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Plenary Sessions

N1-G014

N2-U Hall

September 19 Plenary 1 09:35-10:10 N1-G014

**Impact of environmental factors on individual's health as expressed
in changes in their proteome**

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Environmental pollution is a major risk factor for cancer. In the estimate of the World Health Organization (WHO), over 90% of cancer incidence is closely associated with environmental pollution. Carcinogenic transformation is typically a multistep process that sees cells progress from normal, to pre-cancerous, and finally to the cancerous stage. This progression reflects molecular changes within the cells due to interaction between genes and pollutants. Common viruses, including the Epstein-Barr Virus (EBV) and the human papillomavirus (HPV), are environmental factors that impact upon specific cancer incidence. It is apparent that incidence of cancer in the world exhibits national and regional differences that are likely to reflect the interplay between genetic and environmental factors. In the U.S., oral cancer is by far the most common head and neck cancer; nasopharyngeal cancer (NPC)'s incidence is only 8% of that of oral cancer. By contrast, in China NPC outstrips oral cancer by 200%. Even within China, NPC is largely concentrated in the southeastern regions, including Guangdong and Hong Kong. This highly regional distribution of NPC incidence emphasizes the importance of environmental contribution. This contribution and impact to the proteome will be explored and discussed.

September 19 Plenary 2 10:10 - 10:45 N1-G014

New nitrogen-containing organics species in atmosphere

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Nitrogen-containing organic compounds (NOCs) in air and aerosol play a crucial role in altering the light-absorption properties of particles, thereby impacting regional haze and climate. Many new species were detected due to recently developed high abundance sensitivity mass spectrometers. This study for the first time investigated the diurnal variation, chemical characteristics, and formation pathways of NOCs in ambient air, urban aerosols, cloud water using CI-Orbitrap, a versatile aerosol concentration enrichment system (VACES) coupled with HPLC-Q-TOF-MS and a non-target screening approach, FT-ICR-MS and relative technologies. More than hundreds of new O₃ + NO_x dominated in daytime and NO₃-dominated in nighttime formed NOCs in ambient air, and thousands of new alkyl, cyclic, and aromatic amides, heterocyclic or cyclic amines and aniline homolog series in NOCs in aerosol and cloud water have been revealed. The reaction of ammonium to form imines may be a potential pathway for the formation of aerosol NOCs during nighttime, near two thirds of all CHONs are formed through reactions between NH₃ and carbonyl-containing biogenic volatile organic compound (BVOC) ozonolysis intermediates in cloud. the evolution of CHONs during cloud processes (CPs), which CPs significantly enrich the diversity of CHONs, specifically generating CHONs with O numbers of 1–10 and double bond equivalent (DBE) values of 2–10, which can be described by the formula C_nH_{(2n-16)-(2n)}O₁₋₁₀N₁₋₄. The findings highlight the significant contributions of both primary emissions and ammonium chemistry, particularly amination processes, to the pollution of reduced NOCs in Shanghai's atmosphere.

Keywords

nitrogen-Containing Organics; VACES; aerosol; cloud.

September 20 Plenary 3 09:00 - 09:35 N1-G014

Detection and quantification of legacy and novel PFAS in the urban environment

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Per and polyfluoroalkyl substances (PFAS) are a class of synthetic chemicals that have been incorporated into a range of industrial and domestic products such as AFFFs, cosmetics, household products, medical devices, food contact materials, inks, pesticides, oil production, textiles, leather, and apparel since the 1940s. They have attracted global scientific, regulatory and community attention due to their environmental persistence, bioaccumulative properties and negative impacts of public health and wildlife. A smaller suite of legacy PFAS consists of perfluoroalkyl acids (PFAA), of which the most notorious are perfluoroalkylsulfonic acid (PFOS; $C_8HF_{17}O_3S$) and perfluoroalkyloctanoic acid (PFOA; $C_8HF_{15}O_2$). Global restrictions on the use of PFOA and PFOS have led to the development of thousands of replacement novel PFAS, most without publicly available information on their production, use, environmental distribution and/or toxicology. This talk will focus on PFAS in the Australian environment, including methods of analysis for targeted measurements with LC-QqQ-MS and non-target analysis (NTA) with high resolution mass spectrometry (LC-QTOF). Followed by an examination of PFAS in the Australian urban environment that includes WWTPs and novel sources such as chemical warehouse fires and high-performance motor cars.

September 21 Plenary 4 09:00 - 09:35 N2-U Hall

A 30-year retrospective of POPs in Taiwan from chemical analysis to public communication

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The natural environment and fresh food are indispensable for healthy people as the Chinese ancient proverb “Seven things to open the door” mentions seven daily necessities of the general population: firewood, rice, oil, salt, sauce, vinegar, and tea. Not surprisingly, environmental and food scandals are among high-priority public concerned issues. Public communication can help these scandals in a number of ways as raising awareness of the problem and taking action to demand change, building trust between the public and the organizations involved, holding those responsible accountable, and preventing future scandals.

We have started our POPs works in Taiwan for more than thirty years from identifying the harmful substances involved, studying their pathway to final acceptors, assessing their risks to human health and the environment, and developing standard analytical methods. In some cases, we also worked with policymakers and regulators to develop regulatory and legal solutions. Most importantly, Education about environmental protection or food safety is invisibly practiced during public communications. By so doing, we hope to develop scientifically informed consumers capable of using chemistry information to make decisions or solve problems.

The reported cases include a waste pentachlorophenol manufacturing plant, dioxins in a historical scrap metal and e-waste recycling area Er-Jen Riverside, dioxins from Municipal solid waste incinerators and industrial solid waste incinerators, dioxin-like-compounds in food a total diet study, phthalates in food and daily necessities. Various means are used to convey our findings to the media and concerned public. We learn that providing evidence-based and unbiased information to the public without any potential conflicts of interest is uttermost. Our experience indicates that public communication can play a vital role in protecting consumers' rights and our environment.

September 21 Plenary 5 09:35 - 10:10 N2-U Hall

Omics investigation on adverse effects of dioxin exposure

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The potential risk of dietary exposure to seventeen 2,3,7,8-PCDD/PCDFs and twelve dioxin-like polychlorinated biphenyls (DL-PCBs) of Hong Kong residents was investigated. The concentrations of these persistent organic pollutants in animal origin foods collected in markets were determined. With the food consumption profile of the residents achieved by Food and Environmental Hygiene Department, the dietary exposure to dioxin like compounds and NDL-PCBs was evaluated. By using non-targeted metabolomics approach in conjunction with multivariate data analysis, we found that in aryl hydrocarbon receptor (AhR)-sensitive mouse model-C6, perturbation of metabolic pathways was observed, namely the accumulation of fatty acids and lysophospholipids, the reduced amino acid biosynthesis and the decreased purine metabolism. The metabolomics results were verified with human plasma sample analysis collected from workers in the waste incineration facility.

Keywords

dioxins; metabolomics; biomarkers; human plasma

Young Scientist Award Session

N1-G014

Transformation of mercurous [Hg(I)] species during laboratory standard preparation and analysis: implication for environmental Analysis

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Hg(I), as an important Hg species, controls Hg redox kinetics; however, its metastable nature makes its analysis difficult. Herein, the stability of Hg(I) during laboratory standard preparation and analysis was studied. Gravimetric analysis showed that Hg(I) was stable in its stock solution (1000 mg L⁻¹), yet complete disproportionation of Hg(I) was observed when Hg(I) diluted solution (10 µg L⁻¹) was analyzed using more sensitive liquid chromatography-inductively coupled plasma mass spectrometry (LC-ICPMS). We show that Hg(0) and Hg(II) can react in aqueous phase and give rise to Hg(I) via comproportionation reaction, which was revealed by the density functional theory calculation, suggesting that aqueous Hg(I) is considerably stable. A rapid comproportionation reaction between ¹⁹⁹Hg(0)_{aq} and ²⁰²Hg(II) was further directly observed, however, the separation of Hg(0) and Hg(II) enabled the easy disproportionation of Hg(I) during LC separation process, evidenced by double isotope tracing approach. These results suggest that Hg(I) is a vital Hg species in aqueous solution which can be indirectly quantified using LC-ICPMS protocol. We further show that container material (polypropylene), increasing container headspace, decreasing pH, and increasing dissolved oxygen significantly enhance the transformations of Hg(I) via disproportionation and redox. Thus, storage strategies for stabilizing Hg(I) in a diluted solution were proposed, including glass container, without headspace, and a slightly alkaline solution. Furthermore, the detection of Hg(I) in Hg(I) or Hg(II)-spiked three environmental water samples suggests Hg(I) is an important intermediate during the reduction of Hg(II). These findings provide an applicable approach for aqueous Hg(I) analysis and highlight the significance of metastable Hg(I) on the fate of Hg in aquatic environments.

Keywords

Mercurous mercury (Hg(I)); Disproportionation; Comproportionation; Redox; Storage strategy; Environmental analysis.

Occurrence, origins, and source-specific health risk of PM_{2.5}-bound organophosphate flame retardants in Hong Kong

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Organophosphate flame retardants (OPFRs) are emerging organic pollutants in atmospheric fine particulate matter (PM_{2.5}). Given their potential carcinogenic and neurotoxic effects, they have gained increasing attentions from aerosol scientists in recent years. However, studies on the sources, occurrence, and health risk assessment of PM_{2.5}-bound OPFRs in Hong Kong are lacking. In this study, we optimized a sample pretreatment and GC-APCI-MS/MS method to characterize OPFRs in PM_{2.5} samples over a one-year period in Hong Kong. We successfully apportioned the major sources of OPFRs and quantitatively evaluated the source-specific contributions to both OPFRs and their potential health risks in Hong Kong for the first time. Over 94% of PM_{2.5}-bound OPFRs in the region were primarily emitted, with plastic processing and waste disposal being the leading source (61.0%), followed by marine vessels (14.1%). Our assessment of health risks associated with human exposure to PM_{2.5}-bound OPFRs indicated a low-risk level. However, further source-specific health risk assessment revealed relatively high noncarcinogenic and carcinogenic risks from chlorinated-OPFRs emitted from plastic processing and waste recycling, suggesting a need for more stringent emission control of OPFRs from these sources in Hong Kong.

Keywords

organophosphate flame retardants (OPFRs); PM_{2.5}; source apportionment; source-specific health risk assessment; plastic processing and waste disposal.

Tuesday, September 19
Parallel Session I

Toxicology of PTS
N1-G014

Study on the distinct lipid distribution in mice induced by PFOS and PFOA exposure

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The distribution and metabolic balance of lipids in organisms are essential for their maintenance of normal life activities. Previous studies have shown that perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS) have distinct toxicity, but the differences of lipid distribution caused by PFAS and its molecular mechanism need to be further explored. In this study, we compared the lipid content and distribution in mice following exposure of PFOA and PFOS. Compared to PFOS, PFOA altered a variety of metabolic indicators and increased energy expenditure in mice. All treated mice showed different extent of hepatomegaly and abnormal lipid accumulation, and more hepatic lipids were accumulated in PFOS-exposed mice than PFOA-treated individuals. Specially, PFOS induced lipid droplets (LDs) accumulation in the cytoplasm of hepatocytes, but PFOA resulted in accumulation of nucleus lipid droplets (nLDs). The effects of PFOA and PFOS on LDs generation and transport pathways related to lipid exchange between cytoplasm and nucleus were analyzed with proteomics techniques, and both were found to affect the levels of fatty acid metabolism pathway, cytochrome P450 pathway-related proteins. PFOA also significantly affected aerobic respiration and mitochondrial ATP synthesis coupled proton transport pathway. PFOS significantly affected the glutathione derivative biosynthetic process, cholesterol metabolism and triglyceride metabolism process. Furthermore, it was verified that PFOA can affect the expression levels of key proteins MTP, Ces1d, and Seipin in the molecular pathways related to the formation and aggregation of nLDs in hepatocytes, resulting in the abnormal accumulation of nLDs in mouse hepatocytes based on molecular biology and protein technology. Therefore, the distinct lipid distribution induced by PFOA and PFOS exposure can explain for their different toxic effects in mice. Our study can offer a new insight into evaluation of health effects for PFOA and PFOS, as well as their potential alternatives.

Keywords

perfluorooctanoic acid, perfluorooctane sulfonate, lipid distribution, lipid droplet, nucleus lipid droplets

Effects of endosulfan and OBS on vascular homeostasis and human health

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Endosulfan is a typical persistent organic pollutant (POP), linked to human cardiovascular diseases (CVD). Sodium p -perfluorous nonenoxybenzenesulfonate (OBS) is used as the alternative to perfluorooctanesulfonic acid (PFOS) and becoming one of emerging contaminants. However, the mechanistic understanding of OBS in CVD is limited. Abnormal vascular homeostasis may result in the occurrence of CVD, attributed to dysfunction of vascular endothelial cells. In our study, endosulfan (0.1-20 μM) promotes cell migration, disrupts cytoskeleton and increased endothelial permeability in HUVECs. Base on LD50 in MTT assay, we found that OBS had much higher toxicity than endosulfan in HUVECs with greater impact on vascular homeostasis. Exposure to OBS (0.1~20 μM) resulted in the increase of LDH release, cell adhesion, cell migration and permeability. Transcriptome analysis revealed the up-regulation of 535 genes and down-regulation of 150 genes upon exposure to 20 μM OBS. Disease prediction analysis using Nextbio software suggested that OBS exposure was associated with CVD, particularly coronary atherosclerosis, similar with endosulfan. Our findings provide valuable insights for assessing the cardiovascular toxicity of OBS, chemical management and emission standards.

Keywords

endosulfan; OBS; PFOS; vascular homeostasis; human health

Organochlorine pesticide ban facilitated reproductive recovery of Chinese Striped Hamsters

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Introduction: Organochlorine pesticides (OCPs) have been used worldwide on an enormous scale over the last century but are banned globally due to environmental persistence and ecotoxicity in recent decades. A number of studies have still reported high detection frequency and contaminated levels of these pesticides in various environments. However, long-term effects of OCP-ban for agricultural use in China since 1983 on the reproductive health of small terrestrial mammals have never been evaluated in the field.

Methods: We examined the residue dynamics of OCPs and reproductive performance of Chinese Striped Hamsters (*Cricetulus barabensis*) at population level in North China Plain during 1983-2010. The associations between internal exposure of OCPs and several reproductive performance indexes after adjusting for environmental factors were determined using the generalized linear model.

Results: It showed that the internal exposure levels of OCPs in hamsters drastically decreased from 2900 ± 740 ng/g to 25.2 ± 6.88 ng/g with an average half-life of 5.08 years, coinciding with the observed reproductive recovery of hamsters. The population-based reproductive performance (indexes) of hamsters was significantly and negatively associated with OCP exposure levels after adjusting the contributions from climate (temperature and precipitation) and population density factors, indicating that the ban of OCPs has facilitated the reproductive recovery of hamsters by up to 81% contribution.

Conclusion: Our findings suggest that the OCP ban is effective to restore reproduction of small terrestrial mammals. Integration of population biology and environmental science is essential to assess the impacts of persistent organic pollutants on ecological safety and biodiversity loss under accelerated global change.

Keywords

polybrominated diphenyl ethers; persistent organic pollutants; climate-change; temporal trends; risk-assessment; surface soil

Prediction of carcinogenic effects of persistent toxic substances using neural network model and transcriptome data

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Persistent toxic substances (PTS) pose significant risks to human health and the environment. Understanding the carcinogenic effects of PTS is crucial for effective risk assessment and mitigation strategies. In this study, we propose a novel approach using a neural network model to predict the carcinogenic effects of PTS based on gene expression matrix data obtained through RNA-Seq. To ensure the biological relevance of our predictions, we applied bioinformatic analysis methods to extract features from the RNA-Seq data. By leveraging gene set enrichment, we were able to focus on specific gene sets of interest for targeted analysis. Using a large dataset from The Cancer Genome Atlas (TCGA) database, comprising transcriptome profiles of specific cancer types, we developed a robust neural network model by integrating gene expression profiles. The model was trained and validated on a diverse set of cancer samples, demonstrating its high accuracy in predicting cancer types and identifying potential carcinogenic signatures associated with PTS exposure. Our future work involves expanding the application of our trained model to predict transcriptome changes after exposure to various pollutants. By analyzing differential gene expression patterns and conducting gene set enrichment analysis, we aim to identify specific gene sets and pathways that are enriched in PTS-induced carcinogenicity. This knowledge will contribute to a deeper understanding of the underlying mechanisms and facilitate the development of effective strategies for managing and preventing PTS-related risks. Overall, this study shows the power of integrating advanced machine learning models, large-scale transcriptome datasets, and gene set enrichment analysis for predicting the carcinogenic effects of PTS. The insights gained from this research have significant implications for toxicology, risk assessment, and the development of targeted interventions to mitigate the adverse health effects of PTS exposure.

Keywords

carcinogenicity prediction; neural network; transcriptome; risk assessment

Tuesday, September 19
Parallel Session I

**Occurrence, transport and
fate of PTS**
N1-G018

Semi-rational engineering a biosensor with targeted ligand specificity for the detection of short-chain chlorinated aliphatic hydrocarbons in waters

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Short-chain chlorinated aliphatic hydrocarbons (CAHs), commonly used as industrial reagents and solvents, pose a significant threat to ecosystems and human health as they infiltrate aquatic environments due to extensive usage and accidental spills. Whole-cell biosensors have emerged as cost-effective, rapid, and real-time analytical tools for environmental monitoring and remediation. However, the broad ligand specificity of transcriptional factors (TFs) often prohibits the application of such biosensor. Herein, we employed a Test-Learn-Test (TLT) model to investigate the amino acid residues surrounding the ligand-binding pocket of the alkane-responsive regulator protein AlkS. Leveraging this information, we employed a semi-rational engineering approach to modify the active site of the AlkS, as well as the PalkS and PalkB promoters, and developed a CAHs-sensitive biosensor with significantly reduced background fluorescence using a bidirectional fluorescence-activated cell sorting (FACS) strategy. This biosensor exhibited promising applications in the detection of CAHs in actual water samples, enabling timely environmental pollution warnings.

Keywords

AlkS; whole-cell biosensors; directed evolution; high-throughput screening; chlorinated aliphatic hydrocarbons

Exhaled breath analysis of non-volatile drugs: a review towards practical applications

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Exhaled breath is a promising specimen for in vivo drug analysis, carrying both volatile and non-volatile drugs (NVDs). The analysis of NVDs in exhaled breath is especially valuable due to the clinical prevalence of NVDs. NVDs transfer from the body to exhaled air as part of exhaled breath particles, involving multiple respiratory sites and complex mechanisms linked to breathing maneuvers. The very low concentration of NVDs in exhaled breath poses significant analytical challenges. Breath analysis for NVDs finds utility in drug abuse testing and therapeutic drug monitoring, with a growing body of related studies. This review thoroughly describes the origin of NVDs in exhaled breath, and summarizes the characteristics and limitations of current analytical methods (including offline and online methods) for exhaled NVDs, as well as the applications of breath analysis for NVDs, in order to provide helpful guidance for subsequent basic and translational research.

Keywords

breath analysis; non-volatile drugs; drugs of abuse; drug analysis; therapeutic drug monitoring.

Enhancement of atmospheric nucleation precursors on iodic acid-induced nucleation: predictive model and mechanism

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Iodic acid (IA) has recently been recognized as a key driver for new particle formation (NPF) in marine atmospheres. However, the knowledge of which atmospheric vapors can enhance IA-induced NPF remains limited. The unique halogen bonds (XBs) forming capacity of IA makes it difficult to evaluate the enhancing potential (EP) of target compounds on IA-induced NPF based on widely studied sulfuric acid systems. Herein, we employed a three-step procedure to evaluate the EP of potential atmospheric nucleation precursors on IA-induced NPF. Firstly, we evaluated the EP of 63 precursors by simulating the formation free energies (ΔG) of the IA-containing dimer clusters. Among all dimer clusters, 44 contain XBs, demonstrating that XBs are frequently formed. Based on the calculated ΔG values, a quantitative structure–activity relationship model was developed for evaluating the EP of other precursors. Secondly, amines and O/S-atom-containing acids were found to have high EP, with diethylamine (DEA) yielding the highest potential to enhance IA-induced nucleation by combining both the calculated ΔG and atmospheric concentration of considered 63 precursors. Finally, by studying larger (IA)₁₋₃(DEA)₁₋₃ clusters, we found that the IA-DEA system with merely 0.1 ppt ($\sim 10^6$ cm⁻³) DEA yields comparable nucleation rates to that of the IA-iodous acid system.

Keywords

marine particle formation; iodic acid; QSAR; diethylamine; quantum chemical calculation; atmospheric cluster dynamics simulation

p-Phenylenediamine quinones: analysis, occurrence, and health implications

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p-phenylenediamine (PPDs) antioxidants are a common type of synthetic rubber additives. With the widespread use of rubber products, a large number of PPDs have been released into the environment and detected in different environmental compartments [1,2]. In this study, with advanced mass spectrometry techniques, we have identified a series of quinone transformation products, named PPDs-quinones in atmospheric particulate matters, roadside soil, and surface runoff water in different megacities in China. The identities of newly discovered contaminants were confirmed by using self-synthesized standards. Our results showed that PPDs-quinones exhibited higher environmental levels and human exposure risks than their parent compounds of PPDs. In addition, by using a dithiothreitol assay, we found that PPDs-quinones are a new class of organic components that can induce PM_{2.5} to generate reactive oxygen species. In line with this finding, our results further supported that PPDs-quinones are highly active species, which can induce DNA adducts in mammalian cells and aqueous organisms, which provides a new toxicity mechanism for addressing the health implications of these emerging environmental contaminants.

Keywords

PPD-quinones; mass spectrometry; environmental occurrence; health implications

Tuesday, September 19
Parallel Session II

Toxicology of PTS
N1-G014

Indoor emerging contaminants: exposure status and risks

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As the usage of industrial chemicals continues its upward trajectory, the resultant environmental challenges and threats to human health have grown more dire. Existing environmental research, hindered by limitations such as inadequate sample sizes, limited scope, and a narrow focus on specific chemical contaminants, falls short of meeting the demands of contemporary inquiries into the nexus between the environment and human well-being. In this study, we employed targeted and non-targeted mass spectrometry techniques to analyze indoor contaminants from multiple urban areas in China, and systematically delineated the pollution characteristics and potential health risks associated with a diverse array of contaminants in the Chinese indoor environment. The findings revealed the widespread occurrence of over 600 organic contaminants, including flame retardants, plasticizers, antioxidants, and many others, within indoor environments. These emerging contaminants exhibited complex compositions, characterized by high concentration levels and pronounced regional distribution disparities across China. The current exposure is unlikely cause significant health risks according to the human exposure assessments. However, in vitro toxicity data indicated significant impacts on reproduction, endocrine function, and developmental processes due to indoor environmental contaminants, with no obvious neurological toxicity effects, implying potential health risks to resident humans. This study will facilitate a comprehensive understanding of the pollution characteristics of emerging indoor contaminants nationwide, thereby providing essential data support for research on indoor environmental pollution in China and related health assessments.

Keywords

indoor environment, emerging contaminants, nationwide, occurrence, human exposure

Azole-induced color vision deficiency associated with thyroid hormone signaling

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Azoles that are used in pesticides, pharmaceuticals, and personal care products can have toxic effects on fish. However, there is no information regarding azole-induced visual disorder associated with thyroid disruption. We evaluated changes in retinal morphology, optokinetic response, transcript abundance of the genes involved in color perception and hypothalamic-pituitary-thyroid (HPT) axis, and thyroid hormone (TH) levels in zebrafish larvae exposed to the common azoles, such as climbazole (CBZ) and triadimefon (TDF), at environmentally relevant and predicted worst-case environmental concentrations. Subsequently, the effect of azoles on TH-dependent GH3 cell proliferation and thyroid receptor (TR)-regulated transcriptional activity, as well as the *in silico* binding affinity between azoles and TR isoforms, were investigated. Azole exposure decreased cell densities of the ganglion cell layer, inner nuclear layer, and photoreceptor layer. Zebrafish larvae exposed to environmentally relevant concentrations of CBZ and TDF showed a decrease in optokinetic response to green-white and red-white stripes but not blue-white stripes, consistent with disturbance in the corresponding opsin gene expression. Azole exposure also reduced triiodothyronine levels and concomitantly increased HPT-related gene expression. Molecular docking analysis combined with *in vitro* TR-mediated transactivation and dual-luciferase reporter assays demonstrated that CBZ and TDF exhibited TR antagonism. These results are comparable to those obtained from a known TR antagonist, namely TR antagonist 1, as a positive control. Therefore, the damage to specific color perception by azoles appears to result from lowered TH signaling, indicating the potential threat of environmental TH disruptors to the visual function of fish.

Keywords

ocular toxicity; zebrafish; environmental pollutant; color vision; optokinetic response; signaling pathway.

Assessment of fetal exposure and metabolism of poly- and perfluoroalkyl substances (PFASs): new evidence from pair serum, placenta, and meconium

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Multiple evidences have indicated that prenatal exposure to Poly- and perfluoroalkyl substances (PFASs) have close association with adverse birth outcomes of fetuses. However, the difficult access to human samples limits the understanding of PFASs transport and metabolism across the human placental barrier as well as the accurate assessment the exposure of PFASs to fetal. In the present study, we assess the fetal exposure of 28 PFASs based on pair serum, placenta, and meconium unit. Results showed that 21 PFASs were firstly identified in those four types pair samples, which indicated the prenatal exposure as well as metabolism and excretion of PFASs by the fetal. Specifically, 25 PFASs were detected in meconium samples, with PFOS and PFHxS as the dominant congeners, suggesting the metabolized and excretion of PFASs through meconium. PFASs might easilier metabolism through meconium than that for PFCAs. Based on molecular docking, MRP1, OATP2B1, and ASCT1, and P-gp were identified as the crucial transporters that involve in the dynamic placental transmission of PFASs between maternal and fetal. With the increased of carbon-chain length, both transplacental transfer efficiency and meconium excrete efficiency of PFASs showed a structure-dependent manner. This study reported for the first time that meconium, which is a non-invasiveness and stable biological-matrix, can be strong evidence of prenatal PFASs exposure.

Keywords

ocular toxicity; zebrafish; environmental pollutant; color vision; optokinetic response; signaling pathway.

BDE-47 causes depression-like effects in zebrafish larvae via a non-image-forming visual mechanism

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Depression is a high-incidence mood disorder that is frequently accompanied by sleep disturbances. Circadian disruption triggered by non-image-forming (NIF) visual pathway is accordingly proposed as a new pathogenic factor to improve the conventional monoamine hypothesis of depression. Therefore, we hypothesize that polybrominated diphenyl ethers (PBDEs) which are known to induce visual impairment could promote depression by disrupting the NIF visual system. In this study, zebrafish larvae were exposed to BDE-47 at environmentally relevant concentrations (2.5 and 25 $\mu\text{g/L}$). BDE-47 caused disruptions with a distinct day-night pattern on gene expressions of photopigment melanopsin that dominates the NIF visual system. Mammalian orthologous melanopsin gene *opn4.1* fell to 70% of the normal level at night ($p < 0.05$), but rose to 140%~160% level ($p < 0.01$) in the morning. Such bidirectional difference transmitted to clock genes and neuropeptides in the suprachiasmatic nucleus (SCN) and impacted adjacent serotonin system. However, indicative factors of depression, including *serta*, *htr1aa* and *aanat2*, were unidirectionally increased with 1.3~1.6 fold ($p < 0.05$). They were consistent with changes of nighttime thigmotaxis (increased by 8%, $p < 0.05$) and sleepy hypoactivity (88% for night and 70% for day, $p < 0.05$ for both). The results of melanopsin antagonism also indicated these consequences were possibly due to the combination of direct photoentrainment by melanopsin and circadian disruption originated from melanopsin. Collectively, our findings revealed that BDE-47 exposure disrupted NIF visual pathway and resulted in depression-like effects, which may further exert profound health effects like mood disorders.

Keywords

melanopsin; non-image-forming; depression; BDE-47; circadian rhythm; sleep

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

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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 tracked 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.

Keywords

γ -hexachlorocyclohexane; methane; magnetite nanoparticles; biochar; electro-bioreduction

Acknowledgement

We acknowledge the financial support from the National Natural Science Foundation of China (42225705, 42177006, 41721001), and the Zhejiang Provincial Natural Science Foundation of China (LD21D030001).

Tuesday, September 19
Parallel Session II

**Occurrence, transport and
fate of PTS**
N1-G018

The synergistic associations between methanogenesis and reductive dechlorination, and the simultaneous regulation

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Residues of chlorinated organic pollutants (COPs) in environment is still a major public concern. Reductive dechlorination is the most efficient way for depletion of COPs in paddy soil, where the methanogenesis is usually mass-produced. Both processes are essentially microbial-mediated electron accepting processes and received much attention in last decades, due to their great importance for soil remediation polluted by COPs, and the effect of global warming, respectively. In this report, we applied meta-analyses, incubation experiment and quantum modelling to investigate the associations between reductive dechlorination and methanogenesis. Results indicated the accelerated methanogenesis were commonly synergistically coupled with the accelerated removal of COPs. Some methanogens were showed as the core taxa co-occurring with dechlorinators in the microbial networks of COP-polluted environments. Also, Methanogenic species could promote some COPs dechlorination by regulating cell metabolic functions, e.g., the coenzyme F430 could reduce the activation barrier of reductive dechlorination. Further regulation based on a mixed culture through microbial electrochemical systems (MES) verified the possibility to synchronously regulate these two processes via the application of suitable conductive materials. The addition of biochar is suggested as an advanced win-win approach for rapid removal of COPs and simultaneous decrease of greenhouse gas release in flooded soil. Collectively, our work provides insight into a novel strategy to coordinate methanogenesis that promotes the anaerobic degradation of COPs.

Keywords

γ -hexachlorocyclohexane; methane; magnetite nanoparticles; biochar; electro-bioreduction

Acknowledgement

We acknowledge the financial support from the National Natural Science Foundation of China (42225705, 42177006, 41721001), and the Zhejiang Provincial Natural Science Foundation of China (LD21D030001).

Sensitive immunoassay for small molecule detection in homogeneous solution based on CRISPR-Cas12a

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Sensitive detection of biologically and environmentally relevant small molecules (SM) is essential for many applications, including drug discovery, metabolomics and toxicity, food surveillance, environmental monitoring and clinical diagnosis. Benefiting from the specific target recognition with antibodies, immunoassays are widely used for SM detection in bioanalysis and diagnostics. Discovery of clustered regularly interspaced short palindromic repeat-associated proteins (CRISPR) and their associated proteins (Cas) has revolutionized genome editing. CRISPR-Cas also provides new tools for sensitive detection of nucleic acid and non-nucleic acid targets. Cas12a has crRNA-guided collateral cleavage activity, and can be used for signal amplification in assay developments. Taking advantage of immuno-recognition and CRISPR-Cas12a, here we reported a sensitive CRISPR-Cas12a assisted immunoassay for small molecule detection in homogeneous solution. An active DNA (acDNA) modified with a specific small molecule was used as an affinity probe. Large-sized antibody binding with this acDNA probe inactivates the collateral cleavage activity of CRISPR-Cas12a due to steric effect. When free small molecule target exists, it replaces the small molecule modified acDNA from antibody, triggering catalytic cleavage of DNA reporters by CRISPR-Cas12a, and strong fluorescence is generated. With this strategy, we achieved detection of small molecules, digoxin and folic acid, at picomolar levels by using antibody as recognition elements. This method does not need immobilization, separation, and labeling of antibodies, which greatly simplifies the operation and improves assay speed. We envision this strategy will have broad applications to detection of various small molecules.

Keywords

small molecule detection; immunoassay; CRISPR; free separation.

Development of a rapid detection method for virus nucleic acid based on CRISPR nucleic acid nanotechnology

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The CRISPR nucleic acid nanotechnology, which is characterized by regularly spaced clustered short palindromic repeats, has rapidly developed in molecular diagnostics and become an important tool for amplifying and identifying nucleic acids. The single-tube isothermal detection method based on CRISPR gene editing technology has improved the convenience, sensitivity, and specificity of molecular detection of COVID-19, and expanded its application in environmental monitoring of pathogenic microorganisms. Developing a single-tube isothermal detection method based on the combination of recombinase polymerase amplification (RPA) and loop-mediated isothermal amplification (LAMP) with the CRISPR system can achieve amplification under isothermal conditions, simplify the requirement for specialized equipment, and enable on-site detection. However, the compatibility issue among various systems in homogeneous reactions needs to be addressed first. The RT-LAMP-CRISPR/Cas12a single-tube isothermal detection method involves placing the two systems in separate positions within the same tube, at the bottom and cap, while in the RT-RPA-CRISPR/Cas12a single-tube isothermal detection method, both the RT-RPA and CRISPR/Cas12a systems can react at 37-42°C. By adding RNase H enzyme to release cDNA from the RNA-cDNA hybrid chain and rapidly initiate RPA amplification, the detection capability of low-concentration viral RNA is improved. The developed single-tube isothermal detection technology only requires a temperature-controlled water bath and a handheld UV lamp as auxiliary equipment, and can rapidly and visually detect multiple different gene sites of SARS-CoV-2 virus under isothermal conditions in real-time, achieving the visual detection of virus RNA.

Keywords

SARS-CoV-2; detection of viral nucleic acids; wastewater; graphene oxide; magnetic beads; qRT-PCR

A room-temperature synthesis of nitrogen-rich conjugated microporous polymers for solid-phase extraction of trace synthetic musks

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This study synthesized a conjugated microporous polymer (CMP) at room temperature, which has high surface area, large conjugate system, and nitrogen-rich features. The material was explored as a solid-phase extraction (SPE) column, and it showed a higher extraction efficiency for nitro-musks compared to most commercial columns. Under optimal SPE conditions, a sensitive and efficient method for determining five nitro-musks was established based on gas chromatography–mass spectrometry (GC–MS). The method showed excellent linearity ($R^2 \geq 0.996$), low limits of detection (0.13–0.57 $\text{ng}\cdot\text{L}^{-1}$), good repeatability (1.1–4.0 %, $n = 6$) and was applied to the detection of trace nitro-musks in water and milk samples. The mechanism was further discussed combined with a simulation calculation. The advantages of the proposed method were mainly reflected in the extraction efficiency and sensitivity, which also indicated the potential of CMPs as a sample pretreatment material.

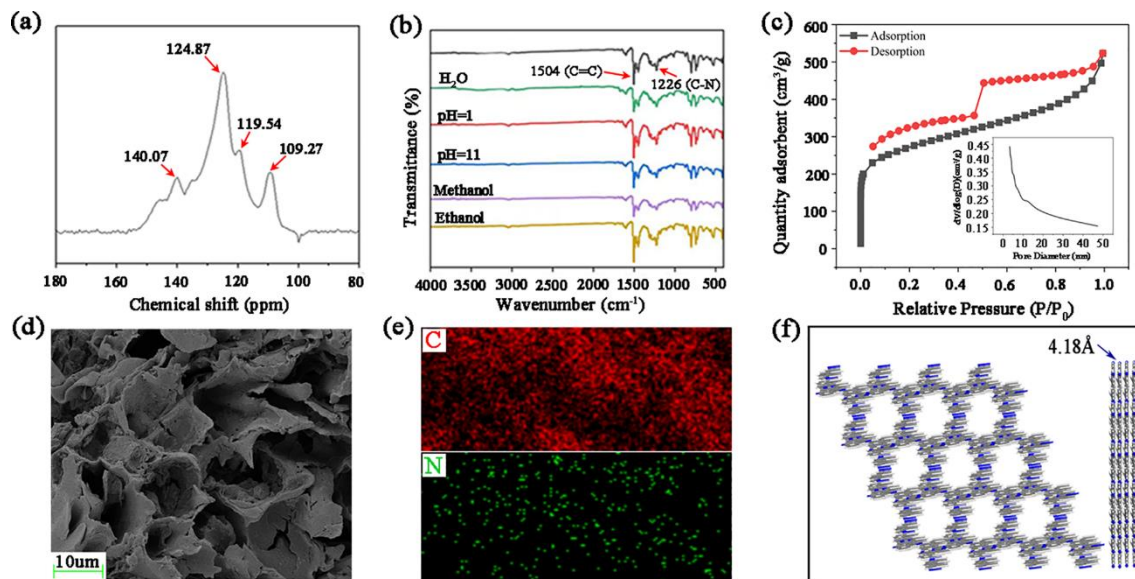


Figure 1 ^{13}C CP/MAS NMR spectrum (a), FT-IR with treatment under various conditions (b), N_2 adsorption–desorption isotherm and pore size distribution (c), SEM (d), EDS (e), Top and side views of the AA stacking mode (f) of TCB-CMPs.

Keywords

conjugated microporous polymers, milk, GC–MS, solid-phase extraction, synthetic musks

Performance enhancement of laser desorption/ionization mass spectrometry by using nanostructures and matrix sublimator

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The type and deposition mode of matrix play critical role in the performance of laser desorption/ionization mass spectrometry (LDI-MS). Here, two methods were developed to enhance the performance of LDI-MS. 1) An integrated matrix sublimation device with synchronous solvent nebulization was developed for matrix deposition. The sensitivity and quality of the images were clearly improved in synchronous mode compared with those of the conventional spray and sublimation methods. The integrated device with both solvent nebulization and matrix sublimation is a useful tool in mass spectrometry image applications. 2) A hybrid of Au NPs decorated graphdiyne (Au/GDY) was fabricated and employed as LDI-MS matrix. The optimized Au/GDY matrix can reliably detect trace sulfacetamide and visualize ex/endogenous components in biological tissues. A novel mechanism system was established to reveal LDI processes of Au/GDY matrix from the perspective of energy conversion and transfer. This work offers an integrated strategy to promote the LDI efficiency based on collaborative coupled thermal field and internal electric field.

Keywords

mass spectrometry; sublimation; nanostructure; laser desorption; ionization; image.

Machine learning-assisted insights into sources and fate of microplastics in wastewater treatment plants

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Wastewater treatment plants (WWTPs) converge multiple sourced microplastics (MPs) and serve as a temporary repository in case of releasing them into the environment. The process involves two critical scientific problems including the source composition of MPs and their fate in WWTPs. Therefore, this study conducted a full-scale investigation in each stage of four WWTPs in Hong Kong, with the results showing that the fate of MPs was mainly affected by their physicochemical characteristics and WWTP parameters. Moreover, three conventional machine learning (ML) methods, namely the multi-label decision tree, random forests, and support vector machine, were also applied for figuring out the source compositions of MPs. The results demonstrated that the sources of MPs were mainly composed of domestic (57.3-59.9%), industrial (21.1-21.7%), coastal (11.2-12.7%), domestic/medical (4.6-5.1%) and domestic/agricultural (2.6-3.8%) sources, respectively. The discovery of domestic/medical-sourced MPs should draw the public's attention to the insufficient management of the used face masks. This study was a novel attempt to utilize ML to explore the fate and sources of MPs in environmental compartments, which provided new insights on developing the MP source tracing approaches from the source management of plastic contaminants.

Tuesday, September 19
Parallel Session III

Toxicology of PTS
N1-G014

Transcriptomic integration analyses uncover common bisphenol A effects across species and tissues primarily mediated by disruption of JUN/FOS, EGFR, ER, PPARG, and P53 pathways

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Bisphenol A (BPA) is a common endocrine disruptor widely used in the production of electronic, sports and medical equipment, as well as consumer products like milk bottles, dental sealants, and thermal paper. Despite its widespread use, current assessments of BPA exposure risks remain limited due to the lack of comprehensive cross-species comparative analyses. To address this gap, we conducted a study aimed at identifying genes and fundamental molecular processes consistently affected by BPA in various species and tissues, employing an effective data integration method and bioinformatic analyses. Our findings revealed that exposure to BPA led to significant changes in processes like lipid metabolism, proliferation, and apoptosis in the tissues/cells of mammals, fish, and nematodes. These processes were found to be commonly affected in adipose, liver, mammary, uterus, testis, and ovary tissues. Additionally, through an in-depth analysis of signaling pathways influenced by BPA in different species and tissues, we observed that the JUN/FOS, EGFR, ER, PPARG, and P53 pathways, along with their downstream key transcription factors and kinases, were all impacted by BPA. Our study provides compelling evidence that BPA indeed induces similar toxic effects across different species and tissues. Furthermore, the investigation sheds light on the underlying molecular mechanisms responsible for these toxic effects. By uncovering these mechanisms, we gain valuable insights into the potential health implications associated with BPA exposure, highlighting the importance of comprehensive assessments and awareness regarding this widespread endocrine disruptor.

Keywords

Bisphenol A; integration analysis; toxicogenomics; lipid metabolism; proliferation; apoptosis.

Multi-omics study of cross-organ responses to air pollution modulating energy balance

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Numerous epidemiological studies have drawn connections between fine particulate matter (PM_{2.5}) and the emergence of metabolic diseases, including cardiovascular disease and non-alcoholic fatty liver, particularly in populations with excessive intake of fat and cholesterol. The influence of air pollution extends significantly, altering biological processes and leading to various metabolic shifts, whereas energy metabolism is pivotal to life and intertwined with nearly all biological functions. Understanding the intricate molecular mechanisms that guide cross-organ communication under these risk factors becomes imperative for grasping how biological systems react to external cues. In the present study, a multi-omics approach was employed to delve into how exposure to PM_{2.5} affects energy balance across different organs. By harnessing the power of multi-omics analysis in studying PM_{2.5} toxicity, we discovered that such exposure could exacerbate the negative impacts of unhealthy diets on cardiovascular health by interfering with the metabolism of other organs. Our findings revealed that PM_{2.5} induces metabolic disorders and injuries in various organs, including alterations in branched-chain amino acid metabolism in the spleen and changes in lipoprotein production and clearance in the liver. These modifications, in turn, accentuated the risks of cardiovascular diseases linked with unhealthy dietary intake. The insights gleaned from this study not only illuminate the underlying mechanisms of PM_{2.5}'s adverse effects on energy balance within circulatory systems but also deepen our comprehension of the compounded risks faced by susceptible individuals on high-fat and/or high-cholesterol diets when exposed to environmental contaminants. This understanding may pave the way for targeted interventions and preventive measures in public health.

Keywords

particulate matter; high fat and high cholesterol; energy metabolism; cardiovascular risk; multi-omics; cross-organ communication.

Airborne PM_{2.5} aggravated high-fat diet-induced hepatic diseases through Sirt3 mediated signaling pathway

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Airborne particulate matter, especially with an aerodynamic diameter less than 2.5 μm (PM_{2.5}), can go directly to the respiratory bronchioles of the lung, and result in respiratory diseases. More recently, the epidemiological studies indicated that PM_{2.5} exposure was also associated with cardiovascular diseases, hepatic diseases and obesity. However, the underlying molecular mechanisms involved in PM_{2.5}-elicited damages are not well elucidated. Therefore, in this study, the liver of high-fat diet (HFD) diet induced obese model after PM_{2.5} exposure were selected to explore the deep molecular mechanisms through multi-omics analysis. Both metabolomic and proteomic studies showed that PM_{2.5} induced oxidative stress and inflammation in the liver by disturbing purine metabolism, glutathione (GSH) metabolism and polyamines. Notably, Sirtuin3 (Sirt3), a mitochondrial deacetylase, was selected as a vital regulator by the enrichment analysis. Previous studies have proved that Sirt3 could regulate redox balance and energy metabolism through reversible acetylation. However, there are no reports of the effects of Sirt3 on the liver after PM_{2.5} exposure. We found that PM_{2.5} and HFD cotreatment significantly reduced the expression of Sirt3 and Sirt3 deficiency aggravated PM_{2.5}-induced oxidative stress and inflammation in the liver by using Sirt3 KO mice model through disturbing the same pathways as in the obese mice. Metabolic flux analysis demonstrated that cells uptook more glutamine to generate GSH and polyamines to resist oxidative stress and inflammation under PM_{2.5} exposure or Sirt3 loss, presenting a negative feedback regulation mechanism. Conversely, we found that Sirt3 overexpression as well as glutamine supplementation repressed PM_{2.5}-caused reactive oxygen species production and pro-inflammatory cytokines release in liver cells. These findings identified Sirt3 as a novel regulator for GSH metabolism and polyamines metabolism and demonstrated the important roles of glutamine in protecting PM_{2.5}-induced oxidative stress and inflammation in the liver for the first time.

Keywords

PM_{2.5}, Sirt3, glutamine metabolism, oxidative stress and inflammation

Nontarget accurate screening and risk assessment of hazard factors in aquatic products

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In this study, a new method for sample pretreatment using improved QuEChERS was established, and 289 organic pollutants with health risks could be identified and quantified through gas chromatography-Orbitrap ultrahigh-resolution mass spectrometry (GC-Orbitrap HRMS). A high-resolution database of 289 environmental pollutants belonging to ten categories, including organochlorine pesticides (OCPs), polycyclic aromatic hydrocarbons (PAHs), phthalates (PAEs), polychlorinated biphenyls (PCBs), and other agricultural chemicals (ACs), was established for the nontargeted screening and quantitative analysis. A simple method for biological sample preparation using improved QuEChERS was proposed by combining a conventional QuEChERS method and a column purification method. After purification using a Florisil column, the lipid content was reduced by 99.9%, which significantly reduces the interference of the matrix effect observed during the analysis. Furthermore, simultaneous high-accuracy qualitative screening and quantitative analysis of the target compounds were performed through high-resolution mass spectrometry (60000 resolution) conducted in the full scan mode. The limit of quantitation was 0.56–57.8 pg/g, presenting a large linear range (~106), and the recovery range was 40%–120%. Due to the ultrahigh resolution and sensitivity of Q Exactive GC-Orbitrap HRMS, the quantitative limits of the target compounds were significantly lower than those achieved through methods based on conventional chromatography and mass spectrometry. Moreover, ultratrace organic contaminants that cannot be detected by conventional methods can be accurately quantified by the proposed method. Sea cucumber samples collected at the breeding site were analyzed using the proposed high-coverage multi-objective analytical method, and more than 100 types of organic pollutants were detected; the mean concentrations of PAHs, ACs, PAEs, and OCPs were 157.8, 153.2, 64.4, and 46.4 ng/g dw, respectively, which were higher than those of other pollutants. Some new contaminants, such as 9-chlorofluorene, 5-chloroacenaphthene, and 3-methylcholanthrene, were detected at very low concentrations for the first time in the sea cucumber samples. The proposed method is simple and efficient, allows the detection of pollutants at very low concentrations, and provides accurate and reliable results. Thus, this nontarget accurate screening method can be widely used for broad-spectrum screening and accurate quantification of contaminants in various aquatic products, providing technical support for food safety control..

Keywords

gas chromatography-Orbitrap high resolution mass spectrometry (GC-Orbitrap HRMS); QuEChERS; nontarget analysis; environmental pollutants; sea cucumber

Tuesday, September 19
Parallel Session III

**Occurrence, transport and
fate of PTS**
N1-G018

Catalytic hydrolysis activity of minerals under water-unsaturated conditions

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Surface properties of minerals play important roles on mediating the migration and transformation of contaminants in the environment. Especially, the mineral surface moisture is one of the key factors affecting the surface properties of minerals, thus would show great impact on the environmental fate of contaminants. However, the previous studies relating to the mineral-water interfacial processes were mostly investigated in aqueous conditions or in slurry systems, without considering the water unsaturated surface moisture conditions, e.g., in the scenarios of upland soils and aerosol particles. The transformation behaviors of contaminants on the mineral surface under the water unsaturated conditions are of great concern.

In previous studies, we have found that various minerals, such as kaolinite, montmorillonite, iron minerals, aluminum oxides, exhibited exceptional catalytic hydrolysis activities when exposed to moderate atmospheric humidity levels (i.e., 33 - 76%), resulted in degradation of antibiotics (i.e., chloramphenicol, CAP) and phthalate esters with orders of magnitude faster rates than those observed in aqueous phase. It is also worth noting that the catalytic mechanism is specific for each mineral and contaminant. For instance, the hydrolysis of CAP on kaolinite surface relayed on the strength of hydrogen-bonding interaction with the alumina octahedral sheet of kaolinite. The hydrolysis of CAP on montmorillonite surface correlated to the interlayer exchange cations, whose polarization capability determines the surface Brönsted acidity of montmorillonite. While, the surface Lewis acid catalytic mechanism was mainly responsible for the hydrolysis of CAP on iron minerals. Further investigation showed that the catalytic performance of hematite is also facet-dependent, related to the atomic array of surface undercoordinated Fe on each facet. Taking dimethyl phthalate (DMP) as an example, the {012} and {104} facets of hematite with the proper neighboring Fe-Fe distance of 0.34-0.39 nm could bidentate coordinate with DMP, thus induce much stronger Lewis-acid catalysis.

All these phenomena strongly supported the specific catalytic activities of minerals under the water-unsaturated conditions. Except the hydrolysis processes, the catalytic redox reactions on mineral surface might be also of great interest, while still far from clear regarding to the influence of surface moisture.

Dynamic study of reactive oxygen species and its environmental application

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Reactive oxygen species (ROS) are produced in many chemical and biological processes. The roles they play differ significantly, depending on the type of ROS and the target molecules they react with. Since ROS are highly reactive, they have been used to decompose chemical compounds of interest. In the area of semiconductor catalysis, the main mechanism of degradation of pollutants or nanoparticles involves light-initiated generation of ROS and their subsequent redox reactions with the chemicals. Therefore, generation and identification of ROS are of great significance to understanding the catalytic degradation mechanisms, improving degradation processes, and eventually utilizing the technology in practical applications.

Few-layer black phosphorus (FLBP) is easily degraded under ambient condition which is an important barrier that plagues the application of FLBP, but its degradation mechanism is not yet well understood. In this work, we surprisingly found the persistent ROS generation was involved with FLBP degradation process even in the dark, and ROS generation patterns and mechanism was revealed by chemiluminescence and density functional theory (DFT). Meanwhile, Rhodamine B (RhB) and methyl orange (MO) can also be removed by FLBP under dark conditions, which further evidence the ROS generation during FLBP self-degradation. This work provides new insights into FLBP self-degradation mechanism and opens opportunities to practically implement FLBP for green catalytic application.

Keywords

ROS; chemiluminescence; self-degradation; environmental application.

Biodegradation of nondesorbable organic pollutants on biochar

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Knowledge of microbial degradation of biochar-adsorbed organic pollutants is essential for recovering adsorption performance of biochars and reducing secondary pollution in soil and underground water remediation. In previous study, desorption of organic compounds from biochars was perceived as a prerequisite for the microbial degradation. However, microbial degradation of the nondesorbable organic compounds on biochars has not been studied. Therefore, aerobic biodegradation of nondesorbable phenanthrene (PHEN) on a wood chip-derived biochar (WBC700, 700°C) by *Sphingobium yanoikuyae* B1 and anaerobic biodegradation of nondesorbable trichloroethylene (TCE) on WBC700 by *Dehalococcoides mccartyi* 195 were both investigated. It was newly observed in this study that the aerobic biodegradation of nondesorbable PHEN was mainly attributed to the $\bullet\text{OH}$ in extracellular fluid of *Sphingobium yanoikuyae* B1, confirmed by the ROS quenching experiment and ESR spectroscopy. The extracellular $\bullet\text{OH}$ was produced through a Fenton-like reaction involved siderophore, H_2O_2 and iron ions, which could be significantly enhanced by WBC700. Differently, it was observed that the anaerobic biodegradation of nondesorbable TCE was mainly attributed to the electron transfer by WBC700, confirmed by the electrochemical experiment. The electrons produced by *Dehalococcoides mccartyi* 195 were accumulated on the surface of biochar and then were transferred to the nondesorbable TCE through the graphitic carbon of WBC700. The obtained results could provide a new insight into the microbial degradation of biochar-adsorbed organic pollutants in soil and ground water remediation.

Keywords

biochar; nondesorbable pollutant; biodegradation; extracellular $\bullet\text{OH}$; electron transfer.

Concentrations, profiles and health risks of organic ultraviolet filters in human milk and food in China: a national study

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UV filters are widely used in consumer products to protect humans and polymers against harmful effects of UV radiation. Previous studies have reported the bioaccumulation and biomagnification potential of these compounds, and toxic effects. Part of UV filters used in cosmetics are prioritized for environmental assessment by the UK Environment Agency. UV-328 is listed as a persistent organic pollutant regulated under the Stockholm Convention. Human milk is an important matrix for assessing human exposure to contaminants, and dietary intake is an important route of human exposure to organic contaminants. This study investigated the concentrations and compound profiles of 15 UV filters in human milk and food in China, and evaluated the current health risks of human exposure to UV filters. Human milk and eight food categories (aquatic foods, cereals, dairy products, eggs, legumes, meat, potatoes, and vegetables) were collected and processed by the China National Center for Food Safety Risk Assessment through the sixth total diet study. These samples were ultrasonically extracted and consecutively purified by GPC and silica gel columns. Organic UV filters were analyzed using GC-MS/MS. The total concentrations of UV filters in human milk ranged from 78 to 846 ng/g lipid weight. UV-P and EHMC were the dominant UV filters in human milk, while UV-328 contributed relatively low. The estimated daily UV filter intake for breastfed infants was below the reference dose. The total dietary concentrations of 15 UV filters ranged from 1.5 to 68.3 ng/g wet weight. Meat contained the highest total UV filter concentration. A significant positive correlation was found between the estimated daily intake of UV filters via animal-origin foods and the concentrations of UV filters in human milk from the same province. Based on the ADME properties and toxicity assessments of UV filters, OC and EHMC have stronger toxic effects *in vivo*.

Keywords

UV filters; food; human milk; China; human exposure.

Formation of environmentally persistent free radicals from thermochemical and photochemical reactions of catechol on atmospheric particulate matter

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Environmentally persistent free radicals (EPFRs) are internationally recognized as an important component of atmospheric fine particulate matter (PM_{2.5}) when assessing its health risks. Catechol, a widely produced organic chemical, is widespread in multiple environmental compartments, including PM_{2.5}. However, the underlying links and key factors affecting the formation of EPFRs from catechol in natural environment and human activities are not fully understood. In this study, in-situ electron paramagnetic resonance (EPR) spectroscopy was used to detect EPFRs formation from catechol during heating and light irradiation. It was found that significant EPFRs including oxygen-centered phenoxy and semiquinone radicals can be formed from catechol. Their half-lives were up to 12.7 months. It indicated that EPFRs were stable and the potential adverse effects on human health if inhaled or ingested through air or diet should be concerned. After photochemical and thermochemical reactions, CaO, CuO, and Fe₂O₃ significantly promoted the formation of EPFRs from catechol when compared to systems without metal oxide. The effects of these metal oxides on EPFRs formation were in the order of CaO > CuO > Fe₂O₃. Besides, X-ray photoelectron spectroscopy (XPS) was applied to investigate the promotional abilities and underlying mechanisms of various metal oxides in EPFRs formation. It was found that after heating, electron transfer occurred between catechol and CuO after heating, resulting in the reduction of Cu(II) to Cu(I) and facilitating the formation of EPFRs. For CaO, the ratio of Ca(OH)₂ increased indicating that catechol and CaO would generate EPFRs by eliminating H₂O. In addition to EPFRs, the highly active free radicals including hydroxyl free radicals and hydrogen free radicals formed from the photochemical reactions of catechol and PM_{2.5} were also discovered. This is of concern because of the adverse effects of these free radicals on human health.

Keywords

environmentally persistent free radicals (EPFRs); catechol; atmospheric fine particulate matter (PM_{2.5}).

Spatial distribution of environmentally persistent free radicals in atmospheric particulate matter during sandstorms

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Sandstorms are global events, occurring around the world. Recently, Asian sandstorms have become increasingly frequent, with high intensity and wide-ranging impacts, significantly affecting people's life. The composition of atmospheric particulate matter (PM) is highly complex, and environmentally persistent free radicals (EPFRs) were found to be stably absorbed on atmospheric PM. Owing to the persistence, toxicity, reactivity of EPFRs on atmospheric PM and the health risks of EPFRs are similar to smoking, EPFRs has attracted more and more attention. However, there is still nobody conducted on a large scale and systematically exploring the spins levels and spatial distribution characteristics of EPFRs during sandstorms across the entire region of China. In this study, we utilized a machine learning model to establish a correlation between conventional air pollution parameters and EPFRs in PM during sandstorms. This model enables the prediction of EPFRs spins levels in PM during sandstorms by utilizing conventional air pollution parameters and meteorological variables. Moreover, using the established machine learning model, we mapped the spatial distribution characteristics of EPFRs in PM within China during sandstorms. It found that during sandstorms, there were significant spatial variations in the distribution of EPFRs in different regions of China. The distribution of EPFRs in northern region exhibited a radiating pattern propagation from the northern border of China, adjacent to southern Mongolia and Inner Mongolia, towards mainland China and extending further. The distribution of EPFRs in southern region exhibited a radiating pattern propagation from the border between Yunnan and the Indochina Peninsula and extending into mainland China. The findings of this study contribute to further understanding the distribution characteristics and potential risks of EPFRs in PM during sandstorms.

Keywords

environmentally persistent free radicals (EPFRs); sandstorms; atmospheric particulate matter (PM).

Characteristics, sources and risk assessment of polycyclic aromatic hydrocarbons in soils, water and vegetables in an e-waste dismantling site and its surrounding farmland

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Dismantling electrical and electronic waste (e-waste) can release various environmental pollutants such as polycyclic aromatic hydrocarbons (PAHs). This study investigated the characteristics, sources and risk assessment of the PAHs in e-waste and its surrounding farmland by analyzing the soil, water and vegetables. The concentrations of PAHs in e-waste were significantly higher compared to surface soils and vegetables, while similar to that in water. In the e-waste site, surface soils, soil columns, vegetables and water varied from 55.4 to 3990 ng g⁻¹ (mean 884 ng g⁻¹), 1.65 to 5060 ng g⁻¹ (mean 697 ng g⁻¹ per soil layer), 2670 to 10200 ng g⁻¹ (mean 4910 ng g⁻¹) and 46.8 to 109 µg L⁻¹ (mean 70.6 µg L⁻¹), respectively. In the farmland outside the e-waste site, surface soils, vegetables and water ranged from 41.5 to 2760 ng g⁻¹ (mean 271 ng g⁻¹), 506 to 7640 ng g⁻¹ (mean 2030 ng g⁻¹) and 56.6 to 89.2 µg L⁻¹ (mean 69.6 µg L⁻¹), respectively. A high proportion of high molecular weight PAHs appeared in soils, vegetables and water both in e-waste and farmland. Positive matrix factorization (PMF), together with diagnostic ratio revealed that PAHs in e-waste mainly arose from sources of vehicle emission and combustion of e-waste materials, while those in the farmland were derived from mixed sources through combustion of coal, grass, as well as wood. Based on the deterministic health risks, workers working in the e-waste facilities were exposed to potential risk, whereas the residents living in the vicinity were exposed to low risk. The sensitivity analyses indicated that exposure frequency and PAH concentrations were the main factors that influenced exposure risk. This study provided more knowledge on influence of PAHs pollution from e-waste dismantling, and will help to assess the growing global environmental and health risks of e-waste.

Keywords

polycyclic aromatic hydrocarbons; e-waste; positive matrix factorization; health risk assessment

Wednesday, September 20
Parallel Session IV

Toxicology of PTS
N1-G014

Synthetic antioxidants as new pollutants: from environmental occurrence to human exposure

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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. 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 Arctic air since 1994. This comprehensive study provides new knowledge on environmental occurrence and human exposure of synthetic antioxidants.

Toxicokinetics and metabolomic disruptions of a new brominated flame retardant TBPH in zebrafish

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Bis(2-ethylhexyl)-2,3,4,5-tetrabromophthalate (TBPH), one of the widely used new brominated flame retardants (NBFRs), is a ubiquitous environmental contaminant that has been raising great concerns over its contamination in aquatic environments and health risks. However, the bioaccumulations and adverse effects of TBPH in different organs of aquatic organisms are rarely known. In this study, adult zebrafish, after exposure to 2 μ M TBPH for 28 days, was found with high bioaccumulation either in male or female organs with the same order of intestine > liver > gonad > brain > muscle. We further investigated the detrimental effects on gut and liver by exposure to 0.2 ~ 200 nM TBPH. The results showed that TBPH induced pathological changes including the declines in villus length, crypt depth and muscular thickness of the gut, as well as the up-regulations of genes related to intestinal barrier. Dysbiosis of gut microbiota were also observed in the exposed fish of both genders. While in the liver, histological changes indicated obvious steatosis without sex difference. However, biochemical indices of liver and blood, which related to lipid metabolism disorders, including TG, TC, LDL and HDL, were significantly changed, especially in male fish. In addition, the transcriptome analysis also revealed that metabolism processes were mainly disrupted in the liver. Moreover, significant increase of glucose in male blood was found, while an opposite trend was determined with the insulin. Taken together, water borne TBPH led to higher accumulation of it in the gut and liver of fish, where generated histological injuries and metabolism disorders of lipid and glucose.

Keywords

NBFRs; TBPH; bioaccumulation; metabolomics disorder; zebrafish.

Evaluation and mechanistic study of multi- and transgenerational toxicity in zebrafish upon exposure to decabromodiphenyl ethane

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The novel brominated flame retardant decabromodiphenyl ethane (DBDPE) has become a ubiquitous emerging pollutant, hence the knowledge of its long-term toxic effects and underlying mechanism would be critical for further risk assessment. Firstly, the multi- and transgenerational toxicity of DBDPE was investigated in zebrafish upon a life cycle exposure at environmentally relevant concentrations. The results indicated significantly increased malformation rate and declined survival rate specifically in unexposed F2 larvae, suggesting a transgenerational development toxicity by DBDPE. The changing profiles revealed by transcriptome and DNA methylome confirmed an increased susceptibility in F2 larvae, and figured out potential disruptions of glycolipid metabolism, mitochondrial energy metabolism and neurodevelopment. The changes of biochemical indicators such as ATP production confirmed a disturbance in the energy metabolism, whereas the alterations of neurotransmitter contents and light-dark stimulated behavior provided further evidence for multi- and transgenerational neurotoxicity in zebrafish. Consequently, the role of mitochondrial dysfunction in DBDPE-induced toxicity was further studied through a short-term exposure and recovery experiment. The results indicated inhibited mitochondrial oxidative respiration accompanied by decreased mitochondrial respiratory chain complex activities, mitochondrial membrane potential and ATP contents upon DBDPE single exposure. However, addition of nicotinamide riboside could effectively restore DBDPE-induced mitochondrial impairments and resultant neurotoxicity, oxidative stress as well as glycolipid metabolism in zebrafish larvae. Taken together, our data suggest that mitochondrial dysfunction was involved in DBDPE-induced toxicity, providing novel insight into the toxic mechanisms of DBDPE as well as other emerging pollutants.

Keywords

Decabromodiphenyl ethane; transgenerational toxicity; metabolism disorder; neurotoxicity; mitochondrial dysfunction.

Lipidomic study on the developmental toxicity of PFAS to zebrafish embryos

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PFASs are persistent environmental contaminants, posing developmental toxicity to fish and human. PFAS-induced lipid metabolism disorders were demonstrated using the zebrafish embryo model, but research on changes of lipid compositions and the influence of these changes on the biological development are insufficient. Herein, lipidomics analysis was performed to reveal the developmental toxicity on lipid metabolism in zebrafish embryos exposed to PFOA or PFOS through microinjection. We observed various abnormal phenotypes, including heart bleeding, pericardium edema, spinal curvature and increased heart rate at 72 h after fertilization, especially in the PFOS exposure groups. Lipidomic profiling found downregulated phosphatidylethanolamines in the exposed embryos, especially those containing a docosahexaenoyl (DHA) chain, indicating an excessive oxidative damage to the embryos. Glycerolipids were mainly upregulated in the PFOA groups but downregulated in the PFOS groups. These aberrations may reflect oxidative stress, energy metabolism malfunction and proinflammatory signals induced by PFASs. Supplement of DHA may not be effective in recovering the lipidomic dysregulations and protecting from the developmental toxicity induced by PFASs, which reflected the complexity of the mechanism. This study has revealed the dysregulations of lipid metabolism related to developmental toxicity induced by PFASs from the aspect of lipidomics, and discovered the underlying molecular mechanisms.

Keywords

PFAS; lipidomics; developmental toxicity; zebrafish embryos.

Ambient particulate matter (PM) exposure triggered liver metabolic reprogramming via cysteine oxidation on Malate Dehydrogenase 2 (MDH2) and Carnitine Palmitoyltransferase II (CPT2)

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Air pollution remains the leading cause of environmental death worldwide. Proper regulation of redox signaling is essential to cellular homeostasis. Epidemiological and experimental evidence demonstrated association between PM exposure and fatty liver diseases featured by reactive oxidative species (ROS) mediated metabolic reprogramming, while exact targets remained vague. By profiling PM-oxidized cysteine residues, we aim to identify oxidation events that contributed to liver metabolic reprogramming in ambient PM exposed mouse model.

A total of 2805 unique Cysteine-containing peptides from 704 proteins were identified and quantified. Multiple cysteine sites on mitochondria enzymes regulating energy metabolism were found significantly oxidized. In silico screening by molecular dynamics revealed key enzymes with reduced substrate/cofactor affinities which modulate mitochondria shuttles or beta oxidation. Targeted metabolomics and activity assay using liver tissues from exposed mice confirmed that reduced MDH activity caused malfunction of malate shuttle, the primary mitochondria shuttle used in liver for NADH/NAD transportation and rebalancing. Consequently, ROS stress increased and glycolysis was repressed. Reduced CPT2 activity was confirmed by accumulated beta-oxidation fatty acids C14-C18. A metabolic reprogramming trends lipogenesis was therefore identified and further confirmed in PM-exposed human liver HepG2 cells using seahorse fuel flex test. Our study, therefore, provides a potential mechanism for PM mediated liver metabolic reprogramming.

Keywords

PM; redox; energy reprogramming; mitochondria shuttle.

The impact of PM_{2.5} exposure on the cardiovascular system and intervention strategies

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Numerous studies from various fields have demonstrated a close association between PM_{2.5} exposure and the occurrence and progression of cardiovascular diseases, making it a significant and modifiable risk factor for cardiovascular dysfunction. However, the long-term effects of PM_{2.5} exposure on cardiovascular damage across different age groups and the underlying mechanisms remain incompletely understood. To address these scientific inquiries, this study established a real-time PM_{2.5} exposure system in Taiyuan city and conducted a 26-week PM_{2.5} exposure experiment on mice from three different age groups (juvenile, adult, and elderly). The study revealed age-related differences in the impact of long-term PM_{2.5} exposure on cardiac function and identified a reduction in taurine content in myocardial cells as a contributing factor to PM_{2.5}-induced cardiac dysfunction in elderly mice. Building upon these findings and integrating existing research, the protective effects of taurine and fish oil supplementation against PM_{2.5}-induced cardiac impairments were further elucidated through epidemiological and toxicological investigations. This research provided new strategies at the individual level to mitigate PM_{2.5} pollution for the elderly population. Additionally, incorporating the latest cardiovascular disease prevention guidelines and analyzing nearly a decade's worth of cardiovascular disease data from Guangzhou residents provided by the Guangzhou Center for Disease Control and Prevention, an artificial intelligence-based big data analysis was employed to establish an atmospheric health risk assessment and early warning system. This study provided fundamental data support for understanding the mechanisms and preventive interventions of atmospheric particulate matter PM_{2.5} exposure on the occurrence and progression of cardiovascular diseases.

Keywords

PM_{2.5}; Cardiovascular system; Adverse effect; Mechanism; Intervention

Wednesday, September 20
Parallel Session IV

Mercury and heavy metals
N1-G018

Long-term trend in atmospheric gaseous elemental mercury concentrations in China

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Long-term observations of atmospheric mercury are important for the evaluation of the effectiveness of the Minamata Convention on Mercury. We continuously measured gaseous elemental mercury (GEM) concentrations at four remote sites in China for more than ten years, i.e., Mt. Waliguan (100.90° E, 36.29° N) during 2008-2022, Mt. Changbai (128.11° E, 42.40° N) during 2008-2022, Mt. Ailao (101.02° E, 2453° N) during 2011-2022, and Mt. Damei (121.57° E, 29.63° N) during 2011-2022. Our observations showed that GEM concentrations in China increased slightly during 2008-2013, and then the GEM concentrations decreased significantly after 2013. The mean GEM concentrations at the four Chinese sites during 2022 were 1.51 ± 0.35 ng m⁻³, which is close to mean concentrations observed in Europe, North America, the Arctic, and the free troposphere in Pacific Ocean during 2021 (Individual means: 1.14 to 1.51 ng m⁻³, overall mean: 1.34 ± 0.11 ng m⁻³, n = 13). During 2013-2022, GEM concentrations in China decreased by 35%, which was much higher than the decreasing rates observed in Europe (9%), North America (10%), the Arctic (6%), and the free troposphere in Pacific Ocean (9%) during 2013-2021. The declines in GEM concentrations in China since 2013 matches well with the decreasing anthropogenic Hg emission in China estimated by Chinese anthropogenic Hg emission inventory, indicating the reduction in anthropogenic Hg emissions in China was the major driver for the GEM declines.

Keywords

gaseous elemental mercury(GEM); mean concentration; atmospheric mercury; anthropogenic Hg emissions; China

Microbial production of methylmercury dictated by nano-scale structure of mercury sulfides

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Mercury is a ubiquitous heavy metal that travels globally. Our research focuses on one of the top concerns of global mercury issues, i.e., production of the neurotoxic methylmercury (MeHg). Decades of research efforts have gone into understanding the mechanisms regulating microbial mercury methylation, the predominant source of MeHg accumulated in the food web. Until recently, we have started to realize that mercury methylation cannot be accurately predicted based on aqueous mercury speciation alone, and solid phase ought to be included in the predictive models for MeHg production. Herein, we demonstrate that nanoparticulate metacinnabar that forms during the early stage of mercury mineralization represents the bioavailable solid phase for mercury methylation, and exposed facet is a crucial parameter determining the methylation potential of nanoparticulate mercury. Moreover, ferrous iron, which co-exists with mercury at environmental “hotspots” for biomethylation, strongly affects MeHg production by modulating the structure and bioavailability of nanoparticulate mercury sulfide. Co-precipitation of mercury–sulfide–iron (Hg–S–Fe) with natural ligands leads to the formation of iron-incorporated metacinnabar nanoparticles that are available for microbial methylation. Sub-surface incorporation of iron influences the nucleation and aggregation of nano-metacinnabar and subsequently dictates its interaction with methylating cells. Overall, these results have provided new insights into understanding the mechanisms of microbial mercury methylation, which will help improve risk assessment and remediation strategy for mercury contamination.

Keywords

mercury; methylmercury; microbial methylation; nanoparticle.

Assessing China's gridded anthropogenic mercury emissions (1978-2020): identifying hotspots of cumulative emission and cross-media impact

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Mercury emissions from anthropogenic sources exist in environmental media for a long time and are transmitted through the food chain to harm human health. In order to investigate the impact of cumulative anthropogenic emissions in China and the influencing factors of cumulative emissions of speciated mercury, we have established an inventory of anthropogenic mercury emissions in China from 1978 to 2020, and obtained a gridded inventory of China's long-term time series based on the spatial allocation system. For spatial allocation of coal power plants, cement productions, non-ferrous metal smeltings, more precise allocation methods that rely on point sources were established. The results show that from 1978 to 2020, the cumulative atmospheric mercury emissions from anthropogenic sources are increasing, reaching a total of 15590 t, of which Hg^0 is 8988 t, accounting for 57.6%. The Hg^{II} is 5936 t, accounting for 38.1%, and the Hg_P is 665 t, accounting for 4.3%. The cumulative mercury emissions are mainly contributed by cement (17%), power plants (17%), industrial boilers (16%), and zinc smelting (14%). In terms of spatial distribution, Hebei, Henan, Jiangsu and Hunan provinces have the most significant cumulative emissions. For grids involving top cumulative emissions (top 5% of the highest emissions, cumulative emissions large than 21475 kg), high continuous emission and high emission in recent years (2014 and after) account for about 15.8%, mainly located in Handan and Tangshan in Hebei Province, Shenyang and Benxi in Liaoning Province, Jiaozuo in Henan Province, Changzhou and Nantong in Jiangsu Province, and Chenzhou and Changsha in Hunan Province. The average proportion of Hg^{II} and Hg_P in these grids is 47%, making it likely to cause significant local harm through deposition. Therefore, additional attention will need to be focused on emissions from these regions in the future.

Keywords

Mercury; Anthropogenic emission inventory; Cumulative emission; China.

Tackling the multiplicity of solutions for the global mercury budget by a coupled atmosphere-land-ocean model

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The effectiveness of reducing the environmental level of mercury (Hg) by controlling anthropogenic emissions depends on the magnitude of re-emissions from the land and ocean, which requires a comprehensive understanding of its global biogeochemical cycle. However, there is a multiplicity of solutions for the global budget, especially the exchange fluxes between the atmosphere and the land/ocean. Recent advances in atmospheric Hg redox chemistry, vegetation uptake, seawater Hg sources, and riverine discharges greatly challenge our understanding of the global Hg cycle, but the overall effects remain understudied. Here, we develop a new coupled atmosphere-land-ocean model and find potentially 40% higher total atmospheric Hg emissions than previously recognized primarily because of higher re-emissions from the ocean. Our results suggest a likely smaller sensitivity of environmental Hg levels to anthropogenic emission changes, stressing that potentially more aggressive emission control is required to decrease Hg levels.

Microbial-induced biomineralization efficiently immobilizes heavy metals in the environment via hydroxycarbonated apatite

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Heavy metal pollution poses a significant threat to the destruction of ecosystems. Microbially induced calcium carbonate precipitation (MICP) is considered to be a promising technology for the treatment of heavy metal contamination. In this study, a novel heavy metal-resistant ureolytic bacterium (N15) was isolated and identified as *Enterobacter ludwigi*. Its performances for immobilizing heavy metals (Cd, Pb, and Zn) in solution and soil were systematically discussed at different treatment conditions. The results showed that initial pH and heavy metal solubility were essential parameters affecting the removal rate and that hydroxyapatite adsorption of heavy metals was the primary removal mechanism for N15. Soil microcosm experiments showed that in addition to increasing the fixation rate of heavy metals in the soil, N15 (plant growth promoting rhizobacteria, PGPR) also helped to improve soil pH, fertility, and enzyme activity and promotes plant growth. Our results emphasized that the excellent ability of strain N15 to remediate heavy metal-contaminated environments while reducing negative environmental impacts and providing long-term economic value.

Keywords

microbially induced calcium carbonate precipitation (MICP); ureolytic bacterium; *Enterobacter ludwigi*; cadmium remediation; adsorption

Migration and transformation characteristics of chromium in soil-paddy system near Guizhou mining area

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Chromium (Cr) contamination in soil-paddy system threatens human health through food chain. The purpose of this study is to explore migration and transformation pathway of Cr in the soil-paddy system near a mining area. The results showed that when paddy plants were grown in contaminated soils, and they can absorb and accumulate Cr in their tissues, particularly in roots and grains. Chromium concentration in rice tissues at mature stage followed the order of $C_{root} > C_{grain} > C_{stem} > C_{leaf}$. During the process of paddy grown from tillering stage to mature stage, Cr content in rhizospheric soil gradually decreased. The elevation of Cr bioavailability promoted its migration from rhizosphere soil to rice roots. Transfer coefficients of Cr from root to stem, leaf and grain at mature stage were 0.46, 0.19 and 0.54, respectively. This study can not only provide a scientific theoretical basis for pollution control of Cr in paddy soil system, but also offer a viable way for enhancing environmental quality and safety management of agricultural products.

Keywords

chromium; soil; paddy; migration and transformation

Acknowledgments

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Parallel Session V

Toxicology of PTS
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Bacteria feeding on antibiotics – eating the poisonous

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We report here on the isolation of bacterial strains, which are not only resistant to the sulfonamide antibiotics, but also degrade and mineralize them. One of these isolates, namely *Microbacterium* sp. strain BR1 is able to feed on SMX as sole carbon and energy source. In this bacterium, the degradation of SMX and structurally related compounds is initiated by an *ipso*-substitution, catalyzed by a flavin-dependent monooxygenase acting in concert with a FMN reductase. The resulting *p*-aminophenol enters the central metabolism through a second monooxygenase activity, which leads to products amenable to ring opening. The cluster of genes involved in this degradation process was identified and each of these three enzymes could be heterologously expressed in *E. coli*. The presence of this gene cluster might represent an additional, yet unknown resistance mechanism for bacteria against sulfonamides. Even though the classic *sulI* gene is present as well in *Microbacterium* sp. strain BR1, its additional capacity to feed on SMX might represent a superior mechanism conferring to the bacterium clear advantages over a modified protein target especially in nutrient limited environments but also in case of human infection. Finally, we discuss the relevance of these findings addressing a series of questions arising from this research. Is the biodegradation of sulfonamides by *Microbacterium* BR1 a single case? Can the catabolism of sulfonamides be considered as a novel resistance to sulfonamides? What are the reciprocal effects of *sadA* and *sulI*? What is the significance of *ipso*-substitution during wastewater treatment? What if bacteria like *Microbacterium* infects human? Can bacteria feed on other antibiotic families? Do catabolic genes involved in the biodegradation of a given antibiotic impact the propagation of genes determining the resistance to this antibiotic and reciprocally?

Keywords

wastewater treatment; resistance to antibiotics; catabolism; *Microbacterium*; sulfonamides; flavin-dependent monooxygenases.

Beyond silver nanoparticle resistance: exploring general stress responses

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The prevalence of silver nanoparticles (AgNPs) and the potential development of AgNP resistance have gained significant attention. However, the underlying mechanism for this phenomenon remains controversial. In this study, we identified two distinct phases during the adaptive evolution in response to lethal doses of AgNP exposure.

Initially, resistance to AgNPs was primarily linked to flagellin-mediated precipitation and enhanced antioxidant activities. However, as the process progressed, persistent cell formation, biofilm production, and up-regulation of the copper (Cu) efflux pump dominated AgNP tolerance, without precipitation. In the later stages, persister levels increased remarkably, reaching magnitudes 1000 times higher than before. Consequently, the evolved cells exhibited substantial tolerance to multidrug treatments. The envelope stress response (cpx and psp) played a crucial role in the evolutionary transition.

Contrary to common belief, the expression of the Cu-efflux pump and osmotic stress response cannot be solely attributed to Ag⁺ exposure. Instead, they were primarily influenced by the transition to anaerobic respiration and membrane deformation induced by NPs, which are part of general stress responses. This transition from relying solely on specific mechanisms, dependent on nanoparticle properties, to a convergent evolution involving general stress responses highlights the potential adaptive strategies bacteria employ for nano-resistance. Our study also emphasizes the potential timeframe for controlling the evolutionary transition to pathogenesis and antibiotic resistance.

Keywords

AgNPs; bacterial evolution; resistance; persister; antibiotic tolerance.

Toxicity evaluation of 1-nitropyrene by using human adult stem cell-derived airway organoids and multimodal imaging analysis

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The toxic effect of air pollution on cells in the human respiratory tract is still elusive. A robust, reliable in vitro model for recapitulating the physiological response of the human airway is needed to obtain a thorough understanding of the molecular mechanisms of air pollutants. Herein, by using 1-nitropyrene (1-NP) as a proof-of-concept, we demonstrate the effectiveness and reliability of evaluating environmental pollutants in physiologically active human adult stem cell-induced airway organoids. Multimodal imaging tools, including live cell imaging, fluorescence microscopy, and MALDI-mass spectrometry imaging (MSI), were implemented to evaluate the cytotoxicity of 1-NP for airway organoids. In addition, lipidomic alterations upon 1-NP treatment were quantitatively analyzed by nontargeted lipidomics. The toxicity of 1-NP was found to be associated with perturbed SM-Cer lipid signaling pathways and CL regulation, which might be caused by the overproduction of ROS. A higher tolerance of 1-NP toxicity compared to cell lines was observed and might reflect a more physiologically relevant response in adult airway epithelium. Collectively, we have established a novel system for evaluation and investigation of molecular mechanisms of environmental pollution in the human airways via combinatory use of human airway organoid and MS-based analyses.

Keywords

human airway organoids; adult stem cell; air pollution; MALDI-MSI; 1-NP.

A new mechanism of reproductive endocrine disruption based on isothiazolinones

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Isothiazolinones are widely used as preservatives and disinfectants due to their potent antibacterial efficacy. However, the unintended exposure of humans and animals has led to increasing concern regarding their health hazards. Isothiazolinones were previously shown to disrupt the endocrine homeostasis and impair reproductive functions, while the underlying mechanism remains ambiguous. In this study, exposure of medaka to a representative isothiazolinone DCOIT significantly elevated the concentrations of GnRH and FSH in female brain, with concomitant stimulation of oogenesis and fecundity, despite that the development of offspring was compromised. An estrogenic activity was induced in the male, which drove the sex ratio towards female dominance. Chem-Seq and proteome analyses demonstrated the disturbances in GPCR, MAPK, and Ca^{2+} signaling cascades by DCOIT. *In vitro* mechanistic exposure identified the pivotal role of MEK and ERK phosphorylation in inducing the endocrine disruptive effects. In addition, DCOIT had a binding affinity to the active pocket of G protein α_i subunit. DCOIT-bound $G\alpha_i$ turned to interact with the mitochondrial calcium uniporter, consequently changing the intracellular Ca^{2+} dynamics and mediating the phosphorylation of MEK and ERK. Furthermore, other isothiazolinone analogues were tested to verify the generalizability of endocrine disrupting mechanism. Depending on the side chain structure and chlorine substitution, OIT, BIT, and DCOIT showed higher potency to bind with $G\alpha_i$, phosphorylate MEK and ERK, and cause imbalance of sex hormones. Overall, this study characterized the consecutive causative occurrence of key molecular events underlying the outcome of endocrine disruption and proposed a novel framework of AOP relevant to reproduction.

Keywords

Isothiazolinones; reproduction; endocrine disruption; $G\alpha_i$; Calcium signaling; MAPK activation.

Multi-dimensional visualization of ingestion, biological effects and interactions of micro(nano)plastics and a representative POP in edible jellyfish

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The pervasive presence and potential hazards of microplastics (MPs) and nanoplastics (NPs) pose significant environmental concerns. However, substantial knowledge gaps persist in understanding the tissue-specific accumulation and dynamic changes of MPs and NPs in aquatic organisms, as well as their interactions with other environmental pollutants such as persistent organic pollutants (POPs). In this study, we employed innovative methodologies including *in vivo* imaging systems (IVIS), radioisotope tracing, and histological staining to investigate the fate and toxicity of fluorescently-labeled MPs/NPs and ¹⁴C-labeled 2,4,4'-trichlorobiphenyl (PCB28) in the edible jellyfish species, *Rhopilema esculentum*. We visualized the ingestion, biological effects, and interactions of these contaminants at cellular, tissue, and whole-body multidimensional levels. Our findings indicate that both MPs and NPs predominantly accumulate in the mouthlets of oral arms, with the majority of ingested MPs/NPs residing in the extracellular environment rather than being internalized into the mesoglea. Interestingly, the presence of MPs or NPs in seawater significantly reduced the bioaccumulation of PCB28 in jellyfish tissue, thereby mitigating physiological alterations, gastric damage, and apoptosis induced by PCB28. This research introduces a multi-dimensional visualization strategy to illustrate the distribution and biological effects of typical pollutants in marine organisms, providing novel insights into the impacts of MPs/NPs on marine ecosystems.

Keywords

microplastics, nanoplastics, jellyfish, fluorescence imaging, persistent organic pollutant, autoradiography

Tolerance mechanisms of *Chlamydomonas* spp. to mercury stress

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Algal growth and metabolism are susceptible to toxic stress of mercury. In order to identify the most tolerance algal strains to mercury stress, chlorophyll a content, chlorophyll fluorescence activity and algal organic matter of 11 algal species belonging to *Chlamydomonas* taxa at different mercury concentrations were screened. The results showed that chlorophyll a content decreased significantly, the photosynthetic activity of cells was significantly inhibited, and the PSII's electron transport was blocked on the donor side (OEC) and the receptor side (QA- to QB) with the increase of mercury ion concentration. EC₅₀ indicated *Chlamydomonas reinhardtii* FACHB-2217 had the highest tolerance to mercury stress with EC₅₀ was 2.746 mg / L, and *Chlamydomonas* sp. FACHB-889 had the worst tolerance to mercury stress with EC₅₀ was 0.793 mg / L. On the other hand, the supply of light energy for normal photosynthetic metabolism under adversity is guaranteed by changing the photosynthetic energy distribution, which could alleviate the stressed cells, enforce its tolerance and ensure the survival. Furthermore, with the increase of concentration of Hg²⁺, concentration of algal organic matter (AOM) from *Chlamydomonas reinhardtii* FACHB-2217 increased, extracellular proteins-like and humic acids increased, intracellular proteins-like first increased and then decreased, and the sensitivity of extracellular organic matter to Hg²⁺ binding was in the order of fulvic acid > protein-like, variation of intracellular organic matter was the opposite. The intra- and extracellular organic matter content and components were significantly affected by mercury stress, the dynamic change of AOM was the cellular response to mercury stress, which can enhance cellular tolerance ability and alleviate the toxicity of mercury. It could be concluded that changing of the photosynthetic energy distribution and the increasing of AOM were algal cell's detoxification mechanism.

Keywords

Chlamydomonas nivalis; mercury; toxic effects; algal organic matter

Wednesday, September 20
Parallel Session V

Mercury and heavy metals
N1-G018

The potential application of mercury isotopic composition in the ocean

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As one of the most important reservoirs of mercury (Hg) on earth, ocean plays a crucial role in mediating the global cycling of Hg. Hg undergoes complex migration and transformation processes (e.g., adsorption/desorption, deposition/resuspension, oxidation/reduction, and methylation/demethylation) between multiple interfaces (e.g., atmosphere-seawater, land-seawater, seawater-sediment, and seawater/sediment-biota) of the ocean. The recently-developed Hg stable isotope approach has shown great advantages in studying the biogeochemical cycling of oceanic Hg. Herein, we overviewed the accurate analytical methods for Hg isotopes in different marine samples, summarized the reported Hg isotope dataset in seawater, sediment/particulate, and biological samples, comprehensively analyzed the fractionation mechanisms of Hg isotopes and their potential applications in tracing marine Hg cycling.

Keywords

Seawater; Marine sediment; Marine biota; Hg stable isotopes; Hg concentrations; Hg speciation

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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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 ($\cdot\text{OH}$) 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 were 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 MeHg and other measured parameters representing the composition of DOM. These results indicate that thiol may be the key functional group in DOM affecting the photodegradation of MeHg in the YS and ECS.

Keywords

methylmercury; photodegradation; dissolved organic matter; thiol; Yellow Sea and East China Sea.

Decreasing mercury levels in consumer fish over the three decades of increasing mercury emissions in China

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Fish consumption is the primary dietary route of human exposure to methylmercury. It has been well documented that elevated mercury concentration in fish in North America and Europe is linked to anthropogenic mercury emissions. China is the world's largest producer, consumer, and emitter of mercury, as well as the world's largest commercial fish producer and consumer. Although mercury pollution in fish in China is currently receiving much attention worldwide, its status remains largely unknown. Here, we conducted a meta-analysis on total mercury concentrations in marine and freshwater fish samples, covering 35,464 samples collected in China over the past 30 years. It is found that, opposite to the increasing emission and documented mercury contamination events, mercury levels in fish have gradually decreased in China over the past 30 years. The results were in sharp contrast to those found in North America and Europe. The mercury concentrations in fish were significantly anticorrelated with the fish catch and fish aquaculture and were inverse to trophic levels. Overfishing and the short lifecycle of aquaculture fish, both reducing the trophic level and the duration of mercury accumulation, were the most likely causes leading to the decline of mercury concentrations found in fish in China.

Keywords

meta-analysis; mercury; fish; spatial–temporal variability; freshwater and marine waterbodies.

Wednesday, September 21
Parallel Session VI

Mercury and heavy metals
N2-U Hall

Identification of mercury-containing nanoparticles in the liver and muscle of cetaceans

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Mercury (Hg) is a highly concerning global threat owing to its properties of persistence, bioaccumulation, and toxicity. However, mercury is distributed as various species in the environment, including inorganic and organic forms, which largely affect its bioavailability, mobility and toxicity. Compared to organic Hg, inorganic Hg (IHg) species are usually ignored for their lower toxicity, lower bioaccumulation and biomagnification. In this study, liver and muscle tissues of cetaceans were collected to identify the presence and characteristics of mercury-containing nanoparticles (Hg-NPs). We found that methylmercury (MeHg) was the dominant species of Hg in muscles, while inorganic Hg (IHg) accounted for 84.4–99.0% (average 94.0%) of Hg in livers. By using transmission electron microscopy (TEM), size exclusion chromatography coupled with inductively coupled plasma mass spectrometry (SEC-ICPMS) and single particle ICPMS (sp-ICPMS), large amounts (9–161 $\mu\text{g/g}$) of Hg-NPs in livers and small amounts (0.1–0.4 $\mu\text{g/g}$) in muscles were observed, indicating that Hg-NPs was an important form of Hg in livers. Both small sized (5–40 nm) and large sized (>100 nm) Hg-NPs were identified, which were mainly complexed with selenium (Se) and sulfur (S) as well as a few cadmium (Cd), lead (Pb) and silver (Ag). This study provided direct evidence of Hg-NPs in marine mammals as well as their chemical form and size distribution, which are helpful for further understanding the biogeochemical cycle and health risk of Hg.

Keywords

mercury; nanoparticle; size distribution; liver; muscle

Health risk and pathways of human methylmercury exposure in China

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Human exposure to methylmercury (MeHg) from fish consumption has been a major concern. Besides, human MeHg exposure through rice consumption has been recently found to be important in some Asian countries. China is the largest country on mercury (Hg) production, consumption, and anthropogenic emission. However, the health risks and human exposure pathways are not fully understood. In this study, we collected 624 fish, 299 rice, and 994 human hair samples from typical Hg-contaminated areas and major fish-rich areas in China. As well, we used MeHg compound-specific stable isotope analyses (MeHg-CSIA) to trace the contribution of human MeHg exposure from fish and rice consumption in these areas. Fish and rice samples showed relatively low Hg levels, except the rice in the Wanshan Hg mining area (WMMA). 85% of hair samples in WMMA, 62% in Zhoushan, 40% in Xiamen, 26% in Qingdao, and 17% in Zinc Smelting Area had THg concentrations exceeding the limit set by the USEPA (1 $\mu\text{g/g}$). The $\Delta^{199}\text{HgMMHg}$ values of the human hair in fish rich areas were comparable to those of fishery foods but not those of rice. Human MeHg exposures were dominated (>80%) by fishery food consumption in fish-rich areas. In four typical Hg-emission areas, we estimated the relative contributions of rice consumption to human MeHg exposure to be $84 \pm 14\%$, $58 \pm 26\%$, $52 \pm 20\%$ and $34 \pm 15\%$ on average in Hg mining area, gold mining area, zinc smelting area and coal-fired power plant area, respectively. Therefore, local population in typical Hg contaminated areas and coastal areas indicated health risk of MeHg exposure. The CSIA approach can be an effective tool for tracking Hg biogeochemical cycle and human exposure.

Keywords

methylmercury; fish; rice; health risk; pathway; mercury isotope

Bioaccumulation and biotransformation of selenium nanoparticles by methanogenic archaeon *Methanosarcina acetivorans*

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As an essential element, selenium plays a very important role in organisms, and selenium nanoparticles (SeNPs) have great application prospects in agriculture and other aspects due to their unique physical and chemical properties. However, as one of the most important root system microorganisms, little is known about the interaction of SeNPs with methanogens, which play an important role in the carbon cycle. Here, we found that appropriate amount of SeNPs could promote the growth and metabolism of *Methanosarcina acetivorans* C2A. Besides, SeNPs entered the cells via the particulate form, and they could form an ecological crown with a surface dominated by methanol metabolism-related proteins as well as chaperone proteins, and were eventually converted intracellularly into inorganic Se (IV) and organic selenium such as selenocysteine and selenomethionine, etc., which participated in the metabolic activities of *M. acetivorans* C2A. In addition, these intracellular selenium species could be released extracellularly and formed forms of selenium species dominated by methylselenocysteine and selenocysteine. These results provide new insights for understanding the internalization and transformation of SeNPs in methanogenic archaea.

Keywords

selenium nanoparticles; methanogenic archaea; biotransformation; bioaccumulation.

Causes of low mercury levels in fish from the Three Gorges Reservoir, China

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Previous studies have suggested that growth dilution may be an important factor contributing to the low fish Hg levels in China. To evaluate the impact of growth rate to Hg bioaccumulation in fish in the Three Gorges Reservoir (TGR), this study used two fish species, *Aristichthys nobilis* (*A. nobilis*) and *Coilia nasus* (*C. nasus*), which differ significantly in their growth rates. A combined bioenergetic-toxicokinetic model was used to simulate methylmercury (MeHg) concentrations in these two species. The model simulations were compared with the field data and showed good fits. It explained 44.0% and 46.5% of the variation in MeHg concentrations in *A. nobilis* and *C. nasus*, respectively. Sensitivity analysis revealed that growth rate accounted for 55.5% and 15.2% of MeHg concentrations in *A. nobilis* and *C. nasus*, respectively. This indicated that growth rate was the most critical factor affecting MeHg concentrations in fast-growing fish, such as *A. nobilis*. However, in species with low growth rate, such as *C. nasus*, the effect of growth rate was not as prominent as that in fast-growing fish. As a result, Hg elimination rates and water temperature could offset the effect of growth, and become the decisive factors for MeHg concentrations in slow-growing fish.

Keywords

growth dilution; Hg; toxicokinetics; bioenergetics.

**Tuesday, September 19 -
Wednesday, September 20**

**Poster Session
N1-G008**

Au@BN-enhanced laser desorption/ionization mass spectrometry and imaging for determination of fipronil and its metabolites

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Gold nanoparticles (AuNPs) represent an attractive inorganic matrix for laser desorption/ionization mass spectrometry (LDI-MS) detection of low-molecular-weight analytes; however, their direct use is hindered by severe aggregation. To limit AuNPs aggregation, hexagonal boron nitride nanosheets (*h*-BNNs) were employed as supports to improve their desorption/ionization efficiency. Thus, Au@BN was synthesized and systematically characterized. It showed low background noise and high sensitivity for LDI-MS of fipronil and its metabolites. Au@BN-assisted LDI-MS was validated using complex samples including blueberry juice, green tea beverage, and fish muscle, achieving low detection limits ($0.05\text{--}0.20\ \mu\text{g}\cdot\text{L}^{-1}$ for liquid media, $0.82\text{--}1.25\ \text{ng}\cdot\text{g}^{-1}$ for fish muscle), wide linear ranges ($0.2\text{--}100\ \mu\text{g}\cdot\text{L}^{-1}$ for liquid media, $3.00\text{--}1000\ \text{ng}\cdot\text{g}^{-1}$ for fish muscle), high reproducibility (7.55%–13.7%), and satisfactory recoveries (82.62%–109.1%). Furthermore, spatial distributions of analytes in strawberries and zebrafish were successfully imaged. This strategy allows for the quantitative analysis of other small molecules in complex substrates.

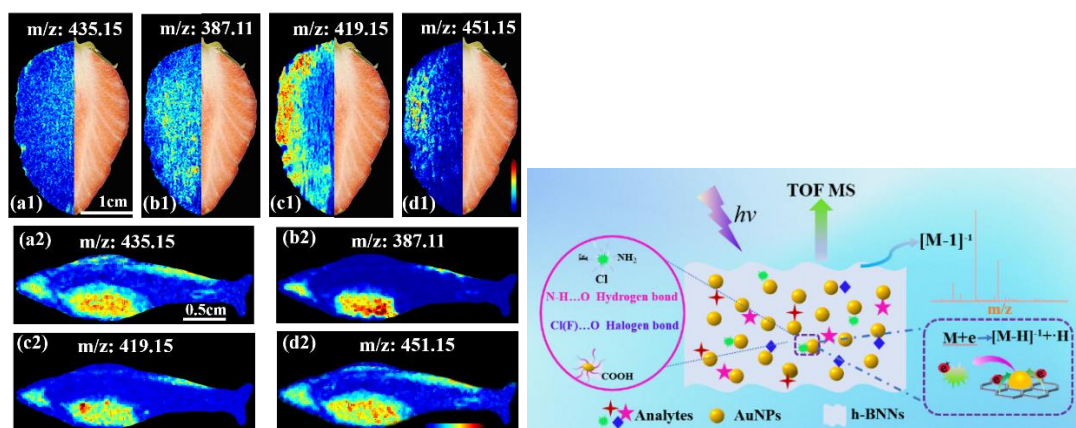


Figure 1 LDI-MSI analysis of the distribution of fipronil and its metabolites in strawberry and zebrafish using the Au@BN matrix and the Desorption/ionization mechanism.

Keywords

fipronil, metabolites, Au@BN, LDI-MS, imaging

Derivatization of N-acyl glycines by 3-nitrophenylhydrazine for targeted metabolomics analysis and their application to the study of diabetes progression in mice

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N-Acyl glycines (NAGlys) are an important class of metabolites in the detoxification system of the human body. They have been used in the diagnosis of several metabolic diseases. Liquid chromatography–mass spectrometry (LC–MS) is the most frequently used NAGlys detection platform. Here, we describe a simple and sensitive method of NAGlys detection by LC–MS in plasma and urine samples. This approach is based on the use of a derivatization reagent, 3-nitrophenylhydrazine. The reaction is quick in aqueous solution, and no quenching step is needed. To expand the coverage of NAGlys when standards are not available, NAGlys were first identified based on high-resolution LC–MS. Quantification was subsequently carried out on triple quadrupole LC–MS. This approach allowed a much broader measurement of NAGlys (41 NAGlys in total), especially when authentic standards are unavailable. Comprehensive analysis of NAGlys with this new method was applied in plasma and urine samples of *db/db* diabetic and non-diabetic *db/m+* control mice. The majority of detected NAGlys were altered with high differentiation ability in plasma and urine samples from diabetic and non-diabetic mice. These identified NAGlys hold the potential to be diagnostic biomarkers for type II diabetes and diabetic complications.

Keywords

N-acyl glycines, LC-MS, 3-nitrophenylhydrazine, *db/db*, plasma, urine

Constructing bifunctional magnetic porous poly(divinylbenzene) polymer for high-efficient removal and sensitive detection of bisphenols

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Due to ultra-low content and serious interferences, the analysis and detection of trace compounds in complex samples received tremendous challenge. Sample pretreatment not only can eliminate interferences, but also can preconcentrate targets, which play important role in analysis of trace targets. In view of widespread existence and toxicity, removal and detection of bisphenols (BPs) is imperative to assess environmental risks and reduce harm to human health. Although many techniques have been reported, constructing fast, sensitive and low cost method remains a challenge. Herein, porous poly(divinylbenzene) polymer was synthesized in-situ on the Fe₃O₄ particles by means of distillation-precipitation polymerization and functioned as sorbents to extract BPs. As the Fe₃O₄@PDVB can induce hydrophobic interactions, π - π stacking interactions and hydrogen interactions that operative cooperatively. Additionally, the porosity of Fe₃O₄@PDVB with large specific surface area is mainly distributed in the outer layer, which promotes faster and better diffusion of the target molecules into the material. As a result, Fe₃O₄@PDVB exhibited extremely fast adsorption rates (in 10 seconds) and high adsorption capacities (1050-1341 mg·g⁻¹), outperformed the previous reported high-end BPs sorbents. Simultaneously, employing Fe₃O₄@PDVB as sorbents, a magnetic solid-phase extraction coupling with liquid chromatographic was developed to detect trace BPs in water. The phase separation and retrieve of sorbents can be easily operated with a magnet, which overcomes the difficulty of separating PDVB from aqueous solution by centrifugal process because of its ultra-light nature in solution. Results indicated that the proposed method presented low detection limits (0.01-0.03 ng·mL⁻¹), high enrichment ability (327-343), and good reproducibility. Moreover, this method showed satisfactory recoveries in the detection of lake water (80.60-116.25%). These findings indicate that Fe₃O₄@PDVB prepared with a facile method presents a promising potential for practical applications and provides new insights into the development of sorbents with low cost, high efficiency and fast removal of bisphenols.

Keywords

sample pretreatment; BPs; porous organic polymer; magnetic solid-phase extraction (MSPE); adsorption

Multi-functional laccase immobilized by MOF-based hydrogel for efficient removal of 2, 4-dichlorophenol

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Laccase has important applications in the field of water pollution control. In order to better exploit the role of laccase in the field of environmental pollution prevention and control, and solve the problem that laccase is easy to be inactivated under extreme temperature and pH, the coating of laccase with PVA/CS-ZIF-8 hydrogel was explored, and the conditions affecting the activity of the embedded laccase were investigated. In this study, laccase molecules were encapsulated into metal-organic frameworks (MOFs) by co-precipitation to obtain Lac@ZIF-8 nanocomposites, and then Lac@ZIF-8 nanocomposites were wrapped in polyvinyl alcohol (PVA)/chitosan (CS) hydrogel networks to prepare highly active, stable and reusable PVA/CS/Lac@ZIF-8 composite hydrogels. The preparation conditions of the composite hydrogels such as laccase dosage, mass ratios of polyvinyl alcohol (PVA) to chitosan (CS), and the number of freeze-thaws were also optimized. Under the optimal immobilization conditions, the absorbance was measured at 420 nm by UV-Vis spectrophotometer using ABTS as the substrate and the immobilized laccase activity was calculated. The prepared PVA/CS/Lac@ZIF-8 composite hydrogels displayed excellent higher stability against a high temperature, and acid than free Lac. Furthermore, these hydrogels exhibited an excellent performance for 2, 4-dichlorophenol removal. And the possible pathway and intermediate of the degradation of 2, 4-dichlorophenol by laccase were determined by GC-MS.

Keywords

laccase; MOF-based hydrogel; immobilization; polyvinyl alcohol; chitosan; 2, 4-dichlorophenol degradation.

Associations between Human Exposure to Typical New Pollutants and Thyroid Cancer

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New pollutants may pose a threat to human health even at low-dose environmental exposure. Thyroid cancer is an endocrine malignancy, and the growth rate of thyroid cancer in China has shown a significant upward trend in recent years. At present, there is limited research on the association between exposure to new pollutants and the incidence of thyroid cancer. In this study, we investigated the association between three typical new pollutants perfluorinated/polyfluoroalkyl compounds (PFASs), novel brominated flame retardants (NBFRs), and organophosphorus flame retardants (OPEs) with thyroid cancer through two case-control studies.

A total of 134 thyroid cancer patients and 185 control participants in Shandong Province from 2016 to 2017 were selected as the study subjects to carry out the correlation study between internal exposure of PFASs and thyroid cancer. The results showed that seven PFASs were widely detected in human serum, with concentrations significantly higher in males than in females. Environmental dose exposure to PFASs had no effect on increasing the risk of thyroid cancer, while PFASs were significantly positively correlated with total cholesterol, total lipid weight, and low-density lipoprotein.

For the novel flame retardants (novel FRs) study, serum samples for 242 thyroid cancer patients and 239 healthy participants were collected. Our results found that pentabromotoluene, 2,3-dibromopropyl 2,4,6-tribromophenyl ether (DPTE), decabromodiphenylethane (DBDPE), tris (2-chloroethyl) phosphate (TCEP), and triphenyl phosphate (TPP) were widely detected in serum samples. DBDPE significantly increased the risk of thyroid cancer in both male and female participants; DPTE and TPP significantly increase the risk of thyroid cancer in women. Novel FRs showed a significant correlation with thyroid hormone levels (TCEP performed a significant negative correlation with triiodothyronine, free triiodothyronine and FT4 and a significant positive correlation with thyroid stimulating hormone), and female exposure to Novel FRs has a higher impact on thyroid hormone than male.

Keywords

new pollutants; PFAS; novel flame retardants; thyroid cancer; human serum.

Parent and halogenated polycyclic aromatic hydrocarbons in serum of coal-fired power plant workers: Levels, sex differences, accumulation trends, and risks

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Workers in coal-fired power plants are at high risk of exposure to polycyclic aromatic hydrocarbons (PAHs) and their halogenated derivatives (HPAHs). HPAHs are emerging persistent organic pollutants and considered to be more toxic than PAHs, yet no studies have investigated such exposure of HPAHs. In this study, the serum concentration levels, sex differences, accumulation trends, and health risks of PAHs and HPAHs in coal-fired power plant workers were investigated. 12 PAHs and 8 chlorinated PAHs (Cl-PAHs), but no brominated PAHs (Br-PAHs), were detected in >80% of serum samples from workers of a coal-fired power plant in eastern China. Serum HPAH concentrations were higher in plant workers (16–273 ng/g lipid) than in people without occupational exposure (12–51 ng/g lipid), and serum PAH and HPAH concentrations both in male and female workers were positively correlated with occupational exposure duration, with an estimated doubling time of 11–17 years. Correlations were found between concentration of \sum_8 HPAHs and \sum_{12} PAHs, but not between 7-chlorobenz[*a*]anthracene (7-ClBaA) and 1-chloropyrene (1-ClPyr) and their respective parent PAHs. Although there was no significant difference in serum concentrations of HPAHs between male and female workers, the associations of HPAHs with various health indicators showed sex differences. In males, total concentrations of PAHs and HPAHs were positively correlated with pulmonary hypofunction and hypertension, but not with abnormal electrocardiogram. The benzo[*a*]pyrene equivalents ratio of \sum_8 HPAHs/ \sum_{12} PAHs was 0.3 ± 0.1 . Among HPAHs in the serum, 9-Clphenanthrene, 7-ClBaA, and 1-ClPyr showed high health risks. This study is the first report on HPAH exposure in coal-fired power plant workers and provides new evidence on the health risks of PAHs and HPAHs in humans.

Keywords

halogenated polycyclic aromatic hydrocarbons (HPAHs); human serum; coal-fired power plant workers; exposure risk; occupational exposure.

Identification of serum metabolites associated with polybrominated diphenyl ethers (PBDEs) exposure in papillary thyroid carcinoma based on a case-control study

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Thyroid cancer is the most common endocrine tumor with a sharply growing incidence worldwide in recent years. Multiple factors including genetics, radiation, iodine, autoimmune diseases and exposure to environmental endocrine disrupting chemicals (EDCs) may be related with incidence of thyroid tumors. Polybrominated diphenyl ethers compounds (PBDEs) have been extensively used in electronic production, soft furnishings, fabrics and paints as a flame-retardant since 1980's. As a typical EDCs, high PBDEs exposure has been reported associated with increase the risk of thyroid cancer. However, interference with metabolic signature in thyroid cancer related to PBDEs exposure has not been studied yet till now.

In this study, 8 congeners of PBDEs were determined in serum from 29 papillary thyroid cancer (PTC) patients and 30 healthy participants by gas chromatography-atmospheric pressure chemical ionization mass spectrometry (GC-APCI-MS/MS) in Table 1. Based on the tertile distribution of total PBDEs concentrations, metabolomics analysis was performed by UHPLC coupled with QExactive Focus Hybrid Quadrupole-Orbitrap Mass Spectrometer (QE Orbitrap MS). The total 29 identified metabolites were correlated with the PBDEs exposure (Partial correlation analysis, $P < 0.05$) in Figure 1. The results showed that PBDEs disturbed the glycerophospholipids, sphingolipids and taurine, *etc.* which demonstrated neurotransmitters, oxidative stress and inflammation were the sensitive pathways in PTC in Figure 2. Furthermore, (+/-)-octopamine and 5-hydroxyindole which linked with neurotransmitters were identified as the potential disturbed metabolite markers for thyroid cancer upon different PBDEs exposure in Figure 3.

This was the first MS-based nontargeted metabolomics findings on PTC with PBDEs exposure and highlighted the evidence for the linkage of PBDEs exposures. Furthermore, our findings prompted deep understanding of the molecular and metabolic mechanisms induced by PBDEs exposure in thyroid cancer and might provide potential effect biomarkers in discriminating malignant lesions from benign ones and early diagnosis.

Keywords

papillary thyroid carcinoma; PBDES; metabolomics; biomarker

Fund programs

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Table 1 Demographic characteristics of the participants based on different PBDEs levels.

Characteristics	Low PBDEs group (n=20)	Median PBDEs group (n=20)	High PBDEs group (n=19)	<i>P</i> -value
PBDEs (ng/g lipid)	3.23 (1.20-5.45)	9.80 (5.69-14.00)	24.48 (14.75-111.11)	<0.05
Age (yrs)	39.05±8.48	42.50±6.70	40.89±8.33	>0.05
Sex				>0.05
Male(n%)	6(30.0%)	12(60.0%)	9(47.4%)	
Female(n%)	14(70.0%)	8(40.0%)	10(52.6%)	
BMI (kg/m ²)	21.30±4.18	22.40±2.15	22.39±2.92	>0.05
Smoking (n%)	4(20.0%)	5(25.0%)	2(10.5%)	>0.05
Drinking (n%)	8(40.0%)	12(60.0%)	11(57.9%)	>0.05
Education Level				>0.05
Primary and below (n%)	1(5.0%)	3(15.0%)	5(26.3%)	
Senior high school and below (n%)	13(65.0%)	9(45.0%)	10(52.6%)	
Junior college and above(n%)	6(30.0%)	8(40.0%)	4(21.1%)	
Iodine nutrition				>0.05
Deficiency (n%)	4(20.0%)	7(35.0%)	3(15.8%)	
Adequate(n%)	6(30.0%)	8(40.0%)	9(47.4)	
Excess (n%)	4(20.0%)	4(20.0%)	3(15.8%)	
Overdose(n%)	6(30.0%)	1(5.0%)	4(21.0%)	

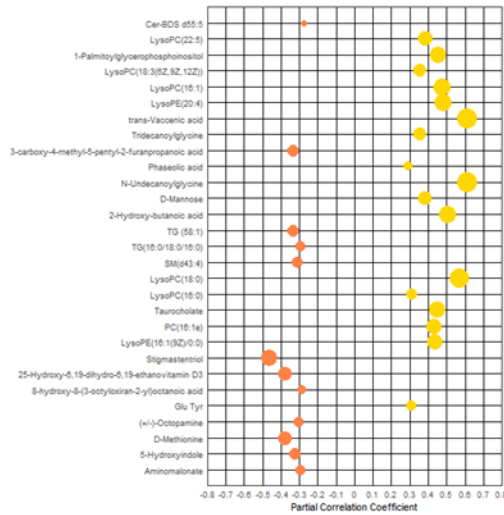


Figure 1 Adjusted partial correlations between the PBDEs and the 29 potential biomarkers. (Bigger point represents stronger correlation and $P < 0.05$)

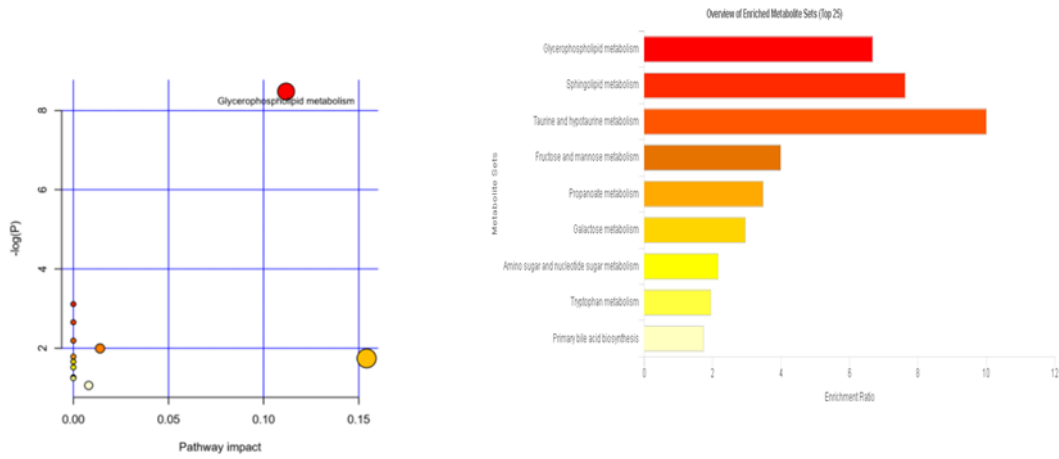


Figure 2 Altered pathways related to PBDEs exposure levels.

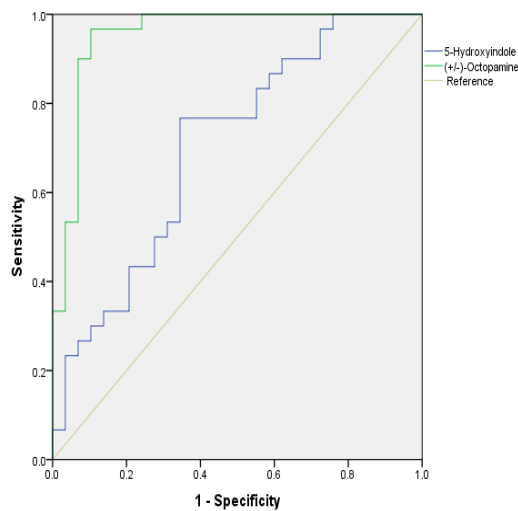


Figure 3 ROC curves of potential metabolic biomarkers for PTC diagnosis.

First evidence of neonicotinoid insecticides in human bile and associated hepatotoxicity risk

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Neonicotinoids (NEOs) are widely applied in agricultural lands and are widespread in different environments, accelerating threats to ecosystems and human health. A number of in vitro/in vivo studies have reported adverse effects of NEOs on mammalian health, but the link between NEO exposure and toxic effects on human liver remains unclear. We randomly recruited 201 participants and quantified eight commercialized NEOs in bile.

High frequency and concentration of detection indicate low degradation of human liver on NEOs. The main NEOs are nitenpyram and dinotefuran, which contribute to about 86% of the total residual levels of eight NEOs, due to the highest solubility in bile and are not degraded easily in liver. In contrast, imidacloprid and thiacloprid are major compounds in human blood, according to previous studies, suggesting that individual NEOs behave differently in blood and bile distribution. There was no statistical difference in NEO residues between cancer and non-cancer participants and among the different participant demographics (e.g., age, gender, and body mass index). The serum hematological parameters -bile acid, total bilirubin, cholesterol and alkaline phosphatase were positively correlated with individual NEO concentrations, suggesting that NEO exposure affects liver metabolism and even enterohepatic circulation. The study first examined the NEO residues in human bile and provided new insights into their bioavailability and hepatotoxicity risk.

Keywords

pesticides; human exposure; liver metabolism; distribution; enterohepatic circulation.

Embryonic exposure to UV-328 impairs the cell cycle in zebrafish (*danio rerio*) by inhibiting the p38 MAPK/p53/Gadd45a signaling pathway

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The benzotriazole UV stabilizer UV-328 is well known for its potent antioxidative properties; however, there are concerns about how it may affect signaling nodes and lead to negative consequences. This study identified the key signaling cascades involved in oxidative stress in zebrafish (*Danio rerio*) larvae and evaluated the cell cycle arrests and associated developmental alternations. Exposure to UV-328 at 0.25, 0.50, 1.00, 2.00, and 4.00 µg/L downregulated gene expression associated with oxidative stress (*cat*, *gpx*, *gst*, and *sod*) and apoptosis (*caspase-3*, *caspase-6*, *caspase-8*, and *caspase-9*) at 3 days postfertilization (dpf). The transcriptome aberration in zebrafish with disrupted p38 mitogen-activated protein kinase (MAPK) cascades was validated based on decreased mRNA expressions of p38 MAPK (0.36-fold), p53 (0.33-fold), and growth arrest and DNA damage-inducible protein 45 α (Gadd45a) (0.52-fold) after a 3- and 14-day exposure alongside a correspondingly decreased protein expression. The percentage of cells in the Gap 1 (G1) phase increased from 69.60% to a maximum of 77.07% ($p < 0.05$) in the 3 dpf embryos. UV-328 inhibited the p38 MAPK/p53/Gadd45a regulatory circuit but promoted G1 phase cell cycle arrest, abnormally accelerating the embryo hatching and heart rate. This study provided mechanistic insights that enrich the risk profiles of UV-328.

Keywords

UV stabilizers; transcriptome aberration; p38 MAPK; cell cycle arrest; apoptosis; zebrafish

Perfluorooctanoic acid-induced metabolic reprogramming impairs intestine health in human intestinal cells

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Intestinal cell metabolism played an important role in intestine health. Perfluorooctanoic acid (PFOA) exposure could disorder intestinal cell metabolism. However, the mechanism of how the three carbon sources interact under PFOA remained unclear. The present study aimed to dissect the interconnections of glucose, glutamine, and fatty acids in PFOA-treated human colorectal cancer cells (DLD-1) using ¹³C metabolic flux analysis. The abundance of glycolysis and tricarboxylic acid (TCA) cycle metabolites was decreased in PFOA-treated cells except succinate, whereas most amino acids abundance was increased. Beside serine and glycine, metabolites labelling from ¹³C glucose was reduced in cells exposed to PFOA, and the pentose phosphate pathway flux was 1.4-fold higher in PFOA-treated cells than in controls. In reductive glutamine pathway, higher labeled enrichment of citrate, malate, fumarate, and succinate in PFOA-treated cells was observed than that of controls. The contribution of glucose to fatty acid synthesis was decreased, while the increase contribution of glutamine to fatty acid was observed. Additionally, more carbon labelling in TCA intermediates from fatty acid β -oxidation was found in PFOA-treated cells. These data indicated that an activation of amino acid and fatty acid depletion might compensate for the loss of glucose function in biomass synthesis and energy metabolism of intestinal cells under PFOA exposure. The ¹³C metabolic flux analysis will be a promising tool to explore metabolic disorder by environmental pollutants.

Keywords

perfluorooctanoic acid; metabolic flux analysis; glutamine metabolism; metabolic remodeling; intestine health; glucose metabolism.

Influence mechanism of sulfur-containing compounds on the formation of POPs during the secondary copper smelting

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Chlorobenzene (CBzs), Polychlorinated Biphenyls (PCBs) and Dioxin (PCDD/Fs) are a kind of persistent organic pollutants (POPs) which usually enter the environment along with flue gas or dust as by-products in the thermal treatment process of industrial production (Zhang et al., 2019; Li et al., 2023). As one of the major industries for priority control of PCDD/Fs emissions in China, the secondary copper smelting also emits a large number of sulfur-containing compounds such as SO₂ which has been reported to influence the formation of PCDD/Fs, but whether it inhibits or promotes the formation of POPs is still controversial (Fujimori et al., 2014). Therefore, it is necessary to study the influence mechanism of sulfur-containing compounds on the formation of POPs. In this study, we investigated the influence of reaction temperature, reaction time, type and content of sulfur-containing compounds on the concentration level, fingerprint distribution characteristics of congener, and gas-solid distribution characteristics of CBzs, PCBs, and PCDD/Fs. In addition, we studied the promotion or inhibition efficiency of sulfur-containing compounds on the formation of CBzs, PCBs and PCDD/Fs, and revealed the influence mechanism of sulfur-containing compounds on the formation of PCDD/Fs. The results can be summarized as follows: (1) the concentrations of CBzs, PCBs and PCDD/Fs increased significantly with a small amount of concentrated sulfuric acid, but showed a downward trend after excessive addition; (2) SO₂ has a significant inhibitory effect on CBzs, while PCBs and PCDD/Fs show a trend of first promotion and then inhibition with the increase of SO₂ concentration; (3) the small amounts of sulfur-containing compounds promote the release of chlorine, while the large amounts of sulfur-containing compounds inhibit the activity of chlorine and catalytic metals.

Keywords

Dioxin; sulfur-containing compounds; influence mechanism.

Occurrence, distribution and special variation of Volatile Methylsiloxanes in the Yangtze River Basin, China

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Due to their chemical stability, hydrophobicity, electrical insulation, and lubricity, Volatile Methylsiloxanes (VMSs) are widely used in various areas of production, such as lubricants, sealants, personal care products, cosmetics and so on. A large number of VMS entering the environment causing widespread concern. Some studies have shown that VMS has persistence, bioaccumulation and toxicity. The Yangtze River is the largest in China, it plays an important role in China's economic and cultural development. Based on a preliminary survey, we found that investigations of VMS in the water environment have mainly focused on natural water bodies and wastewater in north China, with fewer relevant reports for the Yangtze River basin.

In this study, eight cyclic volatile methylsiloxane (CVMS) and seven linear volatile methylsiloxane (LVMS) were measured using SPE followed by GC-MS/MS in water samples collected from the Yangtze River basin to elucidate the distribution of target chemicals. we selected 42 samplings in the upper(9), middle(6) and lower reaches(27) of the Yangtze River basin, including 14 wastewater (P), surface water (S) and source water (C).

CVMS have obvious spatial distribution characteristics in the Yangtze River basin. Probably because of the industrial distribution and hydrodynamics, CVMS concentrations are significantly higher in downstream than upstream and midstream among the three types of water. Among eight CVMS, due to differences in the structural stability of the substances, the concentrations of D6, D7, and D8 were higher than other CVMSs. On the other hand, The spatial distribution of LVMS is not clear, and LVMS concentration levels are significantly lower than CVMS. L7, L8, and L10 are the largest amount of LVMS. The results we detected indicated that pollution control in downstream of the Yangtze River should be strengthened in the future, and more attention should be given to the environmental risk of CVMS.

Keywords

VMS; Yangtze river basin; source water; surface water; wastewater.

Occurrence of and human exposure to benzothiazoles and benzotriazoles in indoor dust in Suizhou and Beijing, China

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Previous experimental and epidemiological studies have shown that benzothiazoles (BTHs) and benzotriazoles (BTRs) may be associated with a variety of adverse health effects. As high-volume production chemicals, they have attracted public concern worldwide. Despite a few studies on these chemicals in different regions or countries, information that pertains to the occurrence and distribution of such chemicals in indoor environment in China is still scarce. Therefore, investigations are needed to extend the knowledge about the occurrence and profiles of these chemicals in indoor dust, and exposure data of these pollutants from derived indoor dust are warranted. Levels of BTHs and BTRs were found higher in dust from Beijing than Suizhou. The median concentrations of \sum_6 BTHs in indoor dust samples from Suizhou and Beijing were 133 and 439 ng/g dw, respectively, whereas the \sum_5 BTRs concentrations from Suizhou and Beijing were 28.4 and 40.1 ng/g dw, respectively. BTH, 2-OH-BTH, 1-H-BTR, and 5-Me-1-H-BTR were the predominant compounds in dust. Human exposure to such chemicals was further evaluated. The intake for population in Suizhou (0.163–0.939 ng/kg bw/day) and Beijing (0.0347–0.200 ng/kg bw/day), China was minor. The obtained results in this study will provide baseline concentrations of such chemicals in indoor environment in China and be able to add insight into human exposure to BTHs and BTRs. It should be noted that this study on concentrations of BTHs and BTRs in Beijing is limited, due to the small sample size. Therefore, larger sample sizes need be examined in future study. In addition to the exposure from dust, other routes of exposure, including foodstuffs, and drinking water, should be investigated to evaluate the total burden of BTHs and BTRs in human body.

Keywords

benzothiazoles; benzotriazoles; dust; distribution; human exposure.

Emerging plasticizers in house dust from multiple countries: an increasing threat to humans

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Following restrictions on phthalate esters (PAEs), a large variety of non-phthalate plasticizers (NPPs) have been employed as substitutes to manufacture consumer products. Knowledge remains limited on the environmental occurrences, fate and human exposure risks of many emerging NPPs. In the present work, we screened for a total of 45 emerging NPPs, alongside the major PAEs, within household dust samples collected from five distinct regions spanning the Asia-Pacific and United States. The results clearly demonstrated ubiquitous occurrences of many NPPs in home environment, particularly acetyl tributyl citrate (ATBC), tricapryl trimellitate (TCTM), trioctyl trimellitate (TOTM), glycerol monooleate (GMO), methyl oleate (MO), and diisobutyl adipate (DiBA). The median total concentrations of NPPs ranged from 17.8 to 252 $\mu\text{g/g}$ in the study regions, while the mean ratios of NPPs to PAEs ranged from 0.19 (Hanoi) to 0.72 (Adelaide). Spatial differences were observed not only for the chemical abundances, but also the composition profiles and the hazard quotient (HQ) prioritization of individual chemicals. The current exposure may unlikely cause significant health risks according to the HQ estimation. However, potential exposure risks cannot be overlooked, due to the lack of appropriate toxic threshold data, the existence of additional exposure pathways, and possible cocktail effects from co-existing NPPs and PAEs.

Keywords

non-phthalate plasticizers; phthalate esters; house dust; multiple regions; human exposure

Nontarget identification of novel organophosphorus flame retardants and plasticizers in rainfall runoffs and agricultural soils around a plastic recycling industrial park

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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.

Keywords

organophosphate esters; novel organophosphorus compounds; precipitation; nontarget screening; plastic recycling and reprocessing

Melting Himalayas and mercury export: results from Everest proglacial Rongbuk River and Trans-Himalayan Koshi River

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Rapid recession of glaciers in the Himalayan region has raised concerns regarding the release of legacy pollutants, including mercury (Hg), and its potential impact on downstream ecosystems. In this study, we conducted continuous and seasonal sampling in the Everest Rongbuk Glacier-fed river and the trans-Himalayan Koshi River, respectively. In the Rongbuk River, the concentrations of total Hg (THg) and methyl Hg (MeHg) were found to be 1.56 ± 0.85 ng/L and 0.057 ± 0.025 ng/L, respectively. These levels were comparable to global background levels and were primarily influenced by the presence of total suspended particulate matter (TSP). Based on the annual runoff and average Hg concentration, the estimated annual export fluxes of THg and MeHg were 441 g and 16 g, respectively, with yield rates of THg and MeHg measured at $1.6 \mu\text{g}/\text{m}^2/\text{year}$ and $0.06 \mu\text{g}/\text{m}^2/\text{year}$, respectively. The overall annual Hg export through meltwater runoff in the Himalayan region was estimated to be approximately 337 kg/year. In the Koshi River, the THg concentration in surface water ranged from 0.64 to 32.96 ng/L, with an average level of 5.83 ± 6.19 ng/L. The THg concentration followed the order of post-monsoon (8.79 ± 7.32 ng/L) > monsoon (6.68 ± 6.12 ng/L) > pre-monsoon (2.18 ± 1.29 ng/L). Particulate Hg (PHg) accounted for an average of 63% of THg and demonstrated a positive correlation with THg across all three seasonal samplings, indicating that the variation in PHg concentration played a significant role in the seasonal and spatial distribution of THg in the Koshi River water. The annual Hg exports and fluxes in the Koshi River were estimated to be 339.04 kg and $3.88 \mu\text{g}/\text{m}^2/\text{year}$, respectively, and are expected to further increase under continuous warming conditions. Our analysis shed light on the environmental impact of glacier retreat in the Himalayas and emphasizes the need of integrated monitoring and research on Hg in glacier runoff and trans-Himalayan rivers.

Keywords

mercury, himalayas, glacier melt, river, export

Toxic effects of PFOA and its alternatives HFPO-DA and HFPO-TA on zebrafish

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Perfluorooctanoic acid (PFOA) has resulted in varieties of biological toxic effects due to its environmental persistence, long-distance migration, and bioaccumulation (Guo et al., 2019; Zhou et al., 2022). The production and application of PFOA are regulated globally. Due to the importance of PFOA in daily life and industrial production, PFOA alternatives have been widely developed. As typical alternatives for PFOA, hexafluoropropylene oxide dimer acid (HFPO-DA) and hexafluoropropylene oxide trimer acid (HFPO-TA) are widely detected in water (Joerss et al., 2020). The current toxicity studies on HFPO-DA and HFPO-TA are mainly focused on terrestrial mammals, and the toxicity on aquatic organisms is still lacking. Moreover, it is unknown whether HFPO-DA and HFPO-TA are less toxic to aquatic organisms than PFOA. Therefore, the toxicity of PFOA and its alternatives HFPO-DA and HFPO-TA on zebrafish embryos and adults were studied from oxidative stress, apoptosis, and immune function. The results showed that reactive oxygen species (ROS) and malondialdehyde contents in embryos and adults were significantly increased. The superoxide dismutase (SOD) activity and 8-hydroxydeoxyguanosine (8-OHdG) content in embryos decreased, while those in adults increased. PFAS induced oxidative damage. PFAS also inhibited apoptosis in both embryos and adults. PFOA exposure only caused immune dysfunction in adults, while HFPO-DA and HFPO-TA exposure disrupted immune homeostasis in both embryos and adults. The integrated biomarker response was used to compare the combined toxicity of PFAS in zebrafish (Sanchez et al., 2013). The ROS content and SOD activity can be used as early warning indicators of PFOA and its alternatives HFPO-DA and HFPO-TA for embryos and adults, respectively. HFPO-DA and HFPO-TA have higher environmental risks and may not be safe alternatives for PFOA. This study provides a reliable basis for evaluating the toxicity of HFPO-DA and HFPO-TA on aquatic organisms and their safety as alternatives to PFOA on aquatic organisms.

Keywords

PFOA alternatives; oxidative stress; apoptosis; immunotoxicity; toxicity comparison.

Effect of flumetsulam alone and coexistence with microplastics on soil microbial carbon and nitrogen cycles: Elucidation of bacterial community structure, functional gene expression, and enzyme activity

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Flumetsulam (FLU) is a representative of the triazolopyrimidine sulfonamide herbicides (El Maataoui et al., 2017). The accumulation of plastic mulch residues is a major source of microplastics (MPs) contamination in agricultural soils (Astner et al., 2019). With the increased use of FLU and the continuous accumulation of MPs, it is possible for these two novel contaminants to co-exist in the soil environment. In the present study, we used brown soil as the test soil and determined the toxicity of FLU at 0.05, 0.5 and 2.5 mg kg⁻¹ alone and in combination with PE MPs (1%) on soil microorganisms. The obtained results demonstrated that the exposure of FLU and FLU+MPs had an inhibitory effect on the numbers of bacteria and fungi. In addition, FLU and FLU+MPs affected the nitrogen cycle in soil, favoring nitrogen fixation and denitrification and inhibiting nitrification. Exposure to FLU and FLU+MPs caused functional bacterial genera changes associated with the nitrogen cycle, altered the expression of related genes, and inhibited urease activity. For carbon cycling in soil, FLU and FLU+MPs exposure increased the relative abundance of carbon cycle-related bacterial genera. The exposure enhanced the carbon fixation capacity of the soil by promoting the expression of the carbon fixation gene *cbbLR*. Compared to FLU exposure alone, exposure to FLU + MPs gave rise to significant differences in soil bacterial community composition, but did not affect carbon and nitrogen cycling. The integrated biomarker response results indicated that the toxicity of FLU and FLU+MPs to soil microorganisms increased with increasing concentrations of FLU. The present experiment clarified the toxicological effects of co-exposure of FLU and MPs on microorganisms and filled the toxicological data gap of FLU.

Keywords

High-throughput sequencing; functional genes; soil enzymes; soil microorganism; integrated biomarker response (IBR).

Highly active complexes of pyrite and organic matter regulate arsenic fate

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Arsenic (As) presents high toxicity and strong carcinogenicity, and its health risks are regulated by its oxidation state and speciation. As can form complexes with the surface of minerals or organic matter through adsorption, affecting its toxicity and bioavailability. However, the regulation effect of the interaction of coexisting minerals and organic matter on As fate remains largely unknown. Here, we discovered that minerals (e.g., pyrite) and organic matter (e.g., alanyl glutamine, AG) can form pyrite-AG complexes, promoting As(III) oxidation under simulated solar irradiation. The formation of pyrite-AG was explored in terms of the interaction of surface oxygen atoms, electron transfer and crystal surface changes. From the perspective of atoms and molecules, pyrite-AG showed more oxygen vacancies, stronger reactive oxygen species (ROS) and a higher electron transport capacity than pyrite alone. Compared with pyrite, pyrite-AG effectively promoted the conversion of highly toxic As(III) to less toxic As(V) due to the enhanced photochemical properties. Moreover, quantification and capture of ROS confirmed that hydroxyl radicals ($\bullet\text{OH}$) played an important role in As(III) oxidation in the pyrite-AG and As(III) system. Our results provide previously unidentified perspectives on the effects and chemical mechanisms of highly active complexes of mineral and organic matter on As fate and provide new insights into the risk assessment and control of As pollution.

Keywords

pyrite; AG; photochemical properties; reactive oxygen specie; As oxidation.

Detoxification of cadmium by algal organic matter of *Microcystis aeruginosa*

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Under cadmium (Cd) stress, bloom-forming cyanobacteria exhibit elevated algal organic matter (AOM) production, which is suspected as a potential detoxification mechanism for algal cells. Thus, this study was conducted to investigate the growth, Cd adsorption and accumulation, and the AOM production of the bloom-forming cyanobacteria, *Microcystis aeruginosa*, under various concentrations of Cd ions. The results indicated that the growth and photosynthetic activity of algal cells were inhibited by cadmium stress. Compared to the control group, the growth rate and the maximal photochemistry efficiency significantly decreased under cadmium stress, while the activities of antioxidant enzymes such as superoxide dismutase (SOD) and ascorbate peroxidase (APX), as well as the content of non-enzymatic antioxidants like reduced glutathione, increased with Cd concentration. The biosorption of cadmium by *M. aeruginosa* ranged from 71.3% to 99.2% and bioaccumulation of cadmium ranged from 0.8% to 29.3% in all cadmium spiked treatment groups. In addition, cadmium stress stimulated the release of AOM. Parallel factor analysis revealed that AOM consisted of one protein-like substance (C1) and three humic acid-like substances (C2, C3, and C4). Under cadmium stress, extracellular protein-like substances increased with the increase of Cd concentration, reaching a maximum increase of 10.18%, whereas intracellular protein-like substances decreased by 29.02% with the increase of Cd concentration. Two-dimensional synchronized fluorescence correlation (2D-SFS-COS) analysis demonstrated that humic acid-like substances exerted a detoxification effect on Cd prior to protein-like substances in extracellular AOM, whereas in intracellular AOM, protein-like substances exerted a detoxification effect on Cd before humic acid-like substances. These findings provide evidence for the detoxification mechanism of AOM against Cd ions.

Keywords

cadmium; *Microcystis aeruginosa*; algal organic matter; PARAFAC analysis; 2D-SFS-COS.

Revelation of mercury-binding proteins in iron-reducing bacteria by *in vitro* thermal shift assays

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Methylmercury (MeHg), leading to significant neurotoxicity, could bioaccumulate via the food chain. Previous research indicates that methylmercury in the environment primarily originates from microbial methylation of inorganic mercury. Gene pairs *hgcAB* are suggested to regulate mercury methylation via acetyl-CoA pathway¹. However, other proteins in mercury methylation pathway remain unrevealed. In this study, we identified binding-proteins of *Geobacter sulfurreducens* PCA potentially related to microbial mercury methylation by using *in vitro* thermal shift assays. There were 22 and 15 proteins identified as binding sites of Hg ions (Hg²⁺) and MeHg, respectively (p value < 0.001, R² > 0.9), in which proteins HgcAB were not identified. Proteins binding with MeHg were involved in translation process, suggesting that ribosomal proteins played important role in transformation and transport of MeHg. Proteins binding with Hg²⁺ showed the function of binding with divalent metal ions (Zn²⁺ and Mg²⁺), which indicated that Hg²⁺ could compete with divalent metal ions for ligands to transport Hg²⁺ inside the cells. Q749N5 and Q747A5, binding both with Hg²⁺ and MeHg, were two potential sites of mercury methylation. Protein Q749N5 could participate in acetate metabolic process, acetyl-CoA biosynthetic process, and phosphorylation. Whereas Q747A5 was an uncharacterized protein, and its specific molecular function is still under investigation. Overall, several Hg-binding proteins related to divalent metal ions ligands were potentially participated in mercury methylation and transportation, providing insights for further investigation of mechanisms of microbial Hg methylation.

Keywords

mercury methylation; mercury-binding proteins; thermal shift assay

Understanding the Hg transformations within organisms

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Organisms are generally considered as Hg “accumulators”, absorbing Hg from the ambient environments and then transferring them to humans along food webs. For past decades, Hg transformations, i.e., methylation/demethylation and reduction/oxidization, are believed to mainly occur in ambient environments, such as in the air, water columns, and sediments/soils. It remains unknown whether and to what extent Hg transformations happen within organisms. This critical knowledge gap leads to the failure in linking Hg in the environments and human exposure, as well as an effective strategy to mitigate Hg risk. Here, we reported the hidden role of organisms as Hg “eliminators”: Significant MeHg demethylation and Hg reduction occur within organisms, including rice plants, algae, etc. These processes largely reduce the Hg contents in organisms and the subsequent Hg flux along food webs, mitigating human Hg exposure risks. Importantly, these transformations were induced by neither light nor microbes, the commonly recognized driving forces of Hg transformations in the ambient environments, suggesting the existence of hidden mechanisms of Hg transformations. Our recent studies highlight the importance of paying attention to the organism-induced Hg transformations and the potential mechanisms, which could largely advance our understanding of Hg biogeochemistry and shape the global Hg cyclings.

Keywords

Hg; biogeochemistry; methylation; demethylation; exposure, reduction.

Transformation of ionic mercury species to nanoparticles in Diatom *Chaetoceros curvisetus*

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Particulate mercury, especially mercury nanoparticles (HgNPs), has been reported to precipitate in anoxic water and exist in marine sediments as the major Hg species (Mazrui, Seelen et al 2018). These species play important roles in marine Hg cycle and flux estimation, in which the biological transformation of Hg is usually ignored or underestimated. As the most widely distributed marine phytoplankton, algae regulate the marine cycle of Hg as a biological pump and 20-90% of dissolved Hg can be transformed into particulate Hg by algae previously (Wu and Wang 2014). However, the detailed knowledge regarding Hg particles formed in algae, such as size and distribution, remains unknown. Herein, the formation, distribution, and excretion of HgNPs were investigated in the diatom *Chaetoceros curvisetus*. Firstly, it was found that HgNPs (24.6-62.2 nm) were formed and partly accumulated inside the diatom cells accounting for 7-11% of total Hg. Then, the size of intracellular HgNPs reduced and small ones (<40 nm) were excreted (10-18% of total Hg). This intracellularly formation and excretion of HgNPs in algae could firstly, contribute to the Hg settling in the water column and eventually Hg burial in sediments; and secondly, promote the recognition to consider the HgNPs as a specific Hg species in flux estimation due to its unique sedimentation behavior compared with ionic Hg. To sum up, those findings could provide important information for better understanding the marine Hg cycle and accurate estimating Hg flux in future studies.

Keywords

Mercury nanoparticles; transformation; diatom; size changes

Topological defects enhanced nonradical oxidation capacity of biochar/peroxydisulfate system

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Persulfates-based nonradical oxidation processes driven by metal-free carbocatalysis are appealing in selective degradation of persistent toxic substances (PTSs). Among various carbonaceous catalysts, biochar (BC) was considered as a potential candidate due to its low cost and environmental friendliness. Several strategies such as heteroatoms doping or regulating oxygen functional groups were explored to optimize the electronic environment of BC to promote its nonradical activity. However, the heavy doping of heteroatoms and excessive oxygen moieties would result in the decrement of the electronic conductivity, which might be unfavorable to the nonradical oxidation. Herein, topological defects were introduced into BC via removing N atoms of N-doped BC (NBC) to improve the nonradical catalytic performance. Compared to the pristine BC and NBC, the introduction of topological defects could achieve up to 36.6- and 8.7-times catalytic activity enhancement for the degradation of tetracycline, respectively. A positively linear correlation between the rate constant (k_{obs}) and topological defects (I_D/I_G) confirmed the crucial role of topological defects. Density functional theory calculations suggested that topological defects enhanced the electron-donating ability of BC by reducing the energy gap, which made the electrons transfer to peroxydisulfate molecules more easily. As a result, holes could be generated on the surface of BC after carbon defects lost electrons, thus inducing the nonradical oxidation of PTSs. This study not only provides a potential avenue for designing efficient biochar-based catalysts, but also sheds light on the mechanism of nonradical oxidation process induced by carbon defects.

Keywords

topological defects; biochar; peroxydisulfate; nonradical oxidation.

Microbial degradation of phenanthrene adsorbed on biochars produced at different pyrolysis temperatures

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As environment-friendly adsorbents with high adsorption capacity, biochars (BC) have been applied to immobilize polycyclic aromatic hydrocarbons (PAHs) in soil remediation. However, the adsorbed PAHs have not been removed completely. It is of great importance to degrade the adsorbed PAHs on biochars. In previous study, microbes can produce extracellular reactive oxygen species (ROS) to degrade the adsorbed-PAHs on a high-temperatures (700 °C) prepared biochar. The extracellular ROS-driven biodegradation of biochar-adsorbed PAHs could be affected by the pyrolysis temperature of biochars, because the pyrolysis temperature can influence the interplay among biochars, microbes and PAHs. However, the effect of pyrolysis temperature on the extracellular ROS-driven degradation has not been studied. Therefore, biodegradation of adsorbed phenanthrene (PHEN) on a wood chip-derived biochar produced at different pyrolysis temperatures (BC150-700) was investigated. Microbes degraded PHEN on BC150-300 after desorption because most of the PHEN on BC150-300 are desorbable. Microbes mainly degraded PHEN on BC400-700 through extracellular ROS because the desorption percentages of PHEN on BC400-700 were ignorable. This could be attributed to the lower contents of dissolved iron element and phenolic group as well as the higher porosity of biochars with higher pyrolysis temperature. The shortage of iron ions promoted the secretion of siderophore to produce more ROS. The decrease of phenolic group on biochars led to the less quenching of ROS. Moreover, the higher porosity of biochars facilitated the transportation of ROS. The obtained results could provide an insight into the extracellular ROS-driven biodegradation of adsorbed PAHs on biochars.

Keywords

biochar; biodegradation; pyrolysis temperature; polycyclic aromatic hydrocarbons.

Counterintuitive oxidation of alcohols at air-water interfaces

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Environmental organic acids not only play critical roles in aerosol formation but also determine water acidity. Oxidation of alcohol is considered to be a vital source of organic acids in the environment. It is known that the oxidation of alcohols by hydroxyl radicals proceeds via H abstraction at their -CH₂- group in the gaseous phase.

By employing advanced molecular simulation techniques, this study shows a rapid and counterintuitive oxidation of alcohols at air-water interfaces. It was found that methanediols (HOCH₂OH) orient at air-water interfaces with an H-atom of the -CH₂- group pointing toward the gaseous phase. Counterintuitively, gaseous hydroxyl radicals do not prefer to attack the exposed -CH₂- group, but the -OH group that forms hydrogen bonds with water molecules at the surface via a water-promoted mechanism, leading to the formation of formic acids. Compared with gaseous oxidation, the water-promoted mechanism at the air-water interface significantly lower free-energy barriers by ~6.7 kcal·mol⁻¹ and accelerate the formation of formic acids.

Overall, the molecular-level insights gained from the study demonstrate that the oxidation of HOCH₂OH as well as other alcohols at the air-water interfaces play a more than expected role in organic acid formation in the environment.

Keywords

Formic acids; molecular simulations.

Angiogenic Activity and Mechanism for Bisphenols on Endothelial Cell and Mouse: Evidence of a Structural-Selective Effect

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Increased epidemiological evidence indicates the association of bisphenol exposure with human vascular disorders, while the underlying mechanism has not been clarified. Here, we sought to unveil the potential angiogenic effect and the underlying mechanism of bisphenols with different structural features using endothelial cells treated with an environmentally relevant concentration of bisphenols (range: 1 nM to 10 μ M) and a C57BL/6 mouse model fed with doses of 0.002, 0.02, 2, and 20 mg/kg BW/day for 5 weeks. Bisphenol A (BPA) and bisphenol S (BPS) at a 1 nM level significantly increased tube formation by 45.1 and 30.2% and induced the microvessel sprouting, while tube length and microvessel sprouting were significantly inhibited by 37.2 and 55.7% after exposure to tetrabromobisphenol S (TBBPS) at 1 μ M, respectively. Mechanistically, TBBPA and TBBPS significantly inhibited the interaction between phosphatidylinositol 3-kinase (PI3K) and thyroid receptor (TR), while BPA and BPS favored the interaction between PI3K and estrogen receptor (ER), resulting in abnormal PI3K signaling with consequent distinct angiogenic activity. BPA- and BPS-induced pro-angiogenic effects and TBBPS showed anti-angiogenic effects due to their distinct disruption on the TR/ER-PI3K pathway. Our work provided new evidence and mechanistic insight on the angiogenic activity of bisphenols and expanded the scope of endocrine disruptors with interference in vascular homeostasis.

Keywords

Bisphenol angiogenesis thyroid receptor estrogen receptor phosphatidylinositol 3-kinase protein interaction

Environmental computational toxicology for risk assessment and designing green alternatives of persistent toxic substances

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While chemicals are essential for modern societies and provide desired benefits, they can be inevitably released into the environment during their lifecycles and pose risks to human and ecological health. The rapid growth in variety and production volume of chemicals can lead to chemicals pollution that exceeds the planetary boundary. Therefore, various environmental computational toxicology studies have been conducted to assess risks of chemical substances, which provides significant support for their sound management.

Apart from risk assessment, environmental computational toxicology should design green alternative chemicals and processes to control risks at sources. Machine learning (ML) can bring innovative solutions for designing green alternatives. Accordingly, a set of green substitution strategies were proposed for persistent toxic substances based on ML, which consists of four components: screening hazardous chemicals, designing low hazardous chemicals, predicting transformation products, and planning green synthetic pathways.

Based on advanced algorithms such as graph neural networks, ML models can be constructed to comprehensively screen environmentally persistent, bio-accumulative, and toxic chemicals. Generative adversarial networks, which can automatically generate molecular structures with specific properties, can also be developed for designing alternatives. Multi-constraint molecular generation models can be employed to design alternatives with both necessary functional properties and low environmental hazards.

Large-scale language models that can be used for organic chemical reaction prediction have also been developed rapidly. The reaction prediction models can also be used in assessing environmental impact of chemicals throughout their life cycles and planning synthetic pathways that meet the principles of green chemistry. With the application of ML-models in molecular design and synthetic process design, a sustainable way that promotes benefits of chemicals and simultaneously minimizes adverse effects to the environment, can be obtained.

Keywords

chemicals, machine learning, risk prevention and control, green alternative design, source management, green chemistry

Screening persistent toxic substances with multimodal deep learning models

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Pursuit of well-being drives mass production and application of synthetic chemicals with various functional attributes. However, some chemicals have deleterious effects on human and ecological health. Therefore, environmental risks of these chemicals (such as persistent toxic substances, PTS) should be assessed and quantified. A premise of PTS risk assessment is to predict the toxicity of chemicals and to identify their toxicity pathways. Deep learning models have been proved to be successful in chemical toxicity prediction. However, interactions between chemicals and organisms are intricate and often involve multiple biological levels and confounders. Most of the previous models adopted single modal data (e.g., molecular structural descriptors) as inputs and ignored the disturbances induced by the chemicals in the organism, leading to poor performance on some toxicity endpoints.

As deep learning advances, multimodal deep learning that can process and fuse data from different modalities are able to capture the complementary information and achieve more robust predictions. Multimodal deep learning models based on chemical and protein structure data could be used to identify PTS and susceptible biomolecules by ranking prediction results. Prediction and identification of critical toxicity pathways can also be achieved by incorporating omics data and high-content data into the models. On this basis, the multimodal models enable cross-species prediction of chemical toxicity by setting a series of rules to distinguish data from different species and encoding them into the models. Therefore, multimodal deep learning models may serve as efficient tools for hazard assessment of PTS by predicting their toxicity on multiple endpoints and elucidating toxicity pathways. Notably, multimodal deep learning is a booming field that needs to be explored for broader applications in toxicology.

Keywords

persistent toxic substances screening; multimodal deep learning; environmental computational toxicology; toxicity pathways; cross-species.

Machine learning-based model with high accuracy and broad applicability domains for screening PMT/vPvM substances

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Persistent, mobile, and toxic (PMT) substances and very persistent and very mobile (vPvM) substances can transport over long distances from various sources, increasing the public health risk. A rapid and high-throughput screening of PMT/vPvM substances is thus warranted to the risk prevention and mitigation measures. Herein, we construct a machine learning-based screening system integrated with five models for high-throughput classification of PMT/vPvM substances. The models are constructed with 44,971 substances by conventional learning, deep learning, and ensemble learning algorithms, among which, LightGBM and XGBoost outperform other algorithms with metrics exceeding 0.900. Good model interpretability is achieved through the number of free halogen atoms (fr_halogen) and the logarithm of partition coefficient (MolLogP) as the two most critical molecular descriptors representing the persistence and mobility of substances, respectively. Our screening system exhibits a great generalization capability with area under the receiver operating characteristic curve (AUROC) above 0.942 and is successfully applied to the persistent organic pollutants (POPs), prioritized PMT/vPvM substances, and pesticides. The screening system constructed in this study can serve as an efficient and reliable tool for high-throughput risk assessment and the prioritization of managing emerging contaminants.

Soil microbial effects on the mineralization, extractable residue, bound residue, and metabolism of a novel vanillin-derived pesticide, vanisulfane

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Vanisulfane, a novel plant antiviral agent, holds significant potential for the prevention and control of viral crop diseases. However, key aspects regarding its fate characteristics, soil transformation pathways, and the influence of microorganisms on its degradation process remain unknown. Here we conducted a comprehensive investigation to study the fate of two different ¹⁴C-labeled positions of vanisulfane in aerobic yellow pine soil using isotope tracer technology combined with HPLC and LC-MS/MS. By comparing its degradation in sterilized and non-sterilized soils, we aimed to elucidate the influence of soil microorganisms. After a 100-day treatment period, we observed distinct differences in the levels of extractable residue, bound residue, and mineralization for the two different ¹⁴C-labeled positions of vanisulfane in both sterilized and non-sterilized soils. The extractable residue ranged from 15.8-17.8% and 35.1-38.3%, while the bound residue ranged from 29.2-34.8% and 34.2-35.5%. Similarly, mineralization was measured at 42.6-49.8% and 27.3-30.6% in non-sterilized and sterilized soils, respectively. The estimated first-order half-lives for vanisulfane were 1.98-2.48 days and 17.00-18.23 days in these soils. Further investigations unveiled that vanisulfane degradation in aerobic yellow pine soil is primarily driven by biological processes, supported by the observed first-order half-lives in both sterilized and non-sterilized soils. Notably, we detected five distinct metabolites of vanisulfane, which were consistent across the two soil conditions. We speculated possible structures for four of these metabolites and proposed a potential degradation pathway involving sulfur arm cleavage, methyl elimination, and oxidation reactions. These findings underscore the substantial contribution of soil microbial activity to the extractable residue, bound residue, mineralization, and overall degradation of vanisulfane in soil. Our study enhances the current understanding of the fate and behavior of this innovative plant antiviral agent, paving the way for further research and effective utilization in crop disease management.

Keywords

soil microorganism; pesticide; vanisulfane; degradation; mineralization; bound residue.

Uptake, translocation and accumulation of decabromodiphenyl ethane in water spinach (*Ipomoea aquatica* Forsk.) and cherry radish (*Raphanus sativus* L.)

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Decabromodiphenyl ethane (DBDPE) is a persistent organic pollutant detected in soil with increasing frequency and concentration in recent years. DBDPE in the agricultural soil may be accumulated by crops and in turn, threaten human health through the food chain. However, the fate and plant uptake of DBDPE in the soil environment is still not well elucidated. In this study, DBDPE was ¹⁴C-labeled to facilitate investigating its fate in soil-plant systems, as well as its dynamic uptake and accumulation by water spinach and cherry radish. Results showed that the vast majority of DBDPE was retained in the soil (>97%) during the 60-day planting time, primarily as extractable residues (>89%), with little bound residues. The analysis of gas chromatography-mass spectrometry (GC-MS) suggested that DBDPE had been present in the soil in its parent state within 60 days, and no metabolites were detected. After being grown in the soil for 60d, the plant uptake of DBDPE was only 0.05-0.07% of the applied compound. Autoradiographic imaging revealed that roots were the predominant part of DBDPE accumulation for both vegetables. For water spinach, the bioconcentration factor (BCF) of DBDPE in different tissues was in the order of roots > stems > leaves; for cherry radish, the order was fibrous roots > fleshy roots > leaves. The translocation factor (TF) values were less than one during the 60 days, suggesting that DBDPE was less prone to translocate in vegetables. The estimated daily intake (EDI) of DBDPE via vegetable consumption was 0.16 and 0.08 ng kg⁻¹ day⁻¹ for water spinach and cherry radish, respectively. This work helps the better understanding of the fate of DBDPE in soil-plant systems, and will contribute to the assessment of its environmental and human health risks.

Keywords

decabromodiphenyl ethane; Carbon-14 tracing; fate; plant uptake; translocation; accumulation.

Additives release from agricultural plastic films in water: experiment and modeling

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Globally, more than 6 million metric tons of agricultural plastic films are used to increase crop yields and reduce the use of water and herbicides, resulting in the contamination of soil and water by plastic debris and additives. However, knowledge of the occurrence and release of additives from agricultural films is limited. In this study, suspect screening with high-resolution mass spectrometry, one-dimensional Fickian diffusion models, and linear free-energy relationships (LFERs) were used to determine the occurrence and mass transfer of various additives from agricultural plastic films. A total of 89 additives were tentatively identified in 40 films, and 62 of them were further validated and quantified. The aqueous concentrations of 26 released additives reached mg L^{-1} after a 28-day incubation at 25 °C. Diffusion models and LFERs demonstrated that the film-water partition coefficient and the diffusivity in polymer, the two critical parameters controlling mass transfer, could be predicted using Abraham descriptors. The findings of this study highlighted the need for future research on the environmental fate and risk assessment of previously neglected additives in agricultural plastic films and other similar products.

Keywords

endocrine disrupting compounds; agricultural plastic; plasticizer; ecological risk; diffusion; release kinetic.

Reduced graphene oxide enhances the transformation of ¹⁴C-Triclosan to non-extractable residues but inhibits its mineralization in paddy soil

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Reduced graphene oxide (RGO) is one of common nanocarriers that is widely used in nanopesticides and nanofertilizers, which is due to its high binding energy with pesticides and the potential for enhancing bioavailability and targeted transport. Triclosan is an antimicrobial agent added in pharmaceuticals and personal care products. Extensive application and release of RGO and triclosan has posed potential risks to the environment and human health. The understanding about the impact of RGO on the fate of triclosan in paddy soil is still limited. Triclosan, with three concentrations (50, 100 and 500 mg kg⁻¹), was employed in the present study to determine its distribution, degradation and mineralization in paddy soil coexisted with RGO. Compared with the control, RGO (500 mg kg⁻¹) significantly inhibited the mineralization of triclosan, and reduced its extractability by 6.5%. The non-extractable residues of triclosan in RGO-contaminated soil (100 and 500 mg kg⁻¹) were 2.9–13.3% greater than that of the control at 112 d. RGO also accelerated the dissipation of triclosan, and its degradation products in both treatments and control were tentatively identified via ¹⁴C-labeling method and LC-QTOF-MS analysis. The concentrations of the major metabolites (methyl-triclosan and dechlorinated dimer) were inversely related with the concentrations of RGO. RGO at 50 mg kg⁻¹ or lower had a negligible effect on the degradation of triclosan in paddy soil. Triclosan was strongly adsorbed onto RGO-contaminated soil, which may play a vital role in the fate of triclosan in RGO-contaminated paddy soil. Interestingly, RGO had little effect on triclosan-degrading bacteria via soil microbial community analysis. This study helps understand the effects of RGO on the transformation of triclosan in paddy soil, which is of significance to evaluate the environmental risk of triclosan in RGO-contaminated soil.

Keywords

reduced graphene oxide; triclosan; transformation; bacteria; adsorption; paddy soil.

Tissue distribution, debromination and human dietary risk evaluation of decabromodiphenyl ether in continuous oral exposed laying hens

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As one of the most widely used brominated flame retardants, Decabromodiphenyl ether (BDE-209) is receiving much attention due to its prevalence and persistence in the environment, with potential adverse effects on human dietary health. This study investigated the specific distribution and metabolic transformation in different tissues of ^{14}C labeling BDE-209 administered at 6.25 mg/day per laying hen, which could facilitate the assessment of chicken products safety. Approximately 79.94% and 88.90% of the radioactivity was excreted following oral exposure to BDE-209 for 4 and 7 consecutive days, respectively. Although the majority of BDE-209 and its metabolites in vivo were observed in the gastrointestinal tract and its contents, they also accumulated in various tissues, ranking as follicle > liver > gallbladder > abdominal fat > blood (concentration, wet weight). Fortunately, muscle (including breast, wings and legs) had a lower proportion of BDE-209 compared to other tissues, with no significant difference between the 4 d and 7 d groups ($p > 0.05$). Levels of BDE-209 in egg yolk were significantly higher than egg white during the experiment ($p < 0.05$), indicating maternal transfer during ovogenesis after intestinal absorption. However, Hazard Quotient (HQ) suggested that there was no cancer risk or management risk of BDE-209 residing in the edible tissues of laying hens in both groups. In addition, excreta GC/EI-MS analysis revealed that BDE-209 was mainly converted to hepta-, octa-, and nona-BDE in laying hens through the removal of 1 to 3 bromine atoms. These results will serve subsequent studies into the bioaccumulation via the food chain and detoxification mechanism in animals of BDE-209.

Keywords

decabromodiphenyl ether (BDE-209); laying hens; tissue distribution; maternal transfer; debromination.

Metabolic analysis of antiviral agent dufulin in aerobic soils assisted by diverse positional ¹⁴C labeling with high specific activity

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Dufulin is a new plant antiviral agent that has achieved large-scale field application. However, little has been reported about its degradation products in soil, which is not conducive to a scientific environmental risk assessment. In this study, the metabolites of ¹⁴C-dufulin labelled at two sites with highly specific activities in aerobic soil were investigated. The results showed that dufulin underwent oxidation, esterification, de-ethylation, and ring opening in the soils, and seven products were identified, of which six were identified with benzyl-labeled dufulin and one with thiazolyl-labeled dufulin. The hydroxyl substitution product M2 was present in three soils except for the acidic red loam soil, and the other five products were detected in all soils. During 120 days of incubation, the percentage of all products did not exceed 10% except M7 in cinnamon soil. Therefore, the residues were defined as dufulin parent and metabolite M7 in cinnamon soil and dufulin parent in red, black and moisture soils. The results of this study provide scientific data for the safe and rational use of dufulin. In addition, multi-site labeling and high specific activity tracers greatly facilitate the environmental metabolism study of dufulin and thus this study could provide methodological references for the investigation of other new pesticides.

Keywords

dufulin; ¹⁴C labeling; aerobic soil; metabolites; transformation pathway

Systematic measures for reducing environmental impacts of chemicals in consumer products

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Chemicals are the building blocks of the goods we use. It was estimated that ca. 350000 chemicals and their mixtures used in the global market. In the European Union, around 62% of the chemicals used were hazardous to health. It is necessary to sound manage synthetic chemicals for advancing sustainable development. Only a limited number of the chemicals have data on their stocks, flows, emission rates, and toxicity, limiting sound management of the chemicals. Textiles, apparel, and footwear products are often composed of synthetic materials, including plastics, synthetic rubbers and synthetic fibers. In production and processing of those synthetic materials, a variety of chemical substances are used, such as additives, processing aids and non-intentionally added substances. Current studies have focused on a limited selection of the substances, mostly well-known hazardous ones or those commonly known for their presence in products. As for textiles, apparel, and footwear products, information on identification, contents, emission rates and toxicity of the substances is still limited. Several environmental systems engineering technologies, such as material flow analysis, life cycle assessment and green chemistry, are promising for providing the information, and supporting sound management of chemicals. The results of our previous study show that the outdoor use of synthetic rubbers, as well as lacquers and paints contributed the highest emissions of Di(2-ethylhexhyl) phthalate (DEHP), a widely used plasticizer, toward environmental matrices in China. Systematic measures for controlling ecological risks of DEHP were proposed. Polyurethane is one of the most versatile materials in the world. Another study provides a material flow analysis coupled with life cycle assessment of polyurethane in China, assessing a variety of environmental and human health impacts across its life cycle. Both studies may provide systematic data and methodology necessary for sound management of synthetic chemicals.

Keywords

chemical management; material flow analysis; multimedia environmental model; ecological risk analysis

Atmospheric secondary pollution chemistry of volatile chemical products

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Volatile chemical products (VCPs) have been recognized as an important source of volatile organic compounds emissions to the atmosphere, making VCPs become new precursors leading to secondary pollution in urban atmosphere. Due to the abundance and limited atmospheric transformation mechanisms of VCPs, it is a challenge to identify priority controlled VCPs for the secondary pollution prevention. Herein, quantum chemical calculations and kinetics modeling were employed to investigate the atmospheric transformation mechanism of four types VCPs (i.e., emerging amines, methylsiloxanes, organophosphates and aromatics), and achieved three innovative achievements:

(1) A machine learning and big-data driven methods to study the atmospheric transformation mechanisms (i.e., oxidation and clustering) of VCPs was developed. The developed methods increase the efficiency of studying the atmospheric oxidation mechanisms and clustering of VCPs by nearly 10-100-fold, providing an effective tool for investigating the atmospheric transformation mechanism of VCPs.

(2) Secondary pollution mechanisms of the selected four types of VCPs were revealed. It was found that these four types of VCPs undergo three novel oxidation mechanisms by employing developed method. More importantly, they can produce low volatile products or highly toxic products (e.g., HCHO, nitrosamines, etc.) via three novel mechanisms. Additionally, we disclosed chemical nature that determines the potential of emerging amines to binary clustering with inorganic acids. Based on the understanding of binary clustering mechanisms, a synergistic clustering mechanism of emerging amines was proposed, which were confirmed by field observation in Beijing.

(3) A predictive model for secondary pollution potential of important VCPs was developed and the priority controlled VCPs were identified. Selecting emerging amines as a representative, we developed four high-throughput models to predict the potential of emerging amines to produce carcinogenic nitrosamine and their potential to clustering with inorganic acids. We found that six emerging amines have high potential for atmospheric secondary pollution and should be prioritized for prevention and control.

Keywords

Volatile chemical products; transformation mechanism; quantum chemical calculation; fine particulate matter; toxic products

The toxic mechanism of 6:2 Cl-PFESA in adolescent male rats: Endocrine disorders and liver inflammation regulated by the gut microbiota-gut-testis/liver axis

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6:2 chlorinated polyfluorinated ether sulfonic acid (6:2 Cl-PFESA), a perfluorooctanesulfonate alternative, has been demonstrated that possesses toxicity for mammals. However, the toxic mechanism of 6:2 Cl-PFESA in mammals is unknown. Herein, adolescent male rats were administered with 50 µg/kg/day 6:2 Cl-PFESA for 28 days (oral gavage) to estimate the toxicity of 6:2 Cl-PFESA and investigate its toxic mechanism. Significant changes in some hematological indicators (e.g., aspartate transaminase and neutrophil) and liver section (inflammatory cell infiltration) indicated that 6:2 Cl-PFESA exposure caused rat hepatotoxicity. Six steroid hormones (e.g., testosterone, progesterone, and cortisol) in serum and thirteen genes in testicles (related to the pathway of steroid hormone biosynthesis) were significantly regulated in 6:2 Cl-PFESA treated rats. This suggested 6:2 Cl-PFESA induced rat endocrine disorders. Compared to the controls, the mean relative abundance of Ruminococcaceae, Pasteurellaceae, Micrococcaceae, and Desulfovibrionaceae was significantly regulated by 1.3-, 0.40-, 0.32-, and 3.2-fold, in the 6:2 Cl-PFESA rats, respectively. 6:2 Cl-PFESA treatment also significantly disturbed 47 gut metabolites (29 up-regulated and 18 down-regulated), mainly including bile acids, short-chain fatty acids, and amino acids. In summary, 6:2 Cl-PFESA induced endocrine disorders and liver inflammation in rats via altering the gut microbiota-gut-testis/liver axis. This study first reveals the toxic mechanism of 6:2 Cl-PFESA in mammals through a multi-omics approach and provides a comprehensive insight into the toxic mechanism of 6:2 Cl-PFESA.

Keywords

PFOS alternative; toxicity mechanism; liver inflammation; endocrine disorder.

Identification of aryl hydrocarbon receptor agonists from real environmental samples

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In this study, sediment samples from an e-waste recycling site have been extracted with accelerated solvent extraction followed by toxicity assay. Using a cell-based genetic reporter assay that utilizes the luciferase reporter gene, aryl hydrocarbon receptor (AhR) agonistic potency in the extracts were measured. The positive samples with high potency have been fractionated using an established method. () In brief, separation of extract using three columns including a cyanopropyl silica column, a nitrophenylpropyl silica column, and a porous graphitized carbon column. According to the cell assay, the active fractions has been performed using both gas chromatography- and liquid chromatography- high resolution mass spectrometry analyses. We then identified 23 AhR agonists in the positive fractions. Benzo [k]fluoranthene and 6-nitrochrysene were the dominant AhR agonists of the AhR activation effects measured in the parent extracts. The major contributor of AhR activity in these sediment samples were petroleum product combustion and biomass combustion. For fractions were collected for unknown AhR-active chemical identification using liquid chromatography or gas chromatography coupled with high resolution mass spectrometry system. We identified 57 AhR agonists in the four fractions, respectively. The identified AhR agonist including 7,12-dimethylbenz [a]anthracene and 8,9,11-trimethylbenz [a]anthracene being the major contributors explained a small potency of the extracts. For the identification most potent AhR agonist, more HPLC columns were required for the optimization of fractionation to purify more potential toxicant.

Influence of dietary status on the obesogenic effects of erythromycin antibiotic on *Caenorhabditis elegans*

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As emerging pollutants, antibiotics were widely detected in environmental matrix (e.g., surface water, soil and sediments) and dietary sources (e.g., chicken and fish). Recently, epidemiological and laboratory studies demonstrated that antibiotics promoted obesity. However, it remained unclear whether the obesogenic effects of antibiotics would be influenced by environment matrix and dietary sources would influence. In present study, erythromycin (ERY) was chosen to represent environmental antibiotics, and *C. elegans* was chosen as the model organism. The ERY exposure was performed with culture medium or pretreated bacteria (both dead and alive bacteria) which referred to environmental and dietary exposure. Results showed that ERY significantly stimulated body width and triglyceride contents in both environmental and dietary exposure. Especially, the stimulation in dietary exposure was more pronounced with live bacteria than dead ones. Furthermore, ERY via environmental exposure inhibited the activities of carnitine acyl transferase (CPT) or acyl CoA synthetase (ACS), indicating decreases of fatty acid β -oxidation (i.e., lipid consumption). However, ERY via dietary exposure stimulated the activity of fatty acid synthetase (FAS) in addition to its inhibition on CPT and ACS. The different effects by dietary exposure could be resulted from influences of ERY on the bacteria where ERY stimulated carbohydrate contents and altered fatty acid composition (especially short-chain fatty acids). Further analysis showed that ERY in environmental exposure upregulated expressions of *daf-2* and *daf-16*, while it in dietary exposure showed downregulation on *daf-2* expressions and upregulation on *daf-16* ones. Summing up, the present study demonstrated the influences of environmental and dietary exposure on the obesogenic effects of ERY, and the involvement of insulin signaling pathways.

Keywords

erythromycin; obesogenic effect; dietary exposure; *C. elegans*; metabolism.

Screening and mechanism profiling of organophosphate esters via adverse outcome pathway

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As the typical emerging contaminants, organophosphate esters (OPEs) have been frequently detected in environmental media. Increasing toxicological studies showed that OPEs could elicit various toxic effects. However, the mechanisms are still unclear and most toxic effects are relatively isolated. Many studies mainly focus on one/several biological levels, lacking the integration of biological effects at multiple levels. Notably, the adverse outcome pathway (AOP) framework is expected to address this challenge by integrating toxicogenic events at different biological levels and supplementing their logical hierarchy or cause-and-effect relationships induced by OPEs through highly cohesive and low-coupling modules. In this study, the mechanism-driven multi-AOPs networks and predictive models were developed to provide theoretical data for OPEs' risk assessment. Transcriptomic technology and computational toxicology were used to explore the critical molecular initiating events (MIEs), key events (KEs), key events relationships (KERs), and adverse outcomes (AOs) disturbed by TPP. And three key AOPs describing mechanisms of toxicity were developed. The weight of evidence (WoE) approach was utilized to assess the evidence-supported postulated AOPs according to the organization for economic co-operation and development (OECD) guidelines. Such screening strategies were useful to predict the toxicity pathway perturbation and identify the alert substructures of OPEs in a high-throughput manner. This study provided theoretical data to elucidate the toxicological effects and assess the toxicity risk, contributing to prevention and control of OPEs.

Keywords

emerging contaminants; organophosphate esters; adverse outcome pathways; computational toxicology; risk prediction and assessment

Redox proteomics reveals a novel mechanism of 1-nitropyrene-induced cytotoxicity

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PM2.5 is the leading environmental risk factor for death globally. 1-Nitropyrene (1-NP) is the most-abundant nitro-polycyclic aromatic hydrocarbons and representative diesel exhaust-sourced component of PM2.5¹. More importantly, 1-NP demonstrates significantly higher cytotoxicity than its structural analogs and precursor². However, although extensively studied, current working mechanisms for 1-nitropyrene are similar to other PAHs, which made it hard to explain the severe cytotoxicity and mutagenicity. In this study, we compare 1-NP with its structural analog 3-nitrofluoranthene and precursor pyrene in human lung epithelial cell lines. An acute ROS accompanied by cell death was observed for 1-NP. Using compound-centric redox proteomics analysis, we showed that 1-NP significantly re-modeled the redox proteome and specifically targeted on ROS reduction pathway. Superoxide dismutase 1 (SOD1) was identified as a potential target. We further demonstrated that 1-NP directly acted on cysteine residue Cys111 and inhibited SOD activity. The position of nitroxide determines its direct target and contributes to the unique mechanism of 1-NP. A novel mechanism for 1-NP cytotoxicity and ROS induction was therefore proposed.

Keywords

redox proteomics; 1-nitropyrene; ROS; superoxide dismutase; PM2.5.

High throughput mass spectrometry-based metabolomics reveal nanoplastics-induced mitochondrial dysfunction in normal human-derived cells

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Plastic particles with a diameter of less than 0.1 μm (nanoplastics (NPs)) have been extensively manufactured and used as engineered nanomaterials. Human activities have resulted in the discharge of large amounts of plastic waste which can continually release secondary NPs. These plastic particles can bioaccumulate in the food chain, which may ultimately result in human exposure. However, the NP-related health impacts on humans are far from understood. Associations between NP exposure and inflammation, immunotoxicity, and neurological dysfunction have been demonstrated in mice. *In vitro* data have shown that the internalization of NPs occurs in various human cell lines, indicating that damage to sensitive organelles especially mitochondria may be a primary mechanism of NP-induced toxicity in cells. The liver and lung are highly involved in metabolism and contain the most well-established metabolic enzymes in humans, while the NP-induced cellular responses of endogenous metabolites in the two vulnerable organs have not been well studied.

In this study, we investigated the effects of 80-nm NPs on mitochondrial functions and metabolic pathways in normal human hepatic cells and lung cells. NP exposure did not induce mass cell death; however, NPs could enter the cells and cause mitochondrial damage was further evidenced by the overproduction of mitochondrial reactive oxygen species, alterations in the mitochondrial membrane potential, and the suppression of mitochondrial respiration. High-throughput mass spectrometry-based metabolomics further confirmed that the most significantly impacted processes were mitochondrial-related. The effects observed at the molecular and cellular levels could be considered predisease events to predict NP exposure outcomes at the tissue and organ levels. Thus, the mitochondrial damage observed in this study might cause cells, and eventually organ tissues, to malfunction. This study provides new insights into NP-induced toxicity mechanisms in human cell lines and offers basic scientific data on the health risks of NP exposure in humans.

Keywords

plastic particles, cytotoxicity, mitochondria, electron transport chain, energy metabolism

Cadmium exposure accelerated the aging process in the nematode *Caenorhabditis elegans*

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The heavy metal cadmium is a persistent environmental toxicant. The health risks caused by cadmium has been received much concern. Long-term chronic exposure to cadmium has been associated high incidence of several chronic diseases including cancer. Aging is defined as progressive functional degeneration, resulting in high incidence of age-related diseases. Although it has been generally accepted that environmental pollution plays important roles in aging processes, the experimental evidence is still insufficient. By using the nematode *Caenorhabditis elegans* as an in vivo model, we investigated whether low doses of cadmium exposure accelerated the aging processes. The results presented here indicated that cadmium exposure reduced lifespan and promoted movement paralysis at the dose of 5.0 and 10.0 μM . Cadmium exposure reduced the pharyngeal pumping rates and prolonged the defecation cycle in a dose-dependent and age-dependent manner. These results indicated that cadmium exposure accelerated functional degeneration in *C. elegans*. By using transgenic worm strains, it was found that cadmium exposure promoted the redistribution of yolk protein, accelerated the accumulation of lipofuscin, and increased the activities of β -galactosidase, all of which are the biomarkers of aging. Finally, we found that cadmium exposure disturbed protein homeostasis and thereby accelerated the aging process in *C. elegans*.

Keywords

cadmium; *Caenorhabditis elegans*; aging; functional degeneration

Environmental occurrence and ecological risks of psychoactive substances

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Psychoactive substances are ubiquitous in the environment at low concentrations, and tobacco, cannabis, etc. are all widely-existing examples. Given their potent biological activity, psychoactive substances are suspected to be harmful to the environment, and reports of their ecological risks are gradually increasing. As an important psychoactive substance, cotinine is prevalent in aquatic environment and its bioactivity could pose health risks to aquatic organisms. However, the underlying mechanisms of its adverse health impacts on aquatic organisms remain poorly understood. The effect of cotinine exposure on the developmental and locomotor behavior of zebrafish (*Danio rerio*) was investigated in this paper, and the toxicity mechanism of zebrafish exposed to 10 µg/L of cotinine six days post fertilization was analyzed using neurotransmitters and overall endogenous metabolism. Exposure to environmentally relevant concentrations of cotinine was found to cause mild developmental toxicity in zebrafish, but it had significant toxic effects on neurobehaviors, including spontaneous movement, touch response, and swimming speed. In addition, the cotinine exposure altered the levels of eight neurotransmitters, including dopamine, serotonin, kynurenine, tyramine, epinephrine, norepinephrine, phenylethylamine, and N-acetylaspartic acid. Using metabolomics technology, we identified significant alterations in thirty metabolites and two pathways (glycine, serine, threonine metabolism and lysine biosynthesis) due to exposure to cotinine. The new findings provide a comprehensive understanding of the ecological risks associated with exposure to cotinine in aquatic environments.

Keywords

Psychoactive substance; distribution; neurobehavioral toxicity; metabolomics.

Direct uptake and intracellular dissolution of HgS nanoparticles: Evidence from a bacterial biosensor approach

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Mercury sulfide nanoparticles (HgS_{NP}), occur widely in oxic and anoxic environments, can be microbially converted to highly toxic methylmercury or volatile elemental mercury, but it remains challenging to assess their bioavailability. In this study, an *Escherichia coli*-based whole-cell fluorescent biosensor was developed to explore the bioavailability and microbial activation process of HgS_{NP}. Results show that HgS_{NP} (3.17 ± 0.96 nm) trigger a sharp increase in fluorescence intensity of the biosensor, with signal responses almost equal to that of ionic Hg (Hg(II)) within 10 h, indicating high bioavailability of HgS_{NP}. The intracellular total Hg (THg) of cells exposed to HgS_{NP} (200 µg L⁻¹) were 3.52-8.59 folds higher than cells exposed to Hg(II) (200 µg L⁻¹), suggesting that intracellular HgS_{NP} were only partially dissolved. Speciation analysis using size exclusive chromatography (SEC)-ICP-MS revealed that bacterial filtrate was not responsible for HgS_{NP} dissolution, suggesting that HgS_{NP} entered cells in nanoparticle form. Combined with fluorescence intensity and intracellular THg analysis, the intracellular HgS_{NP} dissolution ratio was estimated as 22-29%. Overall, our findings highlight the rapid internalization and high intracellular dissolution ratio of HgS_{NP} by *E. coli*, and intracellular THg combined with biosensors could provide innovative tools to explore the microbial uptake and dissolution of HgS_{NP}.

Keywords

mercury sulfide nanoparticles (HgS_{NP}); intracellular dissolution; soluble Hg(II); bioavailability; whole-cell biosensor.

5-hydroxymethyl-2-furfural (5-HMF) might be a potential key toxic component of cigarette smoke that induces male reproductive damage

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It's well known that cigarette smoking (CS) induces male reproductive dysfunction, but the key components and mechanism still remain unclear. Previously, our group had successfully isolated a new component, 5-hydroxymethyl-furfural (5-HMF), from cigarette smoke extract (CSE). It is abundant (comparable to nicotine) in CS, and could be metabolically activated by human CYP2A13, and is speculated as one of the important toxic components in CS. In the present study, the effects of 5-HMF on testicular injury were evaluated *in vitro* and *in vivo*, and the target and mechanism were further explored. The results showed as follows: (1) compared with the rest components of CSE (CSE-O), 5-HMF component (CSE-H) induced obvious testicular spermatogenic disorder and reduced sperm count, and the decrease in the expression of tight junction related proteins, ZO-1 and Occludin, in sertoli cells in mice, which was confirmed by the mice with long-term inhalation of 5-HMF standard. (2) 5-HMF damaged the tightly connected "sandwich" structure and the "anti-penetration" function of the blood-testis barrier (BTB), causing the accumulation of autophagy bodies in Sertoli cells, the increase of autophagy flow, and the upregulation of ATG12, and the elimination of atg12 could significantly alleviate the destruction of BTB and spermatogenesis disorders. (3) 5-HMF could also cause meiosis block in spermatocytes resulting in the decrease in cell numbers, and induce the expression of CYP2A5 in mice, and knockout of cyp2a5 could significantly alleviate the above damages. Further, 5-HMF was proved to be metabolized by CYP2A5 to form the active metabolite DFF and aggravate the damages. In summary, 5-HMF first damage the sertoli cells to cause BTB destruction, which leads large amount of 5-HMF into testis, and then target spermatocyte to cause spermatogenic dysfunction. The study helps enrich the understanding of male reproductive dysfunction caused by smoking, and further suggest that 5-HMF might be an important reproductive toxic component of cigarette smoke.

Keywords

5-hydroxymethyl-2-furfural; cigarette smoking; male reproductive toxicity; cytochrome P450 2A13; metabolic activation

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A simple signal enhancement strategy for Rapid Precoated Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging

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Matrix-assisted laser Desorption/Ionization mass spectrometry imaging (MALDI-MSI) is one of the primary techniques in this area. To increase the throughput of MALDI-MSI, pre-coated approach was introduced to eliminate the time-consuming sample preparation process and improve its utility for applications. In contrast, the pre-coat MALDI-MSI's utility is still limited due to the low ionization yield and appearance of “dark pixels” by the poor tissue-matrix merging. In this study, we propose an easy-to-use and rapid post-processing method (~30 seconds) as a signal enhancement strategy to pre-coated MALDI-MSI. The processing method is to spray a small amount of water or 70% methanol (MeOH) for 15 seconds and subsequent microwave treatment to a tissue-mounted pre-coated ITO slide for 4 seconds. The strategy is demonstrated with 8 μm thickness kidney tissue sections with both MALDI-TOF and MALDI-QTOF. The result shows a 1.5-2-fold signal increase in the lipid region (600-900m/z) and a reduction in the number of empty spectra in both 2,4-Dihydroxybenzoic acid (DHB) pre-coated slide in positive mode and N-(1-Naphthyl)ethylenediamine dihydrochloride (NEDC) pre-coated slide in negative mode after the post-processing treatment. In summary, the proposed strategy increases the signal yield in the lipid region (600-900m/z), and reduces empty spectra and results in better MS imaging quality with an addition ≤ 30 seconds to pre-coated MALDI-MSI sample preparation. We believe this rapid processing method will promote using the MALDI-MSI in applications.