentrations increased with age and peaked in the young and middle-aged adult groups before decreasing in the older age group. This pattern may reflect prevalent exposure to TCS through topical application of personal care products, which is generally more common in young and middle-aged populations. Similar associations have been reported in studies on Korean and Flemish populations. As for parabens, the highest concentrations were often detected in the youngest age groups (0-5 and 5-15y), potentially associated with the use of baby/toddler products such as nappies and sunscreens. When compared to data from other countries, it appears that exposure to bisphenols, parabens, and triclosan in the Australian population is at the higher end. Further research is needed to assess the sources of exposure and their changes over time.

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Exposure Characteristics and Health Risks of Toxic Organic Pollutants in the Urine of Coking Plant Workers: Insights from Non-Target and Target Analyses

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Abstract

Coking contamination in China presents intricate challenges and significant health risks to humans. In this study, we investigated the exposure of coking plant workers to toxic pollutants through non-target and target analyses. Through non-target screening, 32 differential compounds were identified. In addition to common polycyclic aromatic hydrocarbon (PAH) metabolites, several novel compounds were discovered, including quinolin-2-ol, naphthylmethanols, N-hydroxy-1-aminonaphthalene, hydroxydibenzofuran, hydroxyanthraquinone, and hydroxybiphenyl. Target analysis focused on 25 coking-produced aromatic compounds, including those identified through our non-target screening, noted for their high toxicity or frequent presence in coking plants. Hydroxy-PAHs and hydroxy hetero-PAHs were the dominant compounds in exposed workers, with levels significantly higher than those in nearby residents and the control group. Workers from coking, coal preparation, and chemical production processes showed higher concentrations of these compounds. Co-exposure to aromatic compound mixture showed positive effects on DNA damage and lipid peroxidation in workers, with 5-hydroxyisoquinoline and 3-hydroxycarbazole playing significant roles. Moreover, Monte Carlo simulation revealed that coking contamination elevated the carcinogenic risk for exposed workers by 5-fold compared to controls with pyrene, pentachlorophenol, and carbazole contributing the most. Workers in the coking process were identified as being at the highest

risk. This study underscores the imperative to increased attention to the health implications of occupational exposure in coking sites and provides valuable insights for coking contamination control.

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Chronic Kidney Disease of Unknown Etiology (CKDu) in Sri Lanka - The Urgent Need for Multidisciplinary Research

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Abstract

Chronic Kidney Disease of unknown etiology (CKDu) (similar kidney disease epidemics observed in Andra Pradesh (India) and Central America) has emerged as a significant public health challenge in Sri Lanka, predominantly affecting rural agricultural communities. The disease predominantly affects male farmers, often between the ages of 30 and 60, who have no history of diabetes, hypertension, or other known causes of CKD. Research suggests that exposure to agrochemicals, heavy metals (such as cadmium and arsenic), and high levels of fluoride in drinking water may contribute to CKDu. Poor water quality and consumption of hard water have been implicated as potential risk factors. There is ongoing research into genetic predispositions that may make certain populations more vulnerable to CKDu. The role of occupational hazards, including exposure to high temperatures and dehydration, is being studied. None of the hypotheses put forward so far could explain coherently the totality of clinical, biochemical, histopathological findings, and the unique geographical distribution of the disease and its appearance in the mid-1990s.

A multidisciplinary research approach is essential to address the complex and multifaceted nature of CKD in Sri Lanka. Current evidence suggests a convergence of environmental, occupational, genetic, and socio-economic factors contributing to the disease's prevalence. A comprehensive research strategy that integrates epidemiology, environmental science, clinical medicine, toxicology, genetics, sociology, occupational health, economics, policy, and technology is essential for developing effective interventions and sustainable management practices. This paper outlines key areas of focus for multidisciplinary research and emphasizes the importance of collaborative efforts in mitigating the impact of CKDu on affected populations. International collaboration and technological innovation will also play a crucial role in advancing research and implementing effective solutions. By fostering an interdisciplinary framework, we aim to enhance understanding, improve early detection, and implement robust preventive and therapeutic measures to combat CKDu in Sri Lanka.

Keywords: Chronic Kidney Disease of unknown etiology (CKDu); multidisciplinary research; agrochemicals; heavy metals.

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Long term temporal trends of selected persistent organic pollutants in ambient air in Australia, China and Vietnam

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Abstract

Ambient air samples were collected in Brisbane (Australia), Dalian (China), and Hanoi (Vietnam) from March 2013 to February 2018 using polyurethane foam-based passive air samplers for the analysis of polychlorinated biphenyls (PCBs), organochlorinated pesticides (OCPs), polycyclic aromatic hydrocarbons (PAHs) and Chlorinated paraffins (CPs). The mean concentration of $\sum_8$PCBs in Vietnam (158 pg/m³) was significantly higher than in Australia (55 pg/m³) and China (50 pg/m³). PCB-11, PCB-28, and PCB-52 showed increasing annual average trends in Australia, potentially due to continued historical or secondary emissions. $\sum_{15}$OCP levels ranged from 80–1200 pg/m³ in Australia, 100–3200 pg/m³ in China, and 3400–20000 pg/m³ in Vietnam, mainly due to hexachlorobenzene (HCB) and chlorpyrifos. In Australia, annual average concentrations of heptachlor, heptachlor epoxide, and dichloro-diphenyl-trichloroethane (DDT) declined, indicating reduced primary emissions. Atmospheric polycyclic aromatic hydrocarbon (PAH) levels were generally higher during autumn and winter in all countries. Compared to Vietnam (43000 pg/m³) and China (37500 pg/m³), Australia had lower PAH levels (2600–6000 pg/m³). However, increasing trends of phenanthrene, anthracene, and benzo[a]anthracene in Australia highlight the need for continued long-term monitoring of these chemicals. Median atmospheric concentrations of ∑CPs were 0.079 ng m^{-3} in Australia, 1.0 ng m^{-3} in China, and 0.89 ng m^{-3} in Vietnam. Australia's CP levels were consistently low, with no significant differences between the city center and background sites, indicating limited CP usage and production. The highest MCCP concentration was in China, while the highest SCCP concentration was in Vietnam. From 2016 to 2018, SCCP concentrations decreased and MCCP concentrations increased in Brisbane, whereas both SCCPs and MCCPs showed increasing trends in Dalian, suggesting different CP sources in these cities.

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An Enhanced Protocol to Expand Female Exposome and Machine Learning based Prediction for Methodology Application

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Abstract

BACKGROUND: Exposomics on females are quite limited due to the challenging analytical strategies to reveal low-level endocrine disrupting chemicals (EDCs) and their metabolites from heavy matrices of serum and urine samples. This largely overshades the integrity of chemical exposure and thus compromises the understanding of their compound effects on reproductive health.

OBJECTIVES: We developed an enhance protocol, consisting of multi-solid-phase-extraction (multi-SPE) strategy and high-resolution mass spectrometry (HRMS) analysis, to expand female exposome with polar EDCs and their metabolites. We combined extensive EDCs and their molecular descriptors (MDs) to train a machine learning (ML) model for methodology prediction.

METHODS: We developed and validated the multi-SPE protocol with 295 EDCs covering 15 subclasses. The protocol was applied to the serum and urine of 20 women of childbearing age from a cohort of 498 by controlling occupational factors and daily behaviors for high chemical exposure potential. We conducted target screening for 295 EDCs and nontarget identification of unknown chemicals. We created a ML model to predict the applicability of our protocol by considering the MDs of target (n=295) and non-target identified (n=217) chemicals. The key features were identified using the Shapley by quantifying the contribution of each input MD to meta-database (n= 338,233) methodology prediction, and the toxicity potential of the expanded chemical by multi-SPE were further characterized with ToxCast chemicals (n= 6,858) using the trained ML.

RESULTS: Multi-SPE protocol increases quantification of 70 (30%) and 34 (12.0%) target EDCs and identification of 17 (77.2%) and 72 (36.3%) nontarget chemicals (confidence ≥level 3) in serum and urine samples, respectively. The current strategy could expand the exposomics by 30.0% of 33,457 chemicals and 25.0% of 304,776 *in-silico* metabolites based on seven key features. The predictions for the 6,858 ToxCast chemicals suggest that 34% of the substances could be expanded, including some with high toxicological activity.

DISCUSSION: The multi-SPE strategy advances female exposomics by expanding quantification and identification of the internal exposure profiles. This largely promotes the study on the association of EDCs exposure with female reproductive health and adverse outcomes that have been growing to a prevalent issue.

KEYWORDS: EDCs, multi-SPE, targeted, non-targeted, machine-learning, serum, urine

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Exposomics and Health Effects of Toxic Pollutants in Occupationally Exposed Populations in Three Typical Contaminated Sites

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Abstract

Contaminations from typical industries present intricate challenges and potential health risks to humans. In this study, we focused on petrochemical, coking and non-ferrous metal smelting workers to investigate the internal (urine and serum) and external (soil, atmosphere, and water) exposures to toxic pollutants through non-target and target analyses. Our results indicated that PAHs were key pollutants in both environmental samples and exposed workers. However, specific differences were observed. For example, exposed to BTEX, volatile halogenated hydrocarbons, and petroleum hydrocarbons were predominant pollutants in petrochemical sites, PAH derivatives were significant pollutants in coking sites, and metals/metalloids (vanadium, cadmium, arsenic, chromium, tin, antimony, lead, etc.) were notable chemicals in non-ferrous metal smelting sites. Co-exposure to characteristic pollutants at each site significantly affected health indicators related to liver and kidney function, posing serious health threats. This study underscored the imperative need to increase attention to the health implications of occupational exposure at petrochemical, coking and non-ferrous metal smelting contaminated sites. Furthermore, it could serve as a crucial reference to the control of site contamination not only in China but also globally.

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Simultaneous occupational exposure profiles of PAHs and chlorinated paraffins in human serum from non-ferrous metal smelting

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Abstract

In non-ferrous metal smelting, the incomplete combustion of coal releases a significant concentration of polycyclic aromatic hydrocarbons (PAHs). PAHs are well known for their mutagenic, carcinogenic and teratogenic properties, posing serious health risks. In the meantime, the use of metalworking fluids, a primary source of short-chain chlorinated paraffin (SCCPs) emissions in China, contributes significantly to atmospheric pollution during the metalworking process in smelting processes. SCCPs have been also recognized as persistent organic pollutants and listed in the Stockholm Convention since 2017. Therefore, non-ferrous metal smelting workers may be exposed to high concentrations of both PAHs and CPs. To answer this hypothesis, a simultaneous analytical method for those pollutants in human serum is urgently needed. In this study, human serum was pre-treated using acetonitrile for protein precipitation, followed by extraction with a mixture of n-hexane: dichloromethane (v:v, 1:1), and purified using silica gel. This method effectively minimized the matrix effect of lipids and other impurities in the serum samples, ensuring efficient extraction of PAHs and CPs. For the instrumental analysis, PAHs were quantified using GC-MS/MS, and the quantification method for CPs were developed using LC-MS/MS system, where the

chromatographic separation was achieved using a rapid resolution high definition SB-CN threaded column (100mm×2.1mm, 1.8μm). Additionally, SCCPs and MCCPs congeners ($C_{10\text{-}20}Cl_{5\text{-}12}$) were quantified by detecting $[M+CH_3COO]^-$ ions, with ammonium acetate added to the mobile phase. The limit of detection (LOD) of PAHs was obtained as 2.0 $ng \cdot ml^{-1}$, with recoveries and accuracies of 65.5% and 89.6% calculated from spiked quality control samples. The LODs of SCCPs and MCCPs were obtained as 260 $ng \cdot ml^{-1}$ and 190 $ng \cdot ml^{-1}$, respectively, with accuracies of 105.3% and 81.3%, respectively. A total of seven parent PAHs and four halogenated PAHs were detected in the serum collected from population around non-ferrous metal smelting plants, with the highest concentration being 1,5-Cl_2-Anthracene (0.3 $ng \cdot ml^{-1}$). ΣCPs levels in the serum of the exposed population (median, 3328.8 $ng \cdot ml^{-1}$) were found to be significantly higher than those in the control residents (1062.1 $ng \cdot ml^{-1}$). The results indicated increased health risks of occupational exposure of PAHs and CPs in non-ferrous metal smelting site should be further assessed in the future.

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Occupational Exposure Profiles of PAHs and Their Derivatives in human serum from the petrochemical industry

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Abstract

Polycyclic aromatic hydrocarbons (PAHs) have been recognized as major pollutants in the last few decades. However, recent studies have shown increasing concerns on PAH derivatives, such as methylated PAHs (MPAHs), oxygenated PAHs (OPAHs), halogenated PAHs (XPAHs) and heterocyclic PAHs (HPAHs), which may have equal or even greater toxicity than their parent PAHs. It is well known that significant amounts of PAHs and their derivatives are released during oil extraction in petrochemical industry. Therefore, the exposure to PAHs and their derivatives among population in petrochemical industry area should be urgently assessed. In this study, a total of 79 serum samples were collected from a petrochemical plant in North China, including 64 petrochemical workers and 15 residents from the control area. 76 (24 PAHs and 52 derivatives) were analyzed using a GC-MS/MS system, and the results showed that 10 PAHs, two OPAHs, 12 HPAHs , and four XPAHs were detected. Among them, naphthalene showed the highest median concentration (9.27 ng/mL) in the petrochemical workers, followed by acenaphthylene (0.05 ng/mL) and phenanthrene (0.37 ng/mL); In terms of PAH derivatives, 2-methyl-naphthalene, anthraquinone, 5,6-benzoquinline and 5-Br-Ana was found the predominant MPAH, OPAH, HPAH and XPAH, respectively, with the median concentrations of 9.25 ng/mL, 0.62ng/mL, 18.57 ng/mL, 4.09 ng/mL. The highest total concentrations of MPAHs (78.90 ng/ml) were found in the serum of oil workers, followed by PAHs (14.60 ng/ml), HPAHs (41.90 ng/ml) and XPAHs (7.64 ng/ml), the concentration of OPAHs (1.53 ng/ml) was found the lowest. The concentration of PAHs

and MPAHs in serum of these workers was significantly higher than that the residents in the control area. The results showed that PAHs and MPAHs were the most important pollutants in petrochemical industry polluted sites compared with the conventional exposure. This study will provide certain theoretical support for pollution prevention in petrochemical industry, and provide scientific basis for correctly evaluating the environmental impact of PAHs and their derivatives in petrochemical industry plants.

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The impact of various aromatic compounds on human liver and kidney functions in occupationally exposed population from coking industries

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Abstract

Coking industries produce a substantial number of aromatic compounds (ACs), which adversely affect human health. The effects of the physicochemical properties of these ACs on human health have not been fully elucidated. In this cross-sectional study, we utilized data from 389 human urine samples collected at coking industries as compared with 248 residents from the control area, encompassing urinary ACs, molecular descriptors of ACs, and indicators of liver and kidney function. MLR and BKMR models were employed to identify liver and kidney function indicators closely associated with ACs. ACs closely associated with liver and kidney functions were identified through computational analysis employing machine learning algorithms. Using matrix coupling methods to calculate composite indices of chemical descriptors for each sample. Spearman analysis was also conducted for feature selection to identify descriptors strongly correlated with liver and kidney functions. We applied stratified sampling and 5-fold cross-validation to build machine learning models incorporating coupled ACs and descriptors. The models MARS, RF, XGBoost, and KNN were evaluated to determine the optimal machine learning model. The Variable Importance in Projection (VIP) algorithm was used to construct partial dependence plots to explain the outcomes of the optimal model.

The results indicate close relationships between albumin/globulin(A/G) in liver function and uric acid (UA) in kidney function with ACs pollution levels. All machine learning models constructed based on coupled ACs and descriptors outperformed linear regression, and XGBoost method yielding the best fitting results. The VIP algorithm was then utilized to compute the relative importance of ACs and chemical descriptors in the model. Importance analysis revealed that the compounds such as 2-OH-Flu, 4-OH-NNap, 3-OH-CBZ, and 1-OH-Pyr affect liver function, while 1/9-OH-Phe, PCP, 2/3-OH-Phe, and 3/4-moCP affect kidney function. Among the chemical descriptors of these ACs, MATSe7, MATSV6,

and TPSA had relative importance scores of 0.28, 0.17, and 0.12 for liver function damage, while LogP, GATSp5, and MATSV6 had scores of 0.3, 0.285, and 0.285 for kidney function damage. This study indicates that the autocorrelation and spatial effects of atomic or electronic distributions, along with physicochemical properties such as polar surface area and octanol-water partition coefficient within ACs, are linked with liver and kidney damage.

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Metallic contaminants influence the outcomes of male-male competition during precopulatory intrasexual selection

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Abstract

Male-male competition is a component of Darwin's theory of precopulatory intrasexual selection, where males compete for access to resources important for reproduction and successful males pass on traits that endow greater competitive ability to their offspring, thereby exaggerating the trait(s) over evolutionary time. For the first time, we asked whether exposure to metallic contaminants influences the outcomes of male-male competition in shore crabs thereby altering outcomes of intrasexual selection. Crabs were exposed to an environmentally relevant, and a behaviourally relevant, concentration of lead (i.e. Pb, 10 µg/L and 100 µg/L respectively) under laboratory conditions for 96 hours and subsequently allowed to compete for burrow ownership in experimental arenas. Exposed crabs (100 µg/L) were less successful than control crabs in chela size-matched paired competitive interactions, spent less time in burrows and predominantly lost burrow ownership. Further, exposure to Pb contamination (both 10 µg/L and 100 µg/L) negated the size advantage in chela size-asymmetric competitive interactions. This contaminant-induced loss of size-related competitive advantage may result in relaxation in selection pressure on body size and smaller male carapace widths and especially male chela lengths in contaminated locations. Assessment of a range of locations in the wild found a consistent pattern of metal-associated size declines in more contaminated locations.

KEYWORDS: Aggression, Intrasexual selection, Male-male competition, metals, metal(loid)s, Sexual selection.

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Evaluation of the Health Risk Using Multi-pollutant Air Quality Health Index: Case Study in Tianjin, China

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Abstract

Introduction: Air pollution imposes a significant burden on public health. Compared with the popular air quality index (AQI), the air quality health index (AQHI) provides a more comprehensive approach to measuring mixtures of air pollutants and is suitable for overall assessments of the short-term health effects of such mixtures.

Methods: We established an AQHI and cumulative risk index (CRI)-AQHI for Tianjin using single- and multi-pollutant models, respectively, as well as environmental, meteorological, and daily mortality data of residents in Tianjin between 2018 and 2020.

Results and Discussion: Compared with the AQI, the AQHI and CRI-AQHI established herein correlated more closely with the exposure-response relationships of the total mortality effects on residents. For each increase in the interquartile range of the AQHI, CRI-AQHI and AQI, the total daily mortality rates increased by 2.06%, 1.69% and 0.62%, respectively. The AQHI and CRI-AQHI predicted daily mortality rate of residents more effectively than the AQI, and the correlations of AQHI and CRI-AQHI with health were similar. Our AQHI of Tianjin was used to establish specific (S)-AQHIs for different disease groups. The results showed that all measured air pollutants had the greatest impact on the health of persons with chronic respiratory diseases, followed by lung cancer, and cardiovascular and cerebrovascular diseases. The AQHI of Tianjin established in this study was accurate and dependable for assessing short-term health risks of air pollution in Tianjin, and the established S-AQHI can be used to separately assess health risks among different disease groups.

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Health benefits and scenario projections of $PM_{2.5}$ and O_3 pollution in Beijing-Tianjin-Hebei, China

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Abstract

Health benefits and scenario projections of $PM_{2.5}$ and O_3 pollution in Beijing-Tianjin-Hebei, China

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Abstract: Fine particulate matter ($PM_{2.5}$) and ozone (O_3) have become the main atmospheric pollutants in China, which are harmful to human health. In this paper, Beijing-Tianjin-Hebei, a key area of air pollution prevention and control in China, is selected as a research area to analyze the change characteristics of $PM_{2.5}$ and O_3 concentrations and their health effects from 2014 to 2023. Methods such as population health risk impact assessment and monetization evaluation of health effects are used to estimate the potential health benefits of different emission reduction standards in 2030. The results show that: (1) The average annual $PM_{2.5}$ concentration in the Beijing-Tianjin-Hebei region from 2014 to 2023 shows a decreasing trend, while the maximum daily 8-h sliding average (O_3-8 h concentration) of O_3 shows a fluctuating upward trend. (2) Both the number of premature deaths and economic losses attributable to $PM_{2.5}$ pollution showed a downward trend; However, the change of premature death and economic loss due to O_3 pollution showed the opposite trend, and the health risk and economic loss were relatively prominent in Beijing and Tianjin. (3) If the average annual concentration of $PM_{2.5}$ and O_3 reaches the secondary standard limit of the Ambient Air Quality Standards (GB 3095-2012) in 2030, the number of premature deaths attributable to $PM_{2.5}$ and O_3 in Beijing, Tianjin and Hebei will decrease by 23.08% and 20.45%, respectively, compared with 2023. The health economic loss was reduced by 41.23×10^8 yuan (95%CI :33.71×108~48.72×10^8 yuan) and 98.89×108 yuan (95%CI :54.14×108~142.67×10^8 yuan), respectively. Further reduction of $PM_{2.5}$ and O_3 concentrations to higher standards could further avoid the increase in premature deaths and bring significant economic benefits. Research shows that the Beijing-Tianjin-Hebei PM2.5 control has been effective, but the O3 pollution problem is prominent, and the number of health deaths and economic losses caused by it are on the rise. Higher air quality standards should be formulated to effectively improve the health of residents and bring significant economic benefits.

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Arsenic metabolism and methylation efficiency

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Abstract

Inorganic arsenic has been consistently ranked the first on the contaminants priority list of the Agency of Toxic Substances and Diseases Registry (ATSDR). Chronic exposure to inorganic arsenic is known to increase risks of skin lesions, cardiovascular diseases, diabetes, and many types of cancer, such as cancers of the bladder, lungs, and skin. Severity of adverse effect varies among individuals, which could be related to inter-individual differences in arsenic metabolism.

This presentation will discuss metabolism of inorganic arsenic, describe arsenic speciation in human urine, summarize current approaches of assessing methylation efficiency, and emphasize the complexity of metabolism of various arsenic species. Inorganic arsenate and arsenite can be metabolized in humans to produce monomethylarsonic acid (MMA) and dimethylarsinic acid (DMA). Efficiency of arsenic methylation can be estimated using concentrations of individual arsenic species in urine. Concentration ratios and percentages of methylated arsenic species are often calculated from the urinary arsenic speciation data. These methylation efficiency parameters are then used to explore relationships between arsenic metabolism and the health outcomes of arsenic exposure. The interpretation and conclusion of these relationships rely on accurate determination of methylation efficiency. Our research highlights the importance of considering exposure to organic arsenicals and the potential effect of such exposure on the assessment of arsenic methylation efficiency.

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Neonicotinoid Insecticides and Their Metabolites Can Pass Through the Human Placenta Unimpeded

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Abstract

Studies on neonicotinoids (NEOs) exposure in pregnant women and fetuses are scarce, and transplacental transfer of these insecticides is unknown. In this study, parent NEOs (p-NEOs) and their metabolites (m-NEOs) were determined in 95 paired maternal (MS) and cord serum (CS) samples collected in southern China. Imidacloprid (IMI) was the predominant p-NEO in both CS and MS samples, found at median concentrations of 1.84 and 0.79 ng/mL, respectively, whereas *N*-desmethyl-acetamiprid (*N*-dm-ACE) was

the most abundant m-NEO in CS (median: 0.083 ng/mL) and MS (0.13 ng/mL). The median transplacental transfer efficiencies (TTEs) of p-NEOs and m-NEOs were high, ranging from 0.81 (thiamethoxam, THM) to 1.61 (olefin-imidacloprid, of-IMI), indicating efficient placental transfer of these insecticides. Moreover, transplacental transport of NEOs appears to be passive and structure-dependent: cyanoamidine NEOs such as acetamiprid (ACE) and thiacloprid (THD) had higher TTE values than the nitroguanidine NEOs, namely clothianidin (CLO) and THM. Multilinear regression analysis revealed that the concentrations of several NEOs in MS were associated significantly with hematological parameters related to hepatotoxicity and renal toxicity. To our knowledge, this is the first analysis of the occurrence and distribution of NEOs in paired maternal-fetal serum samples.

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New Insights on Free and Conjugated Forms Neonicotinoid Insecticides in Human Serum and Their Association with Oxidative Stress

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Abstract

Following exposure, neonicotinoid insecticides (NEOs) can be metabolized by both Phase I and Phase II reactions catalyzed by human cytochrome P450 enzymes. However, toxicities of parent NEOs and their metabolites are still unclear and little is known about biotransformation rates and pathways of NEOs in humans. In this study, 98 serum samples collected in China were analyzed for free, conjugated and total forms of six parent NEOs (i.e., acetamiprid (ACE), imidacloprid (IMI), clothianidin (CLO), thiacloprid (THD), thiamethoxam (THM) and dinotefuran (DIN)), and four metabolites (i.e., *N*-desmethyl-acetamiprid (*N*-dm-ACE), 1-methyl-3-(tetrahydro-3-furylmethyl) (DIN-U), 5-hydroxy-imidacloprid (5-OH-IMI), olefin-imidacloprid (Of-IMI)). NEOs and their metabolites were detected in all serum samples, and the total median concentrations of free, conjugated, and total forms of 10 NEOs were 2.04, 2.01, and 5.12 ng/mL, respectively. Conjugated forms of NEOs accounted for only half (53%) of the total forms of NEOs. Based on the profiles of Phase I and Phase II metabolites of NEOs in serum, it was found that age is a determinant in Phase I metabolism of DIN and Phase II metabolism of IMI. The Phase II metabolites of NEOs are associated with oxidative DNA damage, and the conjugated forms of IMI, DIN and 5-OH-IMI in serum were significantly positively correlated with oxidative stress. Overall, the amount of NEOs present in conjugated forms in human serum was determined to document the existence of considerable proportion of free forms of these insecticides.

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Placental Transfer of Poly- And Perfluoroalkyl Substances Bisphenol Diglycidyl Ethers (Bdges) and Its Association With Maternal Health in a Population in South of China

Bo Zhang

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Abstract

Despite high production and usage, little is known about human exposure to multiple emerging contaminants. It is essential to determinate the concentration, profiles and more importantly, the transplacental transfer of emerging contaminants in vulnerable pregnant women population. In this study, we determined typical emerging contaminants, per- and polyfluoroalkyl substances (PFAS) and bisphenol diglycidyl ethers (BDGEs), paired maternal and cord serum samples collected from South of China. The study observed multiple types of emerging contaminants, suggesting co-exposure of alternatives, derivatives and legacy ones in pregnant women. The transplacental transfer efficiencies (TTEs) were calculated and further implied the structure-dependent transmission of emerging contaminants between pregnant women and fetuses. The substitution of elements or hydrogen and/or hydrophilic functional groups, as well as formation of hydrated and chlorinated derivatives may alter transplacental transfer efficiencies, leading to different transfer mechanisms. Multiple linear regression analysis indicated significant associations between maternal serum concentrations of emerging PFAS and BDGEs and maternal clinical parameters, especially liver function and erythrocyte-related biomarkers. The newly discovered TTEs in maternal–fetal pairs contribute to a fuller inventory of the transmission activity of contaminants in the human body, ultimately adding to a more significant comprehensive risk evaluation.

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The Silent Threat: PPDs and PPDQs in Healthy and S-NAFLD Cohorts

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Abstract

N, N'-Substituted *p*-phenylenediamines (PPDs) and their quinone derivatives (PPDQs) have been widely detected in the environment, but there is currently limited data on their occurrence in humans. In this study, we conducted the first serum analysis of two PPDs and their characteristic PPDQs in the healthy as well as secondary non-alcoholic fatty liver disease (S-NAFLD) cohorts in South China. Concentrations of four oxidative stress biomarkers (OSBs), such as 8-*iso*-prostaglandin $F_{2\alpha}$ (8-$PGF_{2\alpha}$), 11β-prostaglandin $F_{2\alpha}$ (11-$PGF_{2\alpha}$), 15(R)-prostaglandin $F_{2\alpha}$ (15-$PGF_{2\alpha}$), and 8-hydroxy-2'-deoxyguanosine (8-OHdG) in serum samples were also measured. *N*-(1,3-dimethybutyl)-*N'*-phenyl-*p*-

phenylenediamine (6PPD) and 6PPD quinone (6PPDQ) were the predominant target analytes in healthy and S-NAFLD cohorts, respectively, with the median concentrations of 0.28 and 0.20 ng/mL. Associations between four OSBs and target analytes were examined. Concentration of 6PPD was significant ($p < 0.05$) positively correlated with 8-$PGF_{2\alpha}$, 11-$PGF_{2\alpha}$, 15-$PGF_{2\alpha}$ in the healthy cohort, indicating that 6PPD may be associated with lipid oxidative damage among the target analytes. 6PPD exposure was related with elevated odds of prevalent S-NAFLD in the South China cohort (the crude odds ratio (OR) = 1.515, 95% confidence interval (CI) = 1.124–2.040, *p*-trend < 0.01; the adjusted OR = 1.626, 95%CI = 1.057–2.501, *p*-trend < 0.05). In addition, multilinear regression analysis revealed that the concentrations of 6PPD in serum were associated significantly with total bilirubin (TBIL, $\beta = 0.180$ μmol/L, 95%CI: 0.036–0.396) and direct bilirubin (DBIL, $\beta = 0.321$ μmol/L, 95%CI: 0.035–0.677) related to hepatotoxicity. Furthermore, mediation analysis indicated that 8-$PGF_{2\alpha}$, 11-$PGF_{2\alpha}$, and 15-$PGF_{2\alpha}$ mediated 17.1%, 24.5%, and 16.6% of 6PPD-associated DBIL elevation, respectively. Conclusively, this study provides novel insight into human exposure to and hepatotoxicity assessment of PPDs and PPDQs.

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A Study of the Association Between Neonicotinoid Exposure and Human Obesity

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Abstract

Neonicotinoids are widely used worldwide due to their broad spectrum, high potency and low toxicity. In the past, neonicotinoids were generally considered to be target-safe, whereas existing studies have found that NEOs are toxic to non-target organisms and cause disruption of the human endocrine system. And obesity as a typical endocrine disease, so there may be an association between neonicotinoid exposure and human obesity. In the present study, NEOs were widely detected in human serum samples, and p-NEOs were the most predominant in human exposure, but four m-NEOs were also detected, among which DIN and NIT showed significant differences between normal and obese populations, suggesting that these two types of substances may induce obesity in human beings. We will further analyze the contribution of NEOs to human obesity under single and mixed exposures to screen the key substances, and explore the mechanism of NEOs exposure on human obesity by combining with human energy metabolism indexes.

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The Study on PFAS Contamination Risk in Chinese Drinking Water

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Abstract

Per- and Polyfluoroalkyl Substances (PFASs) are a class of synthetic organic compounds widely used in various industries due to their unique physical and chemical properties. PFASs have garnered global attention due to their environmental persistence and significant impact on ecosystems and human health. Until 2009, the international community through the Stockholm Convention, explicitly banned the production and use of PFOS, which shows the lagging regulatory measures for PFASs. Humans can be exposed to PFASs through various pathways, including diet, drinking water, breast milk, and dust, with drinking water potentially being a major exposure route. Recently, the United States released the first legally binding national drinking water standard for PFASs. However, research on PFASs contamination in drinking water in China remains insufficient, and there is a lack of an accurate, highly sensitive, and simultaneous analysis technique capable of detecting multiple traditional and emerging PFASs in water. The basic data on PFASs concentration levels in urban drinking water in China are also inadequate. This study optimizes a solid-phase extraction combined with a high-performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS) method and develops a simultaneous detection and analysis technique for 40 traditional and emerging fluorinated compounds in water. This technique is applied to a large-scale investigation of PFASs contamination levels in urban drinking water in China, providing a reference for updating and improving China's drinking water standards to supply cleaner, safer, and healthier public drinking water.

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Transformation Products of Neonicotinoids: A Review of Metabolic Pathway, Predicted Toxicity and Human Exposure Assessment

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Abstract

Transformation products of neonicotinoids (t-NEOs), emerging significantly due to global increase used of neonicotinoids (NEOs), show higher environmental presence and toxicity than their parent NEOs (p-NEOs). To date, compared with p-NEOs, fewer systematic summaries and reanalyzes are available for t-NEOs with great environmental concerns. This review aims to comprehensively summarize the current knowledge of t-NEOs, document physical properties and predicted toxicity, and provide an understanding of the metabolic patterns. It also aims to offer new insights into the in/external exposure characteristics of t-NEOs in human and clarify potential health implications based on that evidence, provide noteworthy and prospective recommendations for future studies. Studies published in English prior to 2024 were searched using PubMed, Web of Science, and Google Scholar. No restrictions were placed on the type of health outcome assessed. The toxicological

profiles of t-NEOs diverge significantly from those of their p-NEOs, especially following the removal of nitro or cyano groups. The hydroxylation process, which involves the loss of the nitro group, can elevate mammalian toxicity. Drinking water and food are predominant human exposure pathways, with t-NEOs potentially leading to greater internal exposure levels than p-NEOs. Furthermore, t-NEOs can infiltrate various human tissues, potentially causing adverse effects, where oxidative stress significantly contributes to the toxicity induced by t-NEOs. The studies conducted to date were limited in number with suggestive but inconclusive findings related to t-NEOs toxicity and exposure assessment. Given the constant emerging of t-NEOs, more studies are needed to fully understand their effects on human health.

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The diversity and functional characteristics of seed endophytic bacteria of *Imperata cylindrica*, a pioneer plant of abandoned mine lands

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Abstract

Seed endophytes could improve host plants biotic and abiotic stress tolerance. *Imperata cylindrica* is a dominant pioneer plant in some abandoned mine lands with a higher concentration of heavy metal (HM). To discover the reason for *I. cylindrica*'s extreme environment adaptation, endophytic bacteria of *I. cylindrica*'s seeds from HM heavily contaminated (H) and lightly contaminated (L) sites were studied by both culture-dependent and high-throughput sequencing methods. Culturable results showed that *Pantoea* sp. was unique to site H compared to site L. The functional characteristics assay demonstrated that 100% of seed endophytic bacteria showed phosphorus solubilization, IAA synthesis, nitrogen fixation, or siderophores synthesis capacity. Most interestingly, the isolates of *Pantoea* sp. showed better Cd tolerance than the others. High-throughput sequencing results showed that HM-contamination significantly reduced the richness of endophytic bacteria in seeds, however, it increased the abundance of resistant species. *Massilia* sp. (13.16%) was the dominant genus at site H, and its relative abundance was significantly higher than that of site L ($p < 0.05$, Kruskal-Wallis sum-rank test). Spearman's rank

correlation coefficient analysis showed that *Massilia* sp. showed a significant positive correlation with Zn concentration, indicating that it may have a strong tolerance to Zn. In conclusion, the concentration of HM in the soil significantly affected the seed endophytic bacteria of *I. cylindrica*. Meanwhile, seed endophytic bacteria promoted the colonization and growth of *I. cylindrica* in abandoned mine lands through different functional properties. The survival of *I. cylindrica* in HM severely contaminated environment may mainly be through recruiting more microorganisms with HM-tolerance and growth promotion abilities to colonize the seeds.

Keywords: Heavy metal; Pioneer plant; *Imperata cylindrica*; Seed endophyte

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Exposure Levels of BPA in Overweight and Obese Individuals and Their Relationship with Metabolic Disorders

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Abstract

Obesity, as a multifactorial chronic metabolic disease, is one of the major public health issues of the 21st century. Bisphenol A (BPA) is an endocrine disruptor (EDCs) with estrogenic activity.Exposure to BPA and obesity can lead to metabolic disorders in the human body, thereby endangering health. This study aims to reveal the relationship between obesity and BPA exposure in the serum of overweight and obese individuals and normal individuals, and to explore the relationship between BPA exposure and obesity and metabolic disorders. Method: The research subjects were freshmen and sophomores of Sun Yat sen University, with a total of 41 effective serum samples. This experiment adopts the internal standard method for quantitative

analysis. After pre-treatment, serum samples are tested for BPA concentration using the LC-MS/MS platform to analyze the impact of overweight and obesity populations and BPA exposure on various metabolic indicators. Result: The detection rate of BPA was 100%, with a median and mean of 0.59 and 0.64 ng/mL (0.36-1.69). The levels of serum triglyceride (TG), total cholesterol (TC), fasting blood glucose (GLU) and fasting insulin (INS) in overweight and obese people were significantly increased ($p<0.05$). The serum BPA levels in overweight and obese individuals are significantly higher than those in the normal population, and there is a gender difference. The serum BPA levels in overweight and obese individuals in women are significantly higher than those in the normal population ($p<0.05$). In addition, correlation analysis showed that serum BPA levels were only significantly positively correlated with body weight and BMI ($p<0.05$). There were significant differences in triglycerides, total cholesterol, and low-density lipoprotein between different BPA exposure groups ($p<0.05$). Conclusion: The overweight and obese population has abnormal blood lipids and blood glucose levels, and BPA is widely exposed in the population and is significantly positively correlated with body weight and BMI. BPA exposure may play a certain role in the occurrence and development of obesity. The proportion of BPA exposure in this study is extremely high, and it may induce the development of obesity and lipid metabolism disorders. Therefore, it is recommended to reduce BPA exposure to reduce the risk of overweight, obesity, and lipid metabolism disorders.

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Exposure to per- and polyfluoroalkyl substances, neonicotinoid insecticides, benzotriazoles and benzothiazoles: Associations with human non-alcoholic fatty liver disease

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Abstract

Evidence of the joint association between exposure to multiple environmental chemicals and non-alcoholic fatty liver disease (NAFLD) is scarce. In this study, 281 participants from Zhuhai, China (138 patients with NAFLD vs. 143 healthy participants) were recruited to explore the associations of 40 per- and polyfluoroalkyl substances (PFAS), 11 neonicotinoid insecticides (NEOs), and 8 benzotriazoles (BTRs) and benzothiazoles (BTHs) with the risk of NAFLD. Perfluorooctane sulfonate (PFOS) and its emerging alternatives (6:2 chlorinated polyfluorinated ether sulfonate [6:2 Cl-PFESA] and 8:2 fluorotelomer sulfonic acid [8:2 FTSA]), NEO metabolites (m-NEOs), BTR, and BTH were the predominant PFAS, NEOs, BTRs and

BTHs, respectively. The total median concentrations of PFAS (20.4 ng/mL vs. 7.16 ng/mL) and NEOs (7.24 ng/mL vs. 6.23 ng/mL) in NAFLD group were significantly higher than those in healthy group. Sex differences in PFAS exposure have been observed among patients with NAFLD. 8:2 FTSA and short-chain PFAS were more predominant in female patients with NAFLD, whereas other emerging (i.e., 6:2 and 8:2 Cl-PFESA) and legacy PFAS (i.e., PFOS and long-chain perfluoroalkyl carboxylic acids) easily accumulated in male patients with NAFLD. The results of the multiple linear regression analysis indicated a significant positive association between PFOS and alanine transaminase (ALT) in serum samples from patients with NAFLD (β = 23.2, 95% confidence intervals (CI): 7.82, 38.5). Conversely, negative correlations were observed between 5-hydroxy-imidacloprid (5-OH-IMI) and γ-glutamyl transpeptidase (GGT) (β = −2.73, 95% CI: −5.29, −0.18), as well as between tolyltriazole (TTR) and total bilirubin (TBIL) (β = −0.70, 95% CI: −1.33, −0.08) and direct bilirubin (DBIL) (β = −0.59, 95% CI: −0.98, −0.20). The Bayesian kernel machine regression (BKMR) model revealed a positive joint effect of exposure to PFAS and NEO on elevated NAFLD outcomes, suggesting that exposure to PFAS and NEO might exacerbate the severity of NAFLD. This study fills the knowledge gap between multi-pollutant exposure and NAFLD risk.

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Environment, Pollution, and One Health

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Abstract

By 2050, 70% of human populations will reside in urban areas with a majority living along or immediately upstream from coastlines. Such high population densities elevate local demand for water, energy, food and other resources, including chemicals, for which usage is then concentrated in cities and within the diverse waste streams released from urban centers. Environment and health implications of global megatrends, including water quality intersections with demographic transitions to cities, present challenges and unique opportunities to achieving the United Nations Sustainable Development Goals. For example, empirical safety information is unavailable for the majority of the >350,000 chemicals and chemical mixtures listed for global commerce. Further, aquaculture will play an important role to meet future food demand, but 80% of the global sewage production is not treated before it is released to the environment and subjected to potential reuse. Judicious resource recovery will become increasingly critical; 66% of the world population will live in water stressed regions by 2025. Water reuse is routinely occurring, where inland surface waters and base flows to bays and estuaries can be dominated by or dependent on reclaimed sewage, which includes diverse contaminants of historic and emerging concern. Herein, we have embraced a One Health approach during study of urban ecosystems. For example, comparative pharmacology and toxicology efforts are affording opportunities to identify susceptible organisms and systems to anthropogenic chemicals and natural toxins when targets (e.g., receptors, enzymes) and molecular initiation events leading to adverse outcomes are evolutionarily conserved among species. These comparative approaches are also advancing a predictive understanding of bioaccumulation of nontraditional organic contaminants, which fall outside the applicability domains of

traditional hydrophobic models. Clearly, urban water quality challenges represent an emerging environment and health frontier, which requires multidisciplinary engagement and systems perspectives such as One Health to define mechanisms, to develop interventions, and to implement sustainable management strategies that promote integrative water quality while reducing risks to public health and the environment.

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An Efficient and Rapid Method for Detecting 41 Primary Aromatic Amine Compounds in Serum and Application

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Abstract

Primary aromatic amine (PAAs) are widely used chemical raw materials and chemical products, which are often used in food contact materials, pesticides, adhesives and dyes in daily life. Most PAAs are listed as priority pollutants and one of the key pollutants in water pollution control because of their toxicity and persistence, and their easy diffusion through aerosol and water migration. Studies have shown that many PAAs are known or suspected carcinogens or mutagens, with cytotoxicity and genotoxicity, and can enter the human body through direct skin contact exposure, inhalation exposure and ingestion exposure, thereby causing irreversible damage to the human respiratory system and blood circulation system. Therefore, it is of great significance to explore the analysis methods of the matrix in human body.

In this study, the human serum matrix was selected as the research object, and the liquid-liquid extraction method was used for pre-treatment, combined with high-performance liquid chromatography-tandem mass spectrometry detection technology, and the qualitative and quantitative detection of human serum PAAs could be carried out under relatively mild conditions. In this study, after the optimization of solvent type, extraction pH value, extraction times and the amount of single extraction liquid, the quantitative analysis of PAAs achieved the best results. The optimal conditions for optimization were determined as follows: 0.2mL of serum was used with ethyl acetate as extraction reagent, 80mg of NaCl was added for oscillatory mixing, and 3 mL was added each time for oscillatory extraction. After the operation was repeated twice, the supernatant was collected, nitrogen blown and redissolved. Under optimal conditions, the recovery rates of 41 PAAs in the study were basically maintained between 50% and 130% after calibration, and intra-day RSD and intra-day RSD were maintained between 0 and 25%, which proved that the detection method developed in this study had good accuracy, precision and reproducibility, and could meet the analysis requirements of PAAs in human serum.

Finally, the optimized scheme was used to analyze the actual serum samples, and it was confirmed that various kinds of PAAs were contained in various serum. Among the 41 PAAs analyzed, 20 PAAs were above the detection limit, and the average concentration was 0.025 ng/ml-4.268 ng/mL.

1072

Determination, Distribution, Identification of Migration of Legacy and Currently Used Pesticides in Pomelo Orchard from South China

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Sun, China

Abstract

Pesticides are a broad range of toxic compounds or mixtures of compounds and biological agents that are used extensively around the globe to avert, deter, control, or eradicate and destroy populations of harmful pests.They have contributed considerably to the development of agriculture by reducing crop losses and increasing affordable yields and food quality. Pomelo (Citrus grandis) is a highly popular and juicy member of the citrus family. To combat potential diseases and pests, various pesticides such as Lufenuron and Buprofezin are commonly used. However, their widespread use has led to concerns about the potential risks they pose to human health through consumption and little is known regarding the extent and distribution of pesticide exposure in pomelo. In this study, we measured legacy and currently uesd pesticides in pomelo and corresponding soil and leaf samples collected from two typical pomelo orchards in South China. Our results suggest the wide spread of all pesticides in pomelo orchards of China.As currently used pesticides, Buprofezin and Lufenuron demonstrated higher detection rates and concentrations in soil and leaf samples than other legacy pesticides. The sum mean concentrations of these pesticide (ΣPesticides) in pulp, soil and leaf samples were 2.6 ng/g, 110 ng/g and 307 ng/g respectively, and the pesticide residues in the pulp were much lower than the soil and leaf samples. Currently used pesticides were the most prevalent in both soil and leaf samples but lower than legacy pesticides in the pulp. Pesticides have different spatial distribution and residue patterns in all parts of the pomelo, the spatial distribution of the mean concentration of all pesticides in the pomelo was: Epicarp (216 ng/g) > Mesocarp (9.5 ng/g) > Endocarp (4.4ng/g) > Seed (3.8 ng/g) > Pulp (1.1 ng/g). Significantly positive correlations showed that the sources of pesticides in soil and pulp were common or related. Principal component analysis further indicated that the residue of individual pesticide was primarily associated with the residue found in epicarp, topsoil or deep soil. The residues of different pesticides in the pulp may originate from different migration pathways, such as the epicarp, topsoil, and deepsoil. The residues of Buprofezin in pulp may originate from its use as a currently used pesticide, which migrates from the epicarp to the inner parts of the fruit after being sprayed. Although the cumulative chronic dietary risks of all pesticides via pomelo consumption were much lower than the acceptable daily intake for both the general population, the potential health risk of pesticides via pomelo consumption should raise more public concern considering the high detection rates of legacy and currently uesd pesticides in environment.

1073

Occurrence, Distribution, and Migration of Legacy and Currently Used Pesticides in Pomelo Orchards in South China

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Abstract

Pesticides are a broad range of toxic compounds or mixtures of compounds, as well as biological agents, which are used extensively around the globe to avert, deter, control or eradicate and destroy populations of harmful pests. Pesticides have significantly contributed to the development of agriculture by reducing crop losses and increasing affordable yields and food quality.Citrus are a ubiquitous and beloved commodity worldwide due to their extensive production volume and significant nutritional and economic impact,which are rich in various nutritional components and functional compounds. Pomelo (Citrus grandis) is a highly popular and juicy member of the citrus family. However, little is known regarding the occurrence and distribution of pesticides in pomelo. In this study, we determined the levels of legacy (n = 25) and currently used pesticides (n = 2) in all parts of pomelo (i.e., epicarp, mesocarp, endocarp, pulp, and seed) and paired soil and leaf samples collected from two pomelo orchards in South China. At least one target pesticide was detected in the pomelo fruit, soil, and leaf samples, indicating that these pesticides are ubiquitous. The spatial distribution of the sum up of pesticides in the pomelo parts was in the order of epicarp (216 ng/g) > mesocarp (9.50 ng/g) > endocarp (4.40 ng/g) > seed (3.80 ng/g) > pulp (1.10 ng/g), revealing different spatial distributions in pomelo. Principal component analysis was performed based on the concentrations of the target pesticides in the pulp and paired samples of epicarp, leaf, topsoil, and deep soil to examine the migration pathway of the pesticides in pomelo. Close correlations were found among the target pesticides, and the pesticides in the pulp mainly migrated from the peel, topsoil, or deep soil. We also explored the factors that affected migration and found that the main migration pathway of the non-systemic pesticide (i.e., buprofezin) into the pulp was the epicarp, whereas the systemic pesticide (i.e., pyriproxyfen) was mainly derived from the soil.The residues of different pesticides in the pulp may originate from different migration pathways, such as the epicarp, topsoil, and deepsoil. The residues of Buprofezin in pulp may originate from its use as a currently used pesticide, which migrates from the epicarp to the inner parts of the fruit after being sprayed. The cumulative chronic dietary risks of all the pesticides resulting from pomelo consumption were much lower than the acceptable daily intake values for children and the general population. The potential health risk posed by legacy and currently used pesticides, which are widely and frequently utilized, should be given increased attention.

1136

Advancements in CRISPR Nanotechnology for Imaging Key Molecules in Living Cells

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Abstract

Active CRISPR/Cas12a systems play a pivotal role in genome engineering and diagnostics through their cis-cleavage and trans-cleavage activities. While the activation of CRISPR/Cas12a by RNA remains not clear. Our research reveals a significant breakthrough, demonstrating the effective activation of the CRISPR/Cas12a system by RNA, resulting in enhanced trans-cleavage capabilities. Moreover, the activated crRNA-Cas12a ribonucleoprotein (RNP) displays a preference for trans-cleaving longer sequences, a crucial insight that guided the development of CRISPR nanorobots tailored for operations within living cells. By integrating the crRNA-Cas12a RNP and nucleic acid substrates on gold nanoparticles, we have achieved a substantial increase in local substrate concentration compared to the RNP, leading to accelerated trans-cleavage kinetics. The initiation of these nanorobots by target microRNA bound to the crRNA-Cas12a RNP triggers their trans-cleavage function. Through successive trans-cleavage events on labeled substrates, we observe the generation of amplified fluorescence signals, enabling highly sensitive, real-time imaging of specific microRNA molecules within live cells. These pivotal advancements underscore the vast potential of CRISPR nanorobots in upcoming biomedical applications, paving the way for novel methods to monitor and modulate biological processes within living cellular environments.

27. Environmental Behaviour and Risks of Antibiotic Resistance Genes

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Spatial distribution of antibiotics and antibiotic resistance genes and microbial communities in the Yangtze River

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Abstract

To study the distribution characteristics of antibiotics and antibiotic resistance genes (ARGs) in the water of the Yangtze River, we selected the river's upper, middle, and lower reaches, and estuaries as our research areas. We collected water and sediment samples from 20 sites and analyzed them for 50 antibiotics, 13 ARGs, and microbial communities. The study showed that the highest concentration of Sulfisomidine was found in sulfonamide antibiotics (SAs), with an average concentration of 465.08 ng L^{-1}, in the highest concentration upstream. In fluoroquinolone antibiotics (FQs), Ciprofloxacin had the highest concentration, with an average

concentration of 1392.62 ng L^{-1}. FQs were frequently detected in the environment, 6.7 times that of SAs and 32.8 times that of macrolide antibiotics (MLs). In MLs, Erythromycin had the highest concentration. The level of antibiotic pollution in the Yangtze River's middle and lower reaches was higher than that in the upper reaches and estuaries. This suggests significant spatial variations in the composition of antibiotics in the Yangtze River. In the sediment samples, 16S rRNA, intI1, and 11 ARGs were detected, which, as an important integron, intI1 is ubiquitous in this study area. Studies have shown that environmental pressure can promote sul1 gene transfer among microorganisms. The spatial distribution of sul1 abundance in the study area is similar to that of intI1, indicating that intI1 may be involved in the occurrence and spread of sulfonamide resistance genes in the Yangtze River. Analysis of the relative abundance of ARGs in sediments shows that sulfonamide resistance genes > fluoroquinolone resistance genes > macrolide resistance genes, the results suggest that the sulfanilamide resistance gene was the dominant type. Microbial community structure indicates that at the phylum level, the dominant microorganisms in the sediments were Proteobacteria, Actinobacteria, Firmicutes, Cyanobacteria, and Bacteroidota. Pearson's correlation analysis suggests that antibiotics and environmental factors were significantly positively correlated with ARGs, and antibiotics and ARGs were significantly positively correlated with sediment microorganisms. This shows that there is a potential pressure on ARGs from antibiotics and that microbes provide the driving force for the evolution and spread of ARGs. This study provides a basis for further research on the occurrence and spread of antibiotics and ARGs in the Yangtze River Basin.

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Environmental Multi-media Interfaces are Hotspots of Antibiotic Resistance Revealed by Stimulated Raman Scattering with D_2O Labelling

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Abstract

Antibiotic resistance is currently an unfolding global crisis threatening human health worldwide. While antibiotic resistance genes (ARGs) are known to be pervasive in environmental media, the occurrence of antibiotic resistance at interfaces between two or more adjacent media is largely unknown. Here, we designed a microcosm study to simulate plastic pollution in paddy soil and used a novel method, stimulated Raman scattering coupled with deuterium oxide (D_2O) labelling, to compare the antibiotic resistance in a single medium with that at the interface of multiple environmental media (plastic, soil, water). Results revealed that the involvement of more types of environmental media at interfaces led to a higher proportion of metabolically active bacteria and enrichment of antibiotic resistance bacteria. Genotypic analysis showed that ARGs (especially high-risk ARGs) and mobile genetic elements (MGEs) were all highly enriched at the interfaces. This enrichment was further enhanced by the co-stress of heavy metal (arsenic) and antibiotic (ciprofloxacin). Our study is the first to apply stimulated Raman scattering

to elucidate antibiotic resistance at environmental interfaces and reveals novel pathway antibiotic resistance dissemination in the environment and overlooked risks to human health.

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Biotransformation and toxicity of SMX in phycosphere: Importance of SMX exposure ways in aquatic ecosystems

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Abstract

The widespread use of antibiotics has inevitably led to their increasing release into aquatic systems. Research has shown that the mode of antibiotic entry into water bodies significantly influences their toxicity and ecological risk. In this study, sulfamethoxazole (SMX) was selected to explore its biotransformation and degradation pathways in the phycosphere under different exposure scenarios: single exposure at high concentration (10 mg/L and 1 mg/L) and continuous exposure at low concentration (1 μg/L, 10 μg/L, 20 μg/L, 50 μg/L, and 100 μg/L). The ecological toxicity of various degradation products was also analyzed. Results indicated that accumulation of biomass was significantly promoted by continuous exposure at low concentrations. The increase in EPS in the system with continuous exposure at low concentrations was significantly higher than that in the system with single exposure at high concentration. Additionally, the ROS content in the 100 μg/L SMX group was found to be 1.8 times that of the control group, indicating that continuous exposure exerted greater environmental stress on the system. The removal of SMX in the algae-bacteria system followed the order: biotransformation > biosorption > bioaccumulation. It was observed that the system with continuous exposure at low concentration exhibited higher levels of biosorption compared to the system with single exposure at high concentration. The degradation products of SMX were found to be the same under different treatment methods, with 11 TPs being detected. Side-chain cleavage, oxidation, hydroxylation, and nitration were major degradation pathways. In addition, the toxicity of most degradation products was reduced through degradation. This study elucidates the biotransformation and toxicity of SMX in the phycosphere under different exposure scenarios. These findings contribute to a comprehensive understanding of the ecological risks and dynamic responses of system biota when antibiotics enter aquatic ecosystems through various pathways at different concentrations. New insights are provided for the risk assessment of antibiotics under continuous exposure in river systems.

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Microalgae enhances the adaptability of epiphytic bacteria to sulfamethoxazole stress and proliferation of antibiotic resistance genes mediated by integron

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Abstract

The transmission of ARGs in the microalgae-associated epiphytic bacteria remains unclear under antibiotic exposure, apart from altering the microbial community structure. In this study, *Chlorella vulgaris* cocultured with bacteria screened from surface water was examined to explore the spread of ARGs in the presence of sulfamethoxazole (SMX). The extracellular polymers released by *Chlorella vulgaris* could reduce antibiotic-induced collateral damage to bacteria, thus increasing diversity of the microalgae-associated epiphytic bacteria. The abundances of *sul1* and *intI1* in phycosphere at 1 mg/L SMX dose increased by 290 and 28 times, respectively. Metagenomic sequencing further confirmed that SMX bioaccumulation stimulated the horizontal transfer of *sul1* mediated by *intI1* in the microalgae-associated epiphytic bacteria, while reactive oxygen species (ROS) -mediated oxidative stress induced the SOS response and thus enhanced the transformation of *sul1* in the J group. This is the first study to verify that microalgae protect bacteria from antibiotic damage and hinder the spread of ARGs mediated by SOS response, while the transfer of ARGs mediated by integron is promoted due to the bioaccumulation of SMX in phycosphere. The results contribute to present comprehensive understanding of the risk of ARG proliferation by the presence of emerging contaminants residues in river.

362

Enrichment of antibiotic resistant zoonotic *Aeromonas veronii* by antibiotics-manufacturing wastewater treatment plant and its potential transmission risk to humans and animals

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Abstract

Wastewater released from antibiotics-manufacturing facilities can serve as a major source of antibiotic resistome in the environment. However, the variation of antibiotic resistance genes (ARGs) and bacterial communities along the treatment train of antibiotics-manufacturing wastewater treatment plants (AM-WWTPs) and the associated risks to humans and animals are largely unknown. We used deep metagenomic sequencing to systematically analyze ARGs and bacterial communities following the influent to the effluent through the treatment train of eleven units within a full-scale AM-WWTP receiving wastewater from a β-lactams-manufacturing facility. The bacterial communities and ARG compositions varied significantly among the treatment units, but were significantly correlated. More importantly, two metagenome-assembled genomes of zoonotic *Aeromonas veronii* carrying two resistance genes and multiple virulence factors were significantly enriched in the effluent. The close phylogenetic relationships between these assembled *A. veronii* with the isolates from clinic patients and diseased fish

found in the local area further confirm that *A. veronii* originating from AM-WWTP could potentially transmit to humans and animals. This study reveals a previously unrecognized risk associated with AM-WWTPs, which could contribute to the enrichment and transmission of antibiotic resistant *A. veronii*, a zoonotic pathogen.

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Decadal Trends of Inhalable Antibiotic Resistome in Typical Urban Areas from China

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Abstract

Airborne antibiotic resistance genes (ARGs) were commonly found geographically differentiated in their compositions with influences by seasonal conditions. However, a longitudinal investigation on airborne antibiotic resistome in various geographical locations is still lacking to reveal their evolution under the long-term impacts of climate changes and anthropogenic activities. In this study, we deployed a decade-range (2012–2021) fine particulate matter ($PM_{2.5}$) sampling campaign in three typical cities from different regions of China and adopted an integrated analysis of qPCR and metagenomic sequencing to study the spatiotemporal variations in $PM_{2.5}$-associated antibiotic resistome. Significant geographical differentiation in airborne ARG composition and diversity was observed regardless of sampling time, with ARGs encoding resistance to glycopeptide in north China and to aminoglycoside in south China being major biomarkers that contributed to the differences. This pattern appeared to be majorly affected by the airborne bacterial community (accounting for 12%–26% of the variations in ARG composition and 44%–56% in ARG diversity), followed by source contributions of ARGs and the integrated effects of meteorological conditions and air quality. Despite a higher load of $PM_{2.5}$-associated ARGs in the temperate site, there was a geographically similar trend that the ARG concentration firstly decreased by more than half a magnitude and then rallied in all three sites, as well as the patterns of respiratory pathogens. Our study highlights the relative importance of different driving factors in shaping airborne ARG profiles by ten-year investigations and benefits the understanding of inhalation exposure risks to airborne AMR over the past decade in urban China.

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Characteristics of antibiotic resistance genes in river section and sewage discharge outlets in downstream of the Yangtze River

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Abstract

In order to study the distribution characteristics of antibiotic resistance genes (ARGs) pollution in key river sections and key sewage outlets along the lower reaches of the Yangtze River, samples of 8 river sections and 4 sewage outlets along the lower reaches were analyzed. Metagenomics were used to analyze ARGs and microbial communities in the water samples. The results showed that the types of ARGs in the lower reaches of the Yangtze River mainly resistant to multi-drug, macrolide, and tetracycline. The abundance of tetracyclines and β-lactam resistance genes in the water samples from key sections and sewage outlets in the middle section of the lower reaches of the Yangtze River was relatively high. Microbial analysis at the phylum level indicated that the potential host bacteria for ARGs in water samples were mainly *Proteobacteria* and *Actinobacteria*. PCA analysis was based on the relative abundance of OTUs at the phylum level, the clustering of D2, D4, D6, D7, D10 and DY indicated that the microbial community structure was similar. In sewage samples, the clustering of P1, P3, and P5 samples indicated that there was a small difference in microbial community structure. The D8, DX, and P6 samples showed significant differences in the PC1 axis compared to other samples, indicating a significant difference in microbial community structure. Diversity index analysis showed that the D8, DX, and P6 communities possessed high diversity. This study analyzed the pollution characteristics of ARGs in key river sections and sewage outlets in the lower reaches of the Yangtze River. *g_ Candidatus-Fonsibacter* and *g_ Clavibacter* were significantly associated with multiple ARGs and involved multiple types of antibiotic resistance. The research results provided data support for the distribution a ARGs in water along the lower reaches of the Yangtze River.

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Disinfection enhances antibiotic resistance and human health risks in aerosols

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Abstract

Antibiotic resistance genes (ARGs) and antibiotic resistant bacteria (ARB) in atmosphere could penetrate into human lungs with aerosols, posing more serious potential health risks. Disinfectants, which have been used more during coronavirus disease 2019 (COVID-19), could increase ARGs in bacteria and bacterial resistance to antibiotics, thus causing a more serious global problem of antibiotic resistance. In this study, aerosol samples were collected from four functional regions of Shijiazhuang before (in 2019) and during (in 2020) COVID-19 to analyze the distribution characteristics of ARGs and microbial community structure in aerosols of different functional regions. The results showed that the use of disinfectants decreased the categories of detected ARGs and increased ARGs abundance in different functional regions. Besides, we conducted disinfectants (84 disinfectant) indoor exposure experiments in laboratory conditions. The results indicated that the use of disinfectants increased the abundance of ARGs in aerosols. On the 20 days of disinfection, the absolute abundance of ARGs was more than 1.7 times higher that when no disinfection (day 0), and the absolute abundance of ARGs still increased after the cessation of disinfection for 10 days (day 30), which was more than 1.8 times higher that when no disinfection (day 0). The study of microbial communities found that disinfectants usage reduced bacterial abundance, with the abundance of bacteria dropping by about an order of magnitude after 20 days of disinfection. After disinfection, biodiversity in aerosols decreased (shannon index decreasing from 5.9 to 4.5) and microbial community structure changed, and the relative abundance of *Pseudomonas*, the dominant bacterium, decreased by 18%. In addition, disinfectants usage increased bacterial resistance to antibiotics, with the minimum inhibitory concentration of sulfamethoxazole increasing from 1 mg/L (day 0) to 128 mg/L (day 20). Furthermore, we assessed the human health risks of ARGs in aerosols by analyzing the exposure dose of ARGs in aerosols for female, male and children. It was found that the dose of ARGs by respiration (10^4-10^6 copies/d/kg) was higher than that by skin contact (10^1-10^3 copies/d/kg) in different populations. This study provides theoretical guidance for the rational use of disinfectants and control of antimicrobial resistance.

569

Evolutionary landscapes of antibiotic resistance of E. coli induced by environmental-level antibiotic stresses

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Abstract

Environmental bacteria exposed to low-level antibiotics could derive clinically relevant resistance detrimental to human health. However, the underlying evolutionary landscapes remain poorly understood. Here, we conducted a high-throughput laboratory evolution by exposing a pathogenic, soil-originated *Escherichia coli* to 96 antibiotics widespread in the environment at 10 μg l^{-1} and provided an in-depth analysis of the phenotypic, genetic changes, and gene co-fitness network of the corresponding evolved populations. We found that all evolved populations exhibited resistance to at least one of the eight frequently prescribed antibiotics (up to 349-fold increase). Mutations occurred in 2,432 genes, and the action mechanism of each stressor class predominantly facilitated the direction of resistance evolution. By using transposon sequencing (Tn-Seq), we identified and explored a set of 131 core mutant genes contributing to high-level resistance. The co-fitness network further suggested potential mechanisms employed by various underappreciated mutant genes in conferring high-level resistance, which was validated via gene knockout (e.g., *rtcR* and *hflK*). Spatial analysis of functional enrichment highlighted

underexplored resistance-associated bioprocesses, such as those related to transcriptional reprogramming and carbon/nitrogen/sulfur utilization. 14.6% of the 481 key mutations were detected in the genomes of 1,263 *E. coli* pathogens, and several were prevalent in clinical isolates. These findings are key to unlocking the mechanisms of resistance evolution in complex environmental settings and bridging the clinically relevant mutation and low-level exposure gap

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Mechanism of Resistance to the Chiral Antibiotic Ofloxacin by P. aeruginosa

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Abstract

Antimicrobial resistance (AMR) poses a critical global health threat, contributing to significant morbidity and mortality worldwide. Most antibiotics are derived from natural sources, and resistance arises from the continuous evolution and exchange of resistance genes among humans, animals, and the environment. The use of antibiotics as clinical drugs has created unprecedented selective pressure, drastically altering the conditions for the development and spread of resistance. This selective pressure has facilitated the mobilization and horizontal transfer of numerous antibiotic resistance genes (ARGs) across various disease-causing bacterial species. Additionally, antibiotic concentrations can impact cellular processes, increasing genetic variability and changing cellular behavior. Frequent exposure of bacteria to sub-lethal drug concentrations can stimulate bacterial communities, driving the evolution of resistance. *Pseudomonas aeruginosa*, identified by the World Health Organization (WHO) in 2017 as one of the 12 most dangerous drug-resistant bacteria, is a priority pathogen for new antibiotic development. The aim of this study is to explore how sub-inhibitory concentrations of antibiotics act as intercellular signals and influence the resistance changes in *P. aeruginosa*. We find that *P. aeruginosa* biofilm formation was increased under treatment with sub-inhibitory concentrations of antibiotics and the expression of pyocyanin, LasA, and virulence factors was regulated by quorum sensing. In addition, *P. aeruginosa* was able to increase resistance after biofilm formation through upregulation of efflux pump genes, mutations in fluoroquinolone antibiotic target genes, and horizontal gene transfer.

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Spatio-temporal distribution and dynamics of antibiotic resistance genes in a water-diversion lake, China

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Abstract

The distribution and dynamics of antibiotic resistance genes (ARGs) in water-diversion lakes remain poorly understood. In this study, two comparative in situ investigations of ARG profiles targeting water diversion (DP) and non-diversion periods (NDP) were conducted in Luoma Lake, a vital transfer node for the eastern route of the South-to-North Water Diversion Project in China. And an innovative dynamics-based risk assessment framework covering the horizontal gene transfer (HGT), vertical gene transfer (VGT) and other driving forces (ODF, mainly gene mutation and loss) processes of ARGs was constructed to evaluate their exposure risks to local residents. The results demonstrated significant spatiotemporal variations in ARG contamination and notable differences in the co-occurrence patterns of ARGs and bacterial communities between DP and NDP. Correlations among ARGs with the 16 S rRNA, and mobile genetic elements (MGEs) indicated that the pattern of ARG dissemination in sediments was unchanged between the DP and NDP, with HGT and VGT contributing to ARG dissemination in both periods. However, water diversion altered the pattern in lake water, with HGT and VGT in the NWDP but only HGT in the WDP, which were critical pathways for the dissemination of ARGs. The significantly lower ARG sediment-water partition coefficient in the DP indicated that water diversion could shift the fate of ARGs and facilitate their aqueous partitioning. Partial least squares structural equation modeling was developed to analyze the causal effects of the factors in shaping ARG dynamics and identify the major driving forces in the DP and NDP in the lake. Risk assessment showed that human exposure risk of ARGs (HERA) increased overall with the bacterial carrying capacity in the local environment and peaked when the carrying capacity reached three (NWDP) or four (WDP) orders of magnitude higher than the observed bacterial population. HGT and VGT promoted, whereas ODF mainly reduced HERA in the lake. As the carrying capacity increased, the relative contribution of ODF to HERA remained relatively stable, whereas the dominant mechanism of HERA development shifted from HGT to VGT.

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Using Metagenomic Approaches to Investigate AMR in “One Health” Framework

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Abstract

The proliferation of antibiotic-resistant bacteria and genes has become a globally recognized threat to public health. Antibiotic resistance is not only a clinical issue but also an emerging global environmental

pollution concern. In this study, we employed metagenomic strategies, including the reconstruction of structured databases, bioinformatics network analysis, assembly, and binning techniques to effectively overcome the limitations of qPCR approach. This approach has facilitated the development of a comprehensive methodological pipeline aimed at deciphering antibiotic resistance. Based on the "One Health" framework, we have conducted an exhaustive examination of antibiotic resistance across the interconnected sectors of human, animal, and environmental health. Our analysis of urban water samples from various environments has identified the influent of wastewater treatment plants as a pivotal reservoir for antibiotic resistance. Employing sewage epidemiology principles, a nationwide survey of wastewater treatment plant influents and human fecal contamination has been conducted and has substantiated the intrinsic correlation between antibiotic resistance in these environments and human fecal waste. Furthermore, our investigation into antibiotic resistance within animal gastrointestinal tracts has demonstrated that the use of antibiotics in livestock farming is a significant contributor to elevated environmental antibiotic resistance levels. By integrating multi-omics techniques—encompassing culturomics, metagenomics, transcriptomics, and proteomics—we have unveiled further insights into the molecular underpinnings of antibiotic resistance. Our findings indicate that even trace levels of antibiotics in the environment, at concentrations as low as micrograms per liter, can induce mutations in sensitive bacterial strains, leading to the emergence of resistant strains harboring heritable resistance genetic profiles. Additionally, through prolonged antibiotic exposure experiments, we have identified novel antibiotic resistance genes and provided a profound interpretation of their resistance mechanisms. In conclusion, this study offers a robust methodological framework for the surveillance of environmental antibiotic resistance and imparts critical theoretical insights for the rational management and control of antibiotic resistance in the environment.

28. Environmental Contamination and Control Technology of Per- And Polyfluoroalkyl Substances (PFAS)

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Emerging Polyfluoroalkyl Substances in Contemporary Aqueous Film-forming Foams: Nontarget Identification and Aerobic Soil Transformation

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Abstract

Per- and polyfluoroalkyl substances (PFAS) released from aqueous film-forming foams (AFFF) have attracted increasing global concerns. In this study, a total of 38 PFAS were identified in contemporary AFFF formulations through suspect and nontarget screening using liquid chromatography-high resolution mass spectrometry (HRMS), with emerging fluorotelomer (FT) compounds accounting for 84.8%. Then a mixed AFFF formulation was amended to aerobic soil microcosms for a 150-day incubation period. Among the emerging PFAS, sulfonamide betaine or quaternary amine-based compounds exhibited recalcitrance. In contrast, PFAS containing tertiary amine and thioether moieties underwent significant degradation, with their biotransformation half-life ranging from 2 to 56 days. Based on the

biotransformation products detected by HRMS, the biotransformation pathways of FT and electrochemical fluorination (ECF) PFAS were proposed. Notably, two primary abiotic transformation reactions were observed in the aerobic soil: the hydroxylation of tertiary amine and the oxidation of thioether. Additionally, the response of bacterial, fungal, and archaeal communities in the AFFF-spiked soil was revealed.

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Identification of Bioaccumulative Emerging Per- and Polyfluoroalkyl Substances in Marine Organisms

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Abstract

The trophodynamics of many emerging per- and polyfluoroalkyl substances (PFASs) in aquatic food webs remain poorly understood. Here, seawater and marine organism samples were collected from the northern South China Sea to investigate the trophic biomagnification potential of legacy and emerging PFASs. Significant trophic magnification was observed for 22 PFASs, where the trophic magnification factors of *cis*- and *trans*-perfluoroethylcyclohexane sulfonate (PFECHS) isomers were reported for the first time. Perfluorohexanoic acid was trophic-magnified, possibly attributed to the PFAS precursor degradation.

The toxicokinetics of emerging PFASs have rarely been reported. Here, tissue-specific uptake and depuration kinetics of PFECHS and 6:2 and 8:2 chlorinated polyfluoroalkyl ether sulfonates were studied in marine medaka (*Oryzias melastigma*). Evident bioconcentration was found for these three PFASs in the exposed fish, which showed longer residence times in eyes than in other tissues; *trans*-PFECHS showed higher bioconcentration potential than *cis*-PFECHS, and PFECHS exposure resulted in significant alterations in multiple proteins associated with eye function in medaka.

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Developing New Insights into the Interactions Between Concrete and Per- and Polyfluoroalkyl Substances

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Abstract

The presence of per- and polyfluoroalkyl substances (PFAS) in consumer and industrial products, combined with their harmful health effects, has attracted regulatory attention. A significant source of PFAS contamination is the use of aqueous film-forming foams (AFFF) to combat class B fires at airports, military bases, and firefighter training facilities. Extensive research has investigated PFAS contamination across solid and aqueous matrices as well as biota. Contamination of concrete – an often-overlooked matrix and potential PFAS source – remains underexplored. Concrete, particularly in ground slabs at military bases and airports, is directly exposed to AFFF through various exposure routes. Limited studies have shown significant PFAS presence in concrete from these sites, highlighting its potential for long-term leaching even years after AFFF use. Questions about diffusion rates, the influence of AFFF additives, and concrete-PFAS interactions warrant further investigation. This study aims to understand the physicochemical interactions between concrete and AFFF to better understand PFAS fate upon initial exposure.

Laboratory experiments assessed PFAS contamination in concrete using individual PFAS and a 3M AFFF. PFAS uptake by concrete was evaluated on flat and chipped surfaces to simulate aged concrete. Various PFAS in the AFFF solution were examined using high-resolution mass spectrometry. Results showed no significant concentration decrease in the solutions pooled on concrete surfaces after one year, but PFAS diffusion was detectable within the concrete solid matrix, especially within the top 0.5 cm. Faster penetration was observed in chipped surfaces. A correlation between decreasing PFAS chain length and increased mobility was observed in some cases. Intermittent wetting and drying cycles accelerated PFAS penetration due to wicking, resulting in similar transport rates of PFAS of different chain lengths within concrete. A comprehensive extraction method for PFAS from AFFF-affected concrete was developed and validated through spike-recovery trials. High recoveries for perfluoroalkyl carboxylates and perfluoroalkyl sulfonamides were observed due to generation from precursors, while perfluoroalkyl amido amines showed low recoveries due to rapid degradation. This work provides important insights into PFAS uptake kinetics in concrete and potential transformations at concrete-water interfaces, within concrete, and during extraction.

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Rapid adsorptive removal of emerging and legacy PFASs from water using zinc chloride-modified litchi seed-derived biochar

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Abstract

Per- and polyfluoroalkyl substances (PFASs) have drawn significant attention due to their widespread presence in aquatic environments and their toxicity to organisms. The development of cost-effective and efficient adsorbents for PFASs removal in aquatic systems is crucial. In this study, modified lychee seed biochar was prepared through co-pyrolysis of lychee seed powder and zinc chloride to enhance the removal efficiency of both emerging and legacy PFASs from aqueous solutions. Results indicated that the adsorption efficiencies of L-BC for all studied PFASs were below 40%, while those of M-L-BC were above 95%. Based on the evaluated kinetic and isotherm parameters, the adsorption followed the pseudo-second-order kinetic model (PSO) and the Sips isotherm model, indicating that the adsorption of PFASs primarily occurs via chemical adsorption on the heterogeneous surface of M-L-BC, forming multi-layer adsorption. Additionally, M-L-BC exhibits strong capability in removing PFASs over a wide pH range (3-9). In the presence of coexisting ions, the adsorption efficiency of PFBA is significantly reduced, while other PFASs maintain relatively high levels of adsorption. In the presence of 10mM humic acid, the removal efficiency of short-chain PFASs was notably inhibited, while the effect on long-chain PFASs was less pronounced. Furthermore, M-L-BC demonstrated excellent stability and regeneration performance, maintaining outstanding adsorption efficiency in real water samples and after 5 adsorption-desorption cycles. The results indicated that pore filling electrostatic interaction, hydrogen bonding, and hydrophobic interaction were involved in the adsorption mechanism. Overall, biochar derived from discarded lychee seeds represents a promising and high-quality adsorbent for the effective and sustainable removal of PFASs from water.

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Mouse embryonic stem cells: a novel model to evaluate the neurodevelopmental toxicity of perfluorinated iodine alkanes

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Abstract

Perfluorinated iodine alkanes (PFIs) are a class of perfluorinated substituted straight-chain compounds, containing an even number of carbon atoms, with one or two iodine atoms substituted at one or both ends. As the intermediates in the production of perfluorinated chemicals, the extensive application of PFIs has led to the unintended release and environmental contamination, posing a potential threat to the wildlife and human health. Previous studies have demonstrated that PFIs could exhibit endocrine disrupting effects by specifically binding with estrogen receptors (ERs) and interfering with steroidogenesis, potentially causing environmental health risks. The development of the brain nervous system is related to the health of the whole lifecycle, which is an intricately-regulated hormone-dependent process, and is highly sensitive to the exposure of exogenous endocrine disrupting chemicals (EDCs). Given the typical endocrine disrupting characteristics

of PFIs, whether PFIs have potential neurodevelopmental toxicity is a scientific question of concern. The *in vitro* mouse embryonic stem cell (mESCs) model could be used to investigate the effects of the two typical PFIs on the commitment to neural lineage, hoping to provide the new evidence for the neurodevelopmental toxicities of PFIs, and the related toxicological data may serve well for the evaluation of the environmental risks and health effects of this kind of chemicals.

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Developing a Py-GC/MS Analysis Method for Comprehensive Analysis of PFAS

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Abstract

Per- and polyfluoroalkyl substances (PFAS) have emerged as major environmental pollutants, alongside pharmaceuticals, personal care products, and disinfection byproducts. Because of their environmental persistence, PFAS are frequently detected in environmental samples, with perfluoro octane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) being found in numerous environmental media and human blood during the last decades. Concerns over their persistence and potential harm to human and environmental health have led regulatory efforts in developed countries such as the United States and Europe, with Korea also considering such measures. Given the need for a quick and easy way to determine PFAS in the environment, we propose an integrated PFAS analytical approach based on pyrolysis gas chromatography-mass spectrometry (pyr-GC-MS), which quantifies PFAS in a chemical group rather than individual molecules. The suggested technique uses common target ions from PFAS chemicals such as tetrafluoro ethylene (C_2F_4, m/z=100), pentafluoro cyclopropyl ion ($C_2F_5^+$, m/z = 131) to estimate the overall organic fluorine concentration in the environment. Applying this approach to PFAS analysis allows for quick and simple indirect estimation of environmental PFAS concentrations especially for routine monitoring of PFAS.

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Placental transfer and health risks of legacy and novel per- and polyfluoroalkyl substances near fluorochemical facilities

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Abstract

The levels of legacy per- and polyfluoroalkyl substances (PFAS) have been growing in the environmental matrices and blood of residents living around the fluorochemical industrial park (FIP) in Fuxin of China over the past decade. Although some recent studies have reported occurrence of novel PFAS alternatives in biotic and abiotic matrices near fluorochemical facilities worldwide, little is known about novel PFAS congeners in maternal sera, umbilical cord sera, and placentas from the female residents close to the FIP and their related health risks.

In the present study, 50 paired samples of maternal and cord serum as well as placenta were derived from Fuxin pregnant women at delivery, and 21 target analytes of legacy PFAS in all the samples were analyzed via high-performance liquid chromatography–tandem mass spectrometry (HPLC–MS/MS), revealing that perfluorobutane sulfonate (PFBS), perfluorobutanoic acid (PFBA), and perfluorooctanoic acid (PFOA) were the dominant PFAS contaminants observed in the whole samples. Based upon the suspect screening through high-resolution mass spectrometry (HRMS), 49 novel PFAS assigned to 11 classes were further identified in the Fuxin samples, of which, 20 novel congeners in 4 classes were reported in human blood and placentas for the first time. Moreover, the coefficients for mother-placenta transfer (Rm/p), placenta-newborn transfer (Rp/n), and mother-newborn transfer (Rm/n) of legacy PFAS could be calculated with median values of 1.7, 1.1, and 2.0, respectively, and Rm/p, Rp/n, and Rm/n for each novel PFAS identified were also estimated with the median values of 0.9, 1.2, and 0.8 individually.

Accordingly, novel PFAS contributed 90% of all the legacy and novel PFAS in maternal sera and even occupied 96% of the whole PFAS in both placentas and cord sera. In addition, significant associations were determined among the neonate birth outcomes and serum concentrations of thyroid hormone, sex hormone, and glucocorticoid, together with the levels of certain legacy and novel PFAS in cord sera, potentially posing health risks to newborns in Fuxin.

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Systemic Toxicity Screening of Real-life Mixtures in Poly- and Perfluoroalkyl Substances Detected Consumer Products: An Effect Directed Analysis

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Abstract

The exposure to chemical mixtures in consumer products is a common in daily life, presenting potential systemic hazards to human health. This study aims to bridge the gap in the regulatory framework concerning consumer products by assessing the hazards posed by real-life chemical mixtures. We evaluated the cytotoxicity of real-life mixtures extracted in commonly used consumer products, utilizing six human cell lines representative of systemic organs: liver (HepG2), lung (Beas-2B), brain (SH-SY5Y), immune system (Jurkat), and developmental stages (embryonic stem cells and neural stem cells. Firstly, a targeted chemical analysis of these groups confirmed the presence of significant concentrations of poly- and perfluoroalkyl substances (PFAS). Subsequently, we created artificial mixtures of PFAS at

concentrations matching those found in the consumer products and exposed the same cell lines to these mixtures. The toxicity results of these artificial mixtures were then directly compared with those from real-life product exposures. This comparative analysis revealed that PFAS are major contributors to the toxicity of the mixtures. Our findings underscore the necessity of assessing real-life mixtures in consumer products, providing essential data that could inform regulatory changes and help mitigate environmental and human exposure to hazardous chemicals. Furthermore, this approach enhances scientific comprehension for employing effect-directed analysis on real-life samples, thereby contributing significantly to the implementation of the Green Deal project PANORAMIX.

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Keywords: Real-life mixtures, PFAS, Consumer Products, Effect directed analysis, Mixture Toxicity

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Exterior Building Materials are Sources of Per- and Polyfluoroalkyl substances (PFAS) to the Environment

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Abstract

PFAS are found in over 200 different use categories but we do not know which of those categories contribute significantly to environmental concentrations. We hypothesize that coatings used on exterior building surfaces and outdoor textiles are an important source of PFAS entering the environment. To explore this hypothesis, we followed two steps. First, we developed a combined 1D and 2D diffusion ordered spectroscopy (2D DOSY) fluorine nuclear magnetic resonance (^{19}F-NMR) method to measure total organofluorine (TOF), to distinguish non-polymeric from polymeric PFAS and non-polymeric PFAS composition and determine the major type of PFAS (e.g, fluorotelomer or electrochemical fluorination-based). Liquid or gas chromatography coupled to mass spectrometry (LC-HRMS, GC-MS) analysis were then used to identify specific nonvolatile and volatile PFAS. Second, we assessed changes in PFAS composition in a subset of coatings and outdoor textiles exposed to UV light to simulate weathering. 144 samples analyzed by 1D ^{19}F NMR showed TOF concentrations of 0.1-42, 0.6-2500 and 0.3-74.0, µmol/g in paints, sealants and textiles, respectively. 2D DOSY ^{19}F NMR showed that paints were dominated by 6:2 fluorotelomer (FT) and aromatic trifluoromethyl (Ar-CF_3) based nonpolymeric PFAS, while both side-chain fluorinated polymers (SCFPs) and non-polymers were found in sealants.

LC-HRMS and GC-MS indicated the 6:2 FT non-polymeric PFAS in paints and sealants mainly comprised of 6:2 FT mono-, di-, tri- phosphate esters (6:2 PAP, 6:2 diPAP, 6:2 triPAP) and 6:2 FT di-pyrophosphate. Exposure to UV light either increased the presence of non-polymeric forms consistent with releases from SCFPs or decreased TOF as UV light caused photolytic transformations. These results support the hypothesis that exterior coatings and outdoor textiles can contribute substantial loads of PFAS to the environment.

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Identification of Novel Iodinated Polyfluoroalkyl Ether Acids and other emerging per- and polyfluoroalkyl substances in Soils Using Non-Targeted Molecular Network Method

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Abstract

There is still a vast number of unknown per- and polyfluoroalkyl substances (PFAS) in the environment remains unidentified. Current high-resolution screening methods are still unable to adequately find novel PFAS features without prior structural information. In view of this, a new data-driven algorithm used to calculate the similarity between spectra of PFAS is proposed and applied in generating molecular networks to screen unknown PFAS. Using this approach, 81 PFAS of 12 classes were identified in soil samples collected around an industrial park; several substituted polyfluorinated ether sulfonate (X-PFESA, X=Cl, H, I) have been identified and 12 iodine substituted PFAS are reported for the first time. Standards of four Iodine-substituted polyfluorinated ether sulfonate (I-PFESA) were synthesized for structure confirmation and quantitative analysis, greatly enhancing the understanding of structure and environmental concentration of I-PFAS. Notably, the concentrations of X-PFESA were abnormally high, accounting for 10.8%-94.0% of the total PFAS concentration. Among which, the median concentration of H-PFESA was 63.0 ng/g, far exceeding the median concentrations of legacy perfluoroalkyl carboxylic acids (37.9 ng/g) and legacy perfluoroalkyl sulfonic acid (4.14 ng/g). Through replicating the industrial synthesis route in lab, the environmental source of I-PFESA has been confirmed as a by-product of the production process of 6:2 Cl-PFESA (F53-B) and the pattern of environmental transformation of X-PFESA has also been clarified. According to new PFAS spectra similarity, this study provides new perspectives and a comprehensive understanding for the environmental behavior and transformation of PFAS.

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Pilot-scale removal of PFAS from chromium-plating wastewater by anion exchange resin and activated carbon: Adsorption difference between PFOS and 6:2 fluorotelomer sulfonate

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Abstract

Chromium-plating wastewater is an important source of per- and polyfluoroalkyl substances (PFAS) contamination. Currently, adsorption is considered to be one of the main technologies for the removal of PFAS from wastewater. However, no pilot-scale studies have been conducted to investigate its application in chromium-plating wastewater and the adsorption characteristics of 6:2 fluorotelomer sulfonate (6:2 FTS), the alternative to perfluorooctane sulfonate (PFOS). In this study, we evaluated the removal of PFAS from chromium-plating wastewater by granular activated carbon (GAC) and anion exchange resin (AER) at a pilot-scale. The breakthrough curves of PFOS and 6:2 FTS were similar in GAC columns, but significantly different in AER columns, with PFOS and 6:2 FTS reaching 10% breakthrough at about 45,000 BV and 4,000 BV, respectively. The replacement of 6:2 FTS by PFOS and other coexisting organic substances resulted in the concentrations of 6:2 FTS in the AER effluent reaching up to 3.8 times the influent concentrations. Density functional theory (DFT) calculations showed that the adsorption energy of PFOS on the quaternary amine group of AER was more negative than that of 6:2 FTS, and the weak affinity of AER for 6:2 FTS was closely related to the solvent effect. According to the cost analysis, if 6:2 FTS becomes the target PFAS, AER adsorption will no longer have a cost advantage over GAC adsorption. This study can provide technical support for the adsorptive removal of PFAS from electroplating wastewater and guide the development of efficient adsorbents for PFAS alternatives.

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Occurrence and Fate of Per- and Polyfluoroalkyl Substances (PFAS) in Atmosphere: Size-Dependent Gas-Particle Partitioning, Precipitation Scavenging, and Amplification

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Abstract

Per- and polyfluoroalkyl substances (PFAS) are widely used for various industrial and consumer applications. There is a growing recognition that PFAS have potential to enter the atmospheric

cycling with air masses and entry into the surface of soil and water with atmospheric deposition. However, limited studies on multiphase chemistry of PFAS, as well as complex meteorological conditions and deposition processes, hinder people to fully understand the environmental behaviors and fate of PFAS. Herein, we introduced the environmental factors (e.g. organic matter fraction (f_{om}), ambient temperature) into the understanding for size-dependent gas-particle partitioning (K_{Pi}) and precipitation amplification of PFAS in the atmosphere via the field investigation. Firstly, strong positive relationship was observed between concentration of perfluoroalkyl carboxylic acids (PFCAs) and f_{om} in particle with different size ranges, suggesting f_{om} may be an important factor influencing the size-dependent distribution of PFAS. Secondly, we found that gaseous PFAS tended to transfer into the particles with the ambient temperature decreasing. This trend was likewise showed in negative correlation between K_{Pi} and vapor pressure (P_L) of PFAS. Above results provide new insights into the underlying mechanisms for gas-particle partitioning of PFAS and provide a valuable starting point for the future development of a thermodynamic prediction framework for the environmental fate of PFAS. Furthermore, our results supported that the effectiveness of rainwater in scavenging particle-bound PFAS from atmosphere by washing particles. The decreasing concentration of PFAS in rainwater with the continuous precipitation indicated that below-cloud scavenging might be a primary pathway for incorporation of PFAS into precipitation. In contrast, precipitation was not an effective scavenger for gaseous PFAS and even led to an increase in their concentrations. Therefore, this study emphasizes the significance of precipitation in the cycling and amplification of atmospheric PFAS in environmental multimedia.

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Fatty acid bind proteins are targets for a broad spectrum of organic pollutants

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Abstract

Liver fatty acid binding protein (L-FABP) is known to play a crucial role in regulating the toxicokinetics of per- and polyfluoroalkyl substances (PFAS). We herein unexpectedly discovered that FABPs might be key targets for a much broader of organic pollutants than previously anticipated. In our first study, we synthesized an alkyne chemical probe of triphenyl phosphate. By using chemoproteomics, we identified L-FABP as the selective protein target of triphenyl phosphate which was further validated using recombinant proteins. In the second study, through an affinity selection mass spectrometry approach, we identified multiple chemicals from the ~1200 ToxCast chemical library that bind to L-FABP. Surprisingly, the chemotypes of the newly identified ligands are completely different from those of previously known fatty acid derivative ligands. In the final study, we found that perfluoroether carboxylic acids (PFECAs), rather than legacy PFAS, bind to multiple FABP isoforms with high structural and isoform selectivity. Collectively, our research demonstrates that FABPs are key targets for a broad spectrum of organic

pollutants. Future studies are warranted to clarify the potential toxicological consequences of these binding events.

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6:2 chlorinated polyfluorinated ether sulfonate proved more potent than perfluorooctane sulfonic acid in inducing diabetic kidney disease by regulating PI3K/PDK1/SGK1 signaling pathway

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Abstract

Exposure to perfluoro/polyfluoroalkyl substances (PFASs) is closely associated with the development of diabetes mellitus (DM). Perfluorooctane sulfonic acid (PFOS) is a typical type of PFAS and 6:2 chlorinated polyfluorinated ether sulfonate (F-53B) is an important alternative to PFOS. Diabetic kidney disease (DKD) is one of the most common and serious microvascular complications of DM. To date, the functional significance of F-53B and PFOS in DM and DKD remains unclear. C57BL/6J and db/db mice were exposed to F-53B and PFOS to study the mechanisms of F-53B and PFOS in DM and DKD *in vivo*. Transcriptomics were applied and analyzed between F-53B kidneys and NC kidneys. Mouse podocyte clone 5 (MPC5) cells, mouse mesangial cells (SV40 MES13) cells and human kidney-2 (HK2) cells were utilized to further validate the mechanism *in vitro*. Exposure to F-53B and PFOS resulted in DKD, as evidenced by elevated fasting glucose levels, impaired glucose tolerance, renal impairment, and structural alterationsin renal pathology. Mechanistically, transcriptomics and experimental validation demonstrated that F-53B activates PI3K/PDK1/SGK1 signaling pathway more significantly than PFOS in kidneys and cells. We have demonstrated that F-53B induces diabetic kidney disease by regulating the PI3K/PDK1/SGK1 signaling pathway more significantly than PFOS. The study highlights the critical role of F-53B in managing diabetic kidney disease.

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Effective Defluorination of Hexafluoropropylene Oxide Oligomer Acids under Mild Conditions by UV/Sulfite/Iodide: Mechanisms and Ecotoxicity

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Abstract

It has recently been discovered that HFPO-TA (a processing aid in the production of fluoropolymers) has high levels of bioaccumulation and biotoxicity. Hydrated electrons (e_{aq}^-) have been proposed to be potent nucleophiles that mayde compose PFAS. Unlike previous studies in which the generation of e_{aq}^- was often restricted to anaerobic or highly alkaline environments, in this study, we applied the UV/SO_3^{2-}/I^- process under mild conditions of neutrality, low source chemical demand, and open-air, which achieved effective degradation (81.92%, 0.834 h^{-1}) and defluorination (48.99%, 0.312 h^{-1}) of HFPO-TA. With I^- as the primary source of e_{aq}^-, SO_3^{2-} acting as an I^- regenerator and oxidizing substances scavenger, UV/SO_3^{2-}/I^- outperformed others under mild circumstances. The e_{aq}^- were identified as the main active species by quenching experiments and electron paramagnetic resonance (EPR). During degradation, the first site attacked by e_{aq}^- was the ether bond (C6-O7), followed by the generation of HFPO-DA, TFA, acetic and formic acid. Degradation studies of other HFPOs have shown that the defluorination of HFPOs was accompanied by a clear chain-length correlation. At last, toxicological experiments confirmed the safety of the process. This study updated our understanding of the degradation of newly PFASs and the application of e_{aq}^- mediated photoreductive approaches under mild conditions.

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Optimized Al-Based Electrocoagulation for Effective Removal of Residual Fluoride Ions During Per- and Polyfluoroalkyl Substances (PFASs) Wastewater Treatment

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Abstract

The residual fluorion (F^-) generated during per- and polyfluoroalkyl substances (PFASs) treatment presents a new environmental burden, while minimum attention has been redirected to its removal. In this study, Al-based electrocoagulation (EC) technique was optimized to effectively remove the residual F^- during PFASs wastewater treatment. At EC's optimal operating conditions, it can achieve over 81.7% removal efficiency within 30 min. Furthermore, EC exhibited a stable performance on removing F^- across a wide range of pH (3–11), and could form stable flocs under neutral pH conditions. The in-depth characterization of flocs has revealed the dynamic change of Al-F species along the EC process, and removal mechanisms were proved to be a combination of complexation, ion exchange, hydrogen bonding and precipitation. In addition, the optimized EC showed stable removal efficiency of F^- with the co-existence of multiple PFASs. Hence, we have effectively removed the residual F^- during PFASs wastewater treatment, and provide new insights to better understand the defluorination mechanisms in the EC process.

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Nontarget screening and distribution characteristics of emerging per- and polyfluoroalkyl substances in domestic and semiconductor industrial wastewater at a large scale in China

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Abstract

This study conducted extensive sample collection across China, gathering influent and effluent from typical wastewater treatment plants (WWTPs) in 10 major cities, as well as wastewater from various manufacturing stages at large semiconductor factories located in Beijing, Shanghai, and Ningbo. The all-in-one strategy combining target, suspect screening, and nontarget screening was employed to identify emerging PFAS and explore their distribution patterns. A total of 81 PFAS, categorized into 25 classes with confidence level≥3, were identified. All PFAS were reported for the first time in wastewater from the semiconductor industry in Chinese mainland. Moreover, 14 classes of PFAS, including multiple hydro substituted perfluoroalkyl carboxylic acids (mH-PFCAs), ether-substituted PFCAs (OPFCAs) derivatives, and perfluoroalkyl alcohols (PAs) derivatives, were reported for the first time in semiconductor wastewater. In semiconductor industry wastewater, the highest ΣPFAS concentration (target+nontarget) far exceeded that found in domestic wastewater, reaching up to 12.4 μg/L. Short-chain homologues such as perfluorobutanoic acid (PFBA, 1.20 μg/L), H-PFCAs (n=3-4, 0.647 μg/L), OPFCAs (n=2-4, 3.77 μg/L), and PAs (n=2-3, 0.825 μg/L) were the dominant PFAS. This suggests a significant shift towards the application of short-chain PFAS substitutes in the semiconductor industry. Further analysis of the distribution characteristics of emerging PFAS in semiconductor wastewater reveals distinct patterns in the composition of PFAS with different structural features across various regions. OPFCAs derivatives and PAs derivatives were predominantly found only in semiconductor wastewater from Beijing, with concentrations reaching up to 7.7 μg/L and 2.3 μg/L, respectively. Conversely, semiconductor wastewater from Shanghai predominantly contained a series of mH-PFCAs (0.847 μg/L), while semiconductor wastewater from Ningbo showed almost no detection of emerging PFAS with high concentrations. This suggests that there are variations in the application of emerging PFAS among different semiconductor manufacturing facilities. This study is the first to focus on and reveal the replacement applications of emerging PFAS in the semiconductor industry in Chinese mainland, providing important reference for targeted water treatment of semiconductor wastewater in the future.

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Emerging Per- and Polyfluoroalkyl Ether Carboxylic Acids: Identifacation, Exposure Pathway, and Health Effects

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Abstract

PFAS are a group of emerging pollutants that have received considerable international attention. Since the successive listing of perfluorooctane sulfonate (PFOS), perfluorooctanoic acid (PFOA), perfluorohexane sulfonate (PFHxS), and their related compounds in the Stockholm Convention on Persistent Organic Pollutants, research on PFAS exposure and hazards has become a frontier issue in the global environmental science community. As the largest producer of PFAS, China is in the process of gradually replacing PFOA and PFOS with new types of PFAS compounds. The coexistence of new and legacy PFAS in the environment has complicated pollution issues. Therefore, identifying these emerging PFAS, and further clarifying their baseline exposure and health effects are urgently needed to strengthen the management of emerging pollutants and continuously improve our environment. In this report, we primarily present the research findings of our group over the past five years concerning the identification, exposure pathways, and health effects of new PFAS. By developing multi-functional non-targeted analysis for PFAS, we identified a series of previously unreported per- and polyfluoroether carboxylic acids (PFECAs) and established highly sensitive quantitative methods to unveil their environmental distribution and temporal trends. Furthermore, the exposure pathways of PFECAs in humans differ from those of traditional PFOA/PFOS. Plant-based foods, such as cereals and vegetables, are more significant sources of intake compared to aquatic foods. Emerging epidemiological evidence indicates that PFECA exposure in adults is associated with elevated lipid levels, impaired liver and kidney function, and reduced relative telomere length. Based on ToxPi modeling, some PFECAs may already have become prioritized PFAS in the environment due to their ubiquitous detection, high concentrations, and relatively high risks to ecological and human health.

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An attempt on microbial transformation of Per- and plolyfluoroalkyl substances under anaerobic conditions

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Abstract

Abstract

Per- and polyfluoroalkyl substances (PFAS) constitute a group of synthetic alkyl compounds where hydrogen atoms linked to carbon atoms are wholly or partially substituted by fluorine. PFAS are known for their remarkable hydrophobic properties, exceptional thermal stability, and chemical inertness. Currently, PFAS are extensively employed in both industrial and civilian applications, spanning the realms of chemistry, textiles, leather, firefighting, and everyday detergents. All these compounds are continually discharged into the environment, posing potential threats to organisms and exerting environmental pressures.

In this study, typical PFAS were selected and contaminated site samples were used as inoculation sources for domestication in a specific anaerobic experimental environment, and finally stable defluorinated functional flora was obtained.

Key words: Per- and polyfluoroalkyl substances; Microbial anaerobic reduction; Organohalide-Respiring Bacteria.

Results & discussion

The contanminated soil samples are inoculated into anaerobic media to cultivate defluorinating microbial communities.In the enrichment, PFOS; PFOA; F-53B and Gen-X were served as the electron acceptor in the defluorinating microbial community. Employing lactate or acetate as the carbon source and H2 as the electron donor, the sutdy observed the removal of PFAS. This removal was marked not only by alterations in the concentrations of perfluoro carboxylic acids and perfluoro sulfonic acid compounds within the C4-C7 range but also by variations in fluoride ion levels across different inoculation sources.

The microbial community showed that Firmicutes, Chloroflexi, and Proteobacteria microorganisms play a significant role as the primary functional microbial populations in the anaerobic degradation of PFAS. A multitude of Organohalide-Respiring Bacteria (OHRB) exhibit an obligate reliance on organohalogens, like PCE, for their anaerobic metabolism at the Phylum Chloroflexi. This suggests these microorganisms may contribute to the defluorination process. Furthermore, Methanothrix and Desulfovibrio, which have been detected in the enrichment, have demonstrated their ability to participate in the anaerobic metabolism of organohalogens. Consequently, their involvement may also be pertinent to the removal of PFAS.

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Legacy and Emerging Poly- and Perfluoroalkyl Substances in typical marine mammals from East China Sea: Temporal Trends and Tissue-Specific Accumulation

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Abstract

Poly- and perfluoroalkyl substances (PFASs) are diverse and their contamination characteristics are unclear. Perfluoroalkyl sulfonates (PFSAs), perfluoroalkyl carboxylates (PFCAs), and emerging alternatives and precursors of these compounds were determined in tissues of stranded finless porpoise and whales collected from East China Sea. The results showed that hepatic concentrations of emerging PFASs and some precursors, including chlorinated polyfluorinated ether sulfonates (Cl-PFESAs) as well as fluorotelomer carboxylates (FTCAs) and fluorotelomer sulfonates (FTSAs) were frequently detected in marine mammals. Study on temporal trend indicate The concentrations of 6:2 Cl-PFESA and some short-chain PFASs increased with time between 2009−2010 and 2018−2019. Further, concentrations of legacy PFAS perfluorooctanoate (PFOA) showed a declining trend in finless porpoise, whereas perfluorooctanesulfonate (PFOS) and its precursor (i.e., perfluorooctane sulfonamide [FOSA]) showed an increasing trend with time between 2009−2010 and 2018−2019. Analysis of PFASs in nine different tissues/organs of marine mammal revealed a similar distribution pattern between 6:2 Cl-PFESA and PFOS; however, the tissue distribution patterns differed between PFOA and their alternatives. The estimates of body burdens of PFASs in marine mammals suggested comparable accumulation of PFAS alternatives and legacy PFSAs and PFCAs. This study provides novel information on temporal trends and tissue distribution of emerging PFASs in marine mammals in China.

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Spatial and Temporal Variations of Legacy and Novel Per- and Polyfluoroalkyl Substances (PFASs) in Surface Soils across China during 2002−2021

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Abstract

China aims to actively control the contamination of the globally concerning per- and polyfluoroalkyl substances (PFASs). Evaluation of the current situation can provide a critical reference point for tracking the effectiveness of future progress. Herein, we present the first comprehensive assessment of the spatial and temporal variations of 20 legacy and 54 novel PFASs in Chinese background soils during 2002−2021. Novel PFASs was extensively detected in 98.4% of the samples, with 21 species being first reported, which greatly facilitated the appointment of diverse emission sources that aligned with local industrial structures. However, legacy PFASs still dominated the $\sum_{74}$PFAS profile (median 0.51 ng/g, 0.050−8.33 ng/g). The spatial heterogeneity of soil PFASs was positively driven by economic development and atmospheric deposition but counteracted by shortwave irradiation, enabling the establishment of predictive models to project the national distribution and temporal trends. Elevated PFASs levels were predominantly distributed in the more industrialized eastern and southern regions, as well as other coastal areas with greater precipitations. $\sum_{74}$PFAS was estimated to increase by 0.013 ng/(g·year) over 2002−2021, which would continue alongside economy growth, albeit with greater contributions from

novel alternatives. Our work provides comprehensive baseline and predictive data to inform policies toward PFASs control in China.

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Unravel the defluorination mechanism and structural dependence of per- and polyfluoroalkyl substances (PFAS) by UV/sulfite

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Abstract

Per- and polyfluoroalkyl substances (PFAS) are globally concerning persistent contaminants with various adverse effects. Producing alternatives with retained functionality but minimized adverse impact to the environment and remediation cost serves as a sustainable way to avoid regretful substitution as well as to resolve PFAS contamination. Destructive approaches with complete defluorination of PFAS are thus desired at the emission source. Hydrated electron-based approaches have demonstrated degradability for a wide range of PFAS under ambient conditions, yet the underlying mechanism remains unresolved. We use hydrated electron produced from UV irradiation of aqueous sulfite to initiate reductive hydrodefluorination and break C−F directly under ambient conditions for 42 PFAS in 9 classes. Density functional theory calculations were performed to unravel the structural dependent reactivity and depict the key reaction pathways. In particular, we found PFAS with favored electron transfer accepting moieties (C−Cl, −C=C−, COO^-, and $-(CF_2)_{n\geq 6}$) will promote the degradation by hydrated electron. Of the 35 PFAS achieving complete defluorination, the reaction pathways can be interpreted through two patterns: initial attack of hydrated electrons at the α-C in CF_2COO^- or in the middle of $(CF_2)_n$, resolving the discrepant intermediate profiles and potential delays in defluorination. By achieving complete destruction for most PFAS structures, our results provide practical treatment and remediation technologies to solve the global PFAS control challenge. The unraveled mechanism provides opportunities to establish structure-reactivity prediction models and to design green alternatives with prompt degradability.

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"Machine learning assisted single-molecule sensing of per- and polyfluoroalkyl carboxylic acids isomers"

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Abstract

Emerging pollutants, characterized by their exclusion from current regulatory frameworks, pose significant environmental and health risks due to their widespread distribution, environmental persistence, and potential for bioaccumulation. Precise monitoring is pivotal for the informed management and remediation of these novel contaminants. Single-entity environmental analysis based on nanopore electrochemical sensing introduces an innovative approach to the detection of emerging pollutants. The measurement principle of this method relies on the characteristic currents produced by individual analyte traverse a nanopore, analysis the block currents for qualitative, and statistic the occurrence frequency of electrical signals for quantitative assessments. In this study, we developed a single-molecule monitoring technique using biological nanopores, with perfluorinated and polyfluorocarboxylic acid compounds (PFCA) as the test subjects. By anchoring the PFCA within the nanopore channel of the Aerolysin protein using a peptide probe, we established a structure-activity relationship between the characteristic current intensity and the molecular volume of the analytes. This relationship facilitated the precise prediction of 5 polyfluorinated compounds. Multi-dimensional features of the sample current signal, such as standard deviation, peak-to-peak value, skewness, and kurtosis, were extracted and integrated with a machine learning model, enabling the accurate detection of six types and 17 PFCA isomers with a comprehensive identification accuracy of 99%. Furthermore, the detection limit for trifluoroacetic acid, an ultrashort-chain PFCA, was reduced to 50 ng·L-1, comparable to the state-of-the-art performance.

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Unravel the in-source fragmentation pattern of per- and polyfluoroalkyl substances during analysis by liquid chromatography-high resolution mass spectrometry

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Abstract

In-source fragmentation (ISF) cannot be completely avoided during electrospray ionization of PFAS when analyzed by LC/MS. Despite the extra structural information, ISF results in reduced response of molecular ions, interference of nontarget analysis, and false identification of degradation products that may lead to misinterpretation of reaction mechanisms. Thus, a total of 82 PFASs covering 12 classes were systematically analyzed to identify the structures that undergo ISF and to characterize the fragmentation mechanism. Six classes with carboxylate group, H substitution, Cl substitution, and ether bond were

recognized to undergo significant fragmentation, which varied in fragmentation ratios and pathways. Neutral loss of CO_2 was consistently observed for PFAS containing carboxylate group (-COO^-), with reduced fragmentation ratio for structure with longer perfluorocarbon chain. Whereas HF loss by β-elimination through 6 membered ring with H_2O involved was frequently found when one CH moiety appears in the structure. Terminal CO_2HF loss was found through McLafferty rearrangement for PFdiCAs. For the structures with CH_2 moieties, HF loss by $H^{\cdots}F$ bridge through 6 membered ring was identified. The ether bond was found to be more vulnerable than carboxylate group during electrospray ionization, resulting in low response or absence of molecular ions for ether-PFAS. The calculated bond dissociation energy can only explain the varied fragmentation ratio for carboxylic PFAS, demonstrating the complex mechanism within electrospray ionization. The results provide valuable information to avoid mis-annotation during nontarget analysis of PFAS and benefit product identification in degradation mechanism studies.

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Spatiotemporal variations of emerging and legacy per- and poly-fluoroalkyl substances in surface water of the Bohai Sea

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Abstract

Perfluoroalkyl and polyfluoroalkyl substances (PFAS) have arouse growing concerning due their widely distribution in environment and adverse health effects to ecosystem and human health. Certain PFAS such as PFOA and PFOS have been listed in POPs and thus subject to global restriction in use and produce, in the meanwhile alternatives have been introduced. Emerging perfluorinated compounds such as perfluorinated ether carboxylic acids (PFECAs) have been introduced as alternatives for PFOA, and been widely detected in the coastal and marine environment. In this study, 36 PFAS were examined in the surface water of the Bohai Sea, and the constituent concentrations and compositions of these PFAS were analysed, the spatial distributions were investigated, and the quarterly variations of these PFAS were observed. The concentration of PFAS in the surface water of the Bohai Sea ranged from 15.28 ~ 217.30 ng/L (mean 50.23 ± 30.95 ng/L). The proportions of legacy PFAS and emerging PFAS in the Bohai Sea water were 73.7% and 26.3%, respectively. The highest concentration was perfluorooctanoic acid (PFOA), followed by perfluoro-(3,5-dioxahexanoic) acid (PFO2HxA). Laizhou Bay was the most serious pollution area in the Bohai Sea with quite high concentrations of PFAS. The seasonal distribution showed the highest PFAS level in autumn and the lowest PFAS pollution in summer. The main factors for the low concentration in summer include ocean currents dispersion and rainfall dilution. In the Bohai Sea, the total PFAS concentration has shown an increasing trend and then decreasing trend in recent years, especially for PFOA, with a significant decrease in 2022. However, at the same time, its alternative, PFBA, is showing a rising trend in both

concentration and share. This study increases our knowledge of the pollution of novel pollutants in the Bohai Sea region and provides an understanding of the changes in legacy PFAS.

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Dynamic Characteristics of Per-and Polyfluoroalkyl Substances UnderTidal Influencing in the Estuary

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Abstract

The transport of contaminants in estuaries under tidal influencing is complex. Meanwhile, size fractionation of suspended particulate matter (SPM) influences the mobility and bioavailability of contaminants. Here, we conducted a high-resolution continuous sampling over two tidal cycles in an estuarine maximum turbidity zone (MTZ) with the highest SPM concentrations. Based on the SPM fractionation, we studied dynamic characteristics of dissolved and particulate per- and polyfluoroalkyl substances (PFAS) of different sizes under tidal influencing. The results showed that the predominant SPM size was 1-31 μm (75%, mainly 10-31 μm), but the PFAS tended to be adsorbed by0.22-1μm (60%) and >31 μm (37%) fractions. The PFAS concentration of 1-31 μm increased during flood tides, while the opposite happened during ebb tides. During the rapid flood, SPM (>31 μm) concentration increased but PFAS concentration decreased related to the sediment resuspension. Combined with the Regional Ocean Modeling System (ROMS) model, the daily variation of PFAS flux based on tides was caculated. This study first highlights the varying SPM sizes on PFAS transport in the estuary and provides precise daily flux variation with the hydrodynamic model.

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PFAS in the Environment: A New Method for Analyzing PFAS in Soil

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Abstract

Since the accidental discovery of Teflon in 1938 by Dr. Roy J. Plunkett of DuPont, the water repellency and high surface activity of Teflon-related chemical substances, such as per- and polyfluoroalkyl substances (PFAS), have piqued the interest of the chemical industry due to their excellent chemical stability. Consequently, the use of such related products has recently expanded. However, with the advancement of science, ultra-trace analysis of chemical substances with techniques such as LC-MS/MS has become possible, revealing the adverse effects of PFAS.

The most common PFAS, perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA), are transported long distances through air and water and can cause potential toxicity in humans. Hence, these substances have become a significant concern, especially for human health. Moreover, numerous alternatives to PFAS are being developed, raising concerns about the potential toxicity of these alternatives as well.

While there are ISO and EPA methods for PFAS analysis of water quality, there are very few methods for soil, and those methods have not been verified. In particular, it is extremely difficult to analyze multi-component PFAS from soils with high carbon content, such as volcanic ash soils, making it a significant challenge.

The National Agriculture and Food Research Organization (NARO) has successfully developed the most cost-effective, time-efficient, and simple method for the simultaneous analysis of 30 PFAS in soil. This method will also contribute to the Environmental Contamination and Control Technology of Per- and Polyfluoroalkyl Substances (PFAS).

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Study on the efficient degradation of Per-and Polyfluoroalkyl Substances

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Abstract

Per-and Polyfluoroalkyl Substances (PFASs) are a class of fully fluorinated organic compounds with strong persistence, resistance to biodegradation, endocrine disruption, and immunotoxicity, which have attracted widespread attention and have been included in the Action Plan for New Pollutant Control. PFASs are commonly present in industrial production processes in many countries, such as electrolytic aluminum, fluorine chemicals, semiconductor processing, and coal combustion. Among them, the electrolytic aluminum industry is the main source of CF4 emissions, with an annual emission of about 80000 tons, accounting for about 60% of the total social emissions. CF4 entering the human body will have a certain impact on the cardiovascular system, and its emissions in the atmosphere will cause serious greenhouse effects, with a greenhouse effect value 7390 times that of carbon dioxide. However, PFASs

have strong chemical and thermal stability due to their extremely high C-F bond energy and symmetrical structure, making them difficult to degrade efficiently. Therefore, how to achieve efficient and stable degradation of PFASs gas pollutants is a key scientific challenge that urgently needs to be solved in the treatment of atmospheric pollutants. We propose a charge localization strategy to address the issue of highly symmetrical and non-polar PFASs pollutant molecules, which are difficult to adsorb. By constructing positive charge aggregation sites, the adsorption of CF4 on the catalyst surface is enhanced [1]; A multi-point synergistic strategy has been developed to address the issue of high C-F bond energy and difficulty in breaking bonds in PFASs pollutants. Through the synergistic effect of proton acid and charge localized sites, the stretching and breaking of C-F bonds are promoted, achieving efficient and complete degradation of CF4; Aiming at the problem of strong binding force between catalyst and F and susceptibility to F poisoning, a strategy for in-situ generation of proton acid groups has been developed to promote defluorination and regeneration of active sites, achieving efficient and stable degradation of CF4.

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Occurrence, transport and adsorptive removal of PFAS in electroplating wastewaters

shubo deng

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Abstract

Electroplating industry is an important source of per- and polyfluoroalkyl substances (PFAS) contamination. In this study, we investigated typical electroplating parks and conducted the first full-scale removal of PFAS from chromium-plating wastewater using pore-enlarged granular activated carbon (GAC) and hydrophobic anion exchange resin (AER). The results showed that 6:2 fluorotelomer sulfonate (6:2 FTS) gradually replaced perfluorooctane sulfonate (PFOS) in China's electroplating industry. Conventional wastewater treatment processes cannot effectively remove 6:2 FTS, but the special air flotation process resulted in over 60% of PFOS entering the chromium sludge cake. Based on full-scale evaluation, GAC and AER adsorption were feasible technologies for removing PFAS from chromium-plating wastewater, reducing PFAS discharge by 5,030-8,000 kg/year. This study reveals the current status of PFAS contamination in China's electroplating industry and provides feasible technologies for PFAS control.

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Comprehensive Analysis of PFAS Contamination: Novel Findings and Implications for Future Research

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Abstract

Per- and polyfluoroalkyl substances (PFASs) contamination from Australian firefighting training grounds has led to pollution of groundwater and nearby farmlands, potentially exposing humans, farm animals, and wildlife to complex PFAS mixtures from aqueous film-forming foams (AFFFs). To better characterise human and environmental risk, suspect-screening and nontarget analysis (NTA) was used to identify novel PFAS classes in pooled whole blood and serum samples from cattle exposed to AFFF-contaminated groundwater. Thirty PFASs were identified including three novel compounds and several perfluoroalkyl sulfonamides predominantly in whole blood. Novel PFASs were also identified in groundwater samples contaminated from historic AFFF use. Eighty-eight PFASs were identified in both passive samplers and grab samples, dominated by sulfonate derivatives and sulfonamide-derived precursors. Several classes of ultrashort-chain PFASs were detected for the first time in Australian tap, surface and ground waters, along with several transformation products and two new PFASs. Our findings suggest that current analytical approaches do not comprehensively address the range of PFASs present in these systems, and the potential risk from all PFASs present is likely underestimated. Future studies should include whole-blood analysis with high-resolution mass spectrometry to understand the true extent of PFAS exposure and broaden the scope of PFASs monitored in water systems impacted by AFFFs.

29. Environmental Behaviour and Effects of Emerging Flame Retardants and Plasticizers

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Migration of Phthalate Acid Esters from Plastic Mulch Films and Their Degradation in Response to Ultraviolet Irradiation and Contrasting Soil Conditions

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Abstract

Phthalate acid esters (PAEs) are commonly used plastic additives, which are now ubiquitous in agricultural soils due to plastic being an integral part of intensive agriculture. Dibutyl phthalate (DBP) and di(2-ethylhexyl) phthalate (DEHP) are two of the most common PAEs found in soils, due to the widespread use of plastic mulch films. Degradation of PAEs is primarily attributed to photodegradation and microbial decomposition, yet the impact of the plastic matrix on PAE degradation rates in differing soil conditions is poorly understood. Using ^{14}C-labelled DBP and DEHP incorporated into polyvinyl chloride film, we studied PAE loss and complete degradation rate in soil by monitoring the evolution

of ^{14}C-labelled CO_2. Ultraviolet irradiation, stimulation of microbial activity via organic substrate addition (accelerated bioremediation) and rhizoremediation aimed to accelerate PAEs degradation.

We showed that migration of PAEs from the plastic matrix into soil represents a key rate-limiting step in their bioavailability and subsequent degradation. Incorporating PAEs into plastic film significantly decreased their degradation rates in soil, from 79 % to 21 % and 9 % to <1 % for DBP and DEHP, respectively, over four months, when compared to direct application of PAEs. We attribute the slower degradation of DEHP to its intrinsic low solubility in water compared to DBP. Furthermore, exposure to ultraviolet radiation accelerated PAE mineralisation two-fold, while turnover was also promoted four-fold by the addition of biosolids. However, the presence of plants (rhizoremediation) and other organic residues (straw, grass) failed to promote degradation in soil.

We conclude that the prevailing soil conditions alter the behaviour and fate of individual PAEs in soil but they may persist in soil for much longer than previously thought due to physical trapping within the plastic matrix. This suggests that PAEs may be released from plastics over very long time periods, leading to increasing levels of contamination associated with repeated plastic use.

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Suspect and Nontarget Screening of Organic Pollutants in Purified-, Bottled-, and Tap Water, Using Liquid Chromatography-High Resolution Mass Spectrometry:Involving Flame Retardants, Plasticizers, etc

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Abstract

Concerns over organic pollutants (OPs) in drinking water are increasing. Certain OPs exhibit persistence in aquatic environments, posing significant challenges for their elimination using conventional tap-water treatment methods. Alternative pathways, including water purifiers, cause the potential human exposure to OPs through drinking water. In our previous work, water purified by 12 water purifiers on campus was studied. In this study, four sets of samples were collected: (1) the tap water and water purified by two purifiers on campus for 12 weeks (once a week) ; (2) 21 purified water from public buildings; and (3) 20 bottled water from four water sources; (4) Sonication water-extract of the filter element (cut into different parts) of the water purifier. All samples were pretreated via solid-phase extraction (SPE) and then analyzed to identify OPs through suspect and nontarget screening using liquid chromatography high-resolution mass spectrometry (LC-HRMS). The results show that 18 organic pollutants in different classes have been tentatively identified by MS/MS spectral pattern matching or fragmentation diagnosis. Among them, 16 OPs were tentatively confirmed by standards, and further, 7 OPs were quantified. Briefly, we found four organophosphorus flame retardants (OPFRs) in purified water (up to 1900 ng/L)

and tap water (up to 120 ng/L), e.g., tris (2-chloroethyl) phosphate (TCEP). The plasticizer tributyl citrate (TBC) and the plastic derivative, 1,8-diazacyclotetradecane-2,9-dione (aminohexanoate cyclic dimer, AHCD), were tentatively identified in the purified water. The herbicide hexazinone and the antifungal fluconazole were found in tap water (during 12 weeks, DF=100%). The antifungal fluconazole (DF=70%) and two OPFRs (up to 50ng/L) were found in bottled water. One OPFR, TBC, and 2-hydroxybenzothiazole (used in the rubber industry) were found in the water extract of the purifier filter O-ring. Interestingly, we found that the detected concentration of OPFRs decreased significantly in water purifiers that had been recently maintained, while the detected peak area of AHCD increased significantly. In previous research, OPFRs were found in the O-ring and filter head of the water purifier, while AHCD was derived from the polyamide. Hexazinone and fluconazole were found in tap water and rivers. In conclusion, OPs identified via suspect and nontarget screening can serve as potential targets for drinking water quality monitoring.

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Toxic effects and mechanisms of tri-n-butyl phosphate on the development of zebrafish embryos

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Abstract

As a widely used flame retardant, tri-n-butyl phosphate (TnBP) is frequently detected in water environment and biological samples all over the world. In this study, multiple exposure times (0.2-0.75, 0.75-2.25, 2.25-5.25, 0.2-120, 0.75-120, 2.25-120, and 5.25-120 hpf) and different exposure concentrations (0, 0.625, 1.25, 2.5, 5 and 10 mg/L) were selected, and the aims were to investigate the effects of TnBP on the bioaccumulation, sensitive window, growth and development of zebrafish embryos, the swimming behavior, the apoptosis and the expression of related genes. The results showed that the enrichment rate of TnBP decreased with the prolongation of exposure time in embryos, but the TnBP content decreased significantly in larvae. The sensitivity window of TnBP to zebrafish embryos was 0-0.75 hpf (zygote). TnBP exposure resulted in acute developmental toxicity of zebrafish embryos and significant growth inhibition. The 72 hpf heart rate, 72 hpf hatching rate and 120 hpf body length of zebrafish embryos decreased significantly, the mortality of 120 hpf increased significantly, and the average swimming speed of 120 hpf larvae decreased significantly. The time of death of zebrafish embryos exposed to TnBP was mainly 4-10 hpf. The results of acridine orange (AO) staining and TUNEL detection showed that the apoptotic fluorescence area of 4 hpf zebrafish embryos was significantly increased. TnBP significantly increased Caspase-3 activity in 4 hpf zebrafish embryos and interfered with the expression of apoptosis-related genes. The relative expression levels of *Caspase-3*, *Caspase-8* and *Caspase-9* genes were significantly up-regulated, and the

expression ratio of *Bcl-2* to *Bax* was significantly lymphocyte. The results showed that TnBP could induce apoptosis in 4 hpf zebrafish embryos by regulating the expression of *Bax* and *Bcl-2* genes and Caspase-dependent apoptosis pathway.

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Ornamental Houseplants as Potential Biosamplers for Indoor Pollution of Organophosphorus Flame Retardants

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Abstract

Study on the plants used as biosamplers of airborne semivolatile organic compounds (SVOCs) in the environment remains limited. Furthermore, the contributions of root uptake and foliar absorption on the accumulation of SVOCs within plants are still unclear. Here, we investigated the occurrence, composition, and partitioning behaviors of organophosphorus flame retardants (OPFRs) in indoor dust, air, and ornamental plants to evaluate the possibility of using houseplants as indoor biosamplers of OPFRs. Significant correlation was found between the concentrations of several OPFRs in indoor air and plants, suggesting that ornamental plants can be used as a sentinel for certain OPFRs in the indoor air. We developed a predictive model to assess the partitioning coefficients of OPFRs between indoor air and plant. The lipid content in leaf cuticle instead of leaf organic matter was used to improve the accuracy and reliability of this assessment. The estimated air concentrations were generally comparable with these measured concentrations. We also investigated the contributions of root and foliar (i.e., both gas and particle) uptake pathways to indoor ornamental plants for OPFRs via pot and hydroponic control experiments. The contributions of root uptake to the chemicals in soil cultured plants ranged from 47.5% to 88.5%. We used binary first-order mass conservation equations to calculate the contributions of foliage uptake via gaseous and particle phases to the chemicals with similar K_{ow} in plant leaves. This study suggested that indoor ornamental plants can be potentially used as the biosamplers of SVOCs in the indoor environment. We also provided a novel method for calculating the ratios of different uptake pathways for plants.

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Foliar Exposure of Organophosphate Esters: Mechanisms of Penetration, Transfer, and Multiple Impacts

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Abstract

Organophosphate esters (OPEs) have been frequently detected in plants through foliar spraying and rainwater. The fate of OPEs is affected by their location within the plant and the uptake pathways of these compounds by plants. However, few studies have focused on the uptake pathways, distribution and penetration from the leaf surface and translocation of OPEs in plants following foliar exposure. Herein, to investigate the foliar uptake, accumulation and translocation mechanisms of OPEs in plant, the cucumber (*Cucumis sativus*) and *Lonicera maackii* were selected for OPEs exposure via foliar exposure under control conditions. The results showed that OPEs with higher hydrophilicity tended to reach the mesophyll by stomata (log $K_{ow} \leq 1.44$), and OPEs with log $K_{ow} \leq 3.6$ could enter the mesophyll through aqueous pores when leaf surface humidity increased. Moderately hydrophobic OPEs, such as tris (2-chloroisopropyl) phosphate (TCPP, log $K_{ow} = 2.59$), were more likely to move not only from the cuticle to the mesophyll but also from the mesophyll to the phloem. Strongly hydrophobic OPEs primarily penetrated through lipophilic channels and were difficult to desorb from the cuticle. The penetration and distribution of OPEs from cuticle to mesophyll were influenced by physicochemical property (log K_{ow}, log K_{cw} and molecular volume) of OPEs as well as the compounds (wax, cutin, cutan and polysaccharide) in the cuticles. Young tissue was the primary site for OPEs accumulation after foliar exposure, indicating that growing and developing tissues, such as fruits, may accumulate higher levels of OPEs. These findings contribute to our understanding of the foliar uptake and translocation mechanisms of OPEs by plant.

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Tris(1,3-dichloro-2-propyl) Phosphate Inhibits Early Embryonic Development by Binding to Gsk-3β Protein in ZebrafishZichen Yu, Chunsheng Liu*China University of Geosciences, Wuhan

ZiChen, Yongkang, Ren, Yongjie, Boqun, Liqin, Chunsheng Yu, Zhang, Kong, Xiao, Li, Yu, Liu

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Abstract

Recently, several studies have reported that exposure to tris(1,3-dichloro-2-propyl) phosphate (TDCIPP) results in abnormal development of zebrafish embryos in blastocyst and gastrula stages, but molecular mechanisms are still not clear. This lacking strongly affects the interspecific extrapolation of embryonic toxicity induced by TDCIPP and hazard evaluation. In this study, zebrafish embryos were exposed to 100, 500 or 1000 μg/L TDCIPP, and 6-

bromoindirubin-3'-oxime (BIO, 35.62 μg/L) was used as a positive control. Results demonstrated that treatment with TDCIPP or BIO caused an abnormal stacking of blastomere cells in mid blastula transition (MBT) stage, and subsequently resulted in epiboly delay of zebrafish embryos. TDCIPP and BIO up-regulated the expression of β-catenin protein and increased its accumulation in nuclei of embryonic cells. This accumulation was considered as a driver for early embryonic developmental toxicity of TDCIPP. Furthermore, TDCIPP and BIO partly shared the same modes of action, and both of them could bind to Gsk-3β protein, and then decreased the phosphorylation level of Gsk-3β in TYR·216 site and lastly inhibited the activity of Gsk-3β kinase, which was responsible for the increased concentrations of β-catenin protein in embryonic cells and accumulation in nuclei. Our findings provide new mechanisms for clarifying the early embryonic developmental toxicity of TDCIPP in zebrafish.

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Genotoxicity screening of organophosphate ester flame retardants using machine learning-based quantitative structure-activity relationship (QSAR) models

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Abstract

As the utilization of polybrominated diphenyl ethers (PBDEs) and the broader category of organohalogen flame retardants decreases, the use of organophosphate ester flame retardants (OPFRs) is on the rise. However, their toxicity mechanisms related to genotoxicity remain unknown. Recently, machine learning models have demonstrated the feasibility of efficiently identifying potential toxicity mechanisms of diverse environmental chemicals. In response, this study aimed to screen the potential genotoxic effects of emerging OPFRs using machine learning-based quantitative structure-activity relationship (QSAR) models. Firstly, we compiled a set of OPFRs from the literature. Secondly, we collected genotoxicity data based on OECD test guidelines 471 (Bacterial reverse mutation test) and 473 (In vitro mammalian chromosome aberration test) from the OECD eChemPortal database. Based on these datasets, five algorithms (gradient boosting tree, random forest, multilayer perceptron network, logistic regression, and naïve Bayes) and five molecular fingerprint representations of the chemical structure (MACCS, Morgan, Layered, RDKit, and Pattern) were used to train machine learning models. Finally, the best-performing models, which achieved the highest F1 scores, were selected and used to screen the OPFRs. Among the 49 OPFRs, a few chemicals were predicted to be active by the genotoxicity prediction models. However, many of them showed activity in genotoxicity-related ToxCast bioassays. These chemicals may have the potential for genotoxicity, thus more in-depth assessment is needed. Further experimental evaluation of these chemicals is in progress.

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Key words: Organophosphate flame retardants (OPFRs), genotoxicity, Quantitative structure-activity relationship (QSAR), Machine learning

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A Multifaceted Approach for Assessing Developmental and Neurotoxicity of Bisphenol A and Its Alternatives using Adverse Outcome Pathway (AOP)

Keon Kang, Siyeol Ahn, Jaeseong Jeong, Jinhee Choi

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Abstract

The need for safer alternatives to bisphenol A (BPA) has emerged as health risks associated with it have been identified. Before alternatives can be deemed safe, toxicity assessments must be conducted. This study aims to develop a battery of assays based on the adverse outcome pathway (AOP) framework to evaluate the developmental neurotoxicity (DNT) of BPA and its alternatives. Initially, we screened consumer products containing BPA, bisphenol F (BPF), and bisphenol S (BPS) using the Consumer Product Information Database (CPID), the Chemical and Products Database (CPDat), and the Korean Ecolife database. Subsequently, we constructed an AOP network for DNT using AOP-Wiki and existing literature, linking specific in vitro and in vivo assays to this network to develop a comprehensive battery of assays for evaluating DNT. Screening with human embryonic and neural stem cells for BPA and its alternatives revealed effects on intracellular calcium flux and oxidative stress. Furthermore, the alternatives demonstrated similar adverse effects to BPA, affecting key markers such as IL-6 and BDNF expression. Subsequent testing involved wild-type and mutant strains of Caenorhabditis elegans (ngl-1 and nrx-1), with BPA significantly affecting the behavior of both strains. The relationships between key events were refined using a Bayesian network based on the experimental results. Comparative toxicity was assessed based on the AOP framework, and BPF was found not to be a safe alternative to BPA in terms of DNT. This combined in silico, in vitro, and in vivo approach not only provides a rapid and efficient method for screening DNT but also offers critical insights into the ecological and health impacts of these alternatives.

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Keywords:
Bisphenols, Adverse Outcome Pathway (AOP), Developmental Neurotoxicity (DNT), Bayesian Network (BN), Integrated Testing Strategy (ITS)

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Leaching and Effects of Plastic Additives in Aquatic Ecosystem: Overview and Meta-analysis

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Abstract

Environmental plastic pollution is a critical ecological concern today and specifically regarding the risk of the release of plastic additives (PAs). Leaching from plastic and microplastic waste is a major source of PAs in aquatic ecosystem, which poses threats to aquatic organisms as these additives can persistently migrate through various biological carriers. Over the past decade, research on leaching of PAs has increased rapidly and focused on leachate composition, release kinetics and mechanism, toxicity to organisms, and influencing factors. However, the extensive variety, functions, quantities, and complex compositions of PAs, as well as the variable morphology and property features of plastic polymers present formidable challenges in the monitoring, testing, and assessment. Therefore, our understanding of the fate and impact of PAs on diverse aquatic organisms is still limited. Here, we conducted a meta-analysis of the most up-to-date literature on the leaching and effects of PAs in aquatic ecosystem. From investigation in 49 studies, a total of 6 categories of additives (functional classification), released from about 10 polymers, conducted in 10 types of leaching systems and 8 kinds of leaching medium, exposed to 8 diverse organisms, and observed with 22 biological endpoints were extracted. Laboratory simulations for leaching system include static, dynamic, and specific scenario simulations. Static systems are widely used but may not accurately reflect real conditions. Dynamic systems, including semi-dynamic, continuous flow, and infinite sink setups, are more representative. The infinite sink leaching system, which maintains concentration gradients, has gained popularity. Despite substantial progress, limitations remain in establishing standardized testing methods. Estimation for leaching of additives from polymers into aquatic environments resulted in a moderate level, based on quantitative synthesize effects observed in 12 studies. Some heterogeneity exists between studies, with various factors potentially related to additive structure and properties, polymer features, environmental conditions, and experimental methods. In addition, prospects for new research include integrating non-target screening, various toxicity endpoints, and environmental transformation products into leaching simulations, and exploring better dynamic simulation methods to mimic.

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Metabolomic alterations associated with novel brominated triazine based flame retardant (2,4,6-tris(2,4,6-tribromophenoxy)-1,3,5-triazine (TTBP-TAZ)) exposure

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Abstract

Brominated Triazine-based Flame Retardant (BTFRs) are one of the most promising new types of flame retardants and are being introduced in many aspects of our life. BTFRs has been detected in a variety of environmental media and also in living organisms. However, its toxicity and related molecular mechanisms are still unclear. Previous study of the applicants group revealed that typical BTFR (TTBP-TAZ) exposure can affect lipid storage in rats, which may cause energy metabolism disorder in rats. Whether any metabolic dysregulation may be induced upon TTBP-TAZ exposure under environmentally relevant dosage remains unclear. Thus, systematic study should be conducted to capture more metabolic alterations upon TTBP-TAZ exposure. In this study, we conducted HPLC-HRMS based metabolomic analysis to study the metabolic dysregulation induced by TTBP-TAZ exposure within environmentally relevant exposure dosage. We adopted a data dependent acquisition (DDA) method to balance data credibility and capacity of each acquisition. Moreover, a combination of T3 and Amide chromatographic column were used as complementary separation tools to achieve a more comprehensive coverage of metabolites, achieving an exhaustive inspection of 1859 cellular metabolites identification. Then the dysregulated metabolites were enriched to elucidate the affected pathways and thus evaluate the metabolic disruptions. Finally, more than 50 related genes related to the metabolic disruption pathways were selected to re-evaluate the dysregulation on the transcriptomic level, and joint-network analysis were adopted to elucidate the potential health outcome induced by TTBP-TAZ exposure. TTBP-TAZ exposure can cause disturbance in intracellular energy metabolism balance by interfering with intracellular lipid and amino acid metabolism. Furthermore, the relative quantitative results of RNA expression levels in the relevant pathways aligned with the metabolomics results, and important lipid storage genes such as PLIN were significantly upregulated after TTBP-TAZ exposure. Our study offered an overview of the metabolic disorder induced by environmentally relevant exposure.

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Diastereomer-specific Transformation of Hexabromocyclododecane by Soil Bacterial Communities

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Abstract

As one of the brominated flame retardants listed as POPs, the diastereomer-specific biotransformation of Hexabromocyclododecane (HBCD) can alter the environmental and health effects, which is an urgent need to clarify. In this study, the diastereomer-specific HBCD transformation process and mechanisms by soil bacterial communities were elucidated. The native bacterial communities in the soil exhibited a biotransformation ability specific to diastereomers of HBCD. The soil bacterial communities also produced a diastereomer-specific response. During α- and β-HBCD transformation, Proteobacteria became the dominant phylum to accelerate biotransformation. In contrast, soil bacterial communities responded to γ-HBCD stress by increasing species richness. The Proteobacteria *Acinetobacter hemolyticum* strain HW-2 was isolated and demonstrated isomer specificity for β-HBCD, attributed to the differential expression of the four key genes. Bioaugmentation with strain HW-2 successfully promoted biotransformation of HBCD, expedited isomer selection, and reduced ecotoxicity. Our findings provide an pivotal basis for the use of microorganisms to more reasonably control HBCD in ecosystems.

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In-Vehicle Exposure of Southern California Commuters to Tris(1,3-dichloro-2-propyl) phosphate

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Abstract

Tris(1,3-dichloro-2-propyl) phosphate (TDCIPP) is an additive, organophosphate-based flame retardant (OPFR) introduced within vehicle parts to meet a stringent, federal-level flammability standard within the United States. As TDCIPP is a semi-volatile organic compound, TDCIPP migrates from end-use products, resulting in human exposure to TDCIPP-contaminated air and/or dust within the interior of vehicles. To our knowledge, human OPFR exposure as a function of total commute time had not been evaluated prior to 2019. Therefore, the overall objective of our first, one-week study in 2019 was to leverage silicone wristbands to monitor personal OPFR exposure within a subset of commuter vs. non-commuter undergraduate students (N=88) at the University of California, Riverside. Out of 22 OPFRs analyzed, 13 OPFRs were detected on at least 62 wristbands (70% detection rate). Among these 13 OPFRs, TDCIPP was the only OPFR that was significantly predicted by total commute score, suggesting that longer commutes were associated with increased human exposure to TDCIPP. Therefore, the overall objective of our second, two-week study in 2020 was to determine if a decrease in interior car dust resulted in mitigation of personal TDCIPP exposure for participants (N=49) who spend a significant amount of time in their personal vehicles. Once participants enrolled in the study, participants were distributed across four groups that determined when the participants wiped their car interiors during the two-week study. Interestingly, there was no significant difference in wristband TDCIPP concentrations among the different

wiping groups despite concentrations being higher than those of non-commuters. Therefore, findings from our 2020 study suggest that the correlation between TDCIPP exposure and longer commutes within our 2019 study may have been attributed to direct partitioning from vehicle parts into wristbands via car interior air. Given that Americans within densely populated regions across the United States spend one or more hours commuting on a near-daily basis, there is a critical need to understand the potential human health implications of chronic TDCIPP exposure within vehicles, particularly within traffic-congested areas such as Southern California.

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Comprehensive Characterization of Chlorinated paraffins in Chinese Tires

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Abstract

Chlorinated paraffins (CPs) are widely used as plasticizers, flame retardants, and lubricants in poly(vinyl chloride), polyurethane foam adhesive, and rubber products. However, the presence of CPs in tire products remains scarcely studied. This work investigates short-, median-, and long-chain CPs (SCCPs, MCCPs, and LCCPs, respectively) in paired end-of-life and new tires for sedan, SUV, truck, and van in China. The total CP concentration (C_{10-20}) ranged from 81 to 245 μg/g (mean 137 μg/g) in end-of-life tires produced in 2018 and from 6 to183 μg/g (mean 71μg/g) in new tires produced in 2023. A decreasing trend in CP levels was observed in Chinese tires from 2018 to 2023. SCCPs and MCCPs dominated by C_{13-14} were the primary CPs found in Chinese tires. Evaluation of the tire mass distribution combined with air emission simulation experiment indicated that tire wear emission and air emission contributed approximately 20% and 5%, respectively, to the total CP tire loads over the lifespan of tires. Environmental emissions of CPs from tire wear particles were estimated at 170 tons per year in China.

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Efficient Removal of Phthalic Acid Esters in Soil and Water by Isolated Bacterial Strain and Engineered Biochar from Different Biowastes

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Abstract

Phthalic acid esters (PAEs) are a class of lipophilic chemicals widely used as plasticizers and additives to improve mechanical extensibility and flexibility of various products. Synthesized PAEs, causing potential hazards to ecosystem functioning and public health due to their persistence and toxicity, have been detected in water, soil and sediments. Some PAEs have been designated priority organic pollutants for environmental control by countries such as USA, Europe and China. Therefore, effectively removing PAEs from soil and water is urgently needed to avoid potential environmental risks.

Several remediation strategies, including physical, chemical and biological methods, have been developed for this purpose, each with distinct advantages and limitations. Engineered biochar (EB) has been seen as a promising sorbent in recent years and has displayed an excellent cost advantage. However, the effectiveness of EB in removing PAEs varies greatly with biochar feedstock, pyrolysis conditions, surface modification and soil or water conditions. Microbial degradation utilizes specific bacteria or fungi capable of metabolizing PAEs. It is environmentally friendly and sustainable but can be slow and dependent on environmental conditions.

In this study, a series of experiments were conducted to develop EB from different biowastes and to isolate degrading bacteria from sewage sludge for efficient removal of PAEs in soil and water, and to understand the underlying mechanisms of PAE sorption by biochar and PAE biodegradation by bacteria. The novel sequential activation approach and the green and efficient sequential carbonization method were proposed to upcycle biowastes into EB with high porosity, demonstrating excellent removal performance for PAEs. Pore filling, partitioning, hydrogen bonding and π-π stacking were possible sorption mechanisms. The isolated bacterial strain (LUNF1) could completely remove dibutyl phthalate from wastewater through producing a novel PAE hydrolase (DphBL1), demonstrating its great potential for PAE bioremediation.

This study proposes viable remediation technologies for upcycling biowastes into effective EB for PAE removal, contributing to sustainable biowaste management and environmental pollution mitigation. This study also supports structural modification of PAE hydrolases to improve catalytic efficiency in bioremediation, promoting the development of efficient strategies for PAE remediation in the environment.

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Fate and risk control of plastic additives in soil-plant systems

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Abstract

Plastic additives, such as flame retardants and plasticizers, can be released from plastic products into the soil environment during production, usage, and disposal, subsequently taken up by plants and delivered to animals and humans through food chain, causing adverse effects such as endocrine toxicity, reproductive toxicity, and immunotoxicity. This work was carried out to investigate the occurrence, fate, and risk control of plastic additives in plants. Plant samples from eastern China were collected and analyzed, revealing that the detection frequencies of phthalate esters (PAEs) and bisphenols (BPs) were 100 %, with concentrations in ranges of 3.9-24.0 mg/kg (dw) and 1.2-439.6 μg/kg (dw). Congener-specific uptake, translocation, and metabolism of plastic additives in plants were investigated by plant cultivation and cell culture tests. The results showed that the plastic additives can be rapidly taken up by plants, and different chemicals displayed obvious disparities in the potential of root uptake, translocation, and accumulation. High-resolution mass spectrometry was employed to identify the metabolites of plastic additives in plants, demonstrating the congener-specific biotransformation pathways of plastic additives including hydroxylation, methylation, methoxylation, glycosylation, and glutathionylation. Furthermore, phytohormones were applied to reduce the accumulation of PAEs in plants. The results suggested that foliar spray of phytohormones prominently reduced the accumulation of plastic additives in plants through enhancing the plant metabolism, antioxidant system and photosynthesis. These findings improved our understanding of fate of plastic additives in soil-plant systems, providing scientific guidance for the production and application of plastic additives from the perspective of priority pollutants. In addition, this work proposed a potential avenue to reduce the risk of plastic additives in plants.

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Organophosphate flame retardants and their metabolites in dog food and urine: An exposure assessment through food consumption

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Abstract

The exposure of pets to a variety of chemicals present in the indoor environment raises concerns, as it coincides with an increase in noninfectious diseases among these companion animals. However, there is limited knowledge about the sources and pathways of chemical exposure in pets. In this study, we determined the concentrations and distributions of organophosphate flame retardants (OPFRs) and their

metabolites (mOPFRs) in dog food, as well as in paired urine samples. Furthermore, we assessed the risk of OPFR exposure through the consumption of dog food. Paired food and urine samples (n=47) were collected in Seoul, South Korea, in October 2023. Determination of the six OPFRs and eight mOPFRs, including tris(2-chloroethyl) phosphate (TCEP), tris(1-chloro-2-propyl) phosphate (TCIPP), tris(1-chloro-2-propyl) phosphate (TDCIPP), triphenyl phosphate (TPHP), tri-n-butyl-phosphate (TNBP), tris(2-butoxyethyl) phosphate (TBOEP), di-n-butyl phosphate (DNBP), bis(2-chloroethyl) phosphate (BCEP), bis(2-chloropropyl) phosphate (BCIPP), diphenyl phosphate (DPHP), bis(2-butoxyethyl) phosphate (BBOEP), bis(2-butoxyethyl) hydroxyl-2-butoxyethyl phosphate (3OH-TBOEP), bis(1,3-dichloro-2-propyl) phosphate (BDCIPP), 4-hydroxyphenyl phenyl hydrogen phosphate (4-HO-DPHP), was performed by gas chromatography coupled with mass spectrometry (GC/MS) and liquid chromatography coupled with tandem MS (LC/MS/MS), respectively. The levels of OPFRs in dog food were ranged from 3.27-51.8 ng/g. mOPFRs were detected in all dog urine samples at concentrations ranging from not detected (ND) to 3,208 ng/g. The most frequently detected OPFRs were TnBP and TPhP, both with a detection frequency (DF) of 100%, followed by TBOEP (DF: 85.1%), TCIPP, and TCEP (DF: 80.9%). The major mOPFRs were DPhP (DF: 100%), DnBP (DF: 89%), and BBOEP (DF: 83%). The concentrations of ∑OPFRs in dog food were positively correlated with mOPFR concentrations in urine samples (Spearman correlation, $p < 0.01$). In addition, a significant positive correlation was observed between TBOEP/TPhP levels in dog food and paired mOPFR (BBOEP and DPhP) levels in urine samples (Spearman correlation, $p < 0.01$). The detailed discussion on the occurrence, distribution, the relationship between the levels of OPFRs in pet food and mOPFRs in urine samples, as well as the risk assessment will be presented during the conference.

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Atmospheric transformation chemistry and risks of organophosphate esters

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Abstract

In this talk, I will use two examples to highlight the importance of atmospheric transformation in assessing the environmental and health risks of organophosphate esters (OPEs). These examples include (1) Urban air pollution: atmospheric transformation of organophosphate esters (OPEs) in global megacities; (2) Air pollution in polar regions: atmospheric transformation of organophosphite antioxidants (OPAs) to OPEs in the global atmospheric environment including the Arctic and Antarctic.

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Environmental Exposure Risks and Behaviors of Traditional and Novel Organophosphate Esters

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Abstract

Organophosphate esters (OPEs) are emerging contaminants of significant concern in recent years. Widely used as flame retardants and plasticizers, they have been detected in many environmental and human matrices. This study investigated the contamination characteristics of OPEs and their precursors, organophosphite antioxidants (OPAs), in soil and dust nationwide. The concentrations of novel OPEs (NOPEs) originating from OPAs were significantly higher than those of traditional OPEs. Additionally, OPAs underwent significant photo-transformation on dust, rapidly generating NOPEs. These NOPEs then underwent secondary transformations, including hydroxylation and methylation, resulting in products with more complex toxicity than their parent compounds. Food intake emerged as a more important exposure route than dust and air, with daily intakes of NOPEs from various vegetables being much higher than those of traditional OPEs. Furthermore, NOPEs significantly affected soil microbial ecology, posing high ecological risks.

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Non-targeted screening of organophosphate flame retardants and plasticizers in a river impacted by industrial activity in Eastern China

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Abstract

The processing and production of organophosphate ester (OPEs) flame retardants may release corresponding pollutants into the surrounding environment. However, the pollution profile and impact remain insufficiently studied. This study investigates the occurrence of 40 OPEs in the Dan River impacted by industrial activity in Eastern China, and employs non-target analysis based on high-resolution mass spectrometry to identify novel organophosphorus compounds (NOPs). Thirty-four target OPEs are detected in the water samples, with total concentrations ranging from 62.9 to 1061 ng L^{-1}. Additionally, 26 non-target NOPs were identified, 15 of which were detected in the environment for the first time, including three alkyl OPEs, five aryl OPEs, five organophosphorus heterocycles, and two phosphonates. Bis(2,5-di-tert-butylphenyl) hydrogen phosphate and Neopentyl propyl hydrogen phosphate were commonly found in the water, with concentrations reaching 994 and 1034 ng L^{-1}, respectively. The concentration variations of OPEs along the upstream and downstream of the river indicate significant influence from point source pollution. Organophosphorus heterocycles with similar structures exhibited the same variation trends, suggesting they may originate from the same pollution sources.

These findings suggest that the processing and production of OPE flame retardants are important sources of OPEs and NOPs in water bodies, and the occurrence of NOPs may further increase ecological and human exposure risks.

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Identification of Novel Organophosphate Flame Retardants and Plasticizers Released from a Plastic Recycling Industrial Park Using Target and Nontarget Analysis

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Abstract

Plastic recycling and reprocessing activities have the potential to release organophosphate ester (OPE) flame retardants and plasticizers into the surrounding environment. However, there is limited research on the contamination profiles and impacts of these chemicals. This study aimed to investigate the occurrence and spatial distribution of twenty-eight OPEs and their metabolites (mOPEs) in rainfall runoffs and agricultural soils near a major plastic recycling industrial park in North China. In addition, novel organophosphorus compounds (NOPs) were identified using high-resolution mass spectrometry-based nontarget analysis. The results showed that twenty and twenty-seven OPEs were detected in runoff water and soil samples, respectively, with concentrations ranging from 86.0-2491 ng/L in runoffs and 2.53-199 ng/g dw in soil. Furthermore, this study successfully identified thirteen NOPs, eight of which had not been previously reported in environmental matrices. These NOPs included a chlorine-containing OPE, an organophosphorus heterocycle, a phosphite, three novel OPE metabolites, and two oligomers. Among the NOPs identified, triphenylphosphine oxide and diphenylphosphinic acid were present in both runoffs and soils at remarkably high concentrations, reaching levels as high as 390 ng/L and 40.2 ng/g dw, respectively. In addition, the downwind areas of the industrial park exhibited elevated levels of OPEs and NOPs, with soils having a higher abundance of hydroxylated mOPEs compared to runoffs. These findings indicate that plastic recycling and reprocessing activities are significant sources of OPEs and NOPs. Moreover, the process of biotransformation may further exacerbate the ecological and human exposure risks.

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Accumulation and Transformation of Hexabromocyclododecane Isomers in Arabidopsis

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Abstract

Hexabromocyclododecane (HBCD) has been widely used as a brominated flame retardant in the past decades. Although its use has been banned in recent years, it is still widely present in various environments, and is biotoxic and accumulates and amplifies in organisms. Hence, it is crucial to understand its accumulation and transformation in the environment and organisms. HBCD isomers differ in physicochemical properties, persistence and biotoxicity due to their different structures. Therefore, this study aimed to reveal HBCD isomer accumulation and transformation in plants.

In this study, plant *Arabidopsis thaliana* was planted in soil amended with different isomers of HBCD, with one group added HBCD-degrading bacterium *Acinetobacter hemolyticus* strain HW-2. The results showed that the degradation rate of isomers in soil was different after planting plants. *Arabidopsis* enriched all three HBCD isomers in soil. The accumulation of α-HBCD and β-HBCD was in the order of roots > stems > leaves, and the accumulation of γ-HBCD was the highest in stems. It was speculated that γ-HBCD could be transported upward in *Arabidopsis thaliana*. The transfer and transport capacity of HBCD in plants was: γ-HBCD > β-HBCD > α-HBCD. This study also found that the proportion of enantiomers changed during planting. The ratio of the two enantiomers for each isomer in the soil was close to 1:1 initially, and the ratio of right-handed enantiomers in α-HBCD and γ-HBCD continuously decreased during the upward transport of plants. In addition, the added bacterial strain showed clear impacts on the rhizosphere soil microbial community and soil absorption of HBCD.

In summary, HBCD isomers can be enriched and transferred in *Arabidopsis thaliana*. Our results provide important information for the future management of flame retardants in the environment.

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Organophosphate Esters in Tianshan Glacier Runoff: Occurrence, Degradation, and Flux

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Abstract

Organophosphate esters (OPEs) are a class of chemicals of emerging concern，however, little is known about the environmental behavior, release characteristics, and transformation of OPEs in mid-latitude glacial environments. Therefore, this study investigated the concentration and composition characteristics of organophosphate triesters (tri-OPEs) and organophosphate diesters (di-OPEs) in the runoff of Urumqi No. 1 Glacier and Koxkar Glacier in the Tianshan Mountains, and estimated the output of them from glacial rivers. The total concentration of tri-OPEs was 8565 pg/L in glacier surface meltwater and 6568 pg/L in proglacial rivers. Di-OPEs exhibited lower concentrations, with 99 pg/L and 117 pg/L in glacier surface meltwater and proglacial rivers, respectively. Tri-OPEs exhibited clear diurnal variations, which were presumed to be related to environmental temperature, while di-OPEs did not show obvious trend. The total output flux of tri-OPEs in glacial rivers of the entire Tianshan region was estimated approximately 832 kg/year. Given the continuity of glacial melting and the accumulation of emerging pollutants in glaciers, the process of melting poses an increasing risk to freshwater resources, warranting heightened attention.

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Phthalate Acid Esters (PAEs) in Decoration Materials: Occurrence, Sources and implications of Health Risk

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Abstract

Phthalate acid esters (PAEs) are one of the most widely used plasticizers globally. They are extensively employed in a large number of decoration materials. Decoration materials are recognized to be persistent sources of many pollutants in indoor environment. However, studies on the impact of these materials on PAEs pollution and their effects on human health are limited. In this study, a total of 177 samples were collected from four categories of interior decoration materials (furniture boards, floorings, wall coverings,

paint and coatings). The levels, sources, exposure doses, and potential health risks of PAEs from decoration materials were evaluated. The total concentrations of Σ_9PAE (sum of nine PAEs) in decoration materials ranged from 261 ng/g to 4480000 ng/g. Furniture boards and paint and coatings exhibited relatively higher Σ_9PAE compared to floorings and wall coverings ($p < 0.001$). DEHP was the most abundant PAE in furniture boards and flooring, while DMP and DBP emerged as the predominant PAEs in wall coverings and paint and coatings. Principal component analysis showed that decoration materials are important sources of PAEs in indoor environment. The estimated emission rates of total PAEs from furniture board, floorings, wall coverings, and paint and coatings to the indoor environment were 0.0394, 0.0169, 0.0731, and 0.4447 ng/m²/s, respectively. Based on questionnaire survey data from 675 Chinese households in most regions of China, the daily exposure doses of PAEs from decoration materials for Chinsese residents were estimated. The daily exposure doses of PAEs in Chinese residents were positively correlated with the amount of PAEs in decoration materials, especially in indoor environments where walls are treated with paints, reaching up to 0.0799 μg/kg-day (0.0040-11.1956 μg/kg-day, median and range) for adults and 0.1477 μg/kg-day (0.0073-20.6868 μg/kg-day) for children. Additionally, the exposure doses of PAEs through decoration materials are also correlated with factors such as residential area and housing type. Risk assessment indicated that although certain PAEs posed potential health risks, the exposure levels of PAEs were within acceptable limits. However, residents lived in indoor environment treated with a large amount of decoration materials exhibited relatively higher risks, necessitating targeted risk management strategies. This study provides new insights into understanding the risk associated with PAEs in indoor environments.

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Association of organophosphate flame retardants (OPFRs) exposure with liver function in women of reproductive age

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Abstract

Background: Exposure to environmental pollutants is a significant risk factor for liver. However, studies on the relationship between Organophosphorus flame retardants (OPFRs), an emerging environmental contaminant, and liver function in Female of reproductive age are limited.

Methods: The present study comprised 1026 females of reproductive age were recruited from a reproductive hospital in Henan Province between April and December 2023. The OPFRs, including TPrP, TBEP, TPhP, TMCP, TBP, TDCPP and EHDPP in serum were determined using UPLC-MS/MS. Generalized linear regression and quantile g-computation were utilized to assess the associations between OPFRs Single and mixed exposure with liver function (Total Protein (TP), Albumin (ALB) and Globulin (GLB)).

Results: In the single-exposure model, the quantile 2, 3 and 4 of blood EHDPP (b = -0.08 to -0.16, $P_{trend} < 0.001$), the highest quantile of blood TBP (b = -0.11, 95%CI: -0.15 to -0.07), TBEP

(*b* = -0.07, 95%CI: -0.11 to -0.03), and TDCPP (*b*= -0.10, 95%CI: -0.14 to -0.06) was positively correlated with TP compared to quantile 1. The quantile 2, 3 and 4 of blood EHDPP (*b* = -0.08 to -0.13, $P_{trend} < 0.001$) and TBP (*b* = -0.04 to -0.09, $P_{trend} < 0.001$), the highest quantile of blood TBEP (*b* = -0.06, 95%CI: -0.09 to -0.02), and TDCPP (*b* = -0.07, 95%CI: -0.11 to -0.04) were positively correlated with ALB compared to quantile 1. The quantile 2, 3 and 4 of blood EHDPP (*b* = -0.07 to -0.16, $P_{trend} < 0.001$), the highest quantile of blood TBP (*b* = -0.12, 95%CI: -0.17 to -0.07), TBEP (*b* = -0.07, 95%CI: -0.11 to -0.02), and TDCPP (*b*= -0.09, 95%CI: -0.14 to -0.04) was positively correlated with GLB compared to quantile 1. Mixed-exposure analyses revealed that OPFRs were consistently negatively associated with TP (*b* = -0.09, 95%CI: -0.11 to -0.07), ALB (*b* = -0.07, 95%CI: -0.09 to -0.05), and GLB (*b* = -0.08, 95%CI: -0.11 to -0.06). And EHDPP may be the key OPFRs affecting the TP (49.93%), ALB (49.49%) and GLB (54.92%).

Conclusions: Exposure to OPFRs may be associated with liver function in women of reproductive age. EHDPP is the major contributor to the mixed exposure effect.

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Association of organophosphate flame retardants (OPFRs) exposure with ovarian reserve and in vitro fertilization-embryo transfer (IVF-ET) outcomes in women of reproductive age

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Abstract

Background: Organophosphorus flame retardants (OPFRs) are emerging environmental pollutants with reproductive and endocrine toxicity, whereas studies on the relationship between OPFRs exposure and reproductive health in women of reproductive age are limited.

Methods: The present study comprised 555 females of reproductive age were recruited from a reproductive hospital in Henan Province between April and December 2023. The OPFRs, including TPrP, TBEP, TPhP, TMCP, TBP, TDCPP and EHDPP in serum were determined using UPLC-MS/MS. Generalized linear regression and quantile g-computation were utilized to assess the associations between OPFRs Single and mixed exposure with Ovarian reserve function and in vitro fertilization-embryo transfer (IVF-ET) outcomes. The potential mediating role of ovarian function indicators in the association between serum OPFRs and IVF-ET outcomes were also examined.

Results: In the single-exposure model, the exposure level of blood EHDPP was positively correlated with progesterone (*b*= 0.10, 95%*CI*: 0.01 to 0.20) and Testosterone (*b* = 0.14, 95%*CI*: 0.05 to 0.23), the exposure level of blood TPhP was positively correlated with progesterone (*b*= 0.12, 95%*CI*: 0.03 to 0.20), EHDPP increased the risk of premature ovarian insufficiency in women of childbearing age (*OR*= 3.54, 95%*CI*: 1.42 to 9.82). Mixed-exposure analyses showed that EHDPP is the major OPFRs affecting the risk of premature ovarian insufficiency. Single-exposure analyses showed that the highest quantiles of blood EHDPP was significantly negatively associated with fertilization rate (*b* = -0.06, 95%*CI*: -0.11 to -0.01) and blastocyst formation rate (*b* = -0.06, 95%*CI*: -0.12 to -0.01) in IVF-ET outcomes compared to the lowest quartiles. Mixed-exposure analyses revealed that EHDPP may be the key OPFRs affecting the fertilization rate and blastocyst formation rate of IVF-ET outcomes. The testosterone showed a mediating effect in the decrease of fertilization rate (*b* = -0.39, 95%*CI*: -0.81 to -0.06) and blastocyst formation rate (*b* = 0.58, 95%*CI*: 0.05 to 1.35) caused by EHDPP exposure.

Conclusions: Exposure to OPFRs may be associated with diminished ovarian reserve and adverse IVF-ET outcomes in women of reproductive age. EHDPP is the major contributor to the mixed exposure effect. The testosterone plays a mediating role in the adverse outcomes of IVF-ET caused by EHDPP. This may partly explain the potential mechanism by which OPFRs cause adverse IVF-ET outcomes.

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Implications of Takeaway Food Packaging on Phthalate Acid Esters (PAEs) Exposure in Chinese Youth: Occurrence, Sources, and Health Risks

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Abstract

Takeaway delivery services have surged in popularity among Chinese youth in recent years. Tens of thousands of food delivery services require hundreds of millions of containers annually for packaging. These containers often employ phthalate acid esters (PAEs), the most widely used plasticizers globally, raising potential health concerns due to possible exposure from consuming takeaway food. In this study, a total of 77 samples were collected from seven categories of food packaging from the market. The levels, sources, exposure doses, and potential health risks of PAEs in these takeaway food packaging were assessed. The total concentrations of PAEs in takeaway food packaging ranged from 47.0 ng/g to 316000 ng/g, with a median concentration of 4200 ng/g. DBP, DiBP, DCHP, and DEHP were identified as the predominant PAEs. Among all types of packaging, expanded polystyrene (EPS) containers showed the highest concentrations of PAEs, with a median value of 66000 ng/g. Consumption of food from EPS containers resulted in the highest PAE exposure dose (724 ng/kg-day). Youth using EPS containers faced exposure levels approximately 4 to 154 times higher than those using other types of takeaway packaging.

The contribution of takeaway packaging to human exposure to PAEs was evaluated. Consumption of takeaway food from various takeaway packaging accounted for 0.16% to 24.4% of total dietary exposure to PAEs and 0.03% to 5.03% of overall PAEs exposure in humans. Risk assessment indicated that the exposure levels of PAEs through using takeaway packaging were within established safety limits. Although no significant health risks were identified, concers over PAE hazards remain pertinent. Factors such as high temperatures, high-fat content in food, prolonged storage, and frequent consumption can exacerbate the health risks associated with takeaway packaging materials.

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Structure-dependent Distribution, Metabolism and Toxicity Effects of Alkyl Organophosphate Esters in Lettuce (*Lactuca sativa* L.)

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Abstract

This study provides a comprehensive investigation into the structure-dependent uptake, distribution, biotransformation, and potential toxicity effects of alkyl organophosphate esters (OPEs) in hydroponic lettuce (*Lactuca sativa* L.). Trimethyl, triethyl, and tripropyl phosphates were readily absorbed and acropetally translocated while tributyl, tripentyl, and trihexyl phosphates accumulated mainly in lateral roots. The acropetal translocation potential was negatively associated with log K_{ow} values. Trimethyl and triethyl phosphates are less prone to biotransformation, while a total of 14 novel hydrolysis, hydroxylated and conjugated metabolites were identified for other OPEs using nontarget analysis. The extent of hydroxylation decreases from tripropyl phosphate to trihexyl phosphate, but multiple hydroxylations occurred more frequently on longer-chain OPEs. Further comparative toxicity test revealed that hydrolyzed and hydroxylated metabolites have stronger toxic effects on Ca^{2+}-dependent protein kinases (CDPK) than their parent OPEs. Dibutyl 3-hydroxybutyl phosphate particularly induce the upregulation of CDPK in lateral roots, probably associated with adenine reduction that may play an important role in the self-defense and detoxification processes of lettuce. This study contributes to understanding the uptake and transformation behaviors of alkyl OPEs as well as their associations with toxic effect on lettuce. This emphasizes necessary evaluation of the environmental risk of OPEs, particularly focusing on their hydroxylated metabolites.

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Legacy, current-use brominated flame retardants and phthalate esters in indoor dust and air from Vietnam: An update on the contamination, sources and implications for human exposures

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Abstract

Endocrine active chemicals such as brominated flame retardants (BFRs) and phthalate esters (PAEs), are among contaminants of emerging concerns, which have been used in a wide range of industrial and consumer products. However, comprehensive investigations on the occurrences and human exposure in informal recycling waste areas and indoor micro-environments in developing countries including Vietnam are still limited. This presentation provides a review of recent investigations on the contamination of PBDEs and some current-use BFRs in settle dust and indoor air samples some recycling areas in Vietnam to assess the risks for human exposure. PBDE levels found in dust samples collected from end-of-life vehicle (ELV) workshops (120 - 520 ng/g) and nearby living areas (36–650 ng/g) were generally higher than those in common house dust (25 -170 ng/g). The contamination pattern of other BFRs in dust samples was in the order of urban > rural > ELV, reflecting the current use of these compounds in new consumer products. Decabromodiphenyl ethane (DBDPE) and 1,2-bis(2,4,6-tribromophenoxy)ethane (BTBPE) were the major alternative BFRs. The PAE levels in workplace dust of informal vehicle repair and waste processing workshops (9210 - 153,000 ng/g) were remarkably higher than those in common house dust (580 - 83,700 ng/g), indicating waste processing activities as potential sources of PAEs. PAEs concentrations in indoor air and settle dust samples were found to be higher in homes and hair salons than other micro-environments. Children in ELV recycling sites and urban areas received higher intake doses of PBDEs and DBDPE than adults, with the predominant contribution of dust ingestion as compared to air inhalation pathway. Intake doses estimated for PAEs in different micro-environments such as homes, offices, hair salons, kindergartens and laboratories indicated the dominance of air inhalation, and intakes of children through dust ingestion were higher than those in adults. Further studies should be focused on the accumulation of emerging flame retardant and plasticizer such as organophosphorus esters (OPEs) in indoor air and human samples to gain insights into the fate and possible adverse impacts on human health.

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Pollution profiles, source apportionment, and risk assessment of organophosphate esters in coastal aquaculture waters: typical case studies in China

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Abstract

Organophosphate esters (OPEs) have received considerable attention from researchers due to their widespread presence in environments and toxicities. In China, about 2 million hectares of coastal waters were used for the development of mariculture. However, the current studies on OPEs in China's coastal waters mainly focused on the marginal seas, and less attention is paid to the mariculture areas closely related to seafood quality and human health. In this study, 20 OPEs were monitored in waters and sediments simultaneously in three typical mariculture waters (Yunxi Marine Ranching (YX), Hangzhou Bay (HZB), and Zhelin Bay (ZLB)) around Shandong province, Zhejiang Province, and Guangdong Province, respectively, in China, where the production of aquaculture products occupies the national leading level, and a highly concerned freshwater aquaculture area (Meiliang Bay (MLB) of Taihu Lake). Moreover, OPEs in fishes from ZLB and relevant health risk were evaluated. The ∑OPE concentrations in waters followed the order MLB > YX > HZB > ZLB, with TCIPP, TEP, and TCEP being the dominant OPEs. Significantly higher ∑OPE concentrations were found in sediment in MLB compared to the other three areas with similar levels. The decreasing concentration of OPEs from nearshore to offshore areas in HZB and MLB indicated that terrigenous input is the main source of OPEs. The even distribution of OPEs in YX and ZLB combined with PCA analysis suggested ship traffic or aquaculture activities are also potential sources of OPEs. TCIPP, TPHP, and TCEP were the main OPEs in fishes from ZLB. Hydrophobicity was a key factor affecting the bioaccumulation factors of OPEs. The human exposure to OPEs through consumption of fishes from ZLB had a low health risk now. This study provided important information for risk assessment and pollution control strategies of OPEs in coastal aquaculture areas.

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Microbial transformation of new flame retardants

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Abstract

Due to their low cost and effective flame-retardant properties, HBCD (Hexabromocyclododecane) and PBDEs (Polybrominated diphenyl ethers) have been widely produced and incorporated into flammable materials such as polyurethane foam, building materials, electronic products, and carpets. Despite being

restricted in production and use by several countries and regions, these persistent organic pollutants (POPs) continue to be detected in various environmental and biological media due to their inherent environmental and biological persistence. Research into microbial transformation, a key natural attenuation and remediation method, is urgently needed to understand its processes and mechanisms.

After establishing a reliable method for isolating HBCD isomers in the laboratory, three HBCD isomers were added separately to soil to investigate the isomer-specific transformation processes of α-HBCD, β-HBCD, and γ-HBCD by soil microbial communities. The native soil bacterial communities exhibited a specific biotransformation ability for each HBCD diastereomer. During the transformation of α-HBCD and β-HBCD, Proteobacteria became the dominant phylum, accelerating the biotransformation process. In contrast, soil bacterial communities responded to γ-HBCD by increasing species richness. The Proteobacteria strain *Acinetobacter hemolyticum* HW-2 was isolated and shown to have isomer-specific biotransformation for β-HBCD, attributed to the differential expression of four key genes. Bioaugmentation with strain HW-2 successfully enhanced HBCD biotransformation, expedited isomer selection, and reduced ecotoxicity.

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Environmental transformation and metabolic mechanisms of preservative parabens and their consequences for health effects

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Abstract

The pervasive presence of emerging contaminants (ECs) in environments and their associated adverse effects are underscored. Notably, the increased toxicity observed in the environmental transformation of ECs is often linked to the formation of transformation products (TPs). However, understanding the interaction and formation mechanisms contributing to increased toxicity, particularly concerning estrogenic effects, remains an unresolved challenge. To address this gap, by combining quantum chemical and molecular simulations with experiments, the identification and formation of TPs as well as their molecular interactions of estrogenic effect during the transformation of preservatives parabens such as benzylparaben (BZP). Our results revealed the identification of three previously unknown TPs during the transformation of BZP using a non-targeted analysis. Notably, two of these novel TPs exhibited higher estrogenic activities compared to the parent BZP. Furthermore, the binding free energies (ΔG_{bind}) of the oligomers BZP-o-phenol and BZP-*m*-phenol (-29.71 to -23.28 kcal/mol) were lower than the parent BZP (-20.86 kcal/mol), confirming that their stronger binding affinities to the ERα-LBD. In-depth examination of the formation mechanisms indicated that these toxic TPs primarily originated from the successive cleavage of ester bonds (O-$CH_2C_6H_5$ and -COO group), followed by their combination with BZP*. In summary, this study provides valuable insights into the mechanisms underlying the

formation of toxic TPs and their binding interactions with endocrine-disrupting effects. It offers a crucial framework for elucidating the toxicological patterns of ECs with similar structures.

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Ubiquitous Rubber Vulcanization Accelerators in Dust and Sediment: Sources, Occurrence, Human Exposure and Ecological Risk

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Abstract

Vulcanization accelerators (VAs) serve as crucial additives in synthetic rubber on a global scale. Despite their widespread use, the environmental presence, distribution, and associated exposure risks of VAs remain poorly understood. We compiled a target list and conducted a screening for eight classes encompassing 42 VAs in diverse urban dust samples from South China and in sediment samples across from urban rivers to the open ocean. A total of 40 of the 42 target VAs were detectable across all four studied regions, among which 30 were identified for the first time in the environment. Among the eight structure-classified VA classes, xanthates exhibited the highest concentrations (median: 3810–81,300 ng/g), followed by thiazoles, guanidines, sulfenamides, dithiocarbamates, thiurams, thioureas, and others. The median total concentrations of all target VAs (∑VAs) were determined to be 5060 ng/g in road dust, 5730 ng/g in parking lot dust, 29,200 ng/g in vehicle repair plant dust, and 84,300 ng/g in household dust, indicating the widespread presence of numerous rubber-derived VAs in various urban environments. On the other hand, our study confirmed the environmental occurrence of 34 out of 43 targeted VAs across five sediment regions from urban rivers to the open ocean, with 22 being first-time detections in sediments and thiazole derivatives predominating (median: 7.21–98.4 ng/g dry weight). Total VA concentrations (∑VAs) varied significantly ($p < 0.05$), ranging from 5.12 to 462 ng/g, with urban rivers showing the highest median concentration at 188 ng/g, followed by estuarine (median 81.4 ng/g dw), coastal (median 63.9 ng/g dw), deep-sea (median 10.5 ng/g dw) and ocean (median 8.93 ng/g dw). Assessment of their physicochemical properties suggests that most VAs are potential Persistent, Mobile, and Toxic (PMT) substances, as well as very persistent and very mobile (vPvM) substances. Meanwhile, VAs pose acute and chronic risks to aquatic organisms across large geographical scales, with thiuram VAs being the main risk drivers. This study marked the first systematic effort to identify a wide range of emerging rubber-derived VAs prevalent in urban environments. The findings call for increased attention to these widely utilized but less well-evaluated chemicals in future research and environmental management efforts, underscoring the urgency of targeted monitoring and risk mitigation strategies to safeguard aquatic life and human health from their potential detrimental effects.

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Regulatory role of mitochondrial damage on neurotoxicity and metabolic disorder induced by decabromodiphenyl ether in zebrafish (*Danio rerio*)

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Abstract

As a substitute for decabromodiphenyl ether (BDE-209), decabromodiphenyl ethane (DBDPE) has rapidly increased in concentration in environmental and biological media in China, even surpassing BDE-209, becoming a new pollutant of significant concern. Consequently, it is imperative to unravel the transgenerational/trans-generational toxicity effects of DBDPE upon long-term exposure at environmentally relevant concentrations.

Firstly, we conducted a full life-cycle exposure experiment with zebrafish to reveal the transgenerational/trans-generational toxicity effects of DBDPE. Post-fertilization zebrafish embryos were exposed to environmentally relevant concentrations of DBDPE (0, 0.1, 1, 10 nM) until sexual maturity (F0 generation), and the offspring (F1 and F2 generations) were reared in clean water until sexual maturity. The results demonstrated that full life-cycle exposure to DBDPE induced trans-generational developmental impairments in zebrafish larvae, increasing the susceptibility to diseases in the offspring. DNA methylation and transcriptomic analyses indicated that DBDPE primarily disrupted signaling pathways related to glucose, lipid, and energy metabolism, as well as neurodevelopment in the larvae. Furthermore, changes in biochemical markers, neurotransmitter levels, and locomotor behavior corroborated the trans-generational neurotoxicity of DBDPE.

Subsequently, we conducted a short-term exposure experiment with higher doses to validate the regulatory role of mitochondrial dysfunction in DBDPE-induced neurotoxicity and metabolic disruption. Post-fertilization zebrafish embryos were exposed to DBDPE (0, 50, 100, 200, and 400 μg/L) until 120 hours post-fertilization (hpf). The results showed that DBDPE exposure led to neurotransmitter imbalance, abnormal locomotor behavior, and increased malformation rates in zebrafish larvae, indicative of neurodevelopmental toxicity. Concurrently, metabolomic analyses combined with physiological and biochemical indicators confirmed perturbations in glucose and lipid metabolism. Mitochondrial stress tests revealed that DBDPE exposure significantly inhibited mitochondrial respiratory function in zebrafish larvae, accompanied by reduced levels of mitochondrial respiratory chain complexes, mitochondrial membrane potential, and ATP content. However, co-exposure with NR (a potential mitochondrial protector) significantly alleviated these mitochondrial dysfunction-related abnormalities and restored the impaired functions related to neurotransmitters, locomotor behavior, glucose-lipid metabolism, and oxidative stress.

Keywords: Decabromodiphenyl ethane (DBDPE); Transgenerational toxicity; Metabolic disruption; Mitochondrial damage

30. Innovative Disinfection and Novel Disinfection Byproducts

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Non-targeted analysis of coumarins in source water and their formation of chlorinated coumarins as DBPs in drinking water

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Abstract

Coumarin was detected as one of the most abundant compounds by non-targeted analysis of natural product components in actual water samples prior to disinfection. More importantly, pre-chlorination of humic acid generated 3-hydroxycoumarin and monohydroxy-monomethyl-substituted coumarin with a total yield as high as 10.1%, which suggested the humic substance in raw water is an important source of coumarins. 7-Hydroxycoumarin, 6-hydroxy-4-methylcoumarin, 6,7-dihydroxycoumarin, and 7-methoxy-4-methylcoumarin were identified in raw water by high-performance liquid chromatography tandem high resolution mass spectrometry (HPLC-HRMS) due to only some coumarin standards were commercially available. Their chlorination generated mono-chlorinated and polychlorinated coumarins, whose structures were confirmed by the synthesized standards. These products could form at various dosages of chlorine and pH levels and some with the concentration at 600 ng/L can be stable in tap water for days. 3,6,8-Trichloro-7-hydroxycoumarin, 3-chloro-7-methoxy-4-methylcoumarin, and 3,6-dichloro-7-methoxy-4-methylcoumarin were first identified in finished water with concentrations of 0.0670, 78.1, and 14.7 ng/L, respectively, but not in source water, suggesting that they are new DBPs formed in disinfection. The cytotoxicity of 3-chloro-7-methoxy-4-methylcoumarin in CHO-K1 cells was comparable to those of 2,6-dibromo-1,4-benzoquinone (2,6-DBBQ) and 2,6-dichloro-1,4-benzoquinone (2,6-DCBQ) in TIC-Tox analyses, warranting further investigation into their occurrence and control in drinking water systems.

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Tailoring Polyamide Nanofiltration Membrane with NaHCO3 Addition for Enhanced Rejection and Selectivity of Haloacetic Acids Toward Drinking Water Treatment

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Abstract

Nanofiltration (NF) is a promising strategy in drinking water treatment. To produce high-quality drinking water, toxic disinfection byproducts such as haloacetic acids (HAAs) should be efficiently removed while beneficial minerals such as calcium need to be preserved. However, current NF membranes often show overhigh rejection of essential minerals. Herein, we developed novel NF membranes with tailored polyamide properties for selective rejection/passage of HAAs and minerals. These membranes were fabricated through interfacial polymerization (IP) with $NaHCO_3$ as an additive. The tailored membranes exhibited enhanced negative charge, which benefitted their rejection of HAAs and passage of Ca and Mg. The higher rejection of HAAs (e.g., > 90%) with the lower rejection of minerals (e.g., < 30% for Ca) can lead to higher minerals/HAAs selectivity, which was significantly higher than those of commercially available NF membranes. In addition, the tailored membranes can achieve higher water permeance up to ~24.0 L m^{-2} h^{-1} bar^{-1} (more than doubled compared with the control membrane) thanks to the formation of stripe-like features and enlarged pore size. The simultaneous enhancement in minerals/HAAs selectivity and water permeance would greatly boost water quality and water production efficiency. Our findings provide a novel insight to tailor the properties of NF membranes for highly selective separation in drinking water treatment.

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Identification of emerging disinfection byproducts and screening of key molecules by Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR MS)

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Abstract

Disinfection can produce disinfection byproducts (DBPs), which endanger the safety of drinking water. The regulated DBPs are mainly small molecules with carbon numbers ≤ 2. However, with the development of Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR MS), more unknown macromolecules DBPs have been identified, providing technical support for determining the reaction mechanism of complex dissolved organic matter (DOM) and toxic molecules in the chlorination process. However, in the face of complex mass spectrometry data,

how to parse the key information becomes a challenge. For this purpose, based on the paired mass distance (PMD) between each reactant and product, we constructed a chlorination network of complex DOM. Spearman correlation analysis was used to determine the key molecules, anchor the reaction of key molecular groups, and realize the modularization of the reaction network. In combination with Pubchem database and structure similarity based-Chemical Space Networks (CSNs), the main carbon skeleton of key molecular groups was determined. Through these works, we have realized the accurate screening and in-depth analysis of FT-ICR MS data, which provides an analytical idea for applying FT-ICR MS in disinfection.

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Impact of Microplastics in Source Water on the Formation of Halogenated Disinfection Byproducts During Drinking Water Chlorination and Its Mechanism

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Abstract

Microplastics (MPs) are ubiquitously present in source water and undergo ultraviolet (UV) aging in aquatic environments before entering drinking water treatment plants. The presence of MPs in drinking water can impact the formation of halogenated disinfection byproducts (DBPs) during chlorine disinfection, yet the exact effect of MPs on DBP formation remain unclear. In this study, we conducted an investigation into the influence of non-aged and UV-aged MPs on halogenated DBP formation in drinking water and unveiled the underlying mechanisms. In comparison to source water samples devoid of MPs, the total organic halogen concentration was reduced by 19%-43% and 4%-13% in the drinking water samples containing non-aged and aged MPs, respectively. The differing effects on halogenated DBP formation can be attributed to the alternation in physical and chemical characteristics of MPs following UV aging. Aged MPs exhibited larger surface area with signs of wear and tear, heightened hydrophilicity, surface oxidation, increased oxygen-containing functional groups and dechlorination during the UV aging process. Both non-aged and aged MPs possess the capability to adsorb natural organic matter, leading to a reduction in the concentration of DBP precursors in the source water. However, the release of organic compounds from aged MPs outweighed the adsorption of organics. Furthermore, as a result of the surface activation of MPs through the UV aging process, the aged MPs themselves can also serve as DBP precursors. Consequently, the presence of halogenated DBP precursors in source water increased, contributing to a higher level of DBP formation compared to source water containing non-aged MPs. Overall, this study illuminates the intricate relationship among MPs, UV aging, and DBP formation in drinking water. It highlights the potential risks posed by aged MPs in influencing DBP formation and offers valuable insights for optimizing water treatment processes.

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Synergistic effect of combined UV-LEDs and peracetic acid treatment on inactivation of fungal spores

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Abstract

Photo-driven advanced oxidation process (AOP) with peracetic acid (PAA) has received increasing attention. In this study, a new PAA-based AOP (Ultraviolet light emitting diodes (UV-LEDs)/PAA process) was used to inactivate fungal spores. The synergistic factor of UV-LED_{265}/PAA, UV-LED_{280}/PAA and UV-$LED_{265/280}$/PAA are 1.25, 1.14 and 1.19, respectively for Aspergillus niger. The results indicated the synergistic effect of UV-LEDs/PAA system on spore inactivation, and it can be attributed to the generation of radicals and other synergistic action. The contributions of different mechanisms (UV-LEDs, radicals, synergistic action and PAA) in UV-LEDs/PAA process varied in different disinfection evaluation methods (cultivability, membrane integrity, and oxidative stress). For example, UV-LEDs contributed the most (76-87%) to spore damage in cultivability. The role of radicals (5-33%) and synergies (23-65%) mainly targeted in cell membrane damage. Radicals also can stimulate the increase in intracellular ROS level (4-53%). Compared with UV-LEDs alone, the increased inactivation rate constants (k) of UV-LEDs/PAA on membrane damage (0.08-0.25 cm^2/mJ) was much higher than cultivability and oxidative stress, suggesting that the synergistic effect of UV-LEDs/PAA was mainly reflected in the dramatic destruction of cell membranes (45-74%). In addition, the control efficiency of fungal spores of UV-LEDs/PAA were superior to solar/PAA and LP-UV, and the severe damage of fungal spores by UV-LEDs/PAA can control the spores in viable but not culturable states, suppressed the photoactivation, and decreased the possibility of fungal spore regrowth effectively.

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A flow-through Ti_4O_7 membrane electrode for ballast water disinfection: performance, mechanism, and comparison with Ti/RuO_2-IrO_2 electrode

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Abstract

Electrochemical Advanced Oxidation Processes (EAOPs) present a promising solution for ballast water treatment. However, due to the extremely short half-life of reactive oxygen species, the disinfection active zone is limited to the surface of the electrode, resulting in low disinfection current efficiency of

EAOPs. To address this challenge, this study developed a flow-through electrochemical disinfection system utilizing a Ti_4O_7 membrane electrode. A comparative analysis was conducted against a conventional Ti/RuO_2-IrO_2 electrode to assess the Ti_4O_7 membrane electrode's efficacy in ballast water disinfection. The flow-through mode significantly increased the probability of contact between *E. coli* and the surface of Ti_4O_7 membrane electrode, consequently leading to a notable increase in the inactivation rate from 1.05 min^{-1} to 1.63 min^{-1}, at a current density of 20 mA/cm^2, at a Cl^- concentration of 16.5 g/L, and an initial *E. coli* concentration of 10^7 CFU/mL. Notably, at low current densities, the Ti_4O_7 membrane electrode exhibited superior disinfection performance compared to the Ti/RuO_2-IrO_2 electrode. The predominant disinfection active species in the Ti_4O_7 membrane electrode system were identified as reactive oxygen species, particularly •OH and $•O^{2-}$, contrasting with the abundant generation of active chlorine species (ACSs) observed in the Ti/RuO_2-IrO_2 electrode system. Both electrode systems demonstrated the ability to disrupt the cellular structure of *E. coli*. However, due to the sustained effectiveness of ACSs, the degradation rate of total protein in the Ti/RuO_2-IrO_2 electrode system (40.53%) surpassed that of the Ti_4O_7 membrane electrode system (12.39%). Despite the minimal concentration of ACSs in the Ti_4O_7 membrane system (0.02 mg/L), no bacterial regeneration was observed, highlighting the efficacy of the Ti_4O_7 membrane electrode in preventing bacterial regrowth. This study elucidated a free radical-based disinfection mechanism for the Ti_4O_7 membrane electrode, affirming its feasibility for ballast water disinfection purposes.

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Enhanced Photocatalytic Molecular Oxygen Activation by Efficient Interface Charge Transfer for Antibiotics Degradation and its Disinfection By-products Formation Potential

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Abstract

Abstract:

Antibiotic residues and disinfection by-products (DBPs) formation caused by antibiotic abuse have posed potential risks to water safety and human health. Photocatalytic molecular oxygen activation has garnered widely concerned for its advantages such as low carbon emissions, environmental friendliness, and less secondary pollution. The reactive oxygen species (ROS) with strong oxidation capacity produced from photocatalytic molecular oxygen activation can completely degradation pollutants and inhibit the formation of DBPs precursors, thus achieving the purpose of controlling the DBPs formation potential. However, the limited carriers and the low interfacial charge transfer efficiency in the heterogeneous catalytic system hinder the continuity of the reaction, resulting in lower molecular oxygen utilization and surface chemical reaction efficiency, greatly impeding the process of photocatalytic molecular oxygen activation.

Here, van der Waals (VDW) heterojunction catalyst of oxygen-vacancy-rich (Bi_3O_4Br/rGO) with the synergy of interfacial charge transfer and efficient oxygen adsorption, Z-scheme heterojunction catalyst ($Bi_4V_2O_{11}$/Ag/AgCl) with direction regulation of interface carrier transfer, and photo-coupled peroxymonosulfate system ($Bi_3O_4Br/CuBi_2O_4$ + PMS) with efficient molecular oxygen activation by rapidly utilizing interfacial charges were constructed to investigate the molecular oxygen activation efficiency based on efficient interfacial charge transfer. Various characterization and research methods were used to explore cause and mechanism of the enhancement of molecular oxygen activation efficiency. The molecular oxygen activation efficiency of the Bi_3O_4Br/rGO and $Bi_4V_2O_{11}$/Ag/AgCl was increased by more than 4 times. The degradation efficiency of pollutants is greatly enhanced, and the removal rate can reach more than 80%. In addition, the formation potential of trichloromethane (TCM), dichloroacetic acid (DCAA) and trichloritromethane (TCNM) of TC after the degradation of $Bi_4V_2O_{11}$/Ag/AgCl and $Bi_3O_4Br/CuBi_2O_4$ was obviously reduced.

Key words: Molecular oxygen activation; ROS; Antibiotics degradation; DBPs formation potential; Interface charge transfer

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O_3-BAC based advanced treatment process of drinking water in downstream of China's Yangtze River Basin effectively reduces the formation and toxicity of disinfection by-products

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Abstract

To mitigate the concern of hazardous disinfection by-products (DBPs), a number of drinking water treatment processes have been developed. Prior research separately investigated the distribution

characteristics of DBPs and their precursors across expansive regions, remaining a largely unresolved issue: which process plays a pivotal role in reducing the risk of DBPs? This work undertook field investigations spanning 19 cities within the Yangtze River Basin, comparatively investigated the levels of DBP precursors in source water and (un-) known DBPs in authentic drinking water, alongside the evaluation of drinking water bulk cytotoxicity. It is found that the DBP formation potential of downstream source water was 1.88-fold higher than that of midstream. By contrast, the concentrations of DBPs and bulk cytotoxicity in downstream drinking water were 74% and 59% of those in midstream, respectively. ~72% of downstream cities implemented ozone-biological activated carbon (O_3-BAC) process. The popularization of O_3-BAC process in downstream cities effectively reduces the formation and toxicity of DBPs in drinking water. The synchronized control of carbonous, nitrogenous and chlorinated DBPs, but unsettled brominated DBP issue consolidated this deduction. Molecular characterization revealed that O_3-BAC process decreased the unsaturation and aromaticity of precursors, and eventually reduced the formation and cytotoxicity of DBPs. On average, the unsaturation degree ($(DBE\text{-}O)/C_{wa}$) of unknown features in drinking water decreased by 28% from midstream to downstream. Correlation analysis highlighted the significance of haloacetaldehydes (HALs), as major drivers of toxicity within DBP mixtures, inducing >50% of the DBP-associated cytotoxicity and positively correlated to bulk cytotoxicity of drinking water ($r > 0.99$, $p \leq 0.01$). A variety of (un-) known DBPs effectively managed via O_3-BAC process led to a reduction in the bulk cytotoxicity of drinking water within the Yangtze River Basin, indicating the promising prospect of O_3-BAC process for resilient water supply.

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Revealing the important toxicity driver of drinking water

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Abstract

A recent study indicated that seven classes of regulated and unregulated priority DBPs (one and two-carbon-atom DBPs) just accounted for 16.2% of disinfected water cytotoxicity in the U.S., meaning some of the highly toxic DBPs may be overlooked. In this presentation, a Meta analysis was used to explore the relationship between drinking water DBPs and human bladder cancer. The results suggested that low and higher levels of DBPs caused additional human bladder cancer (OR 1.45 [1.14, 1.85]). In addition, the key contributor to drinking water cytotoxicity was analyzed. Firstly, haloketones (HKs) was found to be a class of overlooked aliphatic DBPs, which may contribute 82% and 14% of calculated and overall drinking water cytotoxicity in US, respectively.Moreover, three classes of unknown aromatic and alicyclic DBPs were identified using non-target analysis, including chlorobenzenediols, chloroguaiacols and halocyclopentadienes. In addition, their concentration, formation, and toxicity were analyzed. The results suggested these three classes of emerging DBPs may use to explore the important contributor of drinking toxicity especially developmental toxicity.

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Formation of Larger Molecular Weight Disinfection Byproducts from Acetaminophen in Chlorine Disinfection

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Abstract

Acetaminophen is widely used to treat mild to moderate pain and to reduce fever. Under the worldwide COVID-19 pandemic, this over-the-counter pain reliever and fever reducer has been drastically consumed, which makes it even more abundant than ever in municipal wastewater and drinking water sources. Chlorine is the most widely used oxidant in drinking water disinfection, and chlorination generally causes the degradation of organic compounds, including acetaminophen. In this study, a new reaction pathway in the chlorination of acetaminophen, i.e., oxidative coupling reactions via acetaminophen radicals, was investigated both experimentally and computationally. Using an ultra-performance liquid chromatograph (UPLC) coupled to an electrospray ionization-triple quadrupole mass spectrometer, we detected over 20 polymeric products in chlorinated acetaminophen samples, some of which have structures similar to the legacy pollutants 'polychlorinated biphenyls'. Both C–C and C–O bonding products were found, and the corresponding bonding processes and kinetics were revealed by quantum chemical calculations. Based on the product confirmation and intrinsic reaction coordinate computations, a pathway for the formation of the polymeric products in the chlorination of acetaminophen was proposed. This study suggests that chlorination may cause not only degradation but also upgradation of a phenolic compound or contaminant.

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Rapid Extraction of Target Analytes from Water by Monolithic Adsorbents

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Abstract

Water contaminants are diverse and present at trace levels in complex matrices. Comprehensive analysis of water contaminants has become increasingly important for exposome studies. The first bottleneck is the complete extraction of all contaminants, specifically small polar compounds in water. In this presentation, I will demonstrate several monolithic adsorbents, such as monolithic hydrophile-lipophile balance (HLB) polymer, silica-based composite and covalent organic framework (COF) film. By

comparing their extraction performance with existing solid phase extraction materials, I will elaborate effects and importance of porous structure and surface property on extraction performance of adsorbents. The results show that (1) the hierarchical porosity enables fast mass transfer; (2) the film adsorbent can allow for high flow rates for rapid extraction; and (3) the surface engineering endows monolithic adsorbents with selective adsorption of small molecules but an anti-fouling feature for large molecules (e.g., proteins, humic acid, pigments). We anticipate this study would be helpful for producing new adsorbents for environmental analysis and others.

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Unveiling the toxicological effects induced by tire-derived chemicals in water disinfection

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Abstract

Tire-derived chemicals are important fractions of the anthropogenic chemical pool due to the ubiquitous occurrence. Previous studies revealed the high ecotoxicity induced by tire-derived chemicals. However, questions arise regarding the health impacts of tire-impacted water upon water disinfection. Using Chinese hamster ovary (CHO) cell cytotoxicity as the metric, we found that disinfection processes including chloramination, chlorination, and ozonation significantly elevated the cytotoxicity of tire-impacted water (4.1-, 3.3-, and 0.4-fold increases, respectively). Their cytotoxicity indices were 3.1-6.5 times as high as disinfected surface waters. Using nontarget analyses, over 8000 features were detected in tire-impacted water, 12% - 23% of which were abated upon oxidation. Through the suspect list matching, 103-204 tire-related chemicals were identified as reactants. The chemicals with moieties of benzothiazoles, phenolics, arylamines, organic acids or esters, and heterocyclics were actively involved in the chemical transformation. Meanwhile, 998-2611 features were formed. The formation of transformation products, especially the high-molecular-weight brominated and iodinated products resulted in elevated levels of cytotoxicity. 32 representative additives were quantified. CHO cell cytotoxicity of synthetic waters prepared by these additives after disinfection shows the same trend with tire-impacted water (i.e., the order of chloramination > chlorination > ozonation). Representative additives and their transformation products contributed to 25%-34% of the cytotoxicity in disinfected tire-impacted water, albeit rather minor in terms of dissolved organic carbon contribution (~5%). Our results highlight the high cytotoxicity induced by tire -derived chemicals in water disinfection, posing a potential threat to human health.

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Temporal Cytotoxicity of Disinfection Byproducts on Human Uroepithelium and Chinese Hamster Ovary Cells

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Abstract

The epidemiological observation linking increased bladder cancer risk to the consumption of chlorinated water highlights potential health implications related to disinfection byproducts (DBPs). It remains unclear what DBPs cause the risks because of the lack of information regarding human toxicological effects and mechanisms of DBPs. Chinese hamster ovary (CHO) cell cytotoxicity of over 100 DBPs has been used for the evaluation of water quality. However, human cell toxicity of DBPs is scarce because of lack of normal cell lines for testing. The immortalized human uroepithelium cell line, SV-HUC-1, exhibits biological characteristics which more closely resembling human bladder cells. Therefore, the objective of this study is to examine the comparative cytotoxicity of 14 unregulated and regulated DBPs on both SV-HUC-1 and CHO-K1 cells using a real time cell electronic sensing (RT-CES) platform. Real time responses enabled the determination of the temporal IC50 and toxicity index (TI, SV-HUC-1/CHO-K1) of DBPs over 72 h of exposure. The temporal comparative results revealed unique variations in cytotoxicity among the 14 DBPs. Except for four DBPs (BAN, TCAN, TriCBQ, and IAN), all the other DBPs showed TI ratios as high as 12 (1-12) and progressively increasing over the 72h exposure period. The results demonstrated that the SV-HUC-1 cells exhibited higher cytotoxicity than the CHO-K1 cells. Cell cycle analysis revealed these DBPs inhibited cell growth at different phases. BAA, IAA, CAN and IAN triggered cytotoxicity on SV-HUC-1 cells by inhibiting mitosis and cell division, whereas in CHO-K1 cells, monoHAAs triggered cytotoxicity by disturbing DNA synthesis. Different DBPs also induced varying reactive oxygen species (ROS) production in a cell dependent manner. The variations in cytotoxicity between SV-HUC-1 and CHO-K1 cells exposed to the same DBPs emphasize the presence of compound-specific and cell-specific mechanisms. This study highlights the need for further investigation into the effects of different mixtures of DBPs on human health.

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Molecular-level insights into natural organic matter and its derived chlorinated disinfection byproducts

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Abstract

Dissolved organic matter (DOM) in water, especially the fluorescent DOM, has high reactivity with chlorine, resulting in toxic disinfection byproducts (DBPs). The effective removal of DOM before disinfection is a critical element in controling the formation of toxic DBPs, which is closely related to the recognition of molecular structures for DOM, especially the fluorescent DOM. However, the limited information about the molecular features of fluorescent DOM left much room for the determination of DBP precursors. In our study, optical characteristics and molecular features of DOM fractions with varying molecular weight were first illuminated by using fluorescence excitation-emission matrix spectroscopy and Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS). Through Spearman's rank correlation analysis of fluorescent components and FTICRMS peak relative intensities, 840 formulae shared by different DOM fractions were associated with corresponding fluorescent components, accounting for 58.64% of FTICR-MS peak intensities of raw water. Most of these 840 molecular features are expected to directly account for the optical properties of aggregates for forming macromolecular fluorescent substances. Given the high chlorine reactivity of fluorescent compounds, these 840 molecular features shed some light on the unknown DBP precursors. Due to the complexity of NOM precursors, the formation mechanisms of DBPs and impact factors such as dissolved oxygen (DO) and chlorine dosages on DBP formation during disinfection, particularly at the molecular level, remain unclear. In our recent studies, source waters underwent chlorination with/without DO as well as at different chlorine dosages were tracked using FT-ICR-MS. Mass difference analysis revealed distinctive DBP formation mechanisms under different DO or chlorine dosages. Our findings highlighted the merits of reducing DO/chlorine dosages for controlling Cl-DBPs and reducing the toxicity of water treated by the chlorine process.

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Neurodevelopmental toxicity induced by 2,6-dichloro-1,4-benzoquinone disinfection byproduct

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Abstract

Background: Halobenzoquinones (HBQs) are an emerging class of disinfection byproducts (DBPs) detected in both disinfected drinking water and swimming pool water. Among HBQs, 2,6-dichloro-1,4-benzoquinone (DCBQ) is the most frequently detected one and has the highest concentration. Toxicological experiments have proved that HBQs are extremely cytotoxic, so the health risks of HBQs cannot be ignored. However, there are relatively few reports on their potential neurodevelopmental toxicity, especially the lack of in vivo studies as the most direct evidence.

Methods: This study adopts an integrated method of in vivo and in vitro experiments. A rat model was established for the entire gestation and lactation period to study the neurodevelopmental toxicity of

DCBQ in offspring rats. SH-SY5Y cells were exposed to DCBQ during differentiation to investigate the effects of DCBQ on cell proliferation, neural differentiation, oxidative damage and apoptosis.

Results:

1. in vivo test: Maternal DCBQ exposure impaired the neurobehavior of offspring rats through open field test and Morris water maze test. After maternal DCBQ exposure, the offspring rats showed disordered and loose neural fiber structure. DCBQ reduced the levels of neurotransmitters in the serum and hippocampus of offspring rats, and decreased the mRNA expression of neurotransmitter receptors in offspring rats. Also, maternal DCBQ exposure induced oxidative damage in cerebral cortex of offspring rats, and up-regulated the mRNA and protein expression levels of Cyt-C, Caspase 9, and Caspase 3 in the cerebral cortex of offspring rats. Additionally, maternal DCBQ exposure induced alterations in intestinal flora and intestinal metabolites in offspring rats.

2. in vitro test: DCBQ had a significant inhibitory effect on the proliferation of differentiating SH-SY5Y cells, inhibited the neural differentiation of SH-SY5Y cells, increased intracellular ROS, decreased mitochondrial membrane potential and increased the rate of apoptosis. After exposure to DCBQ, the mRNA and protein expression levels of Cyt-C, Caspase 9, and Caspase 3 in differentiating SH-SY5Y cells were significantly increased.

Conclusion: Our data indicated that DCBQ exposure induced neurodevelopmental toxicity both in vivo and in vitro, and revealed molecular mechanisms of the neurodevelopmental toxicity of HBQs. It also provides new ideas for further studies of the neurodevelopmental toxic effects and mechanisms of other DBPs.

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Inactivation Characteristics of Antibiotic Resistant Bacteria by Chlorine Disinfection

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Abstract

The transmission of antibiotic-resistant bacteria (ARB) poses a significant health risk to human health, numerous studies have indicated the contamination of ARB in drinking water systems. Water disinfection is a crucial process in controlling microbial contamination. However, the characteristics of ARB inactivation during the disinfection process remain relatively limited. Two strains of ARB, *Bacillus paralicheniformis* and *Stenotrophomonas maltophilia*, were isolated, purified, and identified from home water filtration systems in this investigation. The resistance gene sequences were analyzed and the efficacy of chlorine disinfection and changes in ARB activity were investigated.

Both ARB strains contained multiple antibiotic resistance genes including tetracycline class, macrolides class, fluoroquinolones class, aminoglycosides class, sulfonamides class, cephalosporins class, peptide classes, and glycopeptide classes, they also each contained several virulence genes related to aggression, defense, tolerance functions , lack of specificity and virulence regulation. The chlorine resistance of two ARB strains and the non-resistant control strain *Escherichia coli 13733* decreased successively. The necessary amounts of sodium hypochlorite to accomplish a 3 log drop in viable counts were 125, 150, and 75 mg Cl_2·min/L, the quantities of chloramine needed to achieve a 4 log reduction were 80, 120, and 100 mg Cl_2·min/L accordingly.

Chlorine disinfection induced various cellular responses among these bacterial strains such as reactive oxygen species (ROS) generation, bacterial cell membrane permeability enhancement , extracellular protein release, and increased superoxide dismutase (SOD) activity. During the process of disinfection with chlorine, the activity of the SOD enzyme in *Stenotrophomonas maltephilia* rose by a factor of 5.9, while the leakage ofaromatic organic compounds increased by a factor of 4.3. However, the ROS level produced by *Bacillus paralicheniformis* was considerably lowered by 92%, and the extracellular total protein content was reduced by 63%. During hypochlorous acid disinfections, certain ARBs can transition into a viable but non-culturable (VBNC) condition.

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Understanding molecular-level reactions between permanganate/ferrate and dissolved effluent organic matter

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Abstract

Permanganate [Mn(VII)] and ferrate [(Fe(VI)] oxidations are well-recognized as advanced treatment processes to degrade organic components detected in secondary effluents from municipal wastewater treatment plant (WWTP). However, Mn(VII) or Fe(VI) reactions are sensitive to the water matrix components, especially the dissolved effluent organic matter (EfOM) contained in secondary effluent. Here, we found that Mn(VII) or Fe(VI) hardly mineralize EfOM, but do change its molecular-level composition. Tests with representative trace organic contaminants (TrOCs) spiked to EfOM-rich wastewater effluent showed that Mn(VII) and Fe(VI) preferentially oxidize phenolic TrOCs. UV-vis and fluorescence spectroscopy analyses suggested that molecular properties associated with optical characteristics of reaction solutions are altered by treatment, including decreases in aromaticity, molecular weight, and electron-donating capacity of EfOM. At the molecular-level, the observed phenomenon is ascribed to preferential oxidation of aromatic structures and electron-rich functional groups (e.g., phenolic structures and hydroxyl groups) within EfOM, as well as the transformation and decomposition of macromolecular sulfur- and nitrogen-containing compounds (most likely

proteins or microbial byproduct-like material). These findings advance the application of Mn(VII) and Fe(VI) for optimization and proper control of EfOM of emerging concern within treatment trains being developed for advanced treatment facilities.

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Effects of Graphene Quantum Dot on Formation of Disinfection Byproducts during Chlorination

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Abstract

Graphene quantum dots (GQDs) are widely used in various fields due to their distinctive physicochemical properties, and residual GQDs in aqueous environments may affect the formation of disinfection byproducts (DBPs) when entering the disinfection process. Since GQDs have different structures and small particle sizes from other graphene materials, the effect of GQDs on the formation of DBPs during chlorination may be distinguished from that of common graphene oxide (GO) and graphene. The results showed that trichloromethane (TCM) generated from GQDs increased with increasing concentration, reaching a maximum concentration of 1019.6 μg/L, while GO and graphene form TCM at 99.1 μg/L and 7.0 μg/L, respectively. This also suggests that GQDs has the highest potential for DBPs formation due to the abundance of oxygen functional groups and strong hydrophilicity compared to GO and graphene. Different water chemistry conditions such as Br^- increased the formation of Br-DBPs, however, high pH led to a decrease in TCM generated by GQDs, which is different from other graphene materials, and NaCl concentration has a negligible effect on DBPs. Further, residual GQDs in natural water samples can participate in the formation of DBPs and reduce the concentration of DBPs in the surface water through adsorption, which can be influenced by the diversity of chemical composition and the complexity of microbiological activity in surface water. Therefore, a deeper investigation into the interaction mechanisms between GQDs and DBPs under real water sample conditions is of significant scientific importance for optimizing water treatment processes, reducing the formation of DBPs, and ensuring water quality safety.

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Comparison of the inactivation of harmful protozoa in mariculture by UV/chlorine, UV/monochloramine, and UV/chlorine dioxide: efficiency, mechanism and feasibility

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Abstract

Advanced Oxidation Processes (AOPs) are increasingly being researched and applied for the inactivation of harmful microorganisms, while there is limited research on the inactivation of harmful protozoa in aquaculture water. This study investigated the inactivation efficiency and mechanism of *Uronema marinum* (*U. marinum*) under the treatment of UV/chlorine, UV/monochloramine (UV/NH_2Cl), and UV/chlorine dioxide (UV/ClO_2), and evaluated the feasibility of these processes in marine aquaculture. The inactivation efficiency of *U. marinum* by three AOPs followed the sequence UV/chlorine > UV/NH_2Cl > UV/ClO_2 at an oxidant concentration of 25 μM, and an irradiation wavelength of 254 nm. Furthermore, the concentrations of free radicals (•OH, •Cl, and •ClO) and disinfection by-products (DBPs) generated in the three AOPs exhibited the order same. In the investigation of the inactivation mechanism of *U. marinum*, transcriptomic analysis results indicate that the impact of chlorine-based AOPs on the transcription, translation, and lipid metabolism of *U. marinum* may be crucial factors of the inactivation of *U. marinum*. In addition, Pathological analysis of fish indicates that compared with UV/chlorine and UV/NH_2Cl treatments, tilapia cultured in seawater treated with UV/ClO_2 had lower mortality rates and almost no damage. The results of this study provide valuable fundamental information for the selection and operation of AOPs to deactivate harmful microorganisms in marine aquaculture water.

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Revealing Precursors and New Disinfection Byproducts in Water: Machine Learning Assisted Nontargeted Analysis

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Abstract

Appropriate disinfection of drinking water is effective to prevent waterborne disease. An unintended consequence of the chemical disinfection process is the formation of disinfection byproducts (DBPs), resulting from reactions of disinfectants with organic matter in source water. Epidemiological studies have indicated potential association of chronic DBP exposure with adverse health effects (e.g. increased risk of bladder cancer). Although a few easily detectable DBPs are regulated, they may not be responsible for the adverse health effects. To meet growing water demands while controlling regulated DBP formation, water utilities are applying new disinfectant combinations. In light of these

changes in disinfection practice, we must characterize DBPs that are important to human health effects. Water disinfection unavoidably produces a large number of disinfection products (DBPs). Currently, majority of DBPs (>70%) remained unidentified. Nontargeted analysis using high resolution mass spectrometry (HRMS) can detect a huge number of features in each sample, however, data processing is the bottleneck hampering progress in uncovering new DBPs. This presentation will describe our current development of machine learning assisted analytical techniques for nontargeted analysis of precursors in source water and identification of new DBPs of toxicological importance.

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The environmental behavior and underlying mechanism of polar halogenated disinfection by-products in soil system

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Abstract

Disinfection is an essential process in the treatment of reclaimed water, with chlorine disinfection being widely adopted due to its cost-effectiveness and efficacy. However, the disinfection process can lead to the formation of disinfection by-products (DBPs) through reactions with natural organic matter, anthropogenic pollutants, and halogen ions. Among halogenated DBPs, brominated DBPs demonstrate significantly higher toxicity than chlorinated DBPs. In complex soil environments, polar halogenated DBPs are primarily controlled by soil adsorption due to their reduced reactivity with organic matter. The adsorption and desorption behaviors of three polar halogenated disinfection byproducts, 2,4-dichlorophenol (2,4-DCP), 2,4-dibromophenol (2,4-DBP), and 2,4,6-tribromophenol (TBP), were investigated in four representative vadose zones located in Beijing, Anyang, Hangzhou, and Harbin. Moreover, Common polyethylene (PE) in soil was selected to explore the effect of MPs on the adsorption and desorption behavior of TBP in soil.

The results indicate that adsorption followed pseudo-second order kinetic, and the adsorption thermodynamics fitted Langmuir models well. With the increase of temperature and environmental pH and ionic strength, the adsorption amount of DBPs

in soil decreased. Compared to Anyang and Hangzhou soils those from Beijing and Harbin exhibited higher adsorptive capacity towards these target compounds. Multiple linear regression modeling revealed that soil adsorption was controlled by combined effects rather than single factor. For TBP adsorption, with the increase of microplastics (MPs) dosage the adsorption amount of TBP in soil decreased. Compared with APE, PE has a stronger inhibitory effect on TBP adsorption, because its lower zeta potential weakens its binding ability to TBP anions and soil particles. The adsorption energy (Eads) of TBP/ soil, TBP/MPs, and MPs/ soil systems showed negligible affinity between TBP and MPs, while the interaction between MPs and soil particles was more pronounced. TBP is more likely to adsorb soil particles than MPs, and MPs can compete with TBP for adsorption sites on soil. In addition, the affinity of PE to soil particles was better than APE. These findings would be benefit for the control of DBPs pollution in soils and guarantee the safety of groundwater.

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Potential hygienic risks in household water purifiers: Buildup of antibiotics and antibiotic resistance genes

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Abstract

Contamination of emerging organic pollutants in drinking water become a public health concern. Water treatment plants can not completely remove the emerging organic pollutants at micrograms per liter or nanograms per liter levels. To ensure safe and high-quality drinking water, terminal water purifiers have become increasingly popular in households and public buildings as a means of preventing the intake of emerging organic pollutants.

However, concerns are raised regarding the control efficiency in eliminating emerging organic pollutants. To enhance our understanding of the reliability and potential risks of household water purifiers (HWPs), the removal of antibiotics, and antibiotic resistance genes (ARGs) in terminal household water purifiers was investigated.

The levels of antibiotics and ARGs were between less than the limit of detection (LOD) and 7.9 ng/L and between less than LOD and 3.45×10^5 copies/L, respectively, in tap water. HWPSs with fresh filters had a high efficiency in removing antibiotics and ARGs. However, after long-term operation (e.g., more than three months), some HWPSs had low removal rates of antibiotics and ARGs and some HWPSs released antibiotics and ARGs into the effluents leading to higher levels of antibiotics and ARGs in the effluents than those in the influents. Biofilms were observed on many filters of the investigated HWPSs. ARGs were detected on the filters with relative high abundances. High-throughput sequencing analysis showed that *Alphaproteobacteria* and *Gammaproteobacteria* were the dominant classes. The abundances of *Cyanobacteria*, *Patescibacteria*, *Bacteroidetes*, and *Proteobacteria* were significantly positively correlated with the abundances of ARGs.

Microbial growth and enrichment commonly observed in HWPSs can accelerate the exposure risk posed by antibiotics and ARGs to the consumers of water.

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Toxicity Control of Swimming Pool with High Swimming Loads

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Abstract

The commonly used swimming pool disinfectant in China is sodium hypochlorite. However, the high reactivity of sodium hypochlorite with many kinds of organic pollutants such as urine and sweat of swimmers increases the toxic and harmful substances in the water after disinfection. Therefore, we should look for a new type of disinfectant with high persistence ability and low toxicity after disinfection. This paper explored the mechanism of water toxicity after peracetic acid disinfection under various conditions. The traditional disinfectant sodium hypochlorite was used as the benchmark for comparative analysis. The main conclusions are as follows:

(1) The persistence kinetic models (R^2>0.93) were successfully developed and verified to simulate the decay of peracetic acid and sodium hypochlorite in a swimming pool with high swimming loads. It was found for the first time that human body fluid analogues (BFA) had inhibition on the decay of peracetic acid, among which *L*-histidine and citric acid were the two components that caused the inhibition of the decay of peracetic acid.

(2) The variation of toxicity of peracetic acid for disinfection of swimming pool water was discussed for the first time. It was found that the toxicity of water after peracetic acid disinfection was 11.2-39.4 times lower than that of sodium hypochlorite under different swimming loads, multi-period cumulative disinfection and temperature change. The use of peracetic acid instead of sodium hypochlorite for disinfection improved the chemical safety of swimming pool water.

(3) Total organic carbon, ammonia nitrogen and regional fluorescence integral values were significantly correlated with cytotoxicity, and the correlation between regional IV and V were the highest in the peracetic acid disinfection system (-0.94, -0.86). The above characteristic indexes are selected as the alternative indexes of cytotoxicity, which can be used to predict the water toxicity of swimming pool under different swimming loads, multi-cycle cumulative disinfection and temperature changes.

(4) Fluorophore components 1 and 2 represented by humic acid substances may be part of the toxic substances that lead to the increase of toxicity after peracetic acid and sodium hypochlorite disinfection, while the high toxicity caused by sodium hypochlorite disinfection may be due to the macromolecular structure of component 2.

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Solar-driven transformation behaviors and fate of novel halogenated bisphenols and parabens in environmental and engineered water systems

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Abstract

Bisphenols and parabens are classified as emerging contaminants in global waters, and the ubiquitous emergence of their high-risk halogenated products generated from chlorine-based wastewater disinfection has attracted increasing concern. However, rather limited information is known on their environmental behaviors and fate after discharging into surface waters, and also their degradation behaviors by the solar-based engineering water treatment remain unclear. In this study, the reactivity of halogenated bisphenols and parabens with different photochemically produced reactive intermediates was measured and the quantitative contribution analysis showed the dominance of direct photolysis in abating such compounds in sunlit natural freshwaters. The introduction of the solar/peroxymonosulfate (PMS) system could greatly improve the removal of chlorinated parabens. The high-resolution mass spectrometry analysis of the degradation products suggested that dechlorination, hydroxylation, and ester chain cleavage were the dominant transformation pathways during photolysis and solar/PMS treatment. Furthermore, the *in silico* prediction implied the severe aquatic toxicity of certain products but with enhanced biodegradability. Overall, this investigation filled the knowledge gaps on the reactivity of the halogenated bisphenols and parabens with diverse reactive transients and their quantitative contributions to the photolysis and solar/PMS treatment of these emerging micropollutants in water.

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Experimental and computational studies of transformation products of sulfachloropyridazine during water chloramination

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Abstract

Sulfachloropyridazine (SCP), a widely used broad-spectrum antibiotic, occurs in surface water and it can react with chloramine during disinfection to produce new disinfection by-products (DBPs). This study investigated the kinetics and mechanisms of transformation of SCP to new products during water chloramination and assesses the toxicity of the new products by both experimental and computational approaches. The reaction between SCP and monochloramine follows pseudo-second-order reaction kinetics and the reaction rate constant is 0.012 $\mu mol^{-1}h^{-1}$ at pH 6.0. A pH-dependent kinetic profile was observed as lower pH values facilitate more reactive neutral SCP, which has enhanced reactivity with disinfectant. Such pH-driven behavior significantly influences the structural diversity of the resulting DBPs. A total of eight new DBPs were characterized by LC-MS/MS, including chlorinated derivatives of aniline group, hydroxyl derivatives of the aromatic ring, desulfurization products, sulfonamide cleavage products, and reduced chlorination products of aniline group. Theoretical simulations depicted the formation pathway of each DBP, particularly indicating the chlorinated derivatives at aniline group as a key factor to trigger the desulfurization reaction. Finally, a comparative cytotoxicity assessment was carried out and the results show unexpected heightened cytotoxicity of the transformation products of SCP to Hep G2 cells. In conclusion, this study significantly advances our comprehension of SCP transformation and the associated health hazards during chloramine disinfection, shedding light on the innovation and impact of our findings.

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Effect-directed identification of toxic disinfection byproduct formed during halides-involved UV/chlorine treatment

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Abstract

UV/chlorine as an advanced oxidation process has been proposed for pollutant removal and deep disinfection. However, the coexistence of inorganic ions and natural organic matter (NOM) in the water body may affect the disinfection effect and participate in the formation of toxic disinfection byproducts (DBPs). Phenols were selected as the model compound for NOM to study the DBPs formation and toxicity during the treatment of UV/chlorine in the presence of bromide or iodide at actual water concentration levels. Known DBPs and total organic halogen results showed that phenol treated by UV/chlorine with bromide produced more disinfection byproducts than that of UV/chlorine alone and with iodide. The results of acute toxicity of luminescent bacteria indicated more toxic DBPs were produced during UV/chlorine treatment with bromide. Effect-directed analysis (EDA) was applied for the identification of toxicity drivers in the DBPs. Fractionation coupled to toxicity evaluation prioritized the fractions containing the toxic drives, and high-resolution mass spectrometry was used to identify their structures.

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DBP control in DWTPs in Yangtze River Delta region

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Abstract

The Yangtze River basin, which spans one-fifth of China's land area and serves as a crucial water source for one-third of the nation's population. During long-distance water transport from upstream to downstream, a varied array of dissolved organic matter (DOM) from diverse sources were introduced, leading to a significant fluctuation in DOM properties, and the formation of disinfection byproducts (DBPs) in drinking water treatment plants (DWTPs). Our mission is to ensure the safety of drinking water in this region, specifically from the perspective of DBPs.

The research interests mainly focus on identification, occurrence, formation and control of high-risk DBPs in drinking water. The DOM along the Yangtze River, the important DBP precursors, were well characterized, and a long-term survey on the occurrence of DBPs in the distribution system survey in the Yangtze River Delta from 30 DWTPs were conducted. Drawing from the aforementioned study, a series of control strategies were proposed. O_3-GAC, UV/H_2O_2 -chloramination and multipoint chlorination in distribution system could dramatically reduce DBP formation, and has been successfully applied on a large scale in over 20 major water works in the Yangtze River Delta region, with a total capacity of 7 million tons/day, benefiting a population of over 20 million. This study helped to understand the fate of DOM during the transmission in the Yangtze River, and provided a theoretical foundation for ensuring the quality of drinking water in the Yangtze River Delta region, and it could also provide new perspectives on the control of DBPs in other regions or countries.

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A Novel Heterogeneous Reactivity-Directed Analysis Approach for the Identification of Toxic Disinfection Byproducts in Drinking Water

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Abstract

Disinfection byproducts (DBPs) are associated with adverse health effects but many DBPs which may exist greater toxicities than the regulated DBPs remain uncharacterized. The reactivity directed analysis (RDA) strategy has been developed for the precise identification of predominant toxic DBPs. However, the application of the existing homogeneous RDA approaches remains challenging due to the chemical complexity and low abundance of many DBPs. Additional pre-treatment steps may also cause the loss of some important DBPs. Herein, we propose a heterogeneous RDA approach integrating the enrichment and the reactivity of the thiol probes and DBPs in one step. A mercaptopropionic acid functionalized Zr-metal organic frameworks NU-1008 was chosen as a platform to selectively concentrate and react with the toxic DBPs. The adducts of the DBPs and mercaptopropionic acid was eluted from the NU-1008 by solvent-assisted ligand incorporation and then analyze using the high-resolution mass spectrum to predicted their formulas and structures. The proposed heterogeneous RDA approach may address the shortcomings of the existing RDA approaches and provide a powerful tool for the efficient nontargeted identification of the unknown toxic DBPs.

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Control of Antibiotic Resistant Bacteria by Chlorine or UV Disinfection

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Abstract

Municipal wastewater is a hotspot for proliferation of antibiotic resistant bacteria (ARB), making it a crucial site for effective control of ARB. Chlorine and ultraviolet (UV) are widely used in disinfection of municipal wastewater. In this study, we investigated the control of ARB in real and simulated secondary wastewater effluents by chlorine or UV disinfection. Both UV and chlorine disinfection showed similar removal efficiencies for antibiotic resistant *E. coli* to those for the total *E. coli*. For amoxicillin- and

ampicillin-resistant *E. coli*, UV was more effective, while tetracycline- and azithromycin-resistant *E. coli* were more susceptible to chlorine disinfection. More importantly, through investigation of the change in ARB abundance during UV or chlorine disinfection, we found that chlorine disinfection significantly reduced the relative abundances of all antibiotic resistant *E. coli* tested, whereas UV disinfection significantly increased the relative abundances of all antibiotic resistant *E. coli* tested. These results indicate that chlorine disinfection may exhibit a greater potential for effectively controlling ARB compared to UV disinfection.

463

Exploring Higher Molecular Weight Byproducts of Chlorine Disinfection

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Abstract

The reaction of chlorine, the world's predominant disinfectant, with natural organic matter forms potentially carcinogenic disinfection byproducts (DBPs). For nearly 5 decades, research and regulation has focused on a limited number of 1-2 carbon DBPs, particularly trihalomethanes (THMs) and haloacetic acids (HAAs). Over the past decade, research has highlighted the potentially important contribution to the DBP-associated toxicity of disinfected waters of other unregulated 1-2 carbon DBP classes (e.g., haloacetonitriles) that occur at lower concentrations than THMs/HAAs, but exhibit orders of magnitude higher toxic potencies in in vitro mammalian cell bioassays. However, more recent research that has applied these bioassays to whole disinfected waters has suggested that the poorly characterized fraction of higher molecular weight DBPs may be a more important contributor to toxicity. Recognizing the importance of this higher molecular weight fraction can have important practical implications for water treatment. First, research has indicated that the quality of potable reuse water can be comparable or higher than conventional drinking water, suggesting that purifying municipal wastewater as a drinking water supply can provide a safe and high quality water supply. Second, research has indicated that switching from chlorine disinfection to GAC/chlorine can reduce toxicity to a greater degree than switching to chlorine/chloramine disinfection despite comparable reductions in THM/HAA formation. Third, DBP monitoring tends to focus on high water age portions of the distribution system, where THM/HAA concentrations are maximized. However, toxicity tends to reach maximum levels closer to drinking water treatment plants. These findings highlight the need to characterize components driving the toxicity of disinfected waters within the higher molecular weight DBP fraction. The remainder of the presentation will discuss some of the analytical approaches being pursued, including 1) high resolution mass spectrometry, 2) monoaromatic DBPs, and 3) transformation products from chlorine reactions with monomers bound within polymers.

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Improving drinking water safety: Addressing new impacts, identifying important toxicity drivers, and looking to potable reuse

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Abstract

While consumers are concerned about pharmaceuticals and per- and polyfluorinated alkyl substances (PFASs) in their drinking water, the largest threat is from disinfection by-products (DBPs), which are an unintended consequence of using chemical disinfectants to make water microbially safe to drink. DBPs are formed by the reaction of disinfectants with naturally occurring organic matter, bromide, and iodide, as well as from anthropogenic pollutants, such as pharmaceuticals. DBPs are present at levels that are orders of magnitude higher than other emerging contaminants, and many have been found to be carcinogenic, genotoxic, mutagenic, cytotoxic, or developmentally toxic. DBPs have also been associated with cancer, miscarriage, and birth defects in human epidemiologic studies. However, until recently, most research focused only on the 11 DBPs regulated by the U.S. EPA, and the complex chemical mixture of DBPs in drinking water was largely unknown. This presentation will present a state-of-the-science overview of emerging DBPs, including the discovery of new toxic, bioaccumulative halocyclopentadiene DBPs and new findings on potable water reuse. The ultimate goal is to uncover these risks so that new strategies can be applied to improve the safety of drinking water.

526

Photochemical Degradation of Dissolved Organic Matter under Solar Photolysis of Chlorine: Formation of DBPs, Change of Cytotoxicity and Reactive Species

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Abstract

Since elevated level of residual chlorine was discharged into surface water, more attentions should be paid to the degradation of dissolved organic matter (DOM) by solar photolysis of chlorine in natural waterbodies. However, disinfection byproducts (DBPs) formed from DOM under solar photolysis of chlorine, and changes of cytotoxicity during this process remain unclear. In this study, Solar photolysis of chlorine can not only promote the formation of aliphatic chlorinated DBPs, but also significantly increase the generation of aromatic chlorinated DBPs by 44.7-109% and 81.7-121%, respectively compared with dark chlorination. Unknown total organic chlorine containing in low molecular weight (< 1kD) fraction significantly positively correlated to the cytotoxicity of disinfected water. Several quality parameters (bicarbonate, dissolved oxygen, pH, nitrate, ammonia, bromide and iodide) affecting the radical chemistry and formation of DBPs under solar photolysis of chlorine were also investigated. Reactive species

including $HO^{\bullet}$, $Cl^{\bullet}$, O_3 and reactive nitrogen species (RNS) were responsible for the formation of different DBPs. Especially O_3 increased the formation of most categories DBPs tested in this study, and RNS significantly contributed to the formation of nitrogenous DBPs. This study provided more understanding on the adverse impact of overused chlorine, and reaction mechanisms between reactive species and DOM in the future.

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Germination of chlorine-resistant fungal spores in drinking water: stimulation effect by chlor(am)ination and associated taste & odor issues

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Abstract

Disinfection is a key procedure in drinking water supply systems (DWSSs). Fungi, a group of chlorine-resistant microorganisms, have been frequently detected in DWSSs, leading to potential risks of fungal infections, proliferation of biofilms, off-flavors, and increased chlorine consumption. In recent years, fungal contamination of drinking water has become a forefront issue of great concern in the field of water quality science. However, research on the distribution patterns of fungi in DWSSs, their regrowth characteristics, and the derived water quality risks is still in its early stage.

This study investigated germination behavior of three chlorine-resistant fungal spores (*Penicillium chrysogenum*, *Cladosporium halotolerans*, and *Penicillium spinulosum*) in synthetic tap water (STW) at varying conditions of disinfectants (free chlorine and monochloramine), humic acid (HA), and pH. The germination of *C. halotolerans* spores was surprisingly stimulated by chlor(am)ination, with a ratio of 44.14-67.5%. Stimulation effect was outweighed by inactivation at high *CT* values. Nontargeted metabolomics analysis identified the decrease of several potential self-inhibitors for spore germination by chlor(am)ination. Patterns of significantly changed metabolites and pathways, involving lipid, sugar, and amino acid metabolism, were significantly affected by chlor(am)ination treatment for *C. halotolerans* spores. The results provide new insights into survival strategies and germination mechanisms of fungal spores in DWSSs.

In addition, taste and odor (T&O) are among the most frequently encountered aesthetic issues in drinking water. In this study, the T&O compounds produced by 10 native fungal isolates were investigated from two drinking water treatment plants and a premise plumbing. In total, 17 odorants were identified. These fungal isolates from drinking water have been demonstrated to generate high concentrations of musty/earthy compounds, i.e., musty/moldy 2-methylisoborneol (26-256 ng/L), geosmin, and 2-isobutyl-3-methoxy-pyrazine (3-13 ng/L). The genera with the highest yields of these odorants include *Penicillium*, *Aspergillus*, *Paecilomyces*, and *Alternaria*. UV treatment in premise plumbing significantly (p<0.05) reduced the gene reads count of Ascomycota phylum, and *Aspergillus*, *Fusarium*, *Rhizopus*, and *Trichoderma* genera by 2.3, 3.1, 3.8, and 3.7 times, respectively, indicating that UV might serve as a promising strategy for controlling fungi in drinking water.

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Uncovering Halogenated Nucleotides and Nucleobases as Emerging Disinfection Byproducts in Drinking Water

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Abstract

Constant efforts have been devoted to exploring new disinfection byproducts in drinking water causally related to adverse health outcomes. We proposed that chlorinated nucleic acids may occur as mutagenic DBPs in drinking water which were generated from the reaction between chlorine disinfectants and nucleic acids. 113 halogenated nucleotides were identified after chlorination of four representative nucleotides in the presence of bromide and iodide using a non-targeted ultrahigh performance liquid chromatography-mass spectrometry (UPLC-MS/MS) analysis method. The active sites of nucleotides with chlorine were on the aromatic heterocyclic rings of nucleobases, and the formation of these chlorinated nucleotides involved decarbonization, hydrolysis, oxidation and decarboxylation. A highly sensitive quantitative method was further established for halogenated nucleobases and nucleosides by using solid phase extraction (SPE) coupled with UPLC-MS/MS, and the detection limit were in the range of 0.04–0.86 ng/L. Five halogenated nucleobases were identified as new DBPs in drinking water. 2-Chloroadenine showed the highest cytotoxicity (IC_{50}=9.4 μM), while 5-chlorouracil showed the highest genotoxicity (50% Tail DNA = 411 μM). This study provides the first set of evidence for the occurrence of chlorinated nucleotides and nucleobases as mutagenic DBPs after disinfection of drinking water.

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Transformation-derived Toxicity of Metformin During Water Chlorination: A Potential Health Concern

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Abstract

Metformin, as the first-line medication for type II diabetes, has become a global contaminant because of its widespread occurrence in aquatic environments and demonstrated adverse effects on organisms. Chlorination disinfection is routinely utilized in water treatment plants to eliminate microbial risks and also inevitably transform metformin into concerning chlorinated products. However, rather limited research exists on the transformation products and toxic effects of metformin during chlorination. Here, we identified chlorinated metformin products using high-resolution mass spectrometry, detected the presence of the two chlorinated products (3E)-3-(chloroimino)-N,N-Dimethyl-3H-1,2,4-triazol-5-amine (3,3-CDTA) and N-cyano-N,N-dimethylcarbaminmidic chloride (NCDC) in urban water systems as well as evaluated their toxicity on organisms and cells. It is found that 29 metformin products were formed during chlorination, with over 50% exhibiting higher environmental risk than metformin itself. Based on their formation stability, high environmental risk and refined prepared protocol, 3,3-CDTA and NCDC were successfully prepared. Monitoring of various water systems revealed the in situ production and widespread presence of NCDC. Furthermore, compared to metformin with no observable toxic effects, both 3,3-CDTA and NCDC induced membrane disruption, oxidative stress responses, and abnormal protein expressions in Escherichia coli, suggesting potential adverse effects on microbial communities and human health. Both products caused growth inhibition and photosynthetic damage in Pseudokirchneriella subcapitata, indicating potential aquatic ecotoxicity. Their toxicological responses observed in Caenorhabditis elegans exceeded those of inorganic arsenic, suggesting the terrestrial ecotoxicity of 3,3-CDTA and NCDC. Moreover, decreasing survival rates and destructing intestinal integrity in mice indicate their organ-specific toxicity. The cytotoxicity of 3,3-CDTA and NCDC in liver hepatocellular carcinoma cells was comparable to that of inorganic arsenic, highlighting a potential threat to human health. The findings are of great significance for advancing the understanding of the environmental fate of metformin in water systems and for assessing the health risks associated with metformin throughout its life cycle.

949

Occurrence and fate of *N*-nitrosamines in domestic wastewater treatment plants and their impact on receiving waters

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Abstract

Domestic wastewaters contaminated with *N*-nitrosamines pose a significant threat to river ecosystems worldwide, particularly in urban areas with riparian cities. Despite widespread concern, the precise impact of these contaminants on receiving river waters remains uncertain. This study investigated eight *N*-nitrosamines in wastewater treatment plants (WWTPs) and their adjacent receiving river, the Lijiang River in Guilin City, Southwest China. By analyzing thirty wastewater samples from five full-scale WWTPs and twenty-three river water samples from Guilin, we quantified the mass loads of *N*-nitrosamines discharged into the surrounding watershed via domestic effluents. The results revealed that *N*-nitrosodimethylamine

(10-60 ng/L), *N*-nitrosodiethylamine (3.4–22 ng/L), and *N*-nitrosopyrrolidine (not detected–4.5 ng/g) were predominant in influents, effluents, and sludge, respectively, with the overall removal efficiencies ranging from 17.7 to 65.6% during wastewater treatment. Cyclic activated sludge system and ultraviolet disinfection were effective in removing *N*-nitrosamines (rates of 59.6% and 24.3%), while chlorine dioxide disinfection promoted their formation. A total of 30.4 g/day of *N*-nitrosamine mass loads were observed in the Lijiang River water, with domestic effluents contributing about 31.3% (19.4 g/day), followed by livestock breeding wastewater (34.5%, 12.0 g/day), and unknown sources (24.7%, 7.5 g/day). These findings highlight the critical role of WWTPs in transporting *N*-nitrosamines to watersheds and emphasize the urgent need for further investigation into other potential sources of *N*-nitrosamine pollution within watersheds.

1015

Characterization of Dissolved Organic Matter (DOM) from *Eucalyptus urophylla* litter and Its Impact on Disinfection Byproduct Formation

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Abstract

Impact of leaching leaf on the aquatic environment from the widespread planation of eucalyptus in southern China has received much concern. However, the effects of dissolved organic matter (DOM) released by eucalyptus litter on the physicochemical properties of water are still unknown. In this study, three-dimensional fluorescence spectrum and high-resolution mass spectrometer were used to study the DOM release rule and chemical composition characteristics of eucalyptus litter. The reactivity of different disinfectants and DOM, DBPs formation potential and the structure analysis of unknown halogenated disinfection byproducts were studied. The results showed that with the increase of pH, the release of DOC from eucalyptus litter gradually increased, and the stronger alkalinity and hardness inhibited the release of DOC. Fluorescent DOM consists of four components, mainly protein-like organic compounds. DOM elements are mainly composed of CHO and CHON molecular formulars, in which lignin and lipids account for a relatively high proportion. Coagulation has the best removal effect on DOM, and it has good removal effect on protein-like and humic-like organic matter. Compared with standard Suwannee River Natural Organic Matter (SRNOM), DOM has higher C- and N-DBPs formation potential and reactivity, and was generated by many DBPs such as HAA, THMs and HALs. Chloramines produce more unknown DBPs when used as disinfectants compared to HOCl and ClO_2. This study provides reference basis for water quality risk assessment of water source in eucalyptus forest area and theoretical guidance for treatment process optimization in waterworks.

1131

Biomarkers of DBP exposures and semen quality:Population-based evidence and possible mechanism of action

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Abstract

Disinfection byproducts in drinking water have caused widespread human exposures. Exposure to such chemicals associated with potential health hazards have aroused increasing global concern in drinking water safety. Accumulating toxicological evidence has shown that disinfection byproducts have reproductive toxicity such as damaging male germ cells/organs, altering reproductive hormones, and inhibiting spermatogenesis, but the relevant human evidence is inconsistent. The main reason contributing to the inconsistency is the accuracy of exposure assessment of drinking water disinfection byproducts. We used blood trihalomethane and urine haloacetic acid biomarkers to improve the accuracy of individual exposure assessment, and consistently found that exposure to drinking water disinfection byproducts was associated with reduced semen quality among multiple independent Chinese populations based on different study designs. Furthermore, the possible mechanism of action including oxidative stress, genotoxicity, hormonal changes and individual genetic factors were proposed.

1137

Potential fate of halogenated DBPs in drinking water distribution and storage systems with unlined cast iron/copper pipes: Mechanistic insights and toxicity predictions

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Abstract

Previous studies have reported that zero-valent iron (ZVI) can reduce several aliphatic groups of disinfection byproducts (DBPs) (e.g., haloacetic acids and haloacetamides) effectively, and the removal efficiency can be significantly improved by metallic copper. Information regarding ZVI/Cu combined degradation of different types of halogenated DBPs can help understand the fate of overall DBPs in drinking water distribution and storage systems consist of unlined cast iron/copper pipes and related potential control strategies. In this study, we found that besides aliphatic DBPs, many groups of new emerging aromatic DBPs formed in chlorinated and chloraminated drinking water can be effectively degraded by ZVI/Cu; meanwhile, total organic halogen and total ion intensity were reduced significantly after treatment. Moreover, a robust

quantitative structure−activity relationship model was developed and validated based on the ZVI/Cu combined degradation rate constants of 14 typical aromatic DBPs; it can predict the degradation rate constants of other aromatic DBPs for screening and comparative purposes, and the optimized descriptors indicate that DBPs possessing a lower value of the lowest unoccupied molecular orbital energy and a higher value of dipole moment tend to present higher degradation rate constants. In addition, toxicity data of 47 DBPs (belonging to 18 groups) were predicted by two previously established toxicity models, demonstrating that although most of DBPs exhibit higher toxicity than their dehalogenated products, some DBPs show lower toxicity than their lowly halogenated analogs.

1141

Spatial patterns and environmental functions of dissolved organic matter in grassland soils of China

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Abstract

Soil dissolved organic matter (DOM) is crucial to atmospheric, terrestrial and aquatic environments as well as human life. Here, by characterizing DOM from 89 grassland soils throughout China, we reveal the spatial association between DOM geochemistry in the dry season vs annual ecosystem exchange and cancer cases. The humic-like and high molecular weight (3.4-25 kDa) fractions with lower biodegradability, decline from the northern to the southern regions of China, and are correlated with lower soil respiration and net ecosystem productivity at the continental scale. The < 1.2 kDa and proteinaceous fractions could serve as a geographical indicator of nasopharyngeal cancer incidence and mortality, while the 3.4-25 kDa and humified fractions are potentially associated with pancreatic cancer cases ($P < 0.05$). Our findings highlight that exploiting the environmental functions of soil DOM and mitigating the negative impacts are necessary, and require actions tailored to local soil DOM conditions.

31. Transport, Fate and Effects of Nanoparticles in Environment

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Sythesis and Properties of Simultaneously Visualizing and Quantifying Silver Nanoparticles

Minyi Zhao, Wenhong Fan

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Abstract

With the wide application of nanomaterials, silver nanoparticles(Ag NPs) is inevitably discharged into the environment, and the water environment is one of the most vulnerable environmental media. The complex migration and transformation process of Ag NPs in water environment will affect the toxic effect of it, so it is necessary to trace the migration and transformation process of Ag NPs in environmental and biological media to further study the mechanism of toxicity. This kind of tracking mainly includes two aspects: quantification and localization in organisms or environmental media. Current research methods are difficult to achieve both localization and accurate quantification of Ag NPs, so it is of great significance to develop Ag NPs materials that can realize visualization and quantification at the same time.

In this study, a kind of fluorescent-Ag NPs coated gold material(F-Au@Ag NPs) was designed and synthesized. According to the previous research results of the research group , F-Au@Ag NPs were prepared by using the crystal seed growth method in the normal temperature aqueous phase. The prepared materials have uniform particle size, moderate shell thickness and good fluorescence characteristics. A series of materials were characterized by SEM/TEM, molecular fluorescence spectroscopy, UV-VIS spectroscopy, Zeta potential and DLS, and the differences in morphology, optics and hydraulics of Ag NPs, Au@Ag NPs and F-Au@Ag NPs were compared, and the dissolution and agglomeration kinetics of the three materials were compared. The results show that the physical and chemical properties of the F-Au@Ag NPs are basically the same as the original Au@Ag NPs and Ag NPs with the same particle size, except for the fluorescence properties. The dissolution and agglomeration of F-Au@Ag NPs are basically the same as the original Au@Ag NPs, but there are some differences with Ag NPs. Aquatic organisms with different trophic levels, such as chlamydomonas rheinae, Daphnia magna, zebrafish embryos and larvae, were selected as the test organisms. The visualization and quantitative performance of the labeled materials were systematically evaluated. The results showed that the labeling did not affect the bioaccumulation process of the original silver nanoparticles, and the labeling could achieve the visualization and quantification of Ag NPs in aquatic organisms with different trophic

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Differential leaf-to-root movement, trophic transfer, and tissue-specific biodistribution of metal-based (ceria) and polymer-based (polystyrene) nanoparticles when present singly and in mixtures

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Abstract

Large quantities of nanoparticles (NPs), including engineered nanomaterials and nanoplastics, are continuously being released into the environment. The trophic transfer of NPs through the terrestrial food chain via foliar uptake, presents poorly understood risks, particularly in realistic scenarios involving co-pollution and plant translocation. In this study, we investigated the trophic transfer of NPs through a food chain involving radish shoots and snails, as well as radish roots and snails. We exposed the organisms to single and mixed foliar doses of CeO_2 and self-synthesized deuterated polystyrene (DPS). Compared to single treatments, mixture treatments enhanced the uptake of Ce by plants but had no effect on the uptake of DPS. Additionally, mixture treatments did not impact the translocation of Ce and DPS from shoots to roots. Under NPs mixture exposure, trophic transfer efficiency for Ce (TTF: 0.0209 ± 0.0016) and DPS (TTF: 0.0254 ± 0.0032) decreased significantly in shoot-feeding snails. In root-feeding snails, the trophic transfer factor for Ce (TTF: 0.3316 ± 0.0667) exhibited a significant decrease, whereas the TTF for DPS demonstrated no significant change. Mixture treatments exhibited differential impacts on different body parts of snails, particularly with observed biomagnification of DPS in the digestive glands (TTF: 1.0133 ± 0.2312) and soft tissues (TTF: 1.3171 ± 0.1824) of snails that consumed roots exposed to mixtures. Regarding further biodistribution of Ce and DPS, mixture treatments promoted accumulation efficiency (AE) for Ce while inhibiting the AE value for DPS in shoot-feeding snails. There was however no significant change in AE values for both substances in root-feeding snails. Additionally, regardless of single or mixture treatments, both CeO_2 and DPS displayed a sudden increase in AE value following translocation to the roots. Our study provides insights into changes occurring during trophic transfer due to co-exposure and plant translocation processes associated with nanoparticles; these findings contribute towards enhancing our comprehension regarding their genuine environmental risks.

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Application of Machine Learning in Nanotoxicology: a Critical Review and Perspective

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Abstract

The massive production and application of nanomaterials (NMs) have raised concerns about the potential adverse effects of NMs on human health and the environment. Evaluating the adverse effects of NMs by

laboratory methods is expensive and time-consuming, and often fail to keep pace with the invention of new materials. Therefore, *in silico* methods that utilize machine learning (ML) techniques to predict the toxicity potentials of NMs are a promising alternative approach if regulatory confidence in them can be enhanced. Previous reviews and regulatory OECD guidance documents have discussed in detail how to build an *in silico* predictive model for NMs. Nevertheless, there is still room for improvement in addressing the ways to enhance the model representativeness and performance from different angles, such as dataset curation, descriptor selection, task type (classification/regression), algorithm choice and model evaluation (internal- and external validation, applicability domain and mechanistic interpretation which is key to ensuring stakeholder confidence). This review explores how to build better predictive models; the current state of the art is analyzed via statistical evaluation of literature, while the challenges faced and future perspectives are summarized. Moreover, a recommended workflow and best practices are provided to help in developing more predictive, reliable and interpretable models that can assist risk assessment as well as safe-by-design development of NMs.

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Synthesis of Dual-Labeled Core-Shell Micro/Nanoplastics and Their Behavior and Applications in Complex Environmental Systems

Bo Ren, WenHong Fan, XiangRui Wang

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Abstract

Micro- and nano-plastics (MNPs) have been widely detected around the world, which draw growing attentions to their potential threat to the environment. Although significant progress has been made in the enrichment and toxicity of MNPs, but identifying and quantifying MNPs in complex matrices remain a substantial methodological challenge. Therefore, a synthesis method for core-shell structured MNPs has been developed, which incorporate both fluorescent and metal-based labels. The quantitative protocol exhibited a good linear relationship within the range of 0.05-10 mg/L MNPs ($R^2 \geq 0.987$). This labeling approach ensures that the synthesized MNPs maintain consistency with the surface properties of their unlabeled counterparts, thereby providing a reliable analog for studying environmental interactions without altering the inherent characteristics of the particles. Additionally, the labelled MNPs exhibit excellent stability in aquatic environments including in different bodies of water and aqueous solutions of different pH. Particularly during continuous monitoring over a period of up to one month, stable tracking of the particles was achieved in water-sediment systems. Moreover, laser confocal microscopy was utilized to trace the uptake and distribution of these particles within biological system including the *Tetrahymena thermophila*, *Daphnia magna* and so on. This approach contributes to a better understanding of their potential toxicological effects. Overall, this provides a reliable approach for the easier, accurate, and quantitative detection of micro- and nanoplastics in complex media to facilitate a deeper investigation into the critical parameters of environmental transport and bio-interactions.

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Application of kinetic model to unveil the cellular fate of nanomaterials

Xiangrui Wang, WENHONG Fan, Ying Wang

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Abstract

Understanding the cellular fate of nanoparticles (NPs) including internalization, transformation, degradation and depuration is crucial in cytotoxicity assessment. Especially, most of researches indicated that biotransformation of NPs would critically determine their toxicity effect. Although much progress has been achieved to uncover the biotransformation of NPs, the key factors controlling these kinetics remain unclear. Therefore, a quantification kinetic model based on the biological process was urgently needed. In this study, subcellular imaging of silver nanoparticles (AgNPs) was used to determine the intracellular transfer of AgNPs, and single particle ICP-MS was utilized to track the degradation process. A cellular kinetic model was subsequently developed to describe the uptake, transfer, and degradation behavior of AgNPs. Our model demonstrated that the intracellular degradation efficiency of AgNPs was much higher than that determined by mimicking testing, and the degradation of NPs was highly influenced by the cellular factors. Specifically, deficiencies in Ca or Zn primarily decreased the kinetic dissolution of NPs, while Ca deficiency also resulted in the retardation of NPs transfer. The biological significance of these kinetic parameters was strongly revealed. The model indicated that the majority of internalized AgNPs dissolved with the resulting ions being rapidly depurated. The release of Ag ions was largely dependent on the microvesicle-mediated route. Through changing the coating and size of AgNPs, the model results suggested that size would influence the transfer of NPs into degradation process, while coating affected the degradation kinetic. Overall, the developed model provided a valuable tool for understanding and predicting the impacts of physicochemical properties of NPs and the ambient environment on nanotoxicity.

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The toxicity effect of engineered nanoparticles to aquatic environment

WENHONG Fan, Dingyuan Liang, Ying Wang, Xiangrui Wang

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Abstract

With the wide application of engineered nanomaterials (NMs), there is a growing attention to investigate the toxicity effect of NMs. Although great progress has been achieved to illustrate the underlying mechanism, tracking and precise quantification of NMs in the aquatic environment is still difficult, which make it hardly to understand key factors controlling the transformation process and mechanism of NMs. Therefore, it is urgent to develop techniques to track the environmental transformation and locate the biodistribution of NMs. Here, a gore-shell structure was developed to label nanoparticles (NPs), which maintained the surface property and achieved low detection limit. Several kinds of NPs (e.g. Au@Ag, Au@SiO_2, Au@TiO_2 and Eu@PS) have been successfully prepared. This labelling technique would behave similar biological accumulation with pristine NPs. It was further used to clarify the access path of Ag NPs, which strongly suggest the dominate role of released Ag ions on the bioaccumulation of NPs and toxicity effect. As this technique could easily distinguish NP and ion, it was also applied to develop a kinetic model to describe the biotransformation of Ag NPs in the *Tetrahymena thermophila*. The model supported the fast intracellular dissolution of Ag NPs, and the simulated results were well supported by species analysis using X-ray absorption fine structure. Overall, this work suggested a powerful tool to track the environmental behavior and biological effect of NPs. With the precise determination by core-shell structure, it could be the first time to uncover the unique effect induced by NPs from the possible interfere by released ions or degradation byproducts.

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Biodistribution and toxicity of chelating agent-modified nano zero-valent iron

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Abstract

In recent years, nano zero-valent iron (nZVI), a type of iron-based nanomaterial has played a crucial role in environmental applications such as water treatment and soil remediation. The presence of numerous organic and inorganic chelating agents in water and soil, such as humic substances and phosphates, can adsorb onto nanomaterials and potentially alter their physical, chemical, and biological properties. This alteration can influence their fate, transport, and toxicity of these materials. Hence, when nZVI is utilized in water treatment or soil remediation, it is inevitably influenced by these chelating agents. While nZVI offers numerous benefits for environmental remediation, its potential toxicity to organisms remains incompletely understood. Researchers have extensively studied the modification of nZVI using chelating agents to enhance its reactivity, while little is known about the impact of these agents on the toxicity of nZVI. Given the growing use of nZVI in water and soil remediation, it is crucial to investigate the material's toxicity.

Citric acid (CA) and sodium tripolyphosphate (STPP) have been selected to represent the organic and inorganic chelating agents, respectively, in water and soil. the distribution and toxicity of nanoscale zero valent iron (nZVI) and nZVIs coated with CA and STPP (CA-nZVI and STPP-nZVI) in mice were investigated. nZVIs were primarily found in the livers and spleens, followed by the lungs, hearts, and kidneys. Histologic analysis revealed no significant histopathologic abnormalities or lesions in all organs except the liver at 14th d gavage. nZVIs did not have a noticeable impact on the body weight of the mice

or the weight of their organs. Compared with the control group, there were no significant changes in hematology indexes compared to the control group, the nZVIs groups exhibited varying levels of elevation in alanine aminotransferase, aspartate aminotransferase, and creatinine, suggesting liver and kidney inflammation in mice. The up-regulation of Nuclear Factor erythroid 2-Related Factor 2 and Heme oxygenase 1 in the nZVIs groups may be a response to nZVIs-induced oxidative stress. Immunohistochemical analysis confirmed the inflammatory response induced by the three nZVI groups. Chelating agents did not have a significant impact on the distribution or toxicity of nZVIs in mice. This study contributes to a comprehensive and detailed insight into nZVI toxicity in the environmental field.

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Changes in Gut Microbiota Structure: A Potential Pathway for Silver Nanoparticles to Affect the Host Metabolism

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Abstract

Silver nanoparticles (AgNPs) are one of the most widely used NPs. Their adverse effects on either the host or its gut microbiota (GM) have been examined. Nevertheless, whether the GM plays any role in AgNP toxicity to the host remains unclear. In the present study, AgNPs were administered to mice by oral gavage once a day for 120 days. A significant dose-dependent accumulation of Ag in the liver was observed, with a steady state reached within 21 days. The AgNPs changed the structure of the GM, mainly with respect to microorganisms involved in the metabolism of energy, amino acids, organic acids, and lipids, as predicted in a PICRUST analysis. Effects of the AgNPs on liver metabolism were also demonstrated, as a KEGG pathway analysis showed the enrichment of pathways responsible for the metabolism of amino acids, purines and pyrimidine, lipids, and energy. More interestingly, the changes in GM structure and liver metabolism were highly correlated, evidenced by the correlation between ~23% of the differential microorganisms at the genus level and ~60% of the differential metabolites. This implies that the metabolic variations in liver as affected by AgNPs were partly attributable to NP-induced changes of GM structure. Therefore, our results demonstrate the importance of considering the roles of GM in the toxicity of NPs to the host in evaluations of the health risks of NPs.

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Temporal Dynamics of Copper-Based Nanopesticide Transfer and Subsequent Modulation of the Interplay Between Host and Microbiota Across Trophic Levels

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Abstract

During agricultural production, significant quantities of copper-based nanopesticides (CBNPs) may be released into terrestrial ecosystems through foliar spraying, thereby posing a potential risk of biological transmission via food chains. Consequently, we investigated the trophic transfer of two commonly available commercial CBNPs, Reap2000 (RP) and HolyCu (HC), in a plant-caterpillar terrestrial food chain and evaluated impacts on host microbiota. Upon foliar exposure, leaf Cu accumulation levels were 726 ± 180 and 571 ± 121 $mg \cdot kg^{-1}$ for RP and HC, respectively. HC exhibited less penetration through the cuticle compared to RP (RP: 55.5%; HC: 32.8%), possibly due to size exclusion limitations. While caterpillars accumulated higher amounts of RP, HC exhibited a higher trophic transfer factor (TTF; RP: 0.69; HC: 0.74) and was more likely to be transferred through the food chain. The application of RP promoted the dispersal of phyllosphere microbes and perturbed the original host intestinal microbiota, whereas the HC group was largely host-modulated (Control: 65%; RP: 94%; HC: 34%). Integrating multi-omics analyses and modeling approaches, we elucidated two pathways by which plants exert bottom-up control over caterpillar health. Beyond the direct transmission of phyllosphere microbes, the leaf microbiome recruited upon exposure to CBNPs further influenced the ingestion behavior and intestinal microbiota of caterpillars via altered leaf metabolites. Elevated *Proteobacteria* abundance benefited caterpillar growth with RP, while the reduction of *Proteobacteria* with HC increased the risk of lipid metabolism issues and gut disease. The recruited *Bacteroidota* in the RP phyllosphere proliferated more extensively into the caterpillar gut to enhance stress resistance. Overall, the gut microbes reshaped in RP caterpillars exerted a strong regulatory effect on host health. These findings expand our understanding of the dynamic transmission of host-microbiota interactions with foliar CBNPs exposure, and provide critical insight necessary to ensure the safety and sustainability of nano-enabled agricultural strategies.

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“The Distribution of Nanosilver in Water-sediment and Its Toxicity to Chironomid Larvae”

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Abstract

Silver nanoparticles (Ag NPs), known for their unique properties and strong antibacterial capabilities, are widely utilized. According to data from the “2023 China Nanomaterial Industry Panorama Map,” the

global nanosilver market is projected to reach 170.89 billion RMB by 2028. With the extensive use of nanosilver materials, it is inevitable that they will enter the aquatic environment.

Nanosilver particles that enter the water will settle on the surface of sediments and be ingested by benthic organisms, passing through the food chain into the human body. Therefore, it is crucial to study the presence of Ag NPs in sediments and their toxicity to benthic organisms.

In this study, chironomid larvae were chosen as the indicator organism, and gold-core-labeled nanosilver (Au@Ag NPs) developed in our laboratory were used. Through core-shell localization technology, the environmental behavior and biological effects of AgNPs were continuously tracked and quantified, and their distribution in water and sediments and their biotoxicity to chironomid larvae were studied.

The experiment used 30nm Au@Ag NPs (10nm Au core, 20nm Ag shell) as the pollutant and constructed a water-sediment system using OECD artificial sediments and dechlorinated tap water. Different concentrations of Au@Ag NPs (0ppm, 0.5ppm, 5ppm) were set, with three parallel experiments for each. Initially, a 7-day water-sediment system equilibrium experiment was conducted, with sampling at 1 hour, 1 day, 3 days, 5 days, and 7 days, collecting overlying water and sediment samples. After 7 days, 30 live larvae were added to the system for a 72-hour acute toxicity experiment. The larvae were not fed during the experiment, and their survival was recorded at the end of the exposure period. The surviving larvae were collected and preserved in liquid nitrogen. The metal concentrations in water, sediment, and the larvae were measured, and the concentration of nanosilver particles in the samples was determined using single-particle ICP-MS. The results showed that: 1. The distribution of Au@Ag NPs in the water-sediment two-phase reached equilibrium after 5 days, and particles larger than 13nm had all settled in the sediment after 1 hour. 2. Accumulation of Ag NPs and Au NPs was detected in the chironomid larvae, and the silver-to-gold ratio in the larvae was lower than that of the original material, suggesting the presence of Ag+ excretion during the exposure process.

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Aquatic ecological risk and sensitive toxicity mechanism of tris (2-chloroethyl) phosphate

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Abstract

Organophosphate esters (OPEs) are the main components of organophosphorus flame retardants, which are widely used in industrial and household products to increase the heat resistance and plasticity of products. The wide production and use of OPEs results in high concentrations and potential environmental risks. At present, the research on the toxic effects and mechanisms of OPEs is relatively

weak, and it is difficult to provide theoretical support for the risk management and control of OPEs. This study carried out the sensitivity toxicity screening of OPEs and the reproductive toxicity effect and mechanism of typical OPEs on zebrafish under low-dose long-term exposure. The main research results are as follows:

(1) The environmental concentrations of 15 types of OPEs in the Beiyun and Yongding Rivers in Beijing were detected, with OPEs concentrations ranging from 365.83 to 450.16 ng · L^{-1} in the North Canal and 14.86 to 156.94 ng · L^{-1} in the Yongding River ; The ecological risk assessment results showed that the risk of OPEs to aquatic organisms in the two rivers can be ignored.

(2) Collect and screen environmental surface water data alongside toxicity data pertaining to the effects of TCEP on aquatic organisms. TCEP has the strongest reproductive toxicity to aquatic organisms. When the proportion of species affected by reproductive toxicity is 15, 20, and 25%, the surface water ratio causing its reproductive toxicity is 92.26%, 38.97%, and 4.01%, respectively.

(3) With zebrafish as the model organism, the reproductive toxicity experiment was carried out under long-term low-dose TCEP exposure conditions. The results showed that TCEP had an estrogen effect and could inhibit the normal growth of zebrafish. In the high-concentration exposure group, there were reproductive toxicity effects such as female-male ratio imbalance, abnormal secretion of sex hormones, female zebrafish ovary development degradation, male zebrafish testis area reduction.

(4) Transcriptome analysis of the genes showed that the main mechanism of TCEP-induced reproductive impairment in zebrafish was the significant down-regulation of *cyp17b12a* in males and *cyp19a1a* in females, which led to a decrease in testosterone and estradiol in males and females, and consequently to the development of endocrine dysfunction and impaired reproductive function.

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Application of Few-shot learning based on SMOTE Approach: Predicting toxicity of Nanoparticles in Natural Aquatic Environment

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Abstract

Nanoparticles (NPs) are widely used in various fields due to their exceptional physicochemical properties. However, their toxicity is a concern, especially when they enter the environment and organisms. The toxicity of NPs is influenced by various factors such as their own properties,

hydrochemical conditions, and species information. Among these, hydrochemical conditions play an important role. Most studies on the impact of hydrochemical conditions on the toxic effects of nanomaterials are based on laboratory experiments that focus on a few factors such as pH and hardness. However, there are complex hydrochemical conditions in the natural aquatic environment that make using traditional model methods like regression models and biological ligand models limited in accurately revealing the mechanisms. Maybe new machine learning methods can solve this problem. This study collected natural water samples from the Yong ding River and various locations in downtown Beijing in China, and conducted laboratory experiments on the accumulation of gold NPs (AuNPs) in *Daphnia magna*. The results showed that the accumulation of AuNPs in *Daphnia magna* in Beijing ranged from 0.156 mg/g to 1.455 mg/g. In addition, after detecting the hydrochemical conditions, we planed to use machine learning methods to explore the effects of different hydrochemical conditions on the accumulation of AuNPs in *Daphnia magna*. However, due to the limited experimental data that can not meet the requirements of machine learning dataset, SMOTE method is used to generate virtual samples and then constructed few-shot learning models for predicting AuNPs accumulation. The best models is SVM model when generating 14-fold virtual data (R^2 = 0.99, RMSE = 0.02) , which showed the feasibility and reliability of the SMOTE method. Further feature importance analysis indicates that the elements Al, Se, and Cd were found to have the greatest effect on AuNPs accumulation, suggesting that geological conditions and pollution status are key factors. This study demonstrates the potential of few-shot learning for predicting toxicity of NPs under complex conditions. This breaks the limitat of insufficient experimental data for machine learning and provides a foundation for further research on the toxicity mechanisms and ecological risks of NPs.

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Bioavailability of Ag2S nanoparticles to terrestrial plants: relative importance of different pools

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Abstract

The current and continued burden of nanoparticles (NPs) into the environment is significant, including the release of particles that have been historically stored in soils to various water bodies. However, the reactivity and dynamic nature of NPs transformation processes is poorly understood due to the lack of long-term environmentally relevant experiments that accurately represent ecosystem complexity. Here, we conducted a two-year mesocosm study to quantify silver sulfide NP reactivity and fate using stable isotope tracers, quantifying recent $^{109}Ag_2S$-NPs inputs to the water column from agriculture and wastewater (referred to as “emerging NPs”) and historically stored Ag_2S-NPs in soils (referred to as

"legacy NPs"). The findings indicate that 59.4–89.3% of the silver accumulated in brown rice *Oryza sativ*a L., radish roots *Raphanus sativus* L., and rice borers *Chilo suppressalis* originated from legacy NPs, thereby highlighting the previously uncharacterized significance of legacy NPs in agricultural ecosystems. To minimize human exposure to silver via consumption of food crops, recommended concentrations of legacy NPs in soils should be less than 1.6 μg Ag g^{-1} for rice growth and 0.4 μg Ag g^{-1} forradish growth. Quantifying the contribution of differential pools of silver sulfide NPs is not only important to accurately characterizing the exposure and risk of these materials but also to ensuring the safety and sustainability of agriculture.

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Characterization of Bioaerosol Escape During Solid Waste Disposal in Rural Areas of Northwest China

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Abstract

Abstract: With the promotion of the rural revitalization strategy, ecological livability has become an important guarantee for improving the quality of rural development. The generation and disposal processes of solid waste have become one of the main emission source of bioaerosol pollutants and a major problem in the development of rural ecological environment. Due to the potential health hazards of bioaerosols emitted during solid waste generation and disposal processes to nearby villagers, it is of great significance to investigate their fugitive characteristics. In this study, the emission characteristics of bioaerosols from landfills, livestock and poultry farms, and pit toilets in rural areas of Northwest China were investigated using a portable biological particle sampler. The quantitative microbial risk assessment (QMRA) was also carried out to evaluate the potential impacts of the fugitive bioaerosols on the health of local villagers. The results showed that differences in solid waste types caused large variations in the concentration and particle size of bioaerosols, as well as the community composition of pathogens in bioaerosols. The highest concentrations of bacterial and fungal bioaerosols were found in livestock and poultry farms, at 125,609 CFU/m³ and 11,741 CFU/m³, respectively. A significant seasonal variation was observed in bioaerosol emissions, with concentrations lower in winter months compared to other seasons. The particle sizes of bioaerosols detected in landfills and pit toilets were generally larger than 4.7 μm, while those detected in livestock and poultry farms were relatively small. The main potential or opportunistic airborne pathogen in the livestock and poultry farms was *Corynebacterium*, while *Flavobacterium* and *Lactobacillus* were predominant in landfills and pit toilets. Finally, the health risk assessment results indicated that the health risks of villagers living near solid waste generation and disposal sites were significantly higher than the baseline values. In addition, the potential health risks faced by the elderly and children deserve focused attention.

Keywords: rural; solid waste; bioaerosols; population characteristics; influencing factors

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From joint nanotoxicology assessment to nano-bioremediation technology development

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Abstract

Concerns over the combined risks of nanomaterials (NMs) and co-existing pollutants have led to investigations into co-contamination scenarios. Synergistic, additive, antagonistic, and independent effects are all possible toxic interactions resulting from NMs and co-contaminant exposure. Interestingly, NMs may antagonize the toxicity of co-existing contaminants by adsorption/reductive-oxidation reactions, or decrease toxicity through altered biological processes such as antioxidation, detoxification, or biodegradation, along with the removal of contaminants. These types of interactions clearly suggest the potential use of NMs to facilitate the bioremediation of contaminated sites. Based on this consideration, we put forward a strategy extracting valuable information from joint nanotoxicity studies as an indicator for the development of nano-enabled bioremediation (nano-bioremediation) technologies. We established a new soil remediation strategy using nanoscale zero-valent iron (nZVI) coupled with safe rice-production in a paddy soil contaminated with pentachlorophenol (PCP). The synergistic effect of nZVI-treatment and rice cultivation was identified as nZVI-facilitated rhizosphere microbial degradation of PCP. nZVI was also found to interact with alfalfa and synergistically remediate polychlorinated biphenyl-contaminated agricultural soil. We have also drawn inspiration from nano-bio interaction and established a hybrid remediation framework using nZVI and worms for organochlorines (OCs)-contaminated soil. We found that the exposure to nZVI stimulated the synthesis of reductive biomolecules which significantly mitigated the toxicity of OCs and strongly accelerated nZVI-induced OCs dechlorination by facilitating the reductive dissolution of nZVI oxide shell and electron transfer from Fe^0 core to OCs. I will briefly present these nano-bioremediation technologies and introduce how to develop nano-bioremediation technologies from joint nanotoxicology assessment, with a focus on the interactions among NMs, biota, and pollutants.

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Effects mechanism of biochar application on soil carbon sequestration and alfalfa growth in typical mining areas

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Abstract

Biochar, by modifying the soil microenvironment, has the capacity to enhance soil health and sequester CO_2, thereby influencing the global carbon cycle and soil ecological environment. Recent investigations reveal that biochar derived from cotton byproducts represents a promising amendment for soil enhancement, crucial for both agricultural productivity and environmental sustainability. The present study delves into the mechanisms underlying the impact of biochar application on soil carbon sequestration and alfalfa growth in mining regions. Specifically, it explores (i) the most recent research focal points and trends, (ii) the physical and chemical properties of soil as well as microbial diversity, (iii) the role of biochar in soil reclamation, and (iv) the relevant mechanisms of carbon sequestration. Moreover, the study discusses potential future research directions pertaining to the integration of cotton byproduct-derived biochar into the soil environment. The insights gained from this research offer a scientific foundation for promoting the wider application of cotton byproduct-derived biochar in soil ecological restoration efforts.

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The effects of MPs on the growth of Chinese cabbage in saline-alkali area

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Abstract

Plastics are extensively used in agricultural irrigation and plastic greenhouses. Through mechanisms such as microbial action, weathering, UV photolysis, and hydrolysis, plastics degrade into microplastics, accumulating in farmland soils. Upon entering soils, microplastics alter soil properties, functions, and biodiversity. Moreover, microplastics can transfer through the food chain from lower to higher trophic levels, posing threats to human food security and public health.This study investigates the occurrence of microplastics in the Hetao Irrigation District of Inner Mongolia Autonomous Region, China, and explores their impacts on Chinese cabbage growth in saline-alkali soils.

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Aging effects of titanium dioxide on Cu toxicity to *Daphnia magna*: Exploring molecular docking and significance of surface properties

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Abstract

Titanium dioxide nanoparticles (TiO_2 NPs) are commonly found in cosmetics and personal care products, eventually reaching aquatic environments. The surface properties of TiO_2 NPs may change with aging due to environmental factors such as light, and potentially affect their biological effects in aquatic environments. This study explored the impact of the aging process and varying exposure concentrations on the metal bioaccumulation and toxicity of three commercially available TiO_2 NPs. *Daphnia magna* (*D. magna*) was selected as a model organism, and copper (Cu), a common aquatic metal pollutant, was selected for study.

Various concentrations, types and aging durations of TiO_2 NPs significantly influenced the bioaccumulation of Ti and Cu in *D. magna*, along with the endogenous ROS levels and intracellular antioxidant enzymes activities. The primary difference observed in various types and aging durations of TiO_2 NPs was the change in hydrophobicity. Data analysis indicated that increasing hydrophobicity resulted in decreased Ti bioaccumulation but increased Cu bioaccumulation. These changes correlated with the feeding pattern of *D. magna* and TiO_2 NPs's Cu adsorption capacity. As a filter-feeding animal, *D. magna* ingested more hydrophilic TiO_2 NPs and free Cu compared to hydrophobic TiO_2 NPs and those with adsorbed Cu. Changes of bioaccumulation of TiO_2 NPs and Cu in *D. magna* ultimately affected the activities of antioxidant enzymes such as SOD, CAT, GSH-Px, and the transmembrane protein Na^+/K^+–ATPase.

Molecular docking techniques was used to simulate interactions between TiO_2 NPs and biological enzymes. Molecular docking calculations demonstrated that these enzymes were essentially affected by the hydrophobicity of TiO_2 NPs, although their changing trends were different. The changes of activities of these enzymes were due to the interaction between TiO_2 NPs, Cu, and the amino acid residues near the sites with the lowest binding energy and active center of the enzyme. Such effect was closely related to the hydrophobicity of TiO_2 NPs.

These results indicated that the aging process of TiO_2 NPs altered their hydrophobicity, subsequently influencing the bioaccumulation and toxicity of TiO_2 NPs and Cu in *D. magna*. Our results revealed the intrinsic link between the environmental aging process and biological effects, which were beneficial to the evaluation and prediction of the toxicity of related cosmetics and personal care products.

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Quantitatively Tracking the Distribution of Micro- and Nanoplastics in Ecosystem

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Abstract

We have explored a series of analytical methods to monitor the eco-environmental and biological impacts of micro- and nanoplastics (MNP) pollution. By forming a protein corona to precipitate protein-MNP aggregates, MNPs can be extracted and directly introduced into pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS) for quantification. This approach allows for the quantitative determination of MNPs in soils, sediments, plants, and aquatic animals. Additionally, MNPs were doped with trace amounts of palladium (Pd) to track their presence in ecosystems and living organisms. Using this method, we systematically investigated the uptake and depuration constants of NPs in tilapia and their toxicity to tissues and microbiota. Furthermore, the MNP distribution, bioaccumulation, and trophic transfer were quantitatively explored in a lab-constructed microcosm to mimic real-case scenarios of a freshwater ecosystem. These experimental results address knowledge gaps in the quantitative monitoring of MNPs and help us understand their behavior, facilitating the assessment of their risks in ecosystems and living organisms.

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Foliar uptake pathway of nanoplastics and related mechanisms

Yuting Li, Rui Zhang, Lei Wang, Hongwen Sun, Chunguang Liu

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Abstract

In order to investigate the mechanism of nanoplastic uptake by plant leaves, three plants with different properties of leaves were selected for foliar exposure using amino-modified, carboxyl-modified and unmodified polystyrene nanoplastics and nanosilica to analyze the pathways of nanoplastic uptake in the foliage of different plants as well as the distribution of nanoplastics in the leaves. It was found that all three plant leaves were able to absorb through the cuticle and transport nanoplastics through the plasmodesmata. Corn leaves could absorb nanoplastics through stomata, and cucumber leaves could absorb nanoplastics and nanosilica through trichomes. The absorbed nanoplastics were mainly distributed in the cuticle, cell interstitial space and vascular tissues, and a small amount of nanoplastics were internalized into the chloroplasts or transported to the phloem. No large aggregation of nanosilica was found in the leaves in the nanoplastic silica treatment, suggesting that it was well dispersed in the leaves without significant aggregation, which is a necessary condition for nanosilica to be able to be translocated. Nanoparticles

were not heavily aggregated and well dispersed in the leaves, which is a necessary condition for nanoparticles to be able to be translocated in the leaves.

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Insights Into Quantitative Active Species Responsible for Pollutant Degradation

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Abstract

Nonradical pathways in single atom catalysts are promising processes for contaminant degradation. However, previous studies have focused on qualitatively describing degradation mechanisms, the intrinsic contribution of active species (i.e. singlet oxygen, electron-transfer, high-valent metals) for pollutant degradation remains elusive. Therefore, it is imperative to design single atom catalysts with uniform structure to comprehensively analyze structure-performance relationships and quantitatively uncover the contribution of multiple nonradical pathways. To address this issue, Fe-based single atom catalysts with specific structure were synthesized by a simple and green ball-milling process. They were used to uncover intrinsic contribution of nonradical pathways in the peroxymonosulfate-based advanced oxidation processes toward degradation of pollutants. Identification of active species was carried out via radicals quenching, electrochemical, and peroxymonosulfate decomposition experiments. Then the reaction kinetics and contribution of active species to elimination of pollutants were implemented and quantified. Preliminary results showed that singlet oxygen and electron-transfer were dominant active species. This work deepens the understanding of the mechanisms of non-radical pathways and their quantitative contribution to degradation of organic pollutants.

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Exploring the potential of *in silico* machine learning tools for the prediction of acute *Daphnia magna* nanotoxicity

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Abstract

Introduction

Engineered nanomaterials (ENMs) can be found in numerous applications. Despite having many appealing characteristics for novel applications, ENMs also pose dangers towards the environment, human health and safety. Thorough risk assessment of ENMs is therefore vital to understand their impacts on the environment and humans. However, assessing the risks associated with ENMs is significantly hampered by the fact that a large diversity of ENMs is currently available on the market, without sufficient data available for performing proper risk assessment. This creates a challenge for risk assessment as the properties of ENMs can be manipulated in infinite ways.

In silico methods have gained popularity in recent years as an alternative or complement to traditional risk assessment methods. One of the most applied *in silico* methods are quantitative structure-acitivity relationships (QSARs), where the biological effects of untested substances can be predicted based on their chemical structure.

As the number of experimental data reported in literature grows for ENMs, an opportunity is presented to utilize this data for QSAR development. Here we collected data to build QSARs based on supervised machine learning algorithms to explore the performance of such algorithms on relatively small (*in vivo*) datasets. Another aim was to also investigate which variables are crucial for predicting (*in vivo*) toxicity. The models were limited to only *Daphnia magna* and metallic ENMs as both are the best studied species and materials respectively.

Materials and Methods

Immobilization on ENMs were collected for *D. magna* by conducting a literature research. The extracted data included nano-specific physico-chemical properties (e.g. size, shape, zeta potential) and the exposure conditions (e.g. temperature, pH) of the experiments. Furthemore, molecular descriptors were calculated with the tools made available via the OCHEM database and reduced.

Model performance

Models displayed similar performance across most metrics that were assessed. The random forest, k-nearest neighbors and neural network models consistently performed relatively better than the other algorithms, but only marginally). Furthermore, visual inspection of ROC AUC curves (not shown here) showed similar results but also revealed the models' ability to discriminate excellently between the "very toxic" and "not harmful" classes. The models had some difficulty when it came to predicting the "toxic" class.

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Exploring the Protective Role of Beclin 1 Against Lung Injury Induced by Nanometer Zinc Oxide Based on the Mitophagy Pathway

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Abstract

Exploring the Protective Role of Beclin 1 Against Lung Injury Induced by Nanometer zinc Oxide Based on the Mitophagy Pathway

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Objective: This study aimed to explore the roles and mechanisms of Beclin 1 in lung injury caused by zinc oxide nanoparticles (ZnONPs) from the mitochondrial autophagy pathway, in order to provide a scientific basis for the safe application of ZnONPs and discover new means of intervening in the lung toxicity of ZnONPs.

Methods: Multiple different types of animal models (wild-type, Beclin 1 knockdown, Beclin 1 transgenic, and autophagy-inducing peptide Tat-Beclin 1) and cellular models (wild-type, Beclin 1 knockdown, Beclin 1 overexpression, Beclin 1 point mutation, and autophagy-inducing peptide Tat -Beclin 1), were conducted to detect lung injury, oxidative stress, and cell death at animal and cellular levels, respectively, and to examine mitochondrial autophagy, mitochondrial autophagy molecules, and lysosomal indexes and conduct new target mining, in order to clarify the roles of Beclin 1 in lung injury caused by ZnONPs and to further elucidate the role of Beclin 1 in lung injury caused by ZnONPs through the mitochondrial autophagy modulation. The molecular mechanism of lung injury caused by ZnONPs through mitochondrial autophagy was further elucidated.

Results: Beclin 1 knockdown mice exhibited a more severe degree of lung injury as well as oxidative stress imbalance and lung inflammatory response after ZnONPs exposure compared with control mice.However, the exogenous injection of the autophagy-inducing peptide Tat-Beclin 1 effectively alleviated the lung injury and oxidative stress imbalance caused by exposure to ZnONPs in wild-type mice or Beclin 1 knockout mice, and effectively suppressed lung inflammatory response and reduced lung toxicity.Furthermore, the absence of Beclin 1 resulted in impaired mitochondrial autophagy in lung tissues, and exogenous injection of the autophagy-inducing peptide Tat-Beclin 1 significantly promoted mitochondrial autophagy in wild-type mice or Beclin 1 knockout mice.

Conclusion: The experimental results indicated that Beclin 1 plays an important regulatory role in lung injury caused by ZnONPs, and the targeted activation of Beclin 1 can intervene in lung injury caused by ZnONPs.

Keywords: Zinc oxide nanoparticles; Mitochondrial autophagy; Beclin 1; Oxidative stress; Lung injury

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The models of fate of nanoparticles in the environment

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Abstract

Nanoparticles (NPs) are generated during the production and use of various types of nanoproducts. The NPs that enter into the natural environment will be transported and transformed into other forms of particles by producing many physical and chemical reactions. The tiny size of NPs makes it easy to enter cells, thus posing a threat to various plants and animals as well as to human health, so it is necessary to understand their fate in the natural environment and to assess their environmental risks. However, We reviewed previous articles and found that researchers often consider only a single process, such as the release process or fate process or toxicity assessment process, but there is no model that can track the whole process of NPs. Therefore, we take nano titanium dioxide as an example to try to track the entire process. The study not only deepens the understanding of the environmental behaviour of nano titanium dioxide, but also provides a scientific basis for the environmental risk assessment and management of nanoparticles in China. It is of great significance for the protection of environment and ecosystem security as well as the further development of fate models.

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Mitigation of Cadmium and Arsenic Stress with Copper Oxide Nanoparticles on Rice Plant Growth and Development

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Abstract

Heavy metal pollution remains the primary element of global soil pollution. Cadmium (Cd) and arsenic (As) pollution are the heavy metal main pollutants. Due to their special growth environment and physiological characteristics, rice plants are more likely to absorb Cd and As than other crops. It is urgent to reduce the impact of Cd and As on the yield and quality of rice plants to ensure food safety, since rice feeds half of the world population. Our research projects have studied the germination, seedling growth, and greenhouse cultivation process of rice throughout its lifecycle under artificial soil and actual paddy soil conditions. By introducing copper oxide nanoparticles (nCuO), we aim to alleviate the toxic effects of Cd and As on rice growth and development caused by the independent and combined stresses of these two heavy metals. The study showed that when nCuO was at concentrations of 50 and 100 mg/L, it significantly alleviated the toxicity of Cd and As, promoted rice growth and heading process, increased rice yield, and inhibited the accumulation of Cd and As in rice grains. The project aims to provide basic data and technical support for the safe utilization of contaminated farmland, improvement of agricultural ecological environment, and sustainable development of food security.

32. Microplastics: Current Knowledge and Challenges

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Accurate identification of irregularly shaped micro and nanoplastic (MNP) fragments with sub-micron infrared spectroscopic technique

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Abstract

Over the last decade, micro- and nanoplastics have received significant attention due to their potential effects on living organisms and health-related concerns. The presence of tiny polymer fragments is now ubiquitous; learning their chemical characteristics would allow scientists and engineers to correlate their plastic types with potential toxicological and environmental impacts. To make statistical relevance, large samplings of liquids are required, and recent research projects have demonstrated the feasibility of using artificial intelligence (AI) to sort out spectroscopic data and make desired correlations.

Still, accurate identification of microplastics and nanoplastics can be a daunting task for researchers in both academic and industrial settings. Specifically, these challenges arise from analytical perspective would include (1) the inability of conventional infrared microspectroscopic techniques to output high quality FT-IR data for particulates smaller than 20 μm, (2) misidentification of fragments due to the strong autofluorescence baseline in Raman spectra, and (3) the collection of shear amounts of microplastics in each specimen. As a result of these limitations, the microplastics chemistries below particle sizes of 20 μm are not well understood.

Recent developments of submicron infrared technique (optical photothermal infrared spectroscopy or O-PTIR) have shown promise in overcoming these challenges. This novel infrared-based technique makes use a pump-probe arrangement where the infrared laser source and probe lasers are co-illuminated to the

specimen, where the localized photothermal effect on the surface would be quantified by observing the bending of reflected probe laser light into a far-field visible light detector. This quantity is usually referred to as the wavenumber dependent photothermal amplitude. As the IR laser source tunes over the mid-IR, photothermal amplitudes would be plotted per wavenumber to generate FTIR-like infrared absorption (O-PTIR) spectrum. These submicron IR spectra share high resemblance to standard ideal FT-IR counterparts to enable spectral matching to existing standard spectral libraries to confidently identify unknown fragments. In this contribution, we will disclose the application of submicron infrared measurements towards accurately identifying sub-20 μm microplastics fragments.

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Seasonal microplastics and meiofauna distributions in estuarine sedimentary of Van Uc river, Viet Nam

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Abstract

Microplastics (MPs) are widespread in marine sediments and it becomes an emerging global pollutant due to their potential threats to marine ecosystems. However, studies on MPs in sediments of estuarine and coastal ecosystems of Viet Nam are very limited. Here, we conducted the first study on seasonal abundance, distribution, compositions of microplastics and its impacts on benthic organisms (focused on meiofauna species) in the sediments of Van Uc river in the northern Vietnam. Microplastics and meiofauna were identified from sediments of 12 stations along the Van Uc river in the rainy season (June 2021) and dry season (December 2021). In the collected sediments along the Van Uc estuary, the rainy season had significantly lower number of MPs (4.34 - 5.93 item/g of dry weight) than that of the dry season (12.7 - 17.2 items/g of dry weight) ($p < 0.05$, t-Test). PET, PVC and nylon were the most abundant and frequently detected polymer types in the analyzed samples, whereas PTFE was mainly detected in the upper Van Uc river. Pearson correlation analysis revealed that negative relationship was observed between organic matter with MPs ($r = -0.49$, $p < 0.0001$) and/or meiofauna abundances ($r = -0.59$, $p < 0.0001$). In contrast, MP abundance was positively correlated with sediment grain size ($r = 0,6817$, $p < 0.0001$), whereas, no correlation between meiofauna abundance and grain size was found in this study ($r = 0.1812$, $p > 0.05$). Interestingly, our results showed the presence of MPs in sediments of Van Uc river had positive correlation with the meiofauna abundance ($r = 0.33$, $p < 0.01$). This study provides new insights into the ecological relevance of MP contamination and confirms that meiofauna may serve as seasonal biomarkers of MP contamination in estuarine sediments.

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Assessing the Impact of Virgin and Weathered Solid Microplastics on Zebrafish Larvae: Oxidative Stress, DNA Damage, Accumulation and Developmental Toxicity

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Abstract

Microplastics (MPs) are pervasive pollutants with significant bioaccumulative potential and adverse effects on ecosystems. While past research predominantly focuses on spherical MP models, our study delves into the impact of irregularly shaped, weathered MPs (polystyrene and polyethylene) on zebrafish larvae, aiming for environmental relevance. We emulate natural MP concentrations, using both virgin MP spheres from Sigma Aldrich and weathered MPs produced in the laboratory. After characterizing MPs with various microscopy techniques, our findings demonstrate that both virgin and weathered MPs induce toxic responses in zebrafish larvae, including oxidative stress, DNA damage, and cell death, following a 10-day exposure. Notably, weathered MPs exhibit heightened lethality and malformations, highlighting their substantial environmental impact. This research sheds light on the nuanced toxicity of MPs, emphasizing the importance of considering irregular shapes and environmental weathering in assessing their ecological effects. Understanding the mechanisms underlying MP toxicity is critical for developing effective mitigation strategies and promoting the transition to eco-friendly alternatives, ultimately safeguarding aquatic ecosystems and human health. Keywords: Microplastics, Zebrafish, Developmental Toxicity, Oxidative Stress, DNA Damage Repair, Apoptosis

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A Comprehensive Analysis of Tyre Additive Chemicals in the Moreton Bay Catchment

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Abstract

Tyre wear particles, one of the largest sources of microplastic pollution, raise additional concerns due to their role as environmental carriers of a wide range of incorporated additive chemicals. While these additives are essential for enhancing tyre performance, concerns have been raised about their environmental impact. These chemical compounds from tyres can leach into the surrounding environment, particularly waterways, posing a significant risk to aquatic species. Additives, such as

the antioxidant derivative N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylenediamine-quinone (6PPD-quinone), have been reported to cause aquatic toxicity at concentrations relevant to the environment. 6PPD-quinone has been identified as a contributor to acute toxicity in coho salmon (*Oncorhynchus kisutch*), resulting in mass mortality in the USA. Thus, to assess Australian environmental concentrations, samples were analysed for a suite of 15 common tyre additive chemicals using liquid chromatography tandem mass spectrometry (LC-MS/MS), following previously reported methodologies. Consequently, understanding the concentrations of these additives aids in comprehending their behaviour and fate in the Moreton Bay catchment area, as well as their potential to bioaccumulate in aquatic organisms.

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Developing a Method to Extract, Detect and Quantify Small Antifouling Paint Particles in Sediments Using Accelerated Solvent Extraction and Pyrolysis-Gas Chromatography-Mass Spectrometry

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Abstract

The release of antifouling paint particles (APPs) from maritime activity poses a significant, yet poorly investigated source of contamination in coastal environments. APPs contain toxic biocides as active components and exhibit higher toxicity than other anthropogenic particles. Recent studies focusing on APPs showed that the separation and identification of these particles from the sediment matrix is challenging and fairly limited to large size fractions (>500 μm). Considering the current scenario, the present study aimed to develop and optimize a method to successfully extract, detect, and quantify small APPs from complex environmental matrices using accelerated solvent extraction (ASE) followed by pyrolysis-gas chromatography-mass spectrometry (Pyr-GCMS). The composition of APPs from multiple brands was characterized by Fourier-transformed infrared spectroscopy (FTIR) and Pyr-GCMS. Rosin was detected as a common binder across APPs and selected as a marker. The methylating agent tetramethylammonium hydroxide was added to the paints to improve the detection of rosin-associated markers. The compounds methyl abietate and methyl dehydroabietate were selected as quantifiers. Solubility tests with four solvents (acetone, toluene, ethanol, and dichloromethane [DCM]) showed that DCM dissolved all APPs at room temperature, confirming the suitability of developing a solvent extraction method. Eight-point calibration curves were constructed for methyl abietate and methyl dehydroabietate using different paint brands and the rosin standard. Overall, the R2 of the calibration curves ranged from 0.977-0.994. For the extraction of APPs, spike experiments with a standard rosin solution and pre-cleaned sediments were conducted with an optimized ASE method (180 °C and 1500 psi). The recoveries of methyl abietate ranged from 72-115% depending on the spike concentration. To preliminarily validate the method, sediment samples were obtained from a local marina and boat ramp

and analyzed with our previously optimized method. Methyl abietate and Methyl dehydroabietate were detected and traced back to the presence of APPs. A range of potential natural interferences in the analysis were also tested. The study demonstrated the suitability of coupling ASE and Pyr-GCMS methods for the extraction, detection, and quantification of small APPs in complex matrices, ultimately overcoming the size challenges reported in the literature.

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Do microplastic analysis methods affect our understanding of microplastics in the environment?

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Abstract

Microplastics (MPs) have posed potential risks to ecosystems and human health. Numerous studies have been conducted to help understand the distribution of MPs in the environment. However, a lack of method harmonization leads to discrepancies in results, primarily due to variations in MP extraction procedures and analytical techniques. To address this, two analytical methods – both in active use at different laboratories – were tested and compared against each other. A representative composite water sample was collected from the Danube River, and processed following two different methods. The first method used a multistep enzyme-oxidation-density separation MP extraction protocol, with MPs detected on ZnSe window by micro-Fourier-transform infrared spectroscopy (µFTIR) at a nominal pixel resolution of 5.5 µm. The second method utilized an oxidation-density separation MP extraction method, with MPs filtered on Anodisc filter and detected by µFTIR at a nominal pixel resolution of 25 µm.

The results indicated that these two methods led to different MP abundance and MP mass estimates, but not MP characteristics. It is worth noting that MPs less than filter size were observed in our study. This might be related to the aggregation during the sampling process, and the use of a stirring magnet during the MP extraction process. Only looking at MPs larger than filter size, the first method showed a higher MP abundance, namely 418–2571 MP m^{-3} with MP mass estimates of 703–1900 µg m^{-3}, while the second method yielded 16.7–72.1 MP m^{-3} with mass estimates of 222–439 µg m^{-3}. However, the variability between individual samples was larger than the difference caused by the methods. Looking deeper into the steps of the methods showed that each step contributed differently to the results. The MP isolation procedure contributed slightly to the difference in the result. The use of two different substrates (ZnSe windows versus Anodisc filters) caused a substantial difference between results. This was due to a higher tendency for particles to agglomerate on the Anodisc filters. Finally, the µFTIR settings and nominal resolution caused significant differences in identifying MP size and mass estimate, which showed that the smaller the pixel size, the more accurately the particle boundary can be defined. These findings contributed to explaining disagreements between studies, and addressed the importance of harmonization of methods.

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Definitions, instrumentation and robust analysis methods: Current and future requirements for nano- and microplastics research

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Abstract

Producing reproducible and internationally accepted results in measurement institutes as well as in research and testing laboratories, relies on the use of well-established testing methods and reference materials, in addition to extensive knowledge of the limitations of the measurement instruments themselves. In the rapidly developing field of nano- and microplastics, these requirements are still under development. As nano- and microplastics are predicted to affect a wide variety of areas, including environment, industry, food, human health and agriculture, there is a need for global efforts in developing agreed terminology, test methods and reference materials for both pure materials and those weathered or present in different real-world matrices. Organisations such as the International Organization for Standardization (ISO), the European Committee for Standardization (CEN) and Organisation for Economic Co-operation and Development (OECD) are all involved in developing standards and test guidelines. Some specific tasks include developing standards for: terminology and nomenclature; metrology and instrumentation (including specifications for reference materials); test methodologies and science-based health, safety and environmental practices.

Along with documentary standards and protocols, participation in prenormative research offers the opportunity to benchmark in-house methods with international counterparts and is valuable for validating new measurement techniques and methods for generation of reliable and reproducible results. Organisations such as the Versailles Project on Advanced Materials and Standards (VAMAS) where different technical work areas (TWAs) facilitate such efforts; one of the key activities of VAMAS is the coordination of inter-laboratory comparisons to validate measurement and testing methodology. For nano- and microplastics research, TWA 45 focusses on Micro and Nano Plastics in the Environment.

Australia contributes actively to the international efforts described above and here we share some of our experiences in this rapidly changing space from development of documentary standards, method developments, inter-laboratory comparisons and verification of measurement instruments.

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Effects of erythromycin on biofilm formation and resistance mutation of *Escherichia coli* on pristine and UV-aged polystyrene microplastics

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Abstract

Microplastics (MPs) and antibiotics co-occur widely in the environment and pose combined risk to microbial communities. The present study investigated the effects of erythromycin on biofilm formation and resistance mutation of a model bacterium, *E. coli*, on the surface of pristine and UV-aged polystyrene (PS) MPs sized 1–2 mm. The properties of UV-aged PS were significantly altered compared to pristine PS, with notable increases in specific surface area, carbonyl index, hydrophilicity, and hydroxyl radical content. Importantly, the adsorption capacity of UV-aged PS towards erythromycin was approximately 8-fold higher than that of pristine PS. Biofilms colonizing on UV-aged PS had a greater cell count (5.6×10^{8} CFU mg^{-1}) and a higher frequency of resistance mutation (1.0×10^{-7}) than those on pristine PS (1.4×10^{8} CFU mg^{-1} and 1.4×10^{-8}, respectively). Moreover, erythromycin at 0.1 and 1.0 mg L^{-1} significantly ($p < 0.05$) promoted the formation and resistance mutation of biofilm on both pristine and UV-aged PS. DNA sequencing results confirmed that the biofilm resistance was attributed to point mutations in *rpoB* segment of the bacterial genome. qPCR results demonstrated that both UV aging and erythromycin repressed the expression levels of a global regulator *rpoS* in biofilm bacteria, as well as two DNA mismatch repair genes *mutS* and *uvrD*, which was likely to contribute to increased resistance mutation frequency.

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Nanoplastics induce more severe pulmonary fibrosis than microplastics in mice

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Abstract

Due to the extensive application in production and daily life and the low recycling rate of plastic products, the formed microplastics and nanoplastics have polluted all areas of human life and ecology, which has aroused widespread concern. Inhalation is the main route for people to expose microplastics, but few scholars focused on the impact on the respiratory system. And most studies have reported the biological toxicity of microplastics, while ignoring the nanoplastics with higher concentration. In order to investigate the pulmonary toxicity of micro/nanoplastics, we selected polystyrene (PS), the main plastic type used in current reports, to carry out research. Considering the deposition probability of particles of different sizes in the lungs, PS particles of 80 nm and 2.5 μm were used as representatives of nanoplastics and microplastics. Inhalation of PS microplastics (PS-MPs) and PS nanoplastics (PS-NPs) both caused

lung injury. The lung tissue surface of mice exposed to PS-NPs was covered with gray scar protrusions, and the large number of blue-stained collagen fibers in Masson staining as well as significantly elevated collagen I level in lung tissue indicated that PS-NPs induced more severe pulmonary fibrosis in mice. The proliferation of type II alveolar epithelial cells, the decrease of E-cad and the increase of vimentin and α-SMA in lung tissue indicated that the repair of epithelial injury failed and secondary epithelial-mesenchymal transformation occurred, which promoted collagen deposition. The inflammation located in the alveoli and interstitium of the lungs, which were mainly based on the activation of macrophages, explained the different degree of pulmonary fibrosis caused by PS-NPs and PS-MPs. In PS micro/nanoplastics-induced pulmonary fibrosis, the TGFβ_1/Smad3 pathway, which plays a key regulatory role in fibrotic diseases, is activated, and alveolar epithelial cell senescence is involved. In the last, the increased MDA and decreased T-AOC in lung tissue and the improved effects of mitochondria-targeted antioxidant MitoQ on related indicators revealed the important role of mitochondrial oxidative stress in and the irreversibility of PS micro/nanoplastics-induced pulmonary fibrosis. This work reminds us of the potential hazards of microplastics to human health, especially the need to pay attention to nanoplastics, and provide support for further exploration of lung-related diseases induced by micro/nanoplastics.

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Discussion on toxic effects and mechanisms of acetochlor on parental and offspring zebrafish in the presence of microplastics

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Abstract

Microplastics (MPs) are persistent pollutants that can transfer from parents to offspring and act as carriers for contaminants like acetochlor (ACT), a carcinogenic herbicide. Their presence in water bodies poses significant ecological and health risks. This study involved a 9-week exposure of zebrafish to ACT (purity ≥ 99%) and polystyrene MPs (200 nm and 2 μm). Techniques like HPLC-MS/MS, histopathological analysis, and q-PCR were used to assess bioaccumulation, distribution, reproductive endocrine disruption, and transgenerational toxicity of ACT in the presence of MPs.

Results showed ACT accumulated in zebrafish tissues in the order: intestine > liver > gills > brain > gonad > muscle. Co-exposure to MPs (1.0 mg/L) significantly increased ACT content in tissues, indicating MPs facilitate ACT transport. High concentrations of MPs (1.0 mg/L) reduced spawning further than ACT alone, by 5.77% and 25.39% for MPS and NPS, respectively, likely due to increased ACT levels and gonadal damage.

ACT exposure elevated sex hormone levels (E2 and T) in female zebrafish and E2 in males, with MPs exacerbating these effects, disrupting gametogenesis, sexual development, and reproductive function. On the HPG axis, ACT exposure with MPs elevated E2 levels, stimulating erα and *erβ* gene transcription, while inhibiting key genes like *gnrh2*, *gnrh3*, *fshβ*, *lhβ*, *fshr*, and *lhr*, leading to decreased sperm density and spawning, especially in the ACT + 1.0 NPS group.

The study underscores the reproductive toxicity and developmental hazards of ACT and MPs, showing a synergistic effect that exacerbates the negative impacts. Maternal exposure to ACT and MPs also resulted in transgenerational transfer of ACT, with MPs significantly affecting its accumulation in offspring. This research provides a crucial basis for assessing the environmental risks of these pollutants.

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Mask on Beauty: Mask Wearers at Risks of Inhaling Abundant Respirable Hazards From Leave-on Facial Cosmetics

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Abstract

Previous research has widely neglected the inhalation exposure risks associated with cosmetic powder, a complex mixture of particulate matter with diverse chemical compositions, particularly in the context of wearing masks. This study examines the inhalation risks posed by five face powders, focusing on both particulate matter (including minerals and primary microplastics) and soluble components (such as preservatives and organic UV filters). Our findings indicate that wearing masks significantly increases the inhalation risk of face powders, with the level of exposure being influenced by factors such as particle size, density, and composition. Furthermore, the study reveals distinct behaviors of different powder samples when exposed to various human tissue environments, highlighting the variability in their interaction with biological systems. Analysis of soluble components shows the dissolution of multiple additives from the powders in six bodily fluids, with a greater release observed in the respiratory tract compared to the digestive tract. These results underscore the importance of considering both particulate and soluble components when assessing the respiratory and digestive exposure risks from cosmetic powders. Additionally, understanding the interactions between cosmetic particles and bodily fluids, as well as potential synergistic toxic effects, is essential for ensuring the safety of cosmetic products and protecting public health.

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MNPs/6PPD combined exposure induced visual developmental toxicity and underling mechanisms in zebrafish

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Abstract

Currently micro- and nano-plastics (MNPs) environmental governance faces many challenges, among which the plastic product additive-antioxidant (6PPD) is a natural co-exposure factor of MNPs. Therefore, the new pollutants MNPs and 6PPD have a combined exposure risk, which is especially easy to attack the out tissue of eye, and aggravate the damage to the visual development of organisms and even humans. Based on the neurobehavior and eye tissue damage caused by 80nm polystyrene nanoplastics (PS) and 6PPD exposure to zebrafish, we presently studied the visual developmental toxicity effects of acute and chronic combined exposure to PS80 and 6PPD. The molecular mechanism of visual toxicity induced by combined exposure was elucidated by visual regulation gene expression by double fluorescence labeling transgenic stain and eye tissue transcription sequencing. The results showed that PS80 could coordinate the progression of axial myopia induced by 6PPD in zebrafish embryo and aggravate the developmental damage to eye tissue. In addition, the coexposures also caused changes in motor speed, mirror aggression behavior, cluster behavior and eye movement response of juvenile and adult zebrafish under the condition of subacute exposure dose, and the effects of multiple tests were more obvious in the combined exposure group. GFAP and Oligo2 bicolor fluorescently labeled transgenic zebrafish strains were subjected to the above combined exposure, and then confocal observation of frozen eye tissue showed that the combined exposure group significantly inhibited the expression and arrangement of photoreceptor cells in the retina, and delayed the myelination process of the visual nerve. H&E and TEM observation the co-exposed group damaged the retinal structure, inhibited the development process of rod cell and caused lens structure disorder. In order to explore the underling mechanism RNA-Seq was performed, and we found the 6PPD and the co-exposed groups caused differential expressed genes of 1066 and 5151 in the eye. respectively. The enrichment pathways of 6PPD group manifested in retinol metabolism pathways, while the co-exposure group mainly affected ECM-receptor interaction, Focal adhesion, MAPK and calcium channel signaling pathways, partially explain the variant responses. In conclusion, our results provide new evidence by which new pollutants combined exposure induces visual toxicity and ultimately reduces the fitness and survival of aquatic fish in ecosystems.

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Transport of Plastic Debris from Land to Deep Seas

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Abstract

Riverine runoff has been recognized as one of the most important routes for transporting plastic debris from terrestrial environments to the global ocean. We developed an integrated modeling framework using Human Development Index (HDI) as the main predictor. We further estimated the country-specific riverine plastic outflows from 161 countries. Although India, China, and Indonesia are the largest

contributors to riverine plastic outflows in the world, their per capita contributions rank only 23rd, 79th, and 13th, respectively. Once entering the oceans, plastic debris may undergo a variety of processes and eventually deposit in deep seas, which unfortunately have remained poorly understood. Laboratory simulations were also proved fruitless due to the complex conditions in reality. Previous modeling efforts suggested that plastic debris only oscillate within certain depths of the water column, which was contradicted by recent field measurements on the vertical profiles of plastics in deep seas. Our new model, which considers previously overlooked calcite precipitation accompanied with biofouling on plastic surfaces and a new motion equation for irregular particles under fluid drag, predicts that plastic debris can distribute at all depths along the water column, but ultimately deposit at the seabed and twilight zones. Under similar environmental conditions, the simulated vertical distribution patterns of plastic debris are consistent with recent field measurements in the Pacific Ocean and the Indian Ocean. These results highlight the importance of the seafloor as the final fate of plastic debris.

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A robust method for tire wear microplastics quantification based on pyrolysis gas chromatography mass spectrometry: from batch treads rubber composition survey to multi-scenario samples analysis

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Abstract

Tire wear particles (TWP) are recognized as one of the largest contributors of environmental microplastics, and the ecological risk and organismal toxicity resulting from their environmental release is of continuing widespread concern. Due to the heterogeneity of tread composition, graphical and spectroscopic techniques commonly used for microplastic identification are not suitable for individual identification of TWP. In addition, the persistent presence of interfering substances or instability in environmental media makes the use of inherent elements and molecular markers in tread formulations ineffective for quantifying TWP. The elastomer with the highest content in the tread formulation maintains an inherent percentage of rubber over time in environmental medias, and may be an ideal marker for TWP quantification.

A robust method based on pyrolysis gas chromatography mass spectrometry to quantify and differentiate the mass of passenger car and truck tire treads was developed in this study. The first attempt was made to quantify synthetic rubber in tread by the mass of styrene, butadiene and corresponding derivatives of the pyrolysis monomers of styrene-butadiene rubber and butadiene rubber polymers, and to quantify natural rubber by isoprene, the pyrolysis monomer of natural rubber, and corresponding derivatives. The most abundant compounds of the three monomers and their respective characteristic pyrolysis products were selected as the total pyrolysis markers for quantification. The rubber content of three types of Chinese motor vehicle tire treads was corrected using quantitative curves generated from reference treads of known rubber composition. The results show that the average weight of synthetic rubber in passenger car

treads is about 48 % and natural rubber only about 5 %, while in light truck and all-steel tire treads natural rubber is about 35.5 % and synthetic rubber about 11.5 %. On this basis, specific methods for extrapolation from rubber to TWP mass in environmental samples under four scenarios were extended. Compared with other methods, the accuracy and precision of the established approach were significantly improved (recovery range of 94%~113%). The research results can provide guidance for future accurate quantification of TWP in multi-environmental medias and establishment of the open-source tire database.

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Evaluation of Influential Meteorological and Crop Factors on Historical Mulch-Related Microplastic Pollution in China Using Machine Learning Techniques

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Abstract

Microplastics (MPs) in agricultural soil are an emerging environmental concern, and mulching is a major input source. However, most of the studies approached it from an environmental perspective in terms of soil fauna and soil physiochemical properties. The factors that might affect the release of MPs from mulch remain unanswered. Since crop types and regional climate are closely related to the application of mulch, we hypothesize that these two types of factors would affect the distribution of MPs in agricultural soil. Therefore, the present study aimed to explore the correlation between meteorological and crop factors and mulch-derived MPs. Firstly, the number of MPs was estimated for the rapid expansion period (1993-2012) of mulch usage in China based on a reported empirical method. Subsequently, the Elastic Net (EN) and Random Forest (RF) models were employed to analyze the dataset composed of meteorological variables, crop types, and estimated MPs. The models performed differently at two focal scales. Individual Spearman's correlation analysis with MPs further confirmed the key factors. At the national level, the RF model suggested that the temperatures in September and October were a dominant meteorological factor and the negative correlation coefficients hinted that coldness could increase mulch application and affect the MPs in agricultural soil. Moreover, soybean was ranked the most important crop, which might be because of its heavy cultivation in heavily polluted regions, according to the degree of soybean cultivation in each province. At the regional level, the EN model prevailed, and each region had its own distinct combination of meteorological and crop factors affecting the release of MPs. In general, low temperatures remained important, while moisture-related variables became more important in certain regions. The same negative correlation implied that more arid conditions could affect the extent of MPs contamination among regions. As for crop factors, each region has a distinct composition of crops that might affect the MPs, and they can be positively or negatively correlated with MPs. The negative correlation suggested that there could be potential variances among crops that might affect MPs in certain regions. Overall, the present study provides additional perspective

toward understanding the factors affecting the MPs distribution in agricultural soil and guidance for drafting environmental policy addressing mulch contamination.

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Transfer Behavior, Health Risks, and Research Challenges of Microplastics in Asexually Propagated Crops

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Abstract

As an emerging contaminant, microplastics (< 5 mm, MPs) occur widely in environment and are under the global spotlight. MPs can enter into agro-products through planting chain transmission, with potential health risks. Asexually propagated crops are mainly reproduced through aerial stolons, which are likely to transfer MPs to daughter plants once the mother plant is contaminated with MPs, however, little is known about the ability of asexually propagated crops to take up and accumulate MPs through their roots. We selected a typical asexually propagated plant, the strawberry, for the study. The uptake of MPs in strawberries were investigated by combining mass spectrometry with microscopic imaging analysis. The results showed that MPs could enter the root of the strawberry and transport it to the shoot via the apoplastic pathway; The absorption pathway of MPs in strawberry root was related to the particle size of MPs; MPs accumulated mainly in the roots and only a small quantity transferred to the petiole. Furthermore, considering human health risks, the transport and accumulation of MPs in strawberry fruits still need to be figured out. The current problems and challenges of research on the transfer behavior and health risks of MPs in asexual crops will be proposed, aiming to provide a reference value for predicting the behavior and fate of MPs in the soil-crop system and accurately evaluating their environmental and health risks.

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Pollution Characterization of Microplastics in Urban Rivers Using Laser Direct Infrared Imaging and Multidimensional Ecological Risk Assessment

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Abstract

Microplastics (MPs) are widespread in freshwater environments and have garnered significant attention. However, there remains a lack of understanding regarding MPs pollution in urban rivers heavily influenced by human activities. In this study, we investigated the pollution status of small-sized MPs (<500 μm) in major rivers within Shenzhen, a mega-city in China, by using laser direct infrared (LDIR) imaging technology, analyzed the main water environment drivers, and comprehensively assessed the ecological risk of MPs. The results showed that small-sized MPs were abundant and highly spatially heterogeneous in the surface water and sediments of Shenzhen rivers, with an average abundance of 2305 particles/L and 216 particles/g. Morphologically, all were dominated by the PA, 20-50 μm size group, and the film-form, with each category comprising over 50% of the samples. Similarity analysis revealed significant differences in the MPs community characteristics between surface water and sediment samples. LASSO models and redundancy analysis (RDA) highlighted the relative effects of different water environmental factors on MPs abundance and morphology. Additionally, a comprehensive risk assessment framework was developed, considering the multidimensional MPs characteristics, including abundance, polymer type, shape, size, and toxicity effects. This framework utilized multiple indices to thoroughly evaluate the ecological risk of MP exposure in Shenzhen rivers. The comprehensive risk assessment indicated that most sampling points and river basins in the region were at moderate to high risk levels, with polymer type posing the greatest environmental risk. This study represents the first large-scale survey of MPs pollution in major rivers of Shenzhen, providing valuable insights for understanding and effectively managing MPs potential risks in the water bodies of megacities.

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Sequential analysis of microplastics using Fourier-transform infrared spectroscopy and pyrolysis gas chromatography-mass spectrometry

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Abstract

Accurate identification and quantification of microplastics (MPs) in environmental samples is a challenging environmental problem. Many analytical methods are often complementary. For example, Fourier-transform infrared spectroscopy (FTIR) with a microscope allows the identification of the polymer type and physical dimensions of MPs, whereas thermal analysis such as pyrolysis-gas chromatography/mass spectrometry (Pyr-GC/MS) is desirable for quantifying mass of diverse MPs

including their additives. In this study, analytical protocols combining FTIR and Pyr-GC/MS were attempted for quantifying number, type, and mass of MPs in water samples. The validity of the proposed methods was tested with reference MPs spiked in wastewater influent samples. The mass of the reference MPs estimated using FTIR with a microscope were in good agreement but were slightly lower than those obtained using Pyr-GC/MS likely because of low recovery for smaller MPs (<50 μm) using FTIR. This finding supports the notion that the sequential method can be used to determine both the number and the mass of MPs in diverse environmental samples to compensate limitations of each method.

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Enhanced Leaching of Plastic Additives in a Synthetic Enzyme Solution: Implication for the Roles of Biofilm on Microplastics

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Abstract

Plastic pollution is widespread over the world and has been considered a major concern due to its negative effects on organisms. One proposed mechanism is through the leaching of additives from (micro)plastics. Since additives are not chemically bound to the plastic polymers, they can leach out from plastics, making (micro)plastics as persistent mobile sources of those chemicals. Therefore, understanding the mechanisms of additive leaching processes is crucial for assessing the environmental risk of microplastics. However, in natural environments, various factors influence the leaching processes, including weathering of plastics, degradation of plastic additives, and biofilm formation on plastic surfaces. Nevertheless, the impact of environmental factors on the leaching processes of plastic additives has not been sufficiently explored. In this study, we investigated the effects of biotransformation of plastic additives on leaching processes using homogeneous synthetic enzyme solution. Specifically, we examined the effect of glucuronidation on leaching processes of two benzotriazole UV stabilizers (UV 327 and UV328). Low-density polyethylene (LDPE) fibers with 0.3% UV stabilizers were molded in the lab with a benchtop extruder. These LDPE fibers were incubated with rat S9 fraction with uridine diphosphate glucuronic acid (UDPGA) for maximized glucuronidation process. UV stabilizers leached more in the presence of S9 with UDPGA, indicating the enhancement of leaching via glucuronidation. Since (micro)plastics surfaces are often colonized by biofilm in the environment, the laboratory results in this study hint potential acceleration of leaching of hydrophobic additives although further studies are needed.

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Effects of biofilm on Triclosan adsorption behavior and microbial community of microplastics

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Abstract

Microplastics (MPs) in the environment can be colonized by microbes capable of forming biofilm, which may affect the adsorption capacity of MPs to adsorb organic pollutants. In this study, the sorption behavior of TCS on the biofilm-developed polystyrene (PS) microplastics (VB-PS) and UV-aged and biofilm-developed PS (AB-PS) were compared with the virgin PS (V-PS) and UV-aged PS (A-PS). The results demonstrated that the biofilm could reduce the adsorption abilities onto MPs, While the effect of aging process on the adsorption capacity was not significant. When the solution pH raised, the adsorbed amounts of TCS on all tested PS prone to decline. Based on the 16S rRNA analysis, the diversity, richness of the microbial community with biofilm changed to a certain extent after the adsorption of TCS. These results contribute to a deeper understanding of the synergistic environmental behavior of PS and TCS and provide insights into the combined risk of MPs in the environment.

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Ascertaining appropriate measuring methods to determine tire wear particle pollution on driving school grounds in China

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Abstract

Tire wear particles (TWPs) are garnering increasing attention due to their potential adverse environmental impacts. However, precisely ascertaining TWPs content is challenging due to the complexity and variability of the tire components used in the environment, indicating that more reliable methods to accurately determine TWPs are necessary. In this study, driving school grounds were used as a case study to ascertain an appropriate and reliable method to determine TWPs levels based on a comprehensive comparison between different analytical results using styrene butadiene rubber (SBR), N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD), and zinc (Zn) as analytical markers. Thermogravimetric analysis-Gas chromatography mass spectrometry (TGA-GC-MS) method reliability using SBR was verified and applied to measure TWPs levels on driving school grounds. By reliably converting SBR content to TWPs content, the average TWPs content on driving school grounds was measured at 190.13 ± 101.89 mg/g. The highest TWPs content was 281.83 ± 171.44 mg/g under the reverse stall parking driving programs, while the slope start and stop driving programs was lower at 208.36 ± 124.11 mg/g. Our findings highlight the importance of accurately determining TWPs content

within specific environments while comprehensively exploring associated patterns of change to better understand the environmental risks of TWPs.

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Biaccumulation of microplastics: From microorganism to mammals

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Abstract

Microplastics (MPs) have emerged as contaminants of global concern, with bioaccumulation being a pivotal determinant of their ecological and health impact. Despite this, existing methodologies for visualizing and quantifying the bioaccumulation of MPs are not without their constraints. In recent years, we have pioneered two novel approaches: one leveraging stimulated Raman scattering microscopy (SRS) to visualize MP bioaccumulation in microorganisms, and another employing carbon-14 labeling to quantify MP bioaccumulation in mammals. The SRS method, being label-free, enabled us to delineate the bioaccumulation of minute MPs within protozoa from aquatic ecosystems. Conversely, the 14C-labeling technique facilitated a robust demonstration of MPs' absorption, distribution, metabolism, and excretion in a mammalian model, highlighting dependencies on exposure pathways and particle sizes. Collectively, these advances underscore the necessity for innovative methodologies to comprehensively elucidate the bioaccumulation profiles of MPs across a spectrum of physicochemical attributes.

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An acid/alkaline digestion method for efficient microplastic extraction from wastewaters and other environmental matrices

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Abstract

Accurate analysis of microplastic particles (MPs) in environmental samples requires removal of interferences during sample preparation. Such samples, particularly those from wastewater, are interference-rich and thus particularly challenging, with concentrated sulfuric acid currently deemed impractical as a reagent. Therefore, this study aimed to establish a straightforward, effective, and safe method employing concentrated sulfuric acid and potassium hydroxide to eliminate interferents from environmental matrices, with particular focus on from effluent samples obtained from wastewater treatment plants. We found that 80 % sulfuric acid at room temperature with a

brief contact time of 5 min was viable through a qualitative spot test involving 37 plastics categorized into three types (I, II, and III) based on their polymer structure's oxygen
position. A quantitative assessment revealed that treatments involving H_2SO_4 and KOH (20%, 24 h, 48 ^oC), either separately or in combination, had no discernible physical impact on the overall plastics, except for a subtle one for Type III plastics (e.g., nylon and PMMA) known to be labile under harsh pH conditions. This acid/alkaline digestion (AAD) method, incorporating such conditions for H2SO4 and KOH treatments, yielded a high mass removal efficacy (97.8 ± 2.4 %, n = 13) for eliminating natural particle interferents for primary, secondary, and tertiary effluent samples. Furthermore, the AAD method allowed for the determination of MPs in effluents with
high surrogate particle recoveries (e.g., 95.1% for larger than 500 μm size fraction). This method was also shown to be readily adaptable for other environmental matrices, such as ambient surface water, porous media (e.g., sediment), and aquatic biological tissue (e.g., fish).

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Differential acute lethality of the tire-derived chemical 6PPD-quinone to native Japanese salmonids

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Abstract

N-(1,3-Dimethylbutyl)-*N′*-phenyl-*p*-phenylenediamine-quinone, also known as 6PPD-quinone (6PPD-Q), was recently identified as the toxic chemical that causes acute lethality in coho salmon following exposure to urban road runoff. Due to the ubiquitous use of its parent chemical, 6PPD, 6PPD-Q has been detected worldwide in various environments, such as road dust, stormwater runoff, atmospheric particles, and human urine. Several studies have shown that there were large differences in sensitivity to 6PPD-Q among salmonid species, with variation exceeding 100-fold. We performed 96-h acute toxicity tests of 6PPD-Q with three salmonid species native to Japan: *Salvelinus leucomaenis pluvius*, *Salvelinus curilus*, and *Oncorhynchus masou masou*. Our findings revealed that 6PPD-Q was lethally toxic to *S. leucomaenis pluvius* with a 24-h LC50 of 0.51 μg/L but not to the other two species at environmentally relevant concentrations (< 3.8 μg/L based on time-averaged concentration). Additionally, we measured the concentrations of 6PPD-Q and the suspected monohydroxylated metabolite in brain and gill tissues for the three species. The median internal lethal concentrations (ILC50) of 6PPD-Q were estimated to be 4.0 μg/kg of wet weight in brain and 6.2 μg/kg of wet weight in gill for *S. leucomaenis pluvius*, whereas the tissue concentrations of 6PPD-Q in the other two surviving species exceeded the ILC50 values for *S. leucomaenis pluvius*. These results would be helpful in developing an adverse outcome pathway for urban runoff mortality syndrome induced by 6PPD-Q.

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Estimation of Microplastics Load to the Han River via Highway and Bridge Runoff

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Abstract

With growing concerns on microplastics contamination, quantitative estimation of the environmental load of microplastics is important. Among many nonpoint sources of microplastics, runoff from highways and bridges is regarded as an important pathway to rivers. In this study, we analyzed microplastics in stormwater during 4 rain events in 2023 from two highways and one bridge in Seoul. Collected stormwater samples were subjected to isolation of microplastics, quantification using Fourier-Transform Infrared Spectroscopy (FT-IR) and pyrolysis gas chromatography/mass spectrometry (pyr-GC/MS). We estimated the annual load of microplastics through runoff water from 2 highways along the Han River and 32 bridges to be approximately 3.4×10^{12} particles and 6 tons per year, which corresponds to a significant portion of total microplastics flow through the Han River. Furthermore, our investigation revealed a significant correlation between microplastics and suspended solids, indicating that particle removal during rain events would be important to mitigate microplastics input to the Han River.

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Ferrihydrite regulated tire-wear microplastics biofilm for enhanced nitrogen transformation in surface water

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Abstract

Tire-wear microplastics (T-MPs) are prevalent microplastics in surface water, and ferrihydrite has a strong affinity with MPs which may influence biofilm formation. However, there is a lack of research on the interaction of T-MPs and ferrihydrite on biofilm formation and its function in surface water. In this paper, the T-MPs biofilm formation in the presence of ferrihydrite was characterized from the viewpoint of nitrogen transformation. T-MPs had an adsorption effect on ferrihydrite during biofilm formation and co-exposure resulted in the increase of roughness and decrease of hydrophobicity in the surface of T-MPs, and higher biomass and EPS values. At the same time, the co-exposure had a combined facilitating effect on the denitrification process (12 h removal of nitrate increased by 25.74% compared with single T-MPs). Furthermore, *Thauera*, which plays a key role in nitrogen transformation, was mainly enriched under co-exposure (84%), and these microbial structural changes led to an enhanced nitrogen transformation function (glutamine synthetase, nitronate monooxygenase). The promotion of nitrification and

denitrification processes in the co-exposure of T-MPs biofilm and ferrihydrite was strongly correlated with an increased abundance of key enzymes and functional genes (*napA, nrtC, nirB, nosZ*). Genes associated with nitrate and nitrite reduction (*narG, narI*) exhibited higher abundance in the biofilm of T-MPs compared to the surrounding water. This research provided important insights into the effects of T-MPs co-exposure interactions with ferrihydrite on nitrogen transformation in surface water.

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Next Generation Human Risk Assessment of Micro/Nanoplastics: Applications of the Aggregate Exposure Pathway and Adverse Outcome Pathway

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Abstract

Microplastic particles are ubiquitous in the environment, found everywhere from the air we breathe to the food we eat. Although significant progress has been made in research on environmental microplastics, assessing their risks is still challenging due to the diverse characteristics of microplastics and the variable quality of data, making comparisons difficult. This study aims to evaluate the human health risks of micro- and nanoplastics (MNPs) using the frameworks of the Aggregate Exposure Pathway (AEP) and Adverse Outcome Pathway (AOP). We previously developed a preliminary AEP-AOP framework through a comprehensive review of the occurrence, toxicokinetics, and toxicity of MNPs. Building on this, we assessed and classified exposure and toxicity data to conduct a human health risk assessment. Using QA/QC (Quality Assurance and Quality Control) screening, we selected studies on the presence of MNPs in air, water, and food, as well as toxicity studies. Representative values were identified based on the AEP-AOP framework, with toxicity values using Derived No-Effect Level (DNEL) values. For the risk assessment, particle mass concentrations were converted to particle number concentrations, ensuring compatibility across exposure and toxicity data while accounting for experimental conditions. After thorough analysis, it is clear that the concentrations of MNPs in both air and water are below the DNEL, indicating no immediate health hazards. However, given the overall data and several assumptions, we cannot entirely exclude potential risks from MNPs to humans at current environmental concentrations. Therefore, our findings highlight the need to integrate *in vivo* and *in vitro* data based on the AEP-AOP network, as well as consider toxicokinetics, to achieve a more comprehensive evaluation of human risk from MNPs. This study provides a crucial foundation for the next generation risk assessment of MNPs in environmental media, emphasizing their potential implications for human health within the AEP-AOP framework.

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Keywords: Microplastics, Nanoplastics, Risk assessment, Aggregate exposure pathway, Adverse outcome pathway, Quality assurance

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Retention characteristics and influential factors of microplastics on the leaves of typical urban greening trees

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Abstract

As an emergent pollutant, microplastics have been widely detected in marine, terrestrial and atmospheric environments. It has been demonstrated that plant leaves can trap airborne microplastics. However, the influence of rainfall and leaf characteristics on the retention of microplastics by plant leaves remains unclear. To investigate the effects of leaf properties and rainfall on the trapping and retention of microplastics on leaves, we determined the microplastics on the leaves of five urban trees at two sites under different levels precipitation. Our results show that the abundance of microplastics on tree leaves in the landfill was significantly larger than that in the college campus, with a seasonal difference of fall > summer > spring. The abundance of microplastics on the tree leaves in the landfill and college campus during the sampling period ranged from 0.09 to 0.80 items/cm2 and 0.03 to 0.55 items/cm2, respectively. Leaves with denser groove, larger surface area, higher hydrophilicity, and thicker waxy layers exhibited greater capacity for microplastic retention. In addition, higher intensity and longer duration of rainfall resulted in reduced microplastic retention on leaves.

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On-chip imaging enables fast quantification of microplastic fibers released to water

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Abstract

Fast quantification is the primary challenge in monitoring microplastic fiber (MPF) pollution in water. The process of quantifying the number of MPFs in water typically involves filtration, imaging on a filter membrane, and manual counting. However, this routine workflow has

limitations in terms of speed and accuracy. Here, we present an alternative analysis strategy based on our high-resolution lensless shadow microscope (LSM) for rapid imaging of MPFs on a chip and modified deep learning algorithms for automatic counting. Our LSM system was equipped with wide field-of-view submicron-pixel imaging sensors (>1 cm^2; ~500 nm/pixel) and could simultaneously capture the projection image of >3-μm microplastic spheres within 90 s. The algorithms enabled accurate classification and detection of the numbers and sizes of >7-μm linear and branched MPFs derived from melamine cleaning sponges in each image (~0.4 gigapixels) within 60 s. Importantly, neither MPF morphology (dispersed or aggregated) nor environmental matrix had a notable impact on the automatic recognition of the MPFs by the algorithms. This new strategy had a detection limit of 10 particles/mL and significantly reduced the time of MPF imaging and counting from several hours with membrane-based methods to just a few minutes per sample. The strategy could be employed to monitor water pollution caused by microplastics if an efficient sample separation and a comprehensive sample image database were available.

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Year-round spatial and temporal distribution of microplastics in water and sediments of an urban freshwater system (Jungnang Stream, Korea)

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Abstract

Streams and tributaries are crucial conduits for transporting inland microplastics to rivers and oceans, yet research on these water bodies is limited compared to riverine and marine environments. To better understand microplastic dynamics in these water bodies, detailed spatial and temporal analyses are necessary. This study examined the year-round spatiotemporal variations of microplastics monthly in surface waters and sediments of the Jungnang Stream, a key tributary of the Han River in South Korea. The average microplastic concentrations found were 9.8 ± 7.9 particles per liter in water and 3640 ± 1620 particles per kilogram in sediment. Notably, surface water microplastic levels were significantly elevated during the summer, correlating with increased precipitation and river discharge. The predominant polymers identified were polyethylene, polypropylene, and polyethylene terephthalate, with most microplastics being smaller than 200 μm and primarily fragment-shaped rather than fibrous. The estimated annual microplastic fluxes through surface waters ranged from 1.2 to 207 kg (2.7 to 150 billion particles) for input and 11.3 to 272 kg (17 to 769 billion particles) for output, with over 70% of the output occurring in the summer. The higher microplastic output from the Jungnang Stream compared to the Han River suggests significant transport from water to other environmental compartments, such as sediments. These results emphasize the need for seasonal investigations of microplastic abundances in both surface waters and sediments. Such research is critical for understanding the spatiotemporal distribution and dynamics of microplastics, contributing to water management strategies and policy development for freshwater ecosystems.

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Microplastics result in less mineral protection of soil carbon and higher CO_2 emissions

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Abstract

Microplastic pollution in terrestrial ecosystems threatens to destabilize large soil carbon stocks that help to mitigate climate change. Organic compounds leached from microplastics may be preferentially respired by microorganisms and interfere with the mineral-associated preservation of soil organic carbon. Here we show that microplastic-derived dissolved organic matter (MP-DOM) leads to 21-576% higher CO_2 emissions and 34-83% lower mineral-associated organic carbon in soils than dissolved natural organic matter (NOM), depending on the type of plastic polymer. We identified the underlying mechanisms involved in how MP-DOM shapes carbon cycling by estimating its spectroscopic and molecular signatures and comparing its sorption properties on model minerals with NOM. We found that MP-DOM was 7.96-times more labile, on average, than NOM, making it more accessible for microbial utilization. The lower degree of humification, fewer polar functional groups, and higher H/C ratios in MP-DOM also led to, on average, 3.96- times less sorption with mineral particles. Our findings provide insights into the effects of microplastics on soil carbon storage and highlight their consequences for wider terrestrial carbon cycling and climate warming.

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Photoaging Behavior and Eco-environmental Effects of Typical Micro-/Nanoplastics

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Abstract

Due to the ability of micro/nano plastics (M/NPs) to adsorb and carry various pollutants in aquatic environments, as well as their potential toxic effects, M/NPs have become a global environmental concern. This study introduces the typical environmental behaviors and potential mechanisms of M/NPs. Our results show that differences in environmental media can significantly alter the photoaging process of M/NPs, and the photoaging behavior can significantly affect their physical and chemical properties as well as environmental and ecological effects. First, active substances in the water environment, such as small molecular organic acids, can significantly accelerate the photo-transformation rate of M/NPs through the oxidative hydroxyl radicals produced by photolysis. Additionally, under surface soil conditions, air humidity can significantly alter the formation of surface functional groups during the photoaging process of M/NPs, resulting in significant differences in environmental behavior. Moreover, due to the generation of oxygen-containing functional groups on the surface, photoaged M/NPs can promote the hydrolysis reaction of cephalosporin antibiotics through intermolecular hydrogen bonding. Furthermore, the unsaturated conjugated olefinic structure produced during the photoaging process of M/NPs is prone to π-π^* electron transition, resulting in strong fluorescence characteristics. The two-photon laser confocal scanning microscopy can be used to perform fluorescence imaging analysis of the ingestion, excretion, migration, and accumulation of aged M/NPs in aquatic organisms such as *Daphnia magna*. Therefore, our research will help deepen the understanding of the environmental behavior and ecological effects of M/NPs in natural environments.

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Effects of Microplastics and Organic Fertilizer Regulation on Soil Dissolved Organic Matter Evolution

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Abstract

Microplastics are pollutants with global concern nowadays. However, the effects of microplastics addition to soil as a carbon source and the combined effects of microplastics and organic fertilizer on soil dissolved organic matter (DOM) evolution were still unclear. This study focused on the evolution of DOM in soil with the addition of microplastics, and investigated the variations in the content and composition of DOM in unfertilized and fertilized soil with different particle sizes of microplastics. It was observed that the total organic carbon(TOC) concentration of the soil DOM in the treatment with organic fertilizer and microplastics increased more (129.97-161.43 mg kg $^{-1}$) than that in the treatment with microplastics alone (117.17-131.87 mg kg $^{-1}$), and was higher than that in the original soil (95.65 mg kg^{-1}). According to the humic acid relative abundance in DOM of B1000PE-40 (82.03%), A1000PE-40 (73.66%), B30PE-40 (80.91%) and A30PE-40 (73.90%), the humic acid relative abundance in DOM of the soil samples with microplastics and organic fertilizers addition was found to be higher than those with microplastics addition alone, reaching more than 80% in a short time. In conclusion, the TOC concentration of the soil DOM increased with the addition of microplastics, and the increase was more pronounced when organic fertilizers and microplastics were added together. Moreover, the soil

humification increased to a higher level in the short term with the combined addition of microplastics and organic fertilizers, which maintained during the long-term cultivation process.

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Small-size Polyethylene and Polylactic Microplastic Alterations on Soil Aggregate Frmation with Soil Sterilization

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Abstract

Soil microplastic contamination is emerging as a significant environmental concern affecting soil properties and biota, including soil aggregation. This study aimed to determine the influence of soil microplastics on soil aggregation, their impact through effects on soil microorganisms, and their effects on water and mechanical stability of soil aggregates. Soil incubation experiments were conducted using sterilized and non-sterilized soils with 15-μm polyethylene and polylactic microplastics over one month. Sterilized soils showed more water-stable aggregates, particularly in the 0.25-0.5 mm fraction, with both polyethylene and polylactic MPs significantly increasing this fraction. However, no significant effects of soil sterilization and MP addition were found on mechanical stability. The addition of MPs tended to decrease surface roughness but not significantly. The study provides insights into the complex interactions between microplastics and soil aggregation, suggesting that MP effects may not necessarily be related to their toxicity on soil microbes but could involve various physical interactions.

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Microplastic Pollution Assessment in Surface Water, Sediments, and Fish of River Ravi, Punjab, Pakistan

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Abstract

Microplastics (MPs) are emerging pollutants with detrimental effects on aquatic organisms and human health. The massive generation of plastic waste on land leads to MPs pollution in the aquatic environment. Some reports highlight the abundance of MPs in Pakistan however, no

detailed research has been documented about the presence of MPs in the riverine environment. In this regard, the present study highlights the abundance of MPs in environmental matrices such as surface water, sediments, and fish of River Ravi, Punjab, Pakistan while monitoring the effect of the monsoon and post-monsoon seasons. The MPs in surface water and sediment samples were isolated through wet peroxide oxidation (WPO) digestion and from the gastrointestinal tract (GIT) of fish through 10% KOH, density separation, and filtration followed by microscopic quantification and Fourier Transform Infrared Spectroscopy (FTIR) analysis. The results showed the mean abundance of MPs in surface water in monsoon and post-monsoon seasons were 768 ± 869 MPs/m^3 and 1324 ± 1925 MPs/m^3, whereas, sediments depicted 5323 ± 3792 MPs/kg-dry weight and 2637 ± 2701 MPs/kg-dry weight, respectively. The GIT of fish was found to be contaminated with MPs, with a mean of 28.1 ± 20.7 MPs/individual and 26.8 ± 15.9 MPs/individual at Balloki and Sidhnai barrages, respectively. Fiber was the most abundant shape and Polyester (PES), polyethylene terephthalate (PET), Polypropylene (PP), and Polyethylene (PE) were the common polymer types found in all environmental matrices. In fish, the surface dweller fish and omnivore generalist feeding group exhibited the highest MPs abundance. Based on polymer toxicity assessment, nine fish species were categorized as minor, two species as medium, and four species as high-risk group. Bottom-dwelling fishes were at the highest plastic polymer risk level III due to the presence of a high-density polymer with high toxicity hazards. The high-risk prone fishes are under direct threat from MPs pollution, which may disrupt the ecological integrity of the river ecosystem and human health. Thus, the findings of the current study highlight the urgent need to address plastic pollution issues in River Ravi. Moreover, this is the first study on the spatiotemporal distribution of MPs in River Ravi from Pakistan and indicates the high burden of MPs pollution. Consequently, it will provide scientific information to policymakers and river managers to deal effectively with plastic pollution.

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Effect of microplastics on nitrogen transformation in agricultural soils

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Abstract

The effects of microplastics (MPs) from agricultural plastic films on soil nitrogen transformation, especially denitrification, are still obscure. Here, using a robotized flow-through system, we incubated vegetable upland soil cores for 66 days with MPs from PE mulching film (F-PE) and PVC greenhouse film (F-PVC) and directly quantified the emission of nitrogenous gases from denitrification under oxic conditions, as well as the denitrification potential under anoxic conditions. The impact of MPs on soil

nitrogen transformation was largely determined by the concentration of the additive phthalate esters (PAEs) containing in the MPs. The F-PE MPs with low a level of PAEs (about 0.006%) had no significant effect on soil mineral nitrogen content and nitrogenous gas emission under oxic conditions. In contrast, the F-PVC MPs with high levels of PAEs (about 11%) reduced soil nitrate content under oxic conditions, probably owing to promoted microbial assimilation of nitrogen, as the emission of denitrification products (N_2, NO, and N_2O) was not affected. However, the F-PVC MPs significantly enhanced the denitrification potential of the soil due to the increased abundance of denitrifiers under anoxic conditions. These findings highlighted the disturbance of MPs from agricultural films, particularly the additive PAEs on nitrogen transformation in soil ecosystems.

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"Single-particle sensing of micro- and nano-plastics using conical nanopore"

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Abstract

Nanoplastics (NPs), recognized as an emergent class of pollutants, have garnered considerable scientific interest due to their potential to pose greater environmental health risks than microplastics, primarily attributed to their reduced particle size and elevated quantity density. Traditional analytical methods, including optical imaging, spectroscopy, chromatography, and mass spectrometry, typically focus on either qualitative or quantitative analysis but seldom both concurrently. In contrast, the adoption of conical nanopore-based detection represents a novel approach for the simultaneous assessment of these parameters. This research employed finite element simulation to theoretically investigate the detection capabilities of conical nanopores for NPs. Simulations were conducted to capture the electrical signals of NPs along the central axis and specific off-axis positions, varying by particle size (90, 100, 110, 120 nm) and charge density (-0.005, -0.01, -0.015, -0.02 C/m²), from which 157 characteristic parameters were extracted Among these, ten parameters displaying high single factor correlations with particle size or charge were utilized to classify 16 samples electrical signals via a machine learning model, achieving a classification accuracy of 91.7%. Further refinement of the geometry and testing conditions of the conical nanopores enhanced the classification accuracy to 96%. This study innovatively leverages simulation-based signal analysis over empirical data, facilitating the high-throughput screening of pore interface designs and testing condition optimization, provides a robust theoretical foundation and technical framework for the future application of single-particle detection technologies to NPs assessments in real environmental matrices.

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Insights into the environmental behavior of Para-Phenylenediamines and 6PPD-Quinone in high-cold climate

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Abstract

Tire-road friction can lead to the release of additives through tire surface wear, including Substituted para-phenylenediamines (PPDs) and their transformation products, commonly found in urban environments. 6PPD-Quinone (6PPD-Q), an ozone transformation product known as N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine (6PPD), exhibits high toxicity to fish. High-altitude and cold conditions may influence the formation, transformation, and migration of PPDs under intense ultraviolet radiation, posing unknown risks. Elevated concentrations of 6PPD and 6PPD-Q were detected in road dust and stormwater pipe sediments in Lhasa City (China), with detection rates reaching 100%. In some samples, concentrations of 6PPD (1865 ng/g) and 6PPD-Q (949 ng/g) exceeded levels found in cities like Beijing, Tokyo, and Washington. The conversion rate of 6PPD-Q (1.64) in Lhasa exceeded rates in tropical cities such as Guangzhou (0.4) and Hangzhou (0.5). Factors such as rainfall, ozone exposure, and vehicle type significantly influence transformation processes. Simulation experiments demonstrated rapid entry of 6PPD-Q into the water column via solid-liquid exchange, reaching concentrations 2 to 50 times the LC_{50}. Given the higher environmental risks associated with some transformation products, there is a critical need to address the environmental behavior and risks of tire additives in high-altitude and cold urban areas.

968

Emissions, distribution, and transport of Tire Wear Particles (TWPs) in Tibet, China: Invisible but critical

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Abstract

Tire wear particles (TWPs) are a significant source of microplastics, adversely affecting terrestrial ecosystems and human health. The environmentally fragile Tibetan Plateau is experiencing rapid urban development, yet TWP pollution remains understudied. This study qualitatively and quantitatively analyzed the emission characteristics of TWPs in Tibet, the main region of the Tibetan Plateau, and estimated the TWP flux into its largest river, the Brahmaputra River. Our results indicate that the increasing number of vehicles, particularly heavy-duty trucks, has led to a sharp rise in TWPs emissions since 2016. By 2021, annual TWPs emissions reached 4,600 tons, representing a 120% increase over five years. The urban agglomeration around Lhasa exhibits the highest emission intensity of TWPs. Additionally, the emission range and intensity of TWPs have expanded, with spatial emission patterns aligning with surface NO_2 concentration distributions. Urban roads

influence the spatial distribution of TWPs in water bodies, while township roads determine their distribution in soil. Our model estimates that approximately 1,500 tons of TWPs enter the Brahmaputra River annually. This study provides critical data for assessing TWPs pollution on the Tibetan Plateau and can inform local policy development to mitigate TWPs pollution.

1007

Estimating microplastics' storage in the 'skin' of global freshwater lakes

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Abstract

Abstract: Microplastic contamination in freshwater lakes has grown up to a main concern in recent years. While there is no knowledge about the global distribution and loads of microplastics in the lacustrine environment. We commence to solve this matter based on trawl net method investigations in freshwater lakes. Through redundant analysis (RDA) and structural equation model (SEM), we first identify the main influencing factors that affect the microplastic concentrations in freshwater lakes. Then, we use Machine Learning and number to mass transformation tactics to fill in gaps and reach a global prediction. The cropland ratio in lake basin is proved an important role affecting the microplastic occurrence. Totally, we demonstrate an average microplastic concentration of 0.69 items/m^3 in lakes and reservoirs around the world. The hotspots of lacustrine microplastics gather in east and southeast Asia, India, north back of Black Sea and Nile Delta. The accumulated microplastic load in the 'skin' of lakes and reservoirs is approaching 500 tons, only accounts for a negligible share to the plastic waste generation amount. Africa, North America and Asia are continents with highest microplastic loads, but with different causation (concentration-dependent or lake area-dependent). The giant lakes around world contribute highest microplastic loads. The findings of this study provide a feasible approach to estimate the microplastic loads of global lakes, and assist to make reasonable policies to mitigate the microplastic pollution in freshwaters.

1016

Occurrence and removal of microplastics in different processes of the landfill leachate system

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Abstract

Microplastics (MPs) have been ubiquitously detected in aquatic environments and identified as pollutants of emerging concern. There is a critical need to understand the sources and characteristics of MPs to provide a scientific basis for ecological risk assessment. However, studies on MPs in the landfill leachate system (an important pollution source of MPs) are still limited. In this study, water samples from different treatment sections of landfill leachate system in Beijing were collected to investigate the content, particle size, morphology, species and removal efficiency of MPs. The results showed that: 1) MPs existed in different process stages, and the content of MPs in leachate before treatment was as high as 10^4 MPs/L; 2) After treatment, the content of MPs in leachate decreased exponentially, and the final effluent removal rate was 95%; 3) Different processes have obvious differences in the removal of MPs with different particle sizes, and 90% removal of MPs below 20μm can only be achieved by Reverse Osmosis (RO) treatment; 4) There was no significant difference in the proportion of MPs in morphology. The MPs in leachate before and after treatment were mainly particles, followed by fragments, and the least fibers. 5) MPs with different particle sizes were always significantly correlated with the content of total nitrogen and ammonia nitrogen, while their correlation with the content of COD and suspended matter gradually decreased with the increase of particle size. Granular MPs were significantly correlated with the content of total nitrogen and ammonia nitrogen, while debris and fibers were significantly correlated with the content of COD and suspended matter. Overall, the findings reveal that MP pollution is widespread in landfill leachate treatment systems and difficult to remove completely, especially for MP particles below 20 μm. Therefore, it is necessary to further establish a sound removal process for landfill MP pollution in the future to avoid secondary MP pollution in natural waters caused by landfill discharge.

1021

Environmental exposure pathways of microplastics: primary and risky

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Abstract

The exposure pathways of environmental microplastics are not yet clear for both animals and humans. By using internal exposure monitoring methods, the exposure dose of microplastics to soil animals, fish, and humans can be evaluated. According to external exposure monitoring, it is possible to analyze which exposure pathways contribute the most significant exposure dose. For example, for humans, especially infants, oral intake of indoor dust contributes to the majority of the human exposure dose of polyester plastics. Fish and earthworms have been found to have selective uptake of environmental microplastics, and active feeding significantly increases their intake of microplastics. The absorption of microplastics, especially atmospheric microplastics, by plants may be a crucial link for microplastics to enter the food chain. However, exposure dose often does not equate to exposure risk. Compared to acute effects, the chronic toxic effects of long-term exposure to microplastics may be more worthy of attention. For example, after long-term intake of polylactic acid, the gut microbiota structure of zebrafish changes, enhancing its ability to utilize lactic acid, which may lead to more profound changes in zebrafish energy metabolism.

1023

Machine learning-based evaluation for feature importance of microplastic exposure on freshwater algae

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Abstract

Microplastics (MPs), the plastic debris smaller than 5 mm, are ubiquitous in waterbodies and have been shown to be toxic to aquatic organisms, especially to microalgae. The aim of this study is to predict the effects of MPs on algal growth and evaluate the relative importance of different exposure features of MPs using machine learning models. Based on literature searching, published data were collected. Three integrated machine learning algorithms, Random Forest (RF), Categorical Boosting (CatBoost), and Light Gradient Boosting Machine (LightGBM), were used for the construction of classification prediction models for algal growth. In comparison, the LightGBM model has the best performance. Model interpretability analysis shows that larger MPs showed less effects on algal growth. Our study successfully established prediction models for evaluating the effects of various MPs exposure features on algal growth. It also provides insights for future investigations on MP toxicity in microalgae.

1029

Effects of microplastics on terrestrial plants: a study based on meta-analysis and machine learning

Xu Zhao, Chunguang Liu

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Abstract

Pollution of microplastics has become a global concern with the increasing production and use of plastics. Many researches have demonstrated the adverse effects of microplastics on terrestrial plants, but the research methods and results varied widely and it was hard to draw uniform conclusions. To address this, we conducted a meta-analysis to quantify the magnitude of the impacts of microplastic on crops and developed machine-learning models to predict the adverse effects of microplastics and identify important factors. Hopefully, this study can figure out how microplastics infulence the plants under different experimental conditions, providing reference for risk assessment and policy-making.

1032

Carrier Effect and Risk Assessment of Biodegradable Microplastics on Heavy Metals

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Abstract

Amidst the escalating global crisis of plastic pollution, biodegradable plastics have emerged as a promising alternative due to their theoretical environmental compatibility. However, despite being engineered to decompose under specific conditions, the complete biodegradation of these plastics in natural environments remains challenging. The high content of oxygen-containing functional groups and relatively low mechanical strength in biodegradable plastics predispose them to fragmentation into microplastics under natural conditions, potentially posing a latent risk to ecosystems. Biodegradable microplastics, characterized by a large specific surface area, abundant oxygen-containing functional groups, and a negatively charged surface, exhibit enhanced mobility and the propensity to bind with heavy metals. In this study, we selected polylactic acid (PLA), a widely utilized biodegradable plastic, and compared it with polyvinyl chloride (PVC). Subsequently, batch adsorption experiments and quartz sand-packed column tests were conducted to investigate the impact of these microplastics on the transport behavior of cadmium ions (Cd(II)), a typical heavy metal. The risk of Cd(II)-microplastics to human health was evaluated by in vitro simulated digestion test and Hazard Quotient calculation. Employing Fourier Transform Infrared Spectroscopy, X-ray Photoelectron Spectroscopy, and Zeta potential measurement techniques, we conducted an in-depth analysis of the underlying mechanisms of Cd(II) adsorption by microplastics. The findings revealed that PLA microplastics, endowed with abundant oxygen-containing functional groups, and greater electronegativity, possessed superior mobility and Cd(II) adsorption capacity compared to PVC microplastics. PLA microplastics primarily interact with Cd(II) through complexation and electrostatic attraction, effectively enhancing the transport capability of Cd(II) and exacerbating the risk of oral Cd(II)-PLA microplastics complexes to human health, indicating that biodegradable microplastics could pose a potential threat to the environment and organisms. The insights garnered from this study provide significant scientific evidence for understanding the carrier effects of biodegradable microplastics for heavy metals in subsurface environments. This research holds substantial implications for assessing and refining the environmental impact of biodegradable plastics.

1045

Decoding bioplastics breakdown in natural soils

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Abstract

Global concerns are escalating regarding the environmental impact of biodegradable plastics as their production increases, aiming to substitute conventional petroleum-derived plastics. However, limited knowledge exists concerning their degradation in natural soils. In this study, we investigated the degradation dynamics and mechanisms of two typical biodegradable materials, polyhydroxybutyrate (PHB) and poly(lactic acid) (PLA), alongside one petroleum-derived plastic, polystyrene (PS), in laboratory microcosms and field soils, utilizing metagenomics. PHB exhibited a weight loss of 100% and 58.0 ± 20.3% after 12 weeks of incubation in microcosms and field conditions, respectively, whereas PLA and PS showed minimal to no loss. Metagenomic analysis revealed a significant enrichment of PHB hydrolase genes (phaZ and phaZc) in PHB-treated samples, primarily derived from members of Burkholderiales. Subsequent degradation assays employing Burkholderia isolates supported their role in PHB depolymerization. Based on the identified functional genes and degraders involved in PHB degradation, a degradation pathway was proposed. Our findings lay the foundation to further expedite the bioplastic life cycle within natural environments.

1049

Machine learning analysis and prediction of microplastics on soil properties based on XGBoost

Xudong Xu, Chunguang Liu

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Abstract

This study used XGBoost's machine learning method to analyze the effects of microplastics on various soil characteristics, including soil microbial community, enzyme activity, and basic physicochemical properties. It systematically analyzed and made certain predictions from multiple aspects. Analysis shows that the importance of microplastics on different soil characteristics varies greatly, with microplastic size and concentration having the greatest impact.The results of this study can provide certain theoretical support for the risk management of new pollutant microplastics.

1056

Insights into the interaction mechanism of ciprofloxacin and microplastics

雨轩 刘

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Abstract

To investigate the effect of different water quality conditions on the adsorption of antibiotics by microplastics, three common microplastics were selected: polyethylene (PE), polystyrene (PS), and polyethylene terephthalate (PET), with ciprofloxacin (CIP) as a representative antibiotic. Batch adsorption experiments were conducted to study the adsorption mechanism of microplastics on quinolone antibiotics. Research has found that the adsorption equilibrium time of three types of plastics for CIP is 4 hours, and the adsorption process follows the Langmuir equation. The comparison of their adsorption capacity shows that PET>PE>PS, and the maximum adsorption capacities of the three plastics are PET: 0.62/5ug, PE: 0.56/5ug, and PS: 0.44/5ug. Under acidic conditions, the three types of plastics exhibit better adsorption of CIP. The presence of NaCl accelerates the adsorption reaction process. The results indicate that there are significant differences in the adsorption of CIP by different microplastics, and different water quality conditions affect the adsorption process. This result lays the foundation for the study of microplastics and antibiotic migration in the environment. Compared with the research on microplastic adsorption of antibiotics in literature, this experiment is based on the concentration of antibiotics in surface water, with an initial concentration of 100ug/L, which has more practical application significance. In the future, this can be used as a background to explore the desorption behavior of microplastics after adsorbing antibiotics in the human body, which has a guiding role in maintaining human health.

33. Enhancing Science and Policy Link for New Pollutants Regulation

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Thoughts and Suggestions on the Experience in Fullfilling the Sotckholm Conventionand Reinforcing Treatment and Management of Emerging Pollutants in China

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Abstract

As one of the first signatories to the Stockholm Convention on Persistent Organic Pollutants (hereinafter referred to as the Convention), China has strictly implemented the requirements and obligations of the Convention since 2001, and has gained achievements and experience in the prevention and control of Persistent Organic Pollutants (POPs).2022 China enacted the Action Program for the Control of New Pollutants (hereinafter referred to as the Program). POPs controlled by the Convention are one category of

the new pollutants specified in the Program. The POPs assessment mechanism established by the Convention, as well as the management experience in POPs pollution prevention and control, effectiveness evaluation, etc. gained through compliance, can be replicated and generalized in the field of new pollutants governance and promote synergy between new pollutants governance and compliance. Based on the results and experience of compliance, this paper puts forward three recommendations, namely, to coordinate the research on new pollutant control inventories and strengthen capacity building for screening and assessment; to formulate reasonable and feasible new pollutant prevention and control measures and strengthen pilot demonstrations of control; and to promote capacity building for monitoring new pollutants and establish a mechanism for evaluating the effectiveness of implementation, in order to further strengthen the new pollutant control in China.

184

A comprehensive risk assessment of neonicotinoid exposure in the Yangtze River Basin using an integrated approach: implications for human and ecological health

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Abstract

Neonicotinoids are widely used insecticides that pose significant concerns for both environmental and human health. However, there is a lack of comprehensive evaluation of their accumulation in surface water ecosystems and the exposure of various human groups within these ecosystems using an integrated method. This study evaluated neonicotinoids concentrations and their potential impacts on human and aquatic health in the Yangtze River Basin (YRB), China. Using Relative Potency Factor (RPF), Hazard Index (HI), Monte Carlo Simulation (MCS), and Species Sensitivity Distribution (SSD), we assessed exposure and risk for four human demographic groups and aquatic organisms via dermal contact and mistaken oral intake. Neonicotinoid concentrations ranged from 0.1 to 408.12 ng/L, indicating notable risks (10^{-3} to 10^{-1}) for humans and aquatic species. The Incremental Lifetime Cancer Risk (ILCR) for dermal contact and oral intake was moderate. Specifically, the Hazard Index (HI) for dermal exposure ranged from 1.49×10^{-2} to 0.125, while for accidental oral intake, it spanned from 2.69×10^{-2} to 0.14. These findings highlight the potential for non-carcinogenic risks associated with neonicotinoid exposure. Ecological risk assessments revealed acute and chronic hazardous concentrations (HC5) for 5% of species at 946 ng/L and 338 ng/L, respectively. These findings underscore the urgent need for targeted interventions and policies to mitigate neonicotinoid

exposure and its ecological threats in the YRB, contributing to a global understanding of neonicotinoid risks in surface water ecosystems.

458

Risk Assessment for Biopesticides

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Abstract

Biopesticides are considered as a viable and environmentally friendly alternative to synthetic pesticides. Biopesticides used for plant protection are not a defined group. They consist of a heterogeneous group of substances based on diverse active ingredients and modes of action from biological and natural origin such as microorganisms (bacteria, algae, protozoa, viruses, fungi, baculoviruses), natural organic substances (including botanicals), semio-chemicals (pheromones), double-stranded RNA, peptides and other new substances in development. Although specific data requirements for active ingredients and products containing micro-organisms were developed and came into force in 2021 (i.e. Part B of (EC) regulation No. 1107/2009), the other substances mentioned above are still regulated under Part A of regulation (EC) No. 1107/2009, together with the synthetic pesticides. As a consequence, data requirements linked to the pesticide directive are not fit-for-purpose for biopesticides and their dossiers include many data gaps preventing their allowance on the market. Despite considered as a group of substances with a potentially lower risk profile, a risk assessment is still needed to conclude on a safe use. Such a risk assessment should have a clear focus on the group of substances under evaluation as should have the data requirements. A fit for purpose risk assessment defined by a problem formulation step is considered as an important methodological step forward. This first step in the risk assessment can follow a Pathway to Harm approach containing successive steps, covering the use of a substance, its exposure route, its potential hazards and its risk for the specific protection goals. Each step in such a Pathway to Harm approach needs to be investigated by formulating a risk hypothesis, describing an analysis plan based on the latest methodologies and science, and concluding on the risk. If for one or more of these steps a low resp. unlikely risk is found, it can be concluded that it is very unlikely that harm will occur and that the use is safe. Although an approach using a problem formulation is not new and e.g. US EPA already uses it, it is not applied to the risk assessment for biopesticides in Europe as yet. The presentation uses exemplary case studies to show the application of a problem formulation for biopesticides and how such a Pathway to Harm approach could result into a more fit-for-purpose risk assessment to be applied worldwide.

595

From science-policy interface to science-policy panel: the United Nations' strengthening of the sustainable life cycle management of chemicals

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Abstract

In recent years, the chemical production and waste generation have been rapidly increasing, presenting substantial hazards to the ecosystem and human well-being. To address this issue, a series of multilateral environmental agreements (MEAs) have been developed internationally, that provide essential decision-making support for the appropriate governance of chemicals and wastes in the participating countries. MEAs have established subsidiary bodies known as science-policy interface (SPI) institutions to provide evidence-based support and scientific assessments for environmental policies. However, the existing SPIs face limitations that hinder their ability to tackle the obstacles presented by the vast quantities of chemicals and wastes currently found in the environment. Therefore, the fifth session of the United Nations Environment Assembly made the decision to establish a science-policy panel to promote the effective management of chemicals and waste and to prevent pollution (SPP-CWP). This panel is intended to be an independent intergovernmental body, similar to the Intergovernmental Panel on Climate Change and Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services. The United Nations Environment Programme convened an ad hoc open-ended working group (OEWG) to design strategies for the SPP-CWP. Since 2022, three OEWG meetings have been conducted, and draft documents outlining the panel's scope, functions, operational principles, conflict of interest policy, institutional setup, work processes, and procedures have been formulated. In this article, we analyzed the background and development of the SPP-CWP and provided updates regarding the progress of the panel's establishment. We also suggested future trends for the SPP-CWP. We concluded that SPP-CWP will be a comprehensive and authoritative international body, providing policymakers with exhaustive reports, consequently strengthening the capacity of life cycle management of chemicals. Thus, the panel will effectively reduce or prevent waste production and pollution, promote material circulation, and minimize resource consumption, making significant contributions to the establishment of a circular economy and an environmentally friendly society.

751

Municipal plastic waste disposal and reduction potential of management transformation: Effects of economic development, landfill and recycling in China cities

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Abstract

Municipal plastic waste (MPW) disposal is crucial for sustainable city development. Between 2009 and 2021, China's MPW production nearly tripled, with a per capita increase of 22kg. However, the efficiency of MPW disposal varies depending on economic development and requires improvement. This study analyzed MPW disposal methods and capacities based on historical statistics, revealing a shift from landfill to incineration with incineration rates rising from 11% in 2009 to 47% in 2021.

Cities with higher economic development levels, such as first-tier, emerging first-tier, second-tier, and third-tier cities, have seen a substantial increase in incineration, with incineration overtaking landfill as the main disposal method. Fourth-tier and fifth-tier cities still primarily use landfills. The transformation speed is proportional to the city level, except for the largest first-tier cities. Risk analysis shows second-tier, third-tier, and fifth-tier cities have a higher risk of direct MPW leakage, with the cause being an inability to handle short-term surges caused by tourism. The national plan estimates incineration rates will reach 60% by 2030, with incineration becoming the primary disposal method in most cities.

This study projects continued increases in MPW production and estimates that landfills and interim storage in 23 selected cities will surge from 1,658 to 2,192 kilotons. Scenario analysis demonstrates that enhanced recycling and incineration strategies lead to a 25%-57% reduction in landfill and interim storage MPW by 2030. However, recycling is more sustainable than incineration with a potential reduction over 20% higher under similar production volumes. Fourth-tier and fifth-tier cities still rely heavily on landfills and require increased incineration rates to achieve a 69%-73% and 58%-63% reduction respectively.

Simulation results show emerging first-tier cities require mixed policies when MPW generation increases significantly to achieve reductions. Overall, MPW disposal is critical for sustainable city development, and a shift towards enhanced recycling is necessary to achieve long-term sustainability.

823

River Health -Reflections on a River, its Catchment History and Dealing with Shifting Baseline Syndrome

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Abstract

The catchment and waterways of the Richmond River, North Eastern New South Wales, Australia, have undergone significant changes since European settlement. These include conversion of a large percentage of the catchment from forests to agricultural lands and wetland to drained floodplains. Due to past

activities, the Richmond River is burdened with excessive sedimentation, black water events, and acid sulfate soil exposure. Its degraded condition has diminished the value and cultural diversity communities place on the river, and there is limited understanding of what 'was' to imagine what 'could be.' There is no catchment-wide water quality monitoring program, and funding for monitoring is sporadic and uncertain. Riparian restoration works are largely voluntary and dependent upon landowner consent since over 90% of the riparian zone is privately owned. To realize a trajectory of improvement in river health, landscape-scale initiatives are required that connect stakeholders to common goals that are measurable. Is it too much to ask?

839

Reflections on governance planning and management of emerging pollutants

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Abstract

Emerging pollutants present complex challenges due to their biotoxicity, persistence in the environment, and ability to accumulate in organisms. Addressing these issues requires interdisciplinary approaches that integrate scientific research, policy development, and stakeholder engagement. Effective strategies rely on rigorous risk assessment to prioritize pollutants and improve monitoring technologies for accurate detection. International cooperation is crucial for developing policies that can effectively manage these pollutants. Future efforts should focus on integrating emerging pollutants into broader environmental frameworks, promoting sustainability, advancing pollution prevention technologies, and enhancing public awareness and community engagement.

884

Policies and Legislation for Emerging Contaminants

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Abstract

Global population is affected by air, land and water pollution, problems that have increased due to population growth, economic development and industrialisation.

The World Health Organisation estimates that 99% of the world´s population lives in places where air pollution exceeds WHO guideline limits, causing 6.7 million deaths due to exposure to ambient and household air pollution in 2019. Regarding water pollution, the lack of appropriate wastewater management systems has increased exposure to pollutants. It is estimated that some 44% of all wastewater discharged is untreated or not properly treated, affecting human and environmental health all over the world.

Emerging contaminants, or contaminants of emerging concern, enter the environment through various pathways, including untreated wastewater and treated effluents. Their potential impacts have resulted in increasing scientific, regulatory, and public attention during the past few decades at the global level. This, in turn, has resulted in water quality landmarks such as institutions, pollution control acts, and technology-based solutions.

In Asia, some of the countries where water and wastewater management systems have improved significantly are Singapore and China. In 1970, Singapore monitored 36 water quality parameters; by 2016, this number had increased to 340 parameters, a 940% increase in 53 years. Wastewater quality is based on source control. China has also increased the number of water quality parameters that are measured nationwide to more than 110, nearly three times the earlier number. Both countries have invested in human and technical capacity.

Fundamental to the implementation of water quality management frameworks has been the realisation that multilevel governance agendas that incorporate formal and informal institutions facilitate pollution management planning. Another definite factor has been public awareness and the understanding that populations can contribute towards a cleaner environment.

This presentation will discuss policies and legislation for water quality management systems with examples from developed and developing countries in Asia, limitations for their implementation, and lessons learned. It will also argue that water quality has impacts on public health, environmental protection, and economic growth, and a prerequisite for further economic and social development as well as good quality of life.

1004

Long-term Accumulation and Potential Environmental and Health Impact of Chemicals of Concern in Plastics and Their Wastes from the Plastics Recycling Perspective

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Abstract

Promoting plastic recycling and recyclability is becoming an prevailing policy option to address global plastic pollution. However, plastic recycling may also result in continued presence and accumulation of various chemicals of concern in recycled plastics, introducing long-term risks to the environment and public health. In this study, the distribution of phthalates (PAEs) in plastic products and wastes was identified through systematic sampling and analysis of plastic wastes from typical urban waste transfer stations in China, and it was found that the detection rate of PAEs in types of plastic products aside from PVC was as high as 98.6%, but the concentration of PAEs was relatively low, revealing the extensive contamination of recycled plastics. Our material flow analysis indicates that after 10 years of recycling, the total accumulation and average concentration of PAEs in packaging plastics will be 1.8 and 1.3 times higher, respectively. Based on the detected distribution of PAEs in recycled plastic wastes, it is estimated that the environmental release of PAEs from plastic wastes and plastic leakage from plastic products scrapped in 2020 will reach 1715~2708 tonnes and 324~1040 tonnes respectively, in the next 30 years, under the plastics recycling scenarios, demonstrating that enhancing the recycling of plastics would likely increase the environmental release of PAEs from plastics. This study reveals the long-term presence and accumulation of chemicals of concern in plastics, and the associated risks to the environment and health risks of them with the prospect of plastic recycling policies, suggesting that chemicals of concern in plastics and their wastes will need to be given high priority and consideration in future plastics pollution control policies, including the global plastics treaty under negotiation currently.

1006

Towards a sustainable use of plastics in agriculture: state of knowledge and policy perspectives.

Luca Nizzetto

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Abstract

Plastic offers numerous advantages in terrestrial agriculture, but some of these uses have resulted in extensive pollution of rural landscapes. While Chinese researchers have led the way in uncovering this environmental issue, studies from other regions confirm its global relevance.

Several pieces of evidence that have emerged over the last few years show that macro, meso, and microplastics represent ubiquitous and conspicuous contaminants of soils in several regions. Agricultural plastics are identified as the main sources, especially in areas where mismanagement of mulching film has occurred over the years. New evidence, however, highlights that soils that did not necessarily experience poor mulching practices can still upt to 0.03-0.3% by mass of plastics. These environmental levels broadly overlap with concentrations that can cause significant changes in soil properties, fertility, and the growth and quality of crops, indicating that plastic contamination in agricultural soils may have already diffusely reached a risk zone.

Achieving the sustainable use of plastics in agriculture is, therefore, a crucial goal of national and international policies currently under development. In this context, consensus on needed measures among the stakeholders of the agrifood chain is crucial for the effectiveness of laws and interventions. We

reviewed the positions and narratives from international farmers, NGOs, agricultural plastics industries and environmental scientists. Contrasting positions emerge on aspects such as "rejection," "reduction," and improved recycling of agricultural plastics, as well as regarding the shift towards increased use of (bio-)degradable and compostable plastics. Consensus, however, exists on other issues such as the need for redesigning and properly labeling agricultural plastic products, traceability of waste, improved environmental safety standards, deployment and retrieval practices, as well as innovative waste management approaches. All stakeholders express concern for the environment and agricultural sustainability, advocating for circular solutions.

In the context of global food systems increasingly reliant on plastic, scientists emphasize the need to preserve nature-based and traditional knowledge-based sustainable agricultural practices alongside intensive production systems based on plasticulture. Maintaining such a diversity in practices is necessary to ensure the resilience of food systems.