

ABSTRACT BOOK

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Rethinking Environmental Balance for the Future

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Abstract Book

SETAC Asia-Pacific 15th Biennial Meeting

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1. Environmental and Human Toxicology, and Ecology

1.01.P - Advances and Regulatory Applications of New Approach Methodologies (NAMs) in the Environmental Risk Assessment of Chemicals

1.01.P–Mo001 Fluorescence-Based Bioassay for Metal Stress Profiling in Marine Diatoms

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Trace metals are persistent contaminants in coastal ecosystems, yet toxicity assessments for marine diatoms still rely largely on growth inhibition or single-endpoint responses that provide limited mechanistic resolution. This study developed an integrated fluorescence-based bioassay to characterize metal-specific stress responses in two marine diatoms exposed to four environmentally relevant metals, As, Cr(VI), Hg, and Ni. Chlorophyll fluorescence was used as an indicator of photosystem impairment, while Nile Red-based lipid-body fluorescence was applied as a proxy for metabolic reallocation. Species- and metal-specific EC10 and EC50 values were derived for both fluorescence endpoints, and ROS measurement was used to compare cellular stress responses across metal treatments. The two diatoms showed distinct sensitivity profiles, with the benthic species generally exhibiting higher sensitivity across most metals than the planktonic species. Lipid-body fluorescence responded at lower effect levels than chlorophyll fluorescence for several metals, particularly Hg, As, and Cr(VI), indicating that lipid reallocation may serve as an earlier stress signal preceding photosynthetic dysfunction. The magnitude and direction of divergence between lipid and chlorophyll fluorescence thresholds varied among metals, suggesting metal-specific stress sequencing rather than a uniform toxicity pathway. ROS-based stress patterns provided an additional comparative endpoint supporting the interpretation of metal-dependent cellular stress. By coupling photosystem performance, lipid reallocation, and ROS-based stress assessment, this study provides metal-resolved mechanistic toxicity profiles that cannot be captured by conventional single-endpoint approaches. The correspondence between fluorescence-derived EC values and published growth-based toxicity thresholds further supports the applicability of this framework as a streamlined and mechanistically informative bioassay for marine diatom-based coastal metal risk assessment.

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1.01.P–Mo002 Standardizing Exposure Media to Enhance Rigor and Reproducibility of Zebrafish Embryo-Based Toxicity Assays

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Zebrafish embryos have been widely used as New Approach Methodologies (NAMs) to support chemical toxicity screens, prioritization of xenobiotics for testing in mammals, and hypothesis-driven studies

focused on revealing mechanisms underlying adverse phenotypes. As a result, prior efforts have raised awareness about the need to identify potential sources of intra- and inter-laboratory variability within zebrafish-based assays as well as develop internationally harmonized guidelines for determining the toxicity of chemicals on embryonic stages of zebrafish. Despite key advancements over the last 15 years, these efforts have largely overlooked the influence of ionic composition and strength of exposure media as an experimental variable that may affect the prevalence and/or severity of chemically induced abnormalities, resulting in a potential "blind spot" that may, in part, be critical for increasing the rigor and reproducibility of zebrafish-based assays. Using triphenyl phosphate (TPHP) – a widely used organophosphate ester (OPE) – as a case study, this presentation will focus on summarizing recent studies from our group that highlight the critical role of exposure media in driving phenotypic outcomes following TPHP exposure during embryonic development. Over the last 10+ years, our studies have revealed that TPHP blocks cardiac looping during zebrafish embryogenesis in a concentration-dependent manner, a phenotype that is 1) dependent on epidermal injury, aberrant nuclear receptor signaling, disruption of embryonic osmoregulation, and pericardial edema formation and 2) exacerbated by an increase in the ionic strength of exposure media. However, following immersion of embryos within exposure media, TPHP uptake across the embryonic epidermis is not altered under these varying experimental conditions, as increasing the osmolarity of exposure media with D-mannitol (an osmotic diuretic which mitigates TPHP-induced pericardial edema) and increasing the ionic strength of exposure media (which exacerbates TPHP-induced pericardial edema) do not affect embryonic doses of TPHP. Overall, our findings 1) raise concerns about the potential influence of exposure media on the toxicity of other chemical classes (beyond OPEs) at the morphological, physiological, and/or behavioral level and 2) underscore the need to standardize exposure media used in zebrafish-based chemical toxicity screens and mechanistic studies conducted around the world.

1.01.P–Mo003 Synchrotron-based X-ray fluorescence microscopy for unravelling the toxicology of metals in wildlife: review and future applications

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Synchrotron radiation X-ray fluorescence microscopy (SR-XFM) offers unique capabilities for non-destructive, high-resolution mapping of elemental speciation and distribution within intact tissues. This literature review synthesizes current applications of SR-XFM in evaluating the impacts of metals across a range of wildlife taxa. We examine how the unique capability of SR-XFM to image metal concentrations and speciation at high spatial resolution has advanced our understanding of metal uptake, biodistribution, and speciation in various organisms. This review highlights that few studies utilize SR-XFM in exploring metal distribution in early life stages, however, the spatially resolved imaging data available indicates preferential accumulation in excretory organs and organ primordia in embryos and larvae. These insights have highlighted the potential mechanistic links between metal exposure and adverse developmental outcomes. Methodological considerations, including sample preparation, detection limits, and challenges associated with low-Z element detection, are also discussed. SR-XFM has yet to be widely applied in toxicological studies of many wildlife taxa, including large and anatomically complex marine species such as marine turtles, primarily due to constraints in sample acquisition and preparation. Nevertheless, the application of SR-XFM to unravel the accumulation, biodistribution and toxicity of metals in wildlife could yield substantial benefits for conservation and management. We conclude that SR-XFM represents a valuable, but underutilized, tool in environmental toxicology, offering unprecedented insight into the spatial dynamics of contaminant exposure during early development. We propose a methodology for utilizing this tool for investigating the impact of metal exposure on embryonic development of a threatened marine reptile in ovo.

1.01.P–Mo004 Comparative Effects of DEHP, DEHTP and DINCH on Lipid Metabolism in Zebrafish Larvae

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Di(2-ethylhexyl) phthalate (DEHP) is a well-established disruptor of lipid metabolism, yet its commonly used alternatives, di(2-ethylhexyl) terephthalate (DEHTP) and diisononyl cyclohexane-1,2-dicarboxylate (DINCH), remain insufficiently characterized in terms of their metabolic effects. This study aimed to evaluate disturbances in lipid metabolism following early-life exposure to these plasticizers and to compare their mechanisms with atorvastatin, a cholesterol-lowering pharmaceutical.
Freshly fertilized zebrafish (Danio rerio) embryos were exposed till 7dpf to solvent control (0.01% dimethyl sulfoxide), DEHP, DEHTP, DINCH, or atorvastatin. Plasticizer concentrations were 0.1 and 1.0 milligrams per liter. Endpoints included total cholesterol (TC), high-density lipoprotein cholesterol (HDL), and neutral lipid accumulation measured using Oil Red O (ORO) staining. Gene expression analysis targeted pathways involved in cholesterol biosynthesis, nuclear receptor signaling, and bile acid regulation.
Genes showing significant alterations, including 3-hydroxy-3-methylglutaryl-coenzyme A reductase, low-density lipoprotein receptor a, cholesterol 7 alpha-hydroxylase, and nuclear receptor subfamily 1 group H member 3, were further evaluated using Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS) analysis to assess their conservation and suitability as screening biomarkers.
Exposure to DEHP increased TC levels at 1 mg/L whereas DEHTP and DINCH produced concentration-dependent decreases. Transcriptional analysis revealed consistent downregulation of genes involved in cholesterol biosynthesis and nuclear receptor signaling across plasticizer treatments. In contrast, atorvastatin exposure resulted in upregulation of genes such as the low-density lipoprotein receptor, consistent with its known mechanism of action and in opposition to the responses observed for the alternative plasticizers. The divergent transcriptional responses suggest that these alternatives may not reduce lipid levels through canonical pathways, but instead may disrupt lipid transport and homeostasis through distinct mechanisms.
These findings demonstrate that alternative plasticizers, although less potent than DEHP, can still perturb lipid metabolism during early development. Integration with SeqAPASS analysis provides insight into cross-species biological relevance and supports the application of these genes as screening targets for pathway-based toxicological assessment.

1.01.P–Mo005 A Standardizable 21-day Lemna minuta Bioassay Reveals Time-Dependent Pharmaceutical Toxicity Missed by Acute Testing

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Conventional short-term bioassays underpin most regulatory ecotoxicity frameworks but are fundamentally mismatched to the pseudo-persistent exposure conditions typical of pharmaceutical contaminants in aquatic systems. To address this gap, we developed a standardizable 21-day chronic bioassay using the freshwater duckweed Lemna minuta, integrating a miniaturized 6-well plate format with image-based frond area quantification using a single validated global threshold, enabling reproducible and high-throughput growth measurement across multiple clonal generations.
Applied to twelve pharmaceuticals spanning diverse modes of action, the assay revealed substantial and compound-specific time-dependent toxicity. 21-day EC50 values were significantly lower than 7-day values for the majority of compounds, with acute-to-chronic ratios (ACRs) ranging from 0.9 to 54.4. Candesartan exhibited the most pronounced delayed toxicity (ACR = 54.4), while antibiotics such as levofloxacin and ofloxacin showed minimal temporal change. These divergent profiles highlight that chronic toxicity constitutes an independent dimension of hazard not predictable from acute endpoints

alone.
Species sensitivity distributions constructed by integrating 21-day L. minuta data with published Lemnaceae endpoints yielded PNECs that closely matched independently established regulatory benchmarks for levofloxacin and sulfamethoxazole, and provided a data-driven threshold for climbazole, which currently lacks an EU environmental quality standard. These findings demonstrate that acute assays systematically underestimate pharmaceutical ecotoxicity under environmentally relevant exposure conditions, and establish L. minuta as a scalable platform for integrating chronic plant-based endpoints into risk assessment frameworks.

1.01.P–Mo006 High-Throughput Behavioural Monitoring System Using Daphnia for Mechanistic Environmental Toxicity Assessment

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Current Daphnia-based environmental toxicity testing relies heavily on binary endpoints, often mortality and immobilisation, which lack sensitivity and mechanistic insight. Omics-based NAMs (New Approach Methodologies) offer mechanistic resolution, but lack scalability and direct phenotypic relevance. Bridging this gap is a significant challenge for next-generation risk assessment.
So far, this project has developed a high-throughput behavioural monitoring system using Daphnia magna. The system features controlled climate and exposure conditions, and automated recording of ten 24-well multi well plates. Video tracking software is then used to quantify phenotypic response. The high throughput of the system enables testing of multiple concentrations, chemicals, mixtures, or strains in the same assay.

When developing the system, several key constraints were addressed, including evaporation control, environmental stability, behavioural benchmarking, and reliable tracking across extended (48hr) exposure periods. Benchmarking was conducted using reference chemicals with diverse MoA (Modes of Action) and established toxicity profiles to evaluate sensitivity and reproducibility. On-platform immobilisation was analysed alongside conventional, off-platform immobilisation data to ensure concordance with OECD (Organisation for Economic Co-operation and Development) test guidelines.

Preliminary results show that imazalil-exposed Daphnia showed significantly reduced movement over time compared to controls ($p=0.0321$), and a significant increase in edge preference over time ($p=6.57x10^{-10}$), demonstrating that the platform can track Daphnia <24hrs old and identify behavioural responses to sublethal concentrations.

We aim to observe distinct behavioural signatures across chemicals with differing MoA, enabling mechanistic insight. A particular focus will be on molt-disrupting chemicals, integrating behavioural phenomics with PrecisionTox transcriptomic datasets, investigating whether behavioural responses can be aligned with molting-related Adverse Outcome Pathways.

This work aims to establish behavioural phenomics as a practical and scalable NAM that complements existing approaches by linking organism-level responses to underlying mechanisms. The system provides a platform for high-throughput chemical screening, supporting the development of mechanistically informed risk assessment frameworks, applicable to environmental monitoring and regulatory toxicology.

1.01.P–Mo007 Preliminary Evaluation of Oral Exposure Approach Using Microencapsulated Chemicals in Fish

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The development of New Approach Methodologies (NAMs) has become a global priority in environmental toxicology, driven by the need to reduce the use of vertebrate laboratory animals while maintaining biologically relevant hazard characterization. As part of these efforts, alternative in vivo models and exposure strategies that enable controlled, reproducible dosing are increasingly important. In this study, we explore a oral exposure approach in which chemical substances are encapsulated in microcapsules composed of the biodegradable polymer poly (lactic-co-glycolic acid) (PLGA) and administered orally to fish. This method is intended to support the replacement of mammalian models, such as rodents, with small fish species for chemical hazard and safety assessment. The approach offers several advantages, including reduced animal use, lower space and cost requirements, and direct evaluation of organism-level responses compared with in vitro or in silico methods. Furthermore, microencapsulation enables direct uptake of test substances and facilitates more accurate estimation and control of exposure doses than conventional aqueous exposure. This is particularly relevant for hydrophobic, volatile, or hydrolytically unstable compounds, for which maintaining stable aqueous exposure concentrations is challenging.
To evaluate the feasibility of this approach, chemicals with known toxicity in aqueous exposure tests were encapsulated in PLGA microcapsules and administered orally to medaka (Oryzias latipes). Pyrene and o-terphenyl were selected as model compounds, with reported median lethal concentrations (LC50) for medaka of approximately 1 mg/L and 0.1 mg/L, respectively. The results of oral exposure experiments using microencapsulated compounds are presented and compared with their LC50 values from aqueous exposure studies.

1.01.P–Mo008 Machine Learning-based Assessment of Microplastic Pollution and Human Dietary Risk in Four Commercial Markets Fish Species from Yichang, China

Microplastics (MPs) pose an emerging environmental and public health concern particularly, due to their accumulation in aquaculture species for human consumption. Therefore, the current study considered the abundance, characteristics, and human health risk assessment (HHRA) in four commercially available fish species i.e., Dicentrarchus labrax (Sea bass), Carassius Carassius (Crucian carp), Oreochromis niloticus (Nile tilapia), and Hypophathalmichthys nobilis (Bighead carp) sampled from four various local markets in Yichang, China. A proposed protocol by following (10% KOH, 60 °C, 48 h) used for MPs isolation and characterized using micro-Fourier transform infrared spectrometer (μ-FTIR) and scanning electron microscopy (SEM). The results revealed that the highest average MP abundance (52.5±9.4 items/Kg) was found in sea bass with polymer types dominated by polypropylene (PP) and polyethylene (PE), mainly as black colored fibers within 150-5000 μm size ranges. Moreover, a significant positive correlation (R2 = 0.80; p < 0.001) was observed between fish weight and MPs number. Among the machine learning models, XGBoost and LightGBM exhibited superior predictive performance for MPs accumulation validated by the Taylor diagram. The HHRA also found that estimated annual MPs intake by fish consumption was significantly higher for adult male than for female across all the sampled fish species. In conclusion, sea bass posed the highest exposure risk, followed by Nile tilapia and bighead fish, whereas crucian carp showed the lowest levels of risk to human, which highlights the urgent need for regulatory measurement for the mitigation of MPs contamination in food chain.

1.01.P–Mo009 Development of a Microcapsule-Based Oral Exposure Method for Fish Ecotoxicity Testing

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In chemical safety testing, conventional toxicity tests using mammals have increasingly faced restrictions from the perspective of animal welfare. Therefore, fish-based New Approach Methodologies (NAMs) have attracted attention as alternatives for chemical safety assessment. In fish toxicity tests, aqueous exposure is generally employed; however, maintaining stable exposure concentrations is difficult for chemicals with poor water solubility, volatility, or susceptibility to hydrolysis. Furthermore, fish mainly absorb chemicals through the gills and body surface during aqueous exposure, whereas gastrointestinal absorption is the primary exposure route in mammals. Therefore, oral exposure methods that enable quantitative estimation of exposure doses in fish are needed.

In this study, we aimed to develop an ecotoxicological testing method using microcapsules (MCs) that enables the control and estimation of oral exposure doses in fish. MCs consist of a core material containing the target chemical and a biodegradable shell material. Encapsulation allows target chemicals to be dispersed in water, and fish can be exposed via gastrointestinal absorption through ingestion of MCs. However, key aspects of MC-based exposure systems remain unclear, including MC uptake by fish and the amount of chemical encapsulated in each MC.

We investigated two aspects: (1) estimation of exposure doses in fish using MCs and (2) comparison between aqueous exposure and MC-mediated exposure to perfluoroalkyl carboxylic acids (PFCAs). Using medaka, MC ingestion was evaluated by direct microscopic counting and theoretical estimation using mathematical equations. The amount of encapsulated chemical per MC particle was quantified by gas chromatography-mass spectrometry, and exposure doses were estimated from the product of the encapsulated amount and the number of ingested MCs. We also confirmed whether exposure via MC ingestion occurred and evaluated differences in toxic effects between aqueous and MC-mediated exposure.

As a result, quantitative conversion of estimated exposure doses became possible in the MC-based oral exposure system, facilitating the design and evaluation of the experimental system. Future work will examine the applicability of this method to high-dose exposures exceeding aqueous saturation concentrations and to chemicals that are difficult to evaluate using conventional aqueous exposure systems.

1.01.P–Mo010 From Data Gaps to Regulatory Decisions: A Hybrid NAM Approach for Aquatic Toxicity Assessment of Bisphenols

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The widespread use of bisphenols (BPs) and their substitutes has led to increasing environmental exposure, raising regulatory concerns regarding their safety in aquatic ecosystems. Despite ongoing restrictions on bisphenol A, many alternatives remain insufficiently characterized, creating significant data gaps that challenge regulatory environmental risk assessment frameworks.
This study addresses the urgent need for regulatory-ready New Approach Methodologies (NAMs) that support chemical safety evaluation while aligning with international guidelines (e.g., OECD, ECHA) and

reducing reliance on animal testing. The primary objective was to develop and validate a hybrid in silico-in vitro approach for predicting acute aquatic toxicity of bisphenols, explicitly incorporating parameters relevant for regulatory decision-making, such as ionization and pH-dependent behavior.
To achieve this, a QSAR model based on Partial Least Squares (PLS) regression was developed using curated OECD 202 EC50 data for Daphnia magna. The approach integrates molecular descriptors with the distribution coefficient (logD), reflecting the actual exposure conditions of ionized forms of environmental concern. Descriptors selection via genetic algorithms, combined with rigorous internal validation and applicability domain (AD) assessment, ensured compliance with OECD principles for QSAR validation. The model was further aligned with regulatory classification schemes (EU Directive 93/67/EEC) to enable direct interpretation of toxicity classes.
Results demonstrate strong predictive performance and mechanistic consistency, identifying ionization state and lipophilicity as key determinants of toxicity. Model application to untested bisphenols enabled their classification into regulatory hazard categories. External experimental validation confirmed the reliability of predictions, achieving approximately 80% agreement with observed data. The proposed in silico-in vitro approach supports data gap filling, prioritization, and read-across strategies within regulatory contexts, while adhering to transparency and reproducibility requirements.
In conclusion, this work advances the implementation of NAMs in regulatory environmental risk assessment by providing a robust, validated, and interpretable tool. Its application can facilitate safer chemical management, accelerate decision-making processes, and contribute to the transition toward animal-free, science-based regulatory systems.

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1.01.P–Mo011 Integrating New Approach Methods (NAMs) for Toxicity and Exposure to Support Next Generation Risk Assessment

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Humans and ecological species are exposed to thousands of chemicals, and the potential deleterious impacts of these exposures are largely unknown. There is a recognized need to reduce unnecessary animal testing. Monitoring and biomonitoring data are limited compared to the number of chemicals requiring evaluation and it is not feasible to measure all chemicals in the environment. The increasing demand for efficient risk-based assessment has highlighted limitations in traditional methods and data used for estimating exposure and hazard. The Exposure And Safety Estimation (EAS-E) Suite is as an integrated, freely accessible online platform that consolidates new approach methods (NAMs) for hazard and exposure data to support next generation risk assessment (NGRA) and chemical safety and sustainability. The platform combines curated chemical property databases with OECD-validated models for predicting chemical properties with quantitative in vitro-in vivo extrapolation (Q-IVIVE) models, and multimedia mass balance environmental fate and exposure models. In absence of chemical specific hazard data, the internal Threshold of Toxicological Concern (iTTC) can be used as a conservative default. The highlighted case example applications include the calculation of bioactivity exposure ratios (BERs) and linking in vitro bioactivity data to predicted in vivo exposure. The BER workflow incorporates an in vitro mass balance model to account for chemical disposition in assay systems and general physiologically-based kinetic models to estimate steady-state blood concentrations and administered equivalent doses for

various species. Exposure estimates are generated using high-throughput production-to-exposure modeling that integrates near- and far-field pathways across chemical life cycles, enabling aggregate exposure assessment for humans and a range of representative ecological species. The methods support a "One Health" perspective by linking human and ecological exposure assessments and the practical implementation of NAMs for high-throughput risk-based evaluations for chemical priority-setting.

1.01.P–Mo012 Accelerating Conductor-like Screening Model (COSMO) Workflows with general-extended Tight Binding (g-xTB): A New Computational Approach for Per- and Polyfluoroalkyl Partition Coefficients

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With over 300,000 chemicals currently on the global market, scalable in-silico prediction models are essential for calculating the critical properties needed to assess environmental risk, model transport, and inform regulatory decision-making. Partition coefficients, in particular, are fundamental to these efforts, describing the bulk phase equilibria of chemicals as they navigate environmental compartments. While numerous empirical prediction methods exist, recent literature demonstrates that data-poor and structurally complex chemical families, such as per- and polyfluoroalkyl substances (PFAS), pose significant challenges for traditional Quantitative Structure-Activity Relationships (QSARs).The quantum chemical-based Conductor-like Screening Model for Real Solvents (COSMO-RS) offers a highly accurate alternative based on fundamental thermodynamics; however, standard workflows are often too computationally expensive for high-throughput screening. To address this, we propose an accelerated computational New Approach Methodology (NAM) that leverages newly developed semi-empirical models, specifically the general extended-tight binding (g-xTB) model, alongside more efficient conformational sampling algorithms. We hypothesize that replacing fully quantum-mechanical BP/TZVP optimizations with rapid g-xTB geometry optimizations within the COSMOtherm workflow will significantly reduce computational time while preserving the high accuracy typical of this approach.This ongoing study benchmarks this accelerated pipeline against both experimental data and the standard full quantum-mechanical workflow. As a proof-of-concept case study, this accelerated workflow is being applied to a diverse set of per- and polyfluoroalkyl substances (PFAS), a highly flexible, data-poor class of chemicals that are notoriously problematic for both standard empirical models and computationally expensive full quantum-mechanical simulations. To address the systemic challenge of fragmented information and support cross-sector collaboration, the resulting workflow will be published via GitHub and designed for compatibility with both proprietary COSMOtherm and its open-source counterpart, openCOSMO-RS. Ultimately, this research provides a faster, accessible middle-ground, a robust NAM that enables fast and accurate determination of physicochemical properties for critical emerging contaminants.

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1.01.P–Mo013 Prediction of Species-Specific Estrogen Receptor α Sensitivity to Endocrine-Disrupting Chemicals Across Mammals Using Molecular Dynamics–Derived Bioenergetic Descriptors

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Endocrine-disrupting chemicals (EDCs) can differentially activate estrogen receptor alpha (ERα) across species, complicating cross-species risk assessment. Although ERα is structurally conserved, the mechanistic basis of species-specific sensitivity remains unclear. This study evaluates whether molecular dynamics (MD)–derived bioenergetic descriptors, integrated through interpretable machine learning as

new approach methodologies (NAMs), can predict cross-species variation in ERα transactivation. We combined in vitro luciferase assays using ERα from six mammals (human, dog, cat, mouse, Baikal seal, and killer whale) with in silico modeling, docking, and 100-ns MD simulations. From MD trajectories, we quantified descriptors capturing activation-relevant processes, including Helix 12 (H12) stability (RMSD), ligand binding free energy (ΔG_bind), co-activator recruitment energetics (ΔG_CoAct), and inter-domain dynamics. These descriptors were integrated with experimental EC50 data using an Elastic Net (EN) regression model, enabling feature selection and mechanistic interpretability. In silico site-directed mutagenesis was further performed to assess the functional impact of species-specific amino acid substitutions. Results show that ERα sensitivity is governed not only by ligand binding but by ligand-induced conformational stabilization and co-activator energetics. The EN model achieved robust predictive performance ($R^2 \approx 0.67$) and identified ΔG_CoAct and H12 dynamics as dominant predictors, outperforming traditional docking metrics. Reverse mutations revealed mechanistic decoupling between binding and activation; for example, V368G (mouse G to human V mutation) shifted binding energetics and H12 behavior toward human-like responses. Some mutations enhanced ligand binding but reduced co-activator recruitment, while substitutions at integrative positions (e.g., 316 and 334 corresponding to human ERα) disrupted multiple downstream processes, indicating roles in allosteric signal propagation. Overall, evolutionary divergence in ERα reflects fine-tuning of signaling efficiency rather than simple gain- or loss-of-function effects. By linking MD-derived descriptors with an interpretable predictive algorithm, this study provides a transferable framework for species-specific endocrine sensitivity, advancing NAMs in ecotoxicological risk assessment.

1.01.P–Mo014 Developmental Toxicity of the Emerging Per- and Polyfluoroalkyl Substance Hexafluoropropylene Oxide Tetrameric Acid (HFPO-TeA) in Early Chicken Embryos

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Per- and polyfluoroalkyl substances (PFAS) have been widely used in firefighting foams, food packaging materials, and electronic products. Legacy PFAS, such as perfluorooctanoic acid (PFOA), are widely detected in environmental and biological samples and are increasingly regulated. In contrast, emerging PFAS have been introduced as alternatives, but their toxicological information remains limited. More than 30 PFAS have been detected in wild avian species, highlighting the need to evaluate their potential effects on birds. Among emerging PFAS, hexafluoropropylene oxide tetrameric acid (HFPO-TeA) has raised concern because HFPO homologues show increased bioaccumulation potential and toxicity with increasing chain length. Although HFPO-TeA has been reported to induce cardiotoxicity and hepatotoxicity in post-hatch chickens, its effects on early-stage embryos remain unclear. This study aimed to assess the developmental toxicity of HFPO-TeA in chicken embryos and compare its toxicity with that of PFOA using a shell-less embryo culture system.

Fertilized chicken eggs were treated at the start of incubation with PFOA at 1 mg/kg egg, HFPO-TeA at 0.1 or 1 mg/kg egg, or Milli-Q water as the control. After 55–56 h of incubation, the egg contents were transferred to the shell-less culture system and observed from embryonic days 3 to 9. On day 9, body weight and the weights of the heart, liver, brain, and right eye were measured. Morphological and physiological parameters, including body length, head length, head+bill length, eye diameter, forelimb length, hindlimb length, extraembryonic blood vessel length, and heart rate, were assessed using ImageJ. The survival rates on day 9 were 91.7%, 84.6%, 80.0%, and 75.0% in the control, PFOA, HFPO-TeA-L, and HFPO-TeA-H groups, respectively. PFOA exposure showed no clear effect on body or tissue weights. In contrast, HFPO-TeA significantly decreased body weight and the weights of the brain and eye, suggesting impaired neural development. HFPO-TeA also increased the heart-to-body weight ratio, indicative of altered cardiac development. These findings suggest that HFPO-TeA exerts greater developmental toxicity than PFOA and may preferentially affect neural and cardiac development during

early embryogenesis. This study provides novel toxicological insights into an emerging PFAS and supports the utility of the shell-less chicken embryo culture system as a model for evaluating developmental toxicity of environmental contaminants.

1.01.P–Mo015 Effects of 1-chloropyrene (1-ClPyr), a chlorinated PAH, on the development of ex ovo chicken embryos

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Halogenated polycyclic aromatic hydrocarbons (HPAHs), including chlorinated PAHs (ClPAHs), are formed during incomplete combustion and released into the environment via exhaust emissions. Among HPAHs, 1-chloropyrene (1-ClPyr) has been detected at relatively high concentrations in environmental and biological samples worldwide, including air, soil, microplastic surfaces, and fish. However, its toxicity in animals remains poorly understood. This study evaluated the developmental toxicity of 1-ClPyr in chicken embryos and explored its possible mechanisms using ex ovo embryo culture, transcriptomics, and in silico molecular docking as new approach methodologies (NAMs).

Molecular docking was performed using MOE to estimate the binding affinity of PAHs and HPAHs to the ligand-binding domain of human AHR1, based on interaction energy values (U-dock, kcal/mol). U-dock values were compared with previously reported EC50 values for human AHR activation in a yeast assay. Docking of 1-ClPyr with chicken AHR1, PPARα, and RXRα was also simulated. Fertilized chicken eggs were treated with 1-ClPyr (0.001–1 nmol/g egg) or DMSO at the start of incubation. Embryos were transferred to ex ovo culture after 56 h and observed from embryonic day 3 to 9. Seven phenotypic endpoints were measured, and livers were collected on embryonic day 9 for RNA-seq analysis.

U-dock values showed a significant moderate positive correlation with EC50 values for HPAHs toward human AHR ($\rho = 0.403$, $p = 0.025$). Compared with benzo[a]pyrene, 1-ClPyr showed a weaker AHR-related response, with a U-dock value of -24.80 kcal/mol and an EC50 of 660 nM. In the developmental toxicity test, 1-ClPyr did not significantly affect embryo survival up to ED9. Although some phenotypic endpoints showed temporary changes, no clear dose-dependent effects were observed, suggesting limited phenotypic toxicity at doses up to 1 nmol/g egg.
Transcriptome analysis showed that AHR1 and CYP1A1 mRNA expression unexpectedly decreased in a dose-dependent manner. Pathway analysis indicated effects on PPARα signaling, including significant downregulation of PPARA, RXRA, and downstream genes such as CPT1A, which is involved in mitochondrial fatty acid β-oxidation. Docking analysis suggested that 1-ClPyr can bind to chicken AHR1 and RXRα, whereas its affinity for PPARα appeared weaker than that of known PPARα ligands. Overall, 1-ClPyr may interact with AHR1 and RXRα and disturb AHR1-regulated PPARα signaling in chicken embryos.

1.01.P–Mo016 Toxicity Evaluation of Per- and Polyfluoroalkyl Substances in Human iPS Cell-Derived Neural Progenitor Cells and Neurons

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Per- and polyfluoroalkyl substances (PFAS) are widely distributed in the environment and have been

detected in human serum and brain tissue. Epidemiological, in vivo, and in vitro studies suggest that PFAS exposure may be associated with neurological diseases and developmental disorders. However, few studies have directly compared PFAS-induced neurotoxicity between neural progenitor cells and differentiated neurons in the same system. This study investigated the neurotoxic effects and potential mechanisms of PFOA and PFOS using human iPS cell-derived neural progenitor cells (hNPCs) and hNPC-derived induced neuronal cells (iNCs).

hNPCs and iNCs were exposed to PFOA or PFOS at 0.01–1000 μM for 24–72 h. Cell viability, apoptosis, membrane damage, morphological changes, reactive oxygen species (ROS), and reactive nitrogen species (RNS) were evaluated. RNA-seq was also performed on hNPCs and iNCs exposed to 0.1% DMSO, 800 μM PFOA, or 400 μM PFOS to characterize PFAS-induced gene expression changes.

In hNPCs, cell viability decreased to 10–20% after exposure to 1000 μM PFOA or PFOS, whereas iNC viability was not clearly reduced by either compound at 0.01–1000 μM. Both compounds induced apoptosis in a concentration-dependent manner in hNPCs and iNCs. Significant apoptosis was observed in hNPCs exposed to 10–1000 μM PFOA or 100–1000 μM PFOS and in iNCs exposed to 400–1000 μM PFOA or 500–1000 μM PFOS. Oxidative stress increased at apoptosis-inducing concentrations, and membrane damage increased after exposure to 600–1000 μM PFOA or 800–1000 μM PFOS. These results suggest that PFAS may reduce cell viability through oxidative stress-mediated apoptosis and membrane damage.
Transcriptomic analysis showed clear separation between hNPCs and iNCs with no PFAS exposure by principal component analysis. hNPCs expressed stem/progenitor and proliferation marker genes such as PROM1, whereas iNCs expressed neuronal marker genes such as TUBB3. In hNPCs, PFOA affected cytoplasm-related genes, while PFOS altered genes involved in stress responses and cell adhesion. In iNCs, PFOA affected genes related to growth factors and axis elongation, whereas PFOS disrupted genes associated with PI3K-Akt and integrin signaling. Together, these findings suggest that cell type- and compound-specific gene expression responses may explain differences in PFAS sensitivity and contribute to phenotypic effects, including oxidative stress, apoptosis, and reduced cell viability.

1.01.T - Advances and Regulatory Applications of New Approach Methodologies (NAMs) in the Environmental Risk Assessment of Chemicals

1.01.T01 Regulatory challenges with NAMs under Japan’s Chemical Substances Control Law - Case Studies on Bioaccumulation and Aquatic Toxicity

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New Approach Methodologies (NAMs)—including in silico models, in vitro assays, invertebrate tests, and read-across—are being discussed worldwide as tools to support chemical safety assessment and reduce vertebrate testing. In Japan, the use of NAMs for the new chemical registration under the Chemical Substances Control Law (CSCL) is still limited. The Japanese authorities officially allow the use of NAMs only in two areas: 1) for judging substances that are not readily biodegradable, and 2) for evaluating bioaccumulation. Here we present two case studies applying NAMs for the CSCL registration—one successful case for waiving bioaccumulation tests, and one challenging case for waiving a fish acute toxicity test.

In the first case, we applied read-across for bioaccumulation assessments which is officially accepted. This method is based on comparing similar chemicals using their structure, hydrophobicity (measured log Pow, QSARs), and measured bioconcentration factors in OECD TG 305 studies. By following this guidance, we were able to show that the new substances had low potential for bioaccumulation. The

authorities accepted these evaluations, and the tests were waived.

In the second case, we tried to waive the fish acute toxicity test (OECD TG 203) for a transformation product of a fragrance ingredient. To support the waiver, we submitted data from the RTgill W1 cell line assay (OECD TG 249) and QSAR predictions (ECOSAR and KATE). The RTgill W1 assay—exposing cultured rainbow trout gill cells to six concentrations of a test substance for 24 hours and measuring cell viability— estimated an LC_{50} of 4.13 mg/L for the transformation product, while the parent substance had an LC_{50} of 0.44 mg/L which was in excellent agreement with the in vivo measured value in an OECD TG 203 test (LC_{50}: 1.02 mg/L). The QSAR results (10–11 mg/L) also suggested that the transformation product was less toxic. Although these results were consistent and scientifically robust, the waiver was not accepted.

These two case studies show both the progress and the limits of NAM use in Japan. Read-across for bioaccumulation assessment provides a useful example of how NAMs can be applied. However, other areas such as aquatic toxicity still require further discussion before NAMs can be accepted. Continued cooperation among regulators, researchers, and industry will be essential to expand the use of NAMs and to promote more efficient and animal-free chemical safety assessments in Japan.

1.01.T02 Improving BCF Prediction Accuracy Using OECD TG 319B: Model Evaluation Incorporating Hepatic Metabolism in Common Carp

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The Bioconcentration Factor (BCF) is widely used to assess bioconcentration potential of chemicals, though traditional in vivo testing is time-consuming, costly, and animal-intensive. New Approach Methodologies (NAMs) integrating in vitro metabolism data with in silico models have gained attention. While OECD TG 319B provides a framework for incorporating hepatic metabolism into BCF prediction, the applicability of metabolism-based approaches to common carp (Cyprinus carpio), the model species designated under Japan's Chemical Substances Control Law (CSCL), remains insufficiently explored. This study therefore aimed to evaluate the impact of incorporating hepatic metabolism derived from common carp liver S9 fractions into BCF prediction models (B-compass model and Hendriks model). Fourteen anthropogenic chemicals, including UV stabilizers, pesticides, and other industrial chemicals (log Dow: 3–7), were tested to (i) determine in vitro hepatic metabolic rate constants and (ii) estimate BCF values and assess predictive performance. In vitro assays were conducted by incubating each compound (300 nM) with hepatic S9 fractions at 25°C. Concentrations of chemicals at multiple time points were quantified using LC–MS/MS, and intrinsic clearance (CLint, in vitro) was calculated when a significant concentration decrease over time was observed by liner regression ($p < 0.05$). The obtained metabolic parameters were incorporated into BCF prediction models to evaluate the relative importance of branchial uptake, branchial elimination, hepatic metabolism, and fecal egestion to overall chemical elimination and BCF prediction. Incorporating hepatic metabolism into the B-compass model increased the coefficient of determination (R^2) from 0.29 to 0.39, and decreased the root mean squared logarithmic error (RMSLE) from 3.6 to 2.4, indicating improved model performance. Similarly, in the Hendriks model, R^2 improved from 0.27 to 0.42 and RMSLE decreased from 3.2 to 1.8. The improvement was particularly evident for highly hydrophobic compounds (log Dow > 5) including UV-329, UV-328, triclosan, triclocarban, and carbosulfan in which hepatic metabolism accounted for >80% of total elimination. These results demonstrate that accounting for hepatic metabolism is critical for accurate BCF prediction and support the use of in vitro–in silico integrated approaches for common carp.

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1.01.T03 Transcriptomic Points-of-Departure Benchmarked Against Chronic Data Used in Derivation of Canadian Water Quality Guidelines for Bisphenol A

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Transcriptomic points-of departure show promise as a new approach method that could potentially be used as part of a weight-of-evidence for risk assessment activities by some regulatory bodies. Defined as the concentration at which significant molecular changes occur, derivation of a transcriptomic point-of-departure (tPOD) requires analysis of large gene datasets with multiple discretionary decisions at each step, such as filtering criteria, differential gene analysis parameters, models and methods to derive the tPOD, which may affect the results and lead to uncertainty for use in regulatory decisions. Here, we asked how much tPODs obtained from short-term toxicity studies deviate based on chosen parameters. Specifically, we produced multiple tPODs using various parameters for fish species with chronic data to Bisphenol A and benchmarked these tPODs to the chronic data used in the Canadian federal water quality guideline for the chemical. Eleutheroembryos (50%) for Atlantic salmon (Salmo salar) and rainbow trout (Oncorhynchus mykiss) were within tenfold of the chronic guideline value, but tPODs for zebrafish (Danio rerio) were lower than the chronic guideline value by 2 orders of magnitude. The different tPODs for rainbow trout spanned 1 order of magnitude, but 2 and 4 orders of magnitude for Atlantic salmon and zebrafish, respectively. Across all species, the choice of method to derive tPODs was the factor driving the greatest difference. Given that almost all tPODs were within 2 orders of magnitude of chronic data, our study adds weight-of-evidence for tPODs from short-term fish toxicity tests to support water quality guideline derivation. Further studies, including other taxa of aquatic species (rotifers and daphnia), are planned to eventually derive a species-sensitivity distribution using tPODs.

1.01.T04 Multi-omics profiling of emerging fluorinated lithium-ion battery energy storage chemicals across fish gill, liver, and gonad cell models

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Driven by the global transition toward renewable energy and electric mobility, the rapid expansion of lithium-ion battery (LIB) technologies has increased the environmental release of fluorinated electrolyte components, including per- and polyfluoroalkyl substances (PFAS)-related ionic liquids. Despite their growing production, persistence, and mobility in aquatic systems, their toxicological profiles remain poorly understood.

This study aimed to unveil the toxicity and modes of action of a set of fluorinated LIB-related salts and their mixtures using multi-omics profiling. Rainbow trout (Oncorhynchus mykiss)-derived cell models (liver-RTL-W1, gill-RTgill-W1, gonads-RTG-2) were profiled using Cell Painting-based phenomics, metabolomics, and transcriptomics to generate exposure fingerprints across different cell models. By integrating different omics layers, the study directly linked molecular pathway perturbations to subcellular phenotypic alterations, thereby improving the mechanistic and biological interpretability of high-content imaging data.

Among all compounds, sulfonimides, particularly bis(nonafluorobutanesulfonyl)imide (LiFNFSI), elicited the strongest and most consistent responses across cell lines. LiFNFSI induced extensive

phenotypic perturbations, dominated by mitochondrial alterations (up to ~84% of features), with RNA- and DNA-associated phenotypes represented as prominent secondary targets. Transcriptomic analyses further support the coordinated perturbations of transcriptional and nuclear structural organization, revealing a conserved shift from proliferation and genome maintenance toward proteostasis and stress adaptation, accompanied by suppression of chromatin remodeling pathways. These molecular and phenotypical changes also aligned with metabolomic signatures, linking mitochondrial and nuclear texture alterations to lipid remodeling and mitochondrial energy production.

In conclusion, these findings provide mechanistic insight into the biological impacts of emerging fluorinated energy-storage chemicals and highlight the need for proactive environmental hazard assessment as battery production continues to expand globally. By integrating phenotypic, metabolic, and transcriptomic responses across biologically relevant fish cell models, this work also demonstrates the value of multi-omics approaches for identifying early mechanistic toxicity signatures and supporting the development of safer, more sustainable energy-storage chemicals.

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1.01.T05 Mechanism-Informed Prioritization of Consumer Product Chemicals Using the Adverse Outcome Pathway (AOP) - Based Explainable AI Platform, ToxBAI

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Consumer products contain a wide range of chemicals with diverse functional uses, while toxicological information remains limited for many substances. To address this challenge, this study first constructed a Korean consumer product chemical inventory using the EcoLife Database and then applied ToxBAI, an AOP-based AI toxicity prediction platform developed by our group, as the analytical framework for mechanism-informed hazard prioritization. The inventory was organized into eight functional use categories, which were used as the main units for evaluating endpoint-specific concern patterns.

ToxBAI integrates ToxCast/Tox21 bioactivity assay-based prediction models with OECD Test Guideline-based toxicity endpoint models to support endpoint-level prioritization with mechanistic evidence. Prioritization was conducted for endocrine disruption/developmental and reproductive toxicity (ED/DART), inhalation toxicity, and genotoxicity/carcinogenicity. Chemicals within the applicability domain of ToxBAI were classified into High, Moderate, Low, and Very low priority groups using a qualitative weight-of-evidence framework integrating Tier 1–3 evidence. Prioritization results were evaluated at the functional use category level for each endpoint. To account for differences in category size, both the number and proportion of prioritized chemicals were compared. This approach enabled the identification of functional use categories with relatively elevated concern for specific endpoints, as well as categories showing repeated concern across multiple endpoints. Mechanistic interpretation was further supported by ToxBAI-derived evidence on assays, biological targets, pathways, and evidence tiers.

Overall, this study presents an AOP-based, mechanism-informed prioritization framework for consumer product chemical categories by integrating an EcoLife Database-based inventory with ToxBAI. The proposed framework supports endpoint-specific hazard screening at the functional use category level and may assist in identifying chemical groups requiring further toxicological evaluation and regulatory

consideration.

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1.02.P - Advances in Ecological Risk Assessment Using Population- and Ecosystem-Level Modeling, Experimentation and Monitoring Approaches

1.02.P–Tu001 Perumytilus purpuratus as a Coastal Biomonitor in Chilean Sacrifice Zones: A Developing Country Case Study on Industrial Metal Pollution

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Coastal industrial pollution threatens marine ecosystems and human health across the Asia-Pacific region. In developing nations along the Pacific Rim, the expansion of mining, energy, and manufacturing sectors has accelerated metal discharge into coastal waters, yet standardized biomonitoring programs remain critically underdeveloped, compromising regional risk assessment and evidence-based environmental policy.

Chile exemplifies this challenge: five coastal areas are officially designated as sacrifice zones due to concentrated mining and industrial activities, while surrounding areas remain poorly characterized. This study used Perumytilus purpuratus as a bioindicator — a mussel distributed along approximately 6,000 km of the southeastern Pacific coast, from Ecuador and Peru to southern Chile and Argentina — making it an ecologically relevant sentinel across a broad latitudinal range. Specimens were collected in July 2021 across four Chilean regions (II, III, V, and VIII). Concentrations of ten trace elements (As, Cd, Cu, Fe, Hg, Mo, Ni, Pb, V, Zn) were quantified by ICP-OES following USEPA protocols, and PCA-based clustering classified sites as impacted versus less-impacted.

Northern regions exhibited the highest metal burdens, consistent with mining dominance. In Region V, sacrifice zone sites did not differ substantially from nearby locations, suggesting contamination extends beyond formally designated boundaries. Sites historically designated as reference locations showed unexpected metal levels, questioning their current validity as clean baselines and indicating that reference site designations require systematic reassessment.

This study establishes an updated, standardized baseline for coastal metal contamination in Chile, where biomonitoring data were over 20 years old and methodologically inconsistent. By generating comparable reference values across impacted and previously unstudied sites, this work provides a replicable model for developing nations across the Pacific Rim where similar data gaps persist. While industrialized countries have moved toward mechanistic and molecular approaches, many coastal nations in the Global South are still building the foundational baselines that make such advances possible. Standardized biomonitoring frameworks are urgently needed to bridge this gap and enable the next generation of ecotoxicological research in underrepresented regions.

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1.02.P–Tu002 Machine Learning–driven Prioritization of Micropollutants in River

Water: Integrating Ecological and Human Health Risks from a Two-year Monitoring Campaign

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In this study, the prioritization of micropollutants in river water was performed through a two-year monitoring campaign of 117 organic micropollutants (OMPs) from December 2022 to August 2024, in conjunction with random forest models. A total of 82 OMPs, which include 17 pharmaceuticals, 26 pesticides, 14 organophosphate flame retardants, 14 perfluoroalkyl substances, 10 plasticizers, and 1,2,3-benzotriazole, were detected at least once. Total concentrations ranged from 242 ng/L to 4788 ng/L. Pharmaceuticals (average: 710 ng/L) were the most predominant compounds, followed by pesticides (460 ng/L), organophosphate flame retardants (276 ng/L), and plasticizers (219 ng/L) over this period. To systematically prioritize OMPs relevant to both ecological and human exposure, a machine learning (ML)-optimized Toxicological Prioritization Index (ToxPi) was applied. The ToxPi model combined various variables, such as occurrence characteristics, physicochemical properties, and toxicity indicators. Random forest regression was employed to objectively optimize the weights of variables. In both ecological and human exposure scenarios, the selected model demonstrated stable performance (R2 > 0.76 on both the training and test datasets). The model identified detection frequency and concentration as the most important variables for ecological exposure risk. An embedded molecular structure-based deep learning (DL) model was also used to predict the treatability of detected compounds in drinking water treatment plants. Consequently, for human exposure, carcinogenic potential, acute toxicity, and water treatability emerged as the key variables that drive prioritization. Through the integration of these weighting criteria, seven compounds such as metformin, carbendazim, alachlor, metolachlor, bentazone, T3CPP, and PFHpA were the top 20% in ToxPi score and categorized as the high-priority OMPs in both ecological and human health exposure scenarios.

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1.02.P–Tu003 Finding the Sweet Spot: How Pollutant Persistence, Bioaccumulation and Specificity Shape Aquatic Community Stability

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Chemical pollution is considered one of the greatest threats to biodiversity. It has the potential to alter ecosystem structure and function by impairing organism performance, affecting not only physiological processes but also how individuals interact with other organisms of the same and different species. The chemical structure of pollutants determines their persistence in different environmental compartments, and how they disperse, accumulate in sediments, and bioaccumulate in organisms' tissues. Moreover, the mode of action and specificity of pollutants determine the target species in communities, affecting mortality (or population intrinsic growth rate) when effects are lethal, and physiological or behavioral endpoints when effects are sub-lethal. In contrast to individual- or population-level studies, focusing on the community level enables us to investigate not only direct effects on target species, but also how pollutants impact non-target species via trophic interactions, including processes such as biomagnification and changes in predation pressure.

In this study, we utilized a bioenergetic model for polluted food webs to investigate the effects on aquatic communities of PBT substances with different attributes, including half-life DT50 (Persistence), octanol-water partition coefficient KOW (Bioaccumulation), and effects specificity (Toxicity). We then computed

different compositional and functional stability metrics for every combination of physicochemical properties and effect specificities. Finally, we identified combinations of factor levels that produced the lowest destabilization of aquatic communities. The study therefore contributes to modernize PBT concepts by embedding them in a community-dynamic context, revealing how different property combinations propagate through food webs to alter stability. Such insights can be used to refine environmental quality benchmarks, prioritize substances of concern, and support the design of less disruptive chemicals and management strategies.

1.02.P–Tu004 Study on Effects of Chemicals on Threshold Food Concentrations of Two Daphnia Species

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Ecotoxicity tests currently used in chemical regulatory assessments mainly focus on individual-level endpoints such as survival and reproduction. However, developing simple test methods to evaluate the ecological effects of chemicals at the community level remains an important challenge. Interactions among species are key drivers of community dynamics and should be explicitly considered when assessing chemical impacts on ecological communities. The outcomes of interspecific interactions are determined by the ecological traits of the interacting species. Therefore, assessing the effects of chemicals on species traits that influence interspecific interactions may provide valuable insights into community-level effects. In this study, we focused on interspecific competition for food resources as a representative species interaction relevant to community-level impact assessment. Laboratory experiments were conducted to investigate the effects of zinc and linear alkylbenzene sulfonate (LAS) on the threshold food concentration—defined as the minimum food concentration required to maintain a population and a key trait determining the outcome of food competition—of two Daphnia species, Daphnia magna and Daphnia ambigua. Chronic toxicity tests were performed under combinations of different food concentrations and chemical exposure levels, and threshold food concentrations were estimated for each species at each exposure concentration. Based on the experimental results, we discuss the effects of chemical exposure on the outcomes of interspecific competition between D. magna and D. ambigua.

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1.02.P–Tu005 Biomonitoring of Prenatal Exposure to PCBs, OCPs, and Flame Retardants in Mother–Child Plasma and Its Association with Birth Outcomes

Persistent organic pollutants, including polychlorinated biphenyls (PCBs), organochlorine pesticides (OCPs), and flame retardants (FRs), are persistent and bioaccumulative chemicals that can cross the placenta and may affect fetal development. However, data on combined prenatal exposure, mother–child transfer, and associations with birth outcomes remain limited in Northern European populations.

This study aimed to biomonitor prenatal exposure to PCBs, OCPs, and FRs in paired maternal and cord plasma samples, and to examine their determinants and associations with birth outcomes in a Finnish mother–child cohort. We analyzed 102 paired maternal and cord plasma samples from the NUGEN cohort. Concentrations of 13 PCBs, 6 OCPs, PBDE congeners, DBDPE, and chlorinated FRs were measured and lipid-adjusted. Sociodemographic, dietary, lifestyle, and environmental exposure data were collected by questionnaire, and associations with birth outcomes were assessed using correlation and regression analyses.

PCBs, OCPs, and FRs were detected in both maternal and cord plasma, confirming transplacental transfer. Overall, exposure levels in this Northern Finland cohort were lower than those reported in many other European populations. Maternal age, alcohol use during pregnancy, fish and meat intake, parity, smoking, pre-pregnancy BMI, gestational weight change, vegetable intake, and paternal education were associated with variations in contaminant levels. Maternal fish intake was associated with higher PCB levels in children, whereas high meat intake was associated with higher FR levels. For birth outcomes, some congener-specific associations were observed, including positive associations of maternal BDE-28, maternal BDE-153, cord PCB118, and maternal PCB180 with birth weight or related growth measures. However, most POP concentrations were not consistently associated with adverse birth outcomes, while maternal characteristics such as BMI, smoking, parity, and diet showed broader associations with fetal growth indicators.

In conclusion, this study provides evidence of prenatal exposure to PCBs, OCPs, and FRs and their transfer from mother to child in a low-exposure Finnish cohort. While certain congeners may influence birth outcomes, maternal lifestyle, dietary, and sociodemographic factors appear to play a major role in shaping both exposure profiles and fetal growth. These findings support the value of integrated biomonitoring in maternal-child health risk assessment.

Disclaimer/Disclosure: NA

1.02.P–Tu007 Are We Solving or Creating Problems? Evaluating Chemical vs Biological Pest Control using a Predator-Prey Model

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Managing pest populations effectively requires choosing between rapid chemical intervention and continuous biological control. While both aim to reduce pest densities below economic thresholds, they operate on vastly different temporal scales and ecological mechanisms. This study uses an agent-based predator-prey model to evaluate the long-term pest-suppression capacity of chemical and biological control strategies under varying environmental conditions. The model represents natural enemies (Orius laevigatus) as individuals at different life stages with individual-based properties, and pests (Frankliniella occidentalis) as super-individuals to quantify pest control. Modelled ecological processes include development, reproduction, dispersal, overwintering, mortality, and feeding by nymphs and adults on pests. The temperature of the environment is updated daily, and most of the processes are temperature-dependent. Pesticide effects are implemented using toxicokinetic-toxicodynamic modelling of lambda-cyhalothrin. The modelled landscape includes in-crop and off-crop areas that differ in pesticide exposure concentration after application. All processes occur at 1 m2 resolution and a time step of one day. Pest control strategies include control (only wild natural enemies), chemical (wild natural enemies + two applications of lambda-cyhalothrin), light biological (wild natural enemies + two applications of 1 natural enemy/m2), and heavy biological (wild natural enemies + one application of 10 natural enemies/m2). Model simulations over multiple years predict that chemical control provides an effective short-term pest relief, but causes pest resurgence in the long term, associated with the eradication of natural enemies. In comparison, biological control is more effective over the whole season, as it ensures a smaller pest overwintering population entering the growing season and avoids pest resurgence. This work supports ecologically grounded predictions about how pesticides change average pest densities across different temporal scales relative to wild and facilitated biological pest control, as well as the consequences of pesticide-induced disruption of biological pest control.

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1.02.T - Advances in Ecological Risk Assessment Using Population- and Ecosystem-Level Modeling, Experimentation and Monitoring Approaches

1.02.T01 Persistent Legacy Effects of Historical Metal Mining on Benthic Macroinvertebrate Communities: A 50-Year Assessment of the Upstream of the Watarase River in Japan

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While chemical remediation is a primary goal for restoring mine-polluted rivers, the long-term trajectory of biological recovery remains poorly understood. In this study, we evaluated whether 50 years of reduced metal exposure have successfully restored the benthic macroinvertebrate community to its pre-impact state. We integrated contemporary seasonal field surveys (2022–2023) with a historical field survey dataset spanning before mine closure (1964), immediately prior to closure (1970), and shortly after closure (1973). We assessed water quality and benthic-macroinvertebrate community structure—total abundance and taxon richness—across the mainstream Watarase River and four tributaries. Community-level responses were also evaluated using non-metric multidimensional scaling analysis. Our analysis revealed a significant decoupling between chemical and biological recovery. While trace metal concentrations in the mainstream of the Watarase River have decreased remarkably since the 1960s, no statistically significant associations were observed between structural measures of benthic macroinvertebrates and the extent of trace metal pollution in the 2020s. Multivariate analysis revealed that community structure in the mainstream remains distinctly different from that of the uncontaminated reference rivers—a spatial heterogeneity that has remained fixed for 50 years. Metal-sensitive taxa, such as mayflies in the families Ephemerellidae and Heptageniidae, remain scarce in the mainstream despite recovery from metal contamination. These findings suggest that chemical recovery does not automatically guarantee biological restoration. We identified several potential factors hindering biological recovery, including indirect effects of wastewater treatment, such as biofilm formation in riverbed sediments resulting from calcium hydroxide use in flocculation–sedimentation processes; physical habitat fragmentation caused by river structures designed for erosion control; and increased flood susceptibility associated with historical forest degradation. Our study highlights that to achieve ecological restoration of historically metal-polluted rivers, there is a need for a shift in management from simple reduction of metal concentrations to a comprehensive approach that addresses multiple physical and ecological stressors.

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1.02.T02 Evaluating Population-level Relevance of Current Ecotoxicological Tests Through Elasticity Analysis of Matrix Population Models

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Ecotoxicological tests are usually designed to measure individual-level toxicity, such as impacts on survival rate and fecundity during specific life stages. To evaluate population-level chemical risk,

ecotoxicological test results are often incorporated into theoretical population models. However, because test duration is generally shorter than the lifespan of the test species, some life history stages are omitted from tests, and thus, not all survival and reproduction parameters required for constructing population models are measured. Current test protocols may therefore overlook individual-level chemical impacts crucial for population dynamics, potentially leading to inaccurate risk assessments. In this study, we evaluated the population-level relevance of the test protocols provided by the Organization for Economic Co-operation and Development. We first compiled matrix population models that represented the full life cycles of the test species from published articles in the Web of Science Core Collection. Matrix population models consist of individual-level vital rates, which are age- or stage-specific survival rates and fecundities. We conducted elasticity analysis to evaluate how infinitesimal changes in each vital rate affect the population growth rate. We then aggregated the elasticities of the population growth rate to the parameters measured in the tests. The aggregated elasticity, ranging from 0 to 1, represents the extent to which a slight change in vital rates measured in the test affects the population growth rate, indicating the population-level relevance of the test protocols. The relevance scores for each test were generally below 0.4, but varied depending on the endpoint type and the taxonomic group of the target species. Notably, tests designed for terrestrial invertebrates showed lower population-level relevance than those for the other taxa, indicating a substantial limitation in capturing individual-level toxic impacts that may lead to severe population decline in terrestrial invertebrates. Multiple tests targeting the same species, such as both acute and chronic tests, covered the life history complementarily, and their combined use increased population-level relevance. This study provides an overview of the relevance of current ecotoxicological tests to population-level risk assessment, highlighting key directions to better align with population conservation.

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1.02.T03 Population-level ecological impacts of environmental stressors on Trillium camschatcense revealed by exactLTRE and interstage flows

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Understanding how environmental and chemical stressors influence population dynamics is important for improving ecological risk assessment (ERA) and ecotoxicological assessment. Life table response experiments (LTREs) are widely used to identify how changes in vital rates contribute to variation in population growth rates (λ), but conventional LTREs provide limited information on how stressors alter interstage flows of individuals among developmental stages. The objective of this study was to determine how habitat fragmentation and environmental variation influence stage-specific demographic processes and population performance in Trillium camschatcense, a perennial forest herb in Hokkaido, Japan. To address this question, we developed a new analytical framework that combines exact life table response experiments (exactLTRE) with interstage flow matrices. This framework quantifies how environmental stressors influence population growth and transitions among life stages, thereby providing mechanistic insight into population-level ecological responses. We analyzed long-term demographic data using stage-structured population matrices collected from multiple habitats and years. exactLTRE, combined with interstage flow matrices, was used to quantify exact demographic contributions to changes in both population growth and stage-specific interstage flows. Habitat fragmentation had little net effect on

overall population growth rate. For example, in the smallest fragmented population, increased stasis flows in the 1-leaf and 3-leaf stages were compensated by reduced fecundity flows, resulting in little net change in λ despite substantial changes in demographic flows. Interannual environmental variation had stronger effects on population growth, and warmer years were associated with increased stasis flow in the 1-leaf stage, which substantially contributed to variation in λ. These results demonstrate that interstage flow analysis can reveal substantial demographic reorganization even when net changes in population growth rate are small. By integrating exactLTRE with interstage flow analysis, this framework provides an ecological modeling approach for identifying demographic responses to environmental stressors. The framework also provides a mechanistic approach for assessing population-level consequences of chemical stressors and ecotoxicological impacts in ecological risk assessment under multiple environmental stressors.

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1.02.T04 Adapting the EFSA Birds and Mammals Tier 1 Exposure Framework for Risk-Based Assessment in Australian Agroecosystems: A Regionalised Approach

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The EFSA Tier 1 framework is widely applied for risk-based environmental risk assessment (ERA) of pesticides in birds and mammals; however, it is parameterised using European species and ecological relationships. Application to Asia-Pacific systems may therefore introduce uncertainty where species composition, dietary structure, and spatial patterns of habitat use differ. This study evaluates whether the EFSA Tier 1 exposure assessment framework can be reliably applied to Australian agroecosystems and refines it through regionalisation of key biological parameters within agricultural systems on the premise that region-specific biological parameterisation is required for accurate exposure estimation.

A national dataset of Australian birds and mammals was compiled, incorporating species-specific body weights, dietary classifications, and ecological attributes. Field metabolic rate relationships were derived for marsupials for species level data, demonstrating distinct scaling relationships compared with eutherian mammals. Dietary guild definitions were refined to reflect Australian feeding ecology, particularly for omnivorous species. Spatial analysis of species distributions relative to agricultural land uses was undertaken to identify species plausibly exposed within treated environments.

Results show that Australian species do not consistently align with EFSA model species assumptions. Marsupials exhibit different energetic characteristics, with higher relative energy demand at low body weights and lower demand at larger sizes. In birds, omnivorous diets are dominated by insects and seeds rather than foliage. Spatial screening further indicates that only a subset of species within each feeding guild are likely to be exposed at a national scale.

These differences result in both higher and lower predicted exposure depending on feeding guild and body size when Australian-specific parameters are applied. The approach provides a transparent and generalisable pathway for regionalising biological parameters within established exposure assessment frameworks, improving biological realism while retaining the conservative intent of Tier 1 screening and supporting application in risk-based ERA across Asia-Pacific systems.

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1.02.T05 Influence of Food Web Complexities and Phenotypic Diversity to the Community Response and Resilience under Pollutant Stress

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Many biotic communities respond to environmental stress by changing species composition (presence of particular species and their relative abundances). Such communities are expected to restore the original state after the stress eliminates (resilience) if migration from external source communities and local extinction of composite species are limited. Large community responses coupled with high resilience are postulated to facilitate the community stability and persistence under changing environments. We examined how the community response and resilience depended on community complexities, food web structures, and phenotypic (tolerance trait) diversities by means of simulations of community dynamics using randomly-generated community matrices with some biological constraints. The stress in the simulation imitated insecticide pulse treatments in aquatic mesocosms, and the community states were measured with community weighted mean tolerance among composite species. The results showed negligible effects of community structures, which were measured by maximum chain lengths, and very weak influence of community complexities, which were measured by species richness and connectance, on the community response and resilience. In contrast, phenotypic diversities invariably and largely contributed to the community response regardless of community structures and complexities. Species loss (local extinction) during community responses always reduced the community resilience after stresses. It is indicated that phenotypic (functional) diversities of response traits and maintenance of biodiversity are critical for community persistence through response and resilience exhibited by communities against stressors.

1.03.P - Adverse Outcome Pathways (AOPs): From Mechanistic Insight to Regulatory Impact

1.03.P–We004 Adverse Outcome Pathway (AOP) Development in the Era of Artificial Intelligence (AI)

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The Adverse Outcome Pathway (AOP) framework is increasingly used to organize mechanistic knowledge and support next-generation human and environmental risk assessment. Supported by the OECD AOP programme, the AOP KnowledgeBase (AOP-KB), and integration of New Approach Methodologies (NAMs), AOPs can strengthen biological plausibility, weight-of-evidence evaluation, and regulatory decision-making. However, AOP development remains resource- and time-intensive, relying heavily on expert-driven literature review, evidence synthesis, terminology harmonization, and evaluation of causal relationships. This work explores how artificial intelligence (AI) can support AOP development through a structured human-AI hybrid workflow. We identify key bottlenecks in current AOP workflows, including literature triage, mechanistic evidence extraction, identification of key events and key event relationships, ontology alignment, and evidence integration across heterogeneous data sources. Representative AI approaches are mapped to these stages, including natural language processing for literature mining, ontology-based terminology harmonization, knowledge extraction for mechanistic relationship identification, and large language model-assisted summarization and drafting. Particular emphasis is placed on practical applications of accessible AI tools to support routine AOP development activities, including evidence screening, draft key event description generation, organization of mechanistic information, and identification of biologically relevant pathways. We further discuss how AI may facilitate integration of omics and systems toxicology data into AOP development and improve consistency across AOP documentation and knowledge-sharing platforms. Importantly, we also address

limitations associated with AI-assisted AOP development, including transparency, reproducibility, traceability of evidence, and the risk of generating plausible but unsupported mechanistic relationships. These considerations highlight the continued importance of expert oversight and weight-of-evidence evaluation. Overall, this work demonstrates how AI can improve the efficiency, consistency, and scalability of AOP development while maintaining scientific rigor, supporting broader application of mechanistic and pathway-informed approaches in hazard/risk assessments and regulatory decision-making.

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1.03.P–We005 Behavioral and Transcriptomic Responses to Chronic Diazepam Exposure in Medaka Fish and Their Offspring

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Pharmaceutical contamination in aquatic environments has emerged as a growing concern in recent years. In particular, psychotropic drugs such as anxiolytics and antidepressants may affect fish behavior and physiology even at environmentally relevant concentrations. This study aimed to comprehensively evaluate the effects of chronic exposure to diazepam, a widely used anxiolytic, on behavioral traits and gene expression in medaka fish (Oryzias latipes) and their offspring (F1 generation).

Medaka fish were exposed to diazepam at 0.8 and 8 μg/L under semi-static conditions from hatching to adulthood (~4 months). Behavioral assays, including the shoaling test and Peek-A-Boo test (Takai et al., 2023), were conducted to assess sociality, exploration, activity, and boldness. Locomotor behavior was quantified using video tracking, and transcriptomic analysis (mRNA-Seq) was performed on brain tissues. In addition, F1 offspring derived from exposed parents were reared under non-exposure conditions and subjected to the same behavioral assays, along with a predation test using a natural predator (donko fish, Odontobutis obscura).

No significant effects on growth (body length or weight) were observed in the parental generation. Conventional behavioral endpoints showed no significant differences; however, entropy-based analysis of swimming trajectories revealed increased exploratory behavior and reduced responsiveness to a predator image in diazepam-exposed groups (p < 0.05). Transcriptomic analysis indicated downregulation of genes related to glutamatergic synapses and synaptic vesicle function, suggesting impaired neurotransmission. In contrast, F1 offspring exhibited heightened responsiveness to novel environments and a predator image, particularly in the high-concentration group. Although predation rates were unchanged, exposed-lineage F1 fish tended to be captured more quickly.

These findings suggest that chronic diazepam exposure alters neural function and behavior in the parental generation and may induce transgenerational effects, potentially mediated by epigenetic mechanisms. This study highlights the importance of integrating complex behavioral metrics and multigenerational perspectives into ecological risk assessment of pharmaceuticals in aquatic environments.

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1.03.P–We006 Developmental Toxicity Induced by the Organophosphorus Flame Retardant Tris(2-chloro-1-methylethyl) Phosphate (TCIPP) in Early Chicken Embryos: Disruption of FGF Signaling and Somitogenesis

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Tris(2-chloro-1-methylethyl) phosphate (TCIPP) is a major organophosphorus flame retardant (OPFR) used as an alternative to polybrominated diphenyl ethers and detected in wild bird eggs. It has been reported to affect chicken development, including increased CYP3A37 expression and reduced tarsus length; however, its effects during early embryogenesis remain unclear. This study aimed to evaluate TCIPP-induced developmental toxicity in chicken embryos and clarify the underlying mechanisms using a shell-less embryo culture system.

Fertilized chicken eggs were treated with TCIPP at 50 or 500 nmol/g egg, with DMSO as a vehicle control. After 55–56 h of incubation, embryos were transferred to a shell-less culture system and monitored from embryonic days 3 to 9. Morphological parameters were assessed using ImageJ. Embryos collected on day 4 were analyzed by hematoxylin staining, transcriptome analysis, whole-mount in situ hybridization, and Western blotting. The involvement of FGFR signaling was assessed by co-exposure with the FGFR inhibitor SU5402. Embryos at 18 h of incubation were analyzed for epithelial–mesenchymal transition (EMT)- and mesoderm-related gene expression.

TCIPP significantly reduced embryo survival by day 9 and increased somite angle from days 4 to 6. Among embryos with somite curvature, 71.4% died by day 9, with significantly lower survival than morphologically normal embryos (p < 0.01). Hematoxylin staining revealed dorsal skin rupture and enlarged intersomitic spaces in curved embryos. TCIPP increased FGF8 mRNA and protein expression, with elevated FGF8 expression in the curved somite region. Somite angle was positively correlated with FGF8 mRNA expression (r = 0.64, p < 0.01). Co-exposure with SU5402 further increased the number of curved embryos and FGF8 mRNA expression, suggesting disrupted FGFR signaling may contribute to TCIPP-induced somite curvature. Transcriptome analysis of day 4 embryos showed EMT-related pathway alterations, and RT-qPCR at 18 h revealed changes in EMT-related gene expression, including CDH1, SNAI2, TBXT, and FGF8.

Overall, TCIPP disrupted early avian development by altering FGF8/FGFR signaling and EMT-related processes, leading to abnormal somitogenesis and reduced embryo survival. These findings provide insight into OPFR-induced developmental toxicity and highlight the shell-less chicken embryo culture system as a useful model for assessing developmental toxicity of environmental contaminants.

1.03.P–We001 Developing Transcriptomics-based AOPs Using Statistical Causal Discovery and Weighted Gene Co-expression Network Analysis

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AOP is an established framework for linking molecular initiating events (MIEs) to adverse outcomes (AO) following chemical exposure. However, most published AOPs are still developed primarily through expert judgment, making AOP development time- and labor-intensive. Although high-throughput omics technologies have been proposed as powerful tools to identify early molecular responses and candidate MIE-associated genes and to connect molecular responses with AOs, such analysis remains challenging. In particular, high-throughput omics technologies generate large numbers of candidate variables in response to chemical exposure, many of which may reflect secondary or adaptive responses rather than

events causally linked to AOs. Therefore, data-driven approaches are needed to prioritize biologically plausible upstream molecular events while reducing false-positive causal pathways. This study presents a workflow for developing transcriptomics-based AOPs by combining dose–response modeling, weighted gene co-expression network analysis (WGCNA), and statistical causal discovery (SCD).
We applied this approach to RNA-Seq datasets with known or expected toxicological pathways, newly generated transcriptomic data from pyrene-exposed zebrafish embryos and published rainbow trout data for estrogen receptor agonist exposure. For the pyrene dataset, zebrafish embryos were exposed for 96 h across four concentrations including the control, generating transcriptomic profiles for 60 samples. After filtering low-expression genes and identifying dose-responsive genes, WGCNA was used to reduce dimensionality by grouping co-expressed genes into modules. Module eigengenes, representing the first principal component of each module, were then analyzed by DirectLiNGAM to infer causal ordering among exposure and modules. Benchmark dose metrics were estimated for each module. The module containing known aryl hydrocarbon receptor (AhR)-pathway-related genes, including ahr2, cox2, and sox9b, tended to be inferred as an upstream module. When the same approach was applied to published rainbow trout transcriptomic data for estrogen receptor agonist exposure, modules containing known pathway-related genes such as esr1 were prioritized as an upstream module. These results suggest that the proposed workflow can help reduce transcriptome-wide candidate genes from tens of thousands of genes to a smaller set of prioritized modules and candidate upstream genes.

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1.03.P–We002 A Multi-Omics Framework for Adverse Outcome Pathway-Oriented Toxicological Assessment in Morelet's Crocodiles

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Multi-omics datasets are increasingly used in wildlife ecotoxicology, but interpretation often follows mathematical feature reduction, obscuring adverse outcome pathways (AOP) and their mechanisms. This is critical for non-model wildlife exposed to contaminant mixtures, where exposure, molecular responses and toxicological endpoints must be integrated within AOP framework.
We are developing an AOP-oriented workflow for wild Morelet's crocodiles (Crocodylus moreletii). The framework integrates persistent organic pollutants (POPs), metals, and scute transcriptomes, and blood steroid hormone and metabolomic features while preserving exposure-response interpretability. In a pilot implementation, transcriptomic and metabolomic data are condensed into pathway-level scores before multi-omics integration. These scores represent candidate molecular key events, including xenobiotic metabolism, oxidative stress, immune/inflammatory signaling, endocrine-related responses and metabolic disruption.
Rather than assuming a single exposure-response sequence, the workflow evaluates alternative scenarios related to AOPs. The first scenario tests whether contaminant exposure is associated with key transcriptomic events followed by perturbation of metabolites and hormones. The second scenario tests whether exposure initially alters metabolite and hormone levels, which then affect transcriptomic responses. Multi-block integration and supervised feature selection identify exposure-linked molecular

signatures, and the retained features are traced back to contaminant profiles.
A preliminary assessment using available pilot data suggests that the pathway chosen before feature selection improves biological coherence. This is achieved by organizing candidate signals within interpretable exposure-response structures rather than purely statistical layers. This strategy facilitates the comparison of mechanistic orderings and the prioritization of biomarker sets connected to contaminant space.
This work advances non-lethal crocodilian ecotoxicology by shifting the focus from detecting transcriptomic effects to interpreting molecular toxicology linked to exposure. By combining pathway-level enrichment, scenario-based integration and flexible biomarker prioritization, the framework provides a scalable strategy for identifying candidate key events, generating testable hypotheses and supporting effect-based risk assessment in non-model wildlife exposed to contaminant mixtures.

1.03.P–We003 qAOP Development for Estrogen Receptor Agonism and Reproductive Dysfunction Across Fish and Humans

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A major challenge in applying adverse outcome pathways (AOPs) to chemical safety assessment is that many remain qualitative, fragmented and difficult to translate across species. This is particularly important for endocrine disruption, where estrogen receptor (ER) agonism is a well-defined molecular initiating event, but its downstream links to reproductive dysfunction may differ between humans and wildlife. As a result, human health and environmental assessments are often conducted separately, limiting the use of shared mechanistic knowledge across species.

Here, we develop a cross-species quantitative AOP network framework for ER agonism leading to reproductive toxicity in humans and fish. Evidence will be collected from scientific literature and public toxicological databases, including US EPA CompTox, ECOTOX, ChEMBL and PubChem, with large language models used only to support systematic evidence mining and data extraction. Extracted information will include chemical identity, ER bioactivity, species or test system, exposure conditions, molecular and cellular responses, key events, reproductive endpoints and population-relevant outcomes. These data will be organised within an AOP framework to identify conserved and species-specific key event relationships.

The curated evidence base will then be used to define and parameterise qAOP networks using probabilistic and/or mechanistic approaches. Predictive performance will be evaluated by testing whether early molecular or cellular responses can predict downstream reproductive effects across fish and human-relevant systems. This work provides a practical route to make AOPs more quantitative and cross-species applicable, supporting regulatory decision-making and safer chemical assessment for both human and ecological health.

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1.04.P - Bridging Gaps in Microplastic Ecotoxicology: From Particle Characterization to Reliable Risk Assessment

1.04.P–We008 Detection of Microplastics in Bottom Overlying Water of Semi-

Enclosed Coastal Seas

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Recent studies have revealed that microplastics (MPs) originate not only from urban sources but also from polymer-coated fertilizers used in agricultural fields, eventually entering aquatic environments. Consequently, assessing MP contamination and its ecological impacts in inner bays adjacent to agricultural areas has become a critical concern. Notably, MPs are expected to accumulate in the bottom overlying water layer, where filter-feeding organisms may be particularly vulnerable to exposure. However, identifying and quantifying environmental MPs remains challenging due to considerable variability in their composition, size, shape, and degree of degradation. In this study, we aimed to detect MPs in the bottom overlying water of a semi-enclosed coastal sea.

Field surveys were conducted on four occasions between June and December 2025 at six predetermined stations within the inner region of Ariake Bay, Japan. Seawater samples were collected from a depth of 1 meter above the seafloor using a pump connected to a PVC hose. At each station, over 200 liters of seawater were flushed through the system before collecting a 2-liter sample, which is then processed through the next filtration stage . Each sample underwent filtration through a 2-µm stainless-steel filter, followed by organic matter digestion using H_2O_2 at 60 °C for 48 hours, and density separation employing a NaI solution containing 0.5% polyvinylpyrrolidone (PVP). The supernatant was collected on a 0.2-µm Anodisc filter, and the polymer type, shape, and size of each particle were characterized using µFT-IR spectroscopy and digital microscopy. All procedures were executed under stringent contamination-control conditions.

In four samples, the presence of polypropylene (PP), polyethylene (PE), and polystyrene (PS) were identified, with total microplastic (MP) concentrations ranging from 76 to 495 particles per liter. These findings strongly indicate the presence of MPs in the bottom overlying water of Ariake Bay. Future research should increase the number of sampling stations, replicates, and sample volumes to elucidate the spatiotemporal patterns of MP contamination. Additionally, further investigation into the sources and origins of these MPs is warranted.

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1.04.P–We011 Size- and shape-dependent effects of microplastics on survival, reproduction, and multi-omics responses in the brackish water flea Diaphanosoma celebensis

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Owing to their widespread distribution and persistence, microplastics (MPs) have become a global ecological concern in marine ecosystems. MPs can be readily consumed by marine organisms ranging from zooplankton to fish, negatively affecting growth, reproduction, and behavior. Their toxicity can depend on physical properties, such as size and shape, which affect bioavailability, distribution within the body, and mechanical stress. However, comprehensive understanding of how the size and shape of MPs collectively influence toxicity in marine organisms and of their underlying toxic mechanisms is still limited. Thus, in this study, we investigated acute and chronic toxicity of MPs with different sizes and shapes (fragment-S, 0.5-µm; fragment-L, 5-µm; bead-S, 0.74 to 4.99-µm; bead-L, 3 to 16-µm) in the brackish water flea Diaphanosoma celebensis. In addition, transcriptomic, metabolomic, and lipidomic analyses were conducted to assess molecular alterations induced by MP exposure. The results showed that water fleas consumed MPs regardless of size and shape, but smaller MPs were more readily ingested. In

contrast, fragmented MPs had more severe effects on survival and reproduction than spherical MPs regardless of particle size, with fragment-S showing the highest toxicity. Consistent with phenotypic effects, fragment-S induced the most pronounced molecular alterations among the MP exposure groups. Transcriptomic analysis showed that 1,002 and 704 genes were significantly altered following exposure to 5 mg/L of fragment-S and fragment-L, respectively, whereas only 231 and 95 genes were significantly altered following exposure to bead-S and bead-L, respectively. Gene ontology and pathway analyses revealed that genes associated with ribosomal function were predominantly affected by MP exposure. Moreover, pathways related to genetic information processing, metabolic processes, signal transduction, and organismal systems were commonly affected, but the effects were most pronounced in the fragment-S group. Metabolomic and lipidomic analyses showed that lipid species were predominantly affected by MP exposure, particularly in the fragment-S group. Our findings suggest that MPs can negatively affect small zooplanktonic species by disrupting diverse biological processes, particularly genetic information processing and biosynthetic processes, and that these effects may increase with decreasing particle size and more irregular particle surfaces.

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1.04.P–We012 Measurement of 10, 30, and 100 µm aged-fragmented polyethylene microplastics in exposure water by µFT-IR and its effect on Javanese Medaka (Oryzias javanicus)

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Microplastics (MPs; <5 mm) are widespread in marine environments, with aged, fragmented polyethylene MPs (afPE-MPs) being most common. Yet most laboratory studies use pristine polystyrene beads, which differ from environmental particles in shape, surface chemistry, and density. Consequently, the ingestion, depuration, and sublethal effects of realistic afPE-MPs remain poorly characterized. Irregular, non-fluorescent MPs are also difficult to identify and quantify in water and biological samples, limiting exposure–response assessments.
This study had two objectives: (1) develop a quantitative µFT-IR method for afPE-MPs in water and biological matrices; and (2) assess ingestion, intestinal elimination, and acute toxicity of afPE-MPs (10, 30, 100 µm) in Javanese medaka (Oryzias javanicus).
afPE-MPs were produced by photo-oxidative aging and mechanical fragmentation of low-density polyethylene. Samples were filtered through 5 µm PTFE membranes pretreated with H_2O_2 to remove organic matter, then analyzed by µFT-IR scan mode using polyethylene peaks at 2915, 2850, and 1465 cm^{-1}.
Two experiments followed OECD Test Guideline No. 305. Experiment 1: medaka were exposed to 30 µm afPE-MPs for seven days, followed by three-day depuration to assess intestinal elimination. Experiment 2: acute toxicity tests used 10, 30, and 100 µm afPE-MPs at 0 and 10 mg/L, with concentrations measured in water and intestines.
The µFT-IR method reliably quantified afPE-MPs in both matrices, demonstrating its utility for irregular, non-fluorescent particles. Intestinal afPE-MP levels declined gradually during depuration, with elimination slower than reported for spherical polyethylene microbeads, suggesting that irregular fragments are retained longer in the gut. No acute toxicity occurred at 10 mg/L; however, measured water concentrations varied significantly with particle size, reflecting heterogeneous suspension behavior. These findings show that µFT-IR enables exposure assessments based on measured rather than nominal

concentrations. Slow intestinal elimination indicates that irregular afPE-MPs present a different exposure profile than spherical microbeads commonly used in laboratory studies. This study advances MP ecotoxicology by providing a validated quantification method and exposure–response data for environmentally realistic aged-fragmented polyethylene, supporting more realistic ecological risk assessments of marine microplastic pollution.

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1.04.P–We013 Effects of Exposure to Capsule Microplastic Fragments From Polymer-Coated Fertilizers on the Survival, Behavior, and Neurotransmitter Levels of Japanese Medaka (Oryzias latipes)

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Polymer-coated fertilizers (PCFs) are widely utilized in Japanese agriculture, yet their degradation releases capsule microplastic (CMP) fragments into aquatic environments at concentrations up to 0.78 mg/L. The toxicity of microplastics is well-documented, including neurobehavioral toxicity and gut damage. However, the potential impact of CMP on aquatic species remains unknown. To fill this research gap, this study investigated whether environmentally relevant concentrations of CMP fragments could adversely affect the survival, behavior, and neurotransmitter levels of fish. In our study, juvenile Japanese medaka (Oryzias latipes) were exposed to CMP fragments (average size: 36 μm) at concentrations of 0.08 and 0.8 mg/L for 28 days. We assessed survival rates and quantified behavioral traits using DeepLabCut video tracking. To handle data gaps, missing coordinate values were reconstructed through interpolation using the SciPy library, ensuring trajectory continuity. For the behavioral analysis, we focused on changes in the average feeding rate and shoal size. The average feeding rate was defined as the amount of Artemia nauplii consumed in 1 min per fish, while the average shoal size was measured by the area occupied by the fish. Neurotransmitter levels in the eyes and brain were analyzed using high-performance liquid chromatography coupled with triple-quadrupole mass spectrometry (HPLC-MS/MS). Our findings reveal that exposure to both concentrations significantly reduced feeding rates and altered ocular glutamine levels. This suggests that visual impairment and associated changes in neurotransmitters may underlie the observed behavioral anomalies by impairing the ability to recognize food. Furthermore, exposure to CMP at 0.8 mg/L significantly reduced survival rates, potentially as a result of cumulative physiological stress in fish. As the first report of CMP-induced toxicity in fish, these findings identify CMP as an environmental pollutant of increasing concern. This study provides critical empirical data for the risk assessment of agriculture-derived plastics and highlights the urgent need to monitor CMP-related ecological shifts in agricultural watersheds. Further research combining histological and molecular analyses is needed to explore the potential mechanisms underlying the toxicity of exposure to capsule microplastic fragments derived from polymer-coated fertilizers.

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1.04.P–We014 Disruption of the Cholinergic Neurotransmission System in Medaka (Oryzias latipes) Exposed to Polystyrene Microplastics

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Mcroplastics (MPs; <5 mm), cause behavioral abnormalities in fish, yet the molecular mechanisms of

MP-induced neurotoxicity remain unresolved. The cholinergic system, governing learning, memory, and motor control, relies on acetylcholine (ACh), regulated by choline acetyltransferase (ChAT) and acetylcholinesterase (AChE); choline is supplied via dietary phosphatidylcholine (PC). Because MPs have hydrophobic surfaces that adsorb lipids, we hypothesized that polystyrene MPs (PS-MPs) sequester intestinal PC, depleting choline and disrupting cholinergic neurotransmission.

This study (i) assessed whether environmentally relevant PS-MP concentrations affect AChE and ChAT expression in Japanese medaka (Oryzias latipes), and (ii) provides the first direct in vivo evidence of PC adsorption onto PS-MPs in the fish gut. Polystyrene magnetic microspheres (1.0 μm) enabled clean recovery of MPs from biological matrices. Adult medaka were exposed for 14 days to 0, 0.04, or 0.1 mg/L PS-MPs (24 fish/group); brain and intestinal tissues were analyzed by qRT-PCR. PC adsorption was evaluated in vitro in fed-state simulated intestinal fluid (50 mg/L PS-MPs, 24 h) and in vivo at 5 mg/L PS-MPs for two days. Six major PC species were quantified by LC–MS/MS with PC22:0 as internal standard ($\alpha = 0.05$).

Intestinal AChE was significantly downregulated in the low-MP group, with a similar trend at the high concentration; brain ChAT was reduced in the low-MP group. In simulated intestinal fluid, PC adsorption was concentration-dependent, with peaks ~100- and ~400-fold above controls in low- and high-MP groups. PC species were also detected on PS-MPs from medaka feces and intestines. Based on daily feed intake of 1.3% body weight, ~0.8–1.4% of dietary PC was adsorbed onto PS-MPs and excreted.

These findings suggest a coherent mechanism: ingested PS-MPs adsorb intestinal PC, reducing absorption and enhancing fecal excretion, thereby lowering choline availability and altering AChE/ChAT expression. We propose that MPs act not only as conventional vectors introducing hydrophobic contaminants but also as reverse vectors extracting essential nutrients from the body. Because effects occurred at 0.04 mg/L—already documented in natural waters—this mechanism may already affect wild fish. The reverse vector concept advances MP ecotoxicology, indicating that risk assessments should consider both toxicants MPs introduce and nutrients they remove.

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1.04.P–We015 Linking Exposure Pathways to Ecological Risk: A Multi-Species Perspective on Microplastics Uptake and Toxicological Relevance in Estuarine Biota

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Microplastics (MPs) are increasingly recognized as persistent, biologically available contaminants in aquatic systems, yet their ecological and human health implications remain difficult to resolve. While occurrence data in biota are rapidly expanding, the field lacks integration between particle characteristics, exposure pathways, and organism-specific responses, limiting the reliability of risk assessment. This study addresses this gap by examining how estuarine-associated organisms translate MPs exposure into biologically meaningful risk signals. Multiple representative taxa from tropical estuarine systems, including bivalves, crustaceans, and gastropods, were analyzed to capture distinct exposure pathways encompassing filtration, respiration, and sediment interaction. MPs were quantified and characterized by morphology, size, color, and polymer composition, and evaluated using complementary risk indicators, including estimated daily intake (EDI), contamination magnitude (CMPI), and polymer hazard index (PHI). Distinct uptake and risk patterns were observed across taxa. Bivalves exhibited size-dependent accumulation, indicating chronic filtration exposure and direct implications for seafood safety. Crustaceans showed substantial MPs retention in gill tissues, highlighting a critical but underexplored respiratory exposure pathway associated with physical stress and contaminant transfer. Gastropods

reflected baseline contamination linked to localized anthropogenic inputs, with dominant fiber and fragment morphologies associated with urban runoff and fishing activities. Across all taxa, particle type strongly influenced risk interpretation, with fibers and fragments presenting greater potential for contaminant sorption and biological interaction. These findings demonstrate that toxicological relevance cannot be inferred from particle abundance alone but emerges from the interaction between particle properties and biological uptake mechanisms. Integrating multiple bioindicator taxa provides a more robust and ecologically meaningful assessment of MPs exposure and risk. This study advances MPs ecotoxicology by linking particle characteristics to exposure pathways within a unified framework, supporting the development of predictive, data-driven approaches for environmental monitoring, risk assessment of MPs pollution in estuarine systems.

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1.04.P–We016 Initiatives of World Ocean Plastic Planning Center (PLA PLA) in Saga Prefecture: An Integrated Five-Function Hub for Coastal Plastic Pollution

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Marine plastic pollution is a global challenge affecting ecosystems, fisheries, and tourism. Saga Prefecture, Japan, is notably impacted due to oceanographic conditions. The Ariake Sea coast, with Japan's largest tidal range, receives significant riverine debris, while the Genkai Sea and Matsuura coasts gather transboundary debris from East and Southeast Asia. Saga Prefecture is establishing the World Ocean Plastic Planning Center,—PLA PLA—opening in June 2026 at Cape Hado, Karatsu City. The name signifies a planning venue and a casual visit spot. The initiative evolved from beach cleanups by prefectural staff (2018–2024) and Governor Yoshinori Yamaguchi's work on transboundary debris. Building on the 2017 "Mori-Kawa-Umi-Bito" Project and the SAGĀNA Project with ANA, the concept was formalized in 2022 with a design budget approved in FY2024. The center will have five functions: exhibition, recycling, hands-on experience, research, and international cooperation. Located in a renovated 1978 rest facility in Genkai Quasi-National Park, it uses locally sourced Saga timber. Environmental features include roof photovoltaics, battery storage, high-insulation glazing, and high-efficiency HVAC, earning Net Zero Energy Building certification. Rainwater is reused for washing plastics, and local electric-arc furnace slag is used in pavement. A washing area near the entrance lets visitors experience marine debris firsthand, emphasizing prevention. Pre-opening activities generated momentum. The inaugural International Symposium "Minna no Umi" (January 2025) exceeded participation targets, with speakers from UNEP, UN-Habitat, and other institutions. The International Exchange Program in Saga (June 2025) involved Indonesian interns and local volunteers, with bilingual certificates for sustained awareness. Outreach at the UNEP Bangkok seminar and Expo 2025 Osaka–Kansai advanced collaboration. Three factors enabled realization: Cape Hado's status as the "Route Grand Bleu" terminus, funding via nuclear-siting grants and bonds, and human factors including leadership and grassroots activities. PLA PLA may be the first facility integrating five functions with regional, environmental, and international perspectives, aiming to inspire global resonance and catalyze region-led movements, showing local governments can advance marine plastic solutions and model community-driven international action.

1.04.P–We007 Development and characterization of an environmentally relevant micro- and nanoplastics library for cytotoxicity evaluation

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As emphasized in the Sustainable Development Goals (SDGs), growing global attention has been directed toward the potential adverse health effects associated with plastic pollution, particularly microplastics (MPs, <5 mm) and nanoplastics (NPs, <1 μm). The identification of these particles in various human tissues and biological samples strongly indicates that human exposure is widespread and likely unavoidable. Environmental MPs/NPs (collectively referred to as MNPs) exhibit substantial diversity in their physicochemical properties, including differences in polymer type, particle size, morphology, and surface chemistry. Despite this complexity, most existing toxicological evaluations rely on idealized model particles, typically spherical and smooth, which fail to accurately represent real-world environmental conditions. To overcome this limitation, we developed a comprehensive MNPs library that integrates physicochemical characteristics representative of environmental particles. In this study, we systematically characterized the constructed MNPs library, performed comparative analyses with environmental samples, and assessed the cytotoxic potential of the particles. The library was designed using five widely used plastic polymers—polyethylene (PE), polystyrene (PS), polypropylene (PP), polyvinyl chloride (PVC), and polyethylene terephthalate (PET). Particles were prepared with controlled variations in size (MPs and NPs), morphology (fragment, fiber, and sphere), and surface condition, including oxidative degradation induced by vacuum ultraviolet irradiation. Comparative analysis with environmental MNP datasets revealed that the particles in our library closely mimic the morphology and surface characteristics observed in real environmental samples. Furthermore, cytotoxicity evaluations demonstrated that MNPs with surface degradation induced measurable toxic responses across multiple cell lines, whereas non-degraded particles exhibited minimal cytotoxicity. These findings underscore the importance of incorporating environmentally relevant surface properties into safety assessments. In future studies, we plan to further expand the MNPs library to cover a broader range of materials and conditions, and to deepen the evaluation of their biological effects. The MNPs library developed in this work will be made available to the research community upon request through collaborative arrangements (Contact: haga-y@phs.osaka-u.ac.jp).

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1.04.P–We009 Ecotoxicological Effects of Aged and Fragmented Polyethylene Microplastics on Marine Algae and Crustaceans with Consideration of Actual Particle Concentrations

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Microplastics (MPs) are widespread contaminants in marine environments, and numerous studies have investigated their impacts on aquatic organisms. However, many previous studies have used non-aged spherical MPs, which may differ from MPs found in natural environments. In addition, their observed effects in these studies may have included the influence of the plastic additive agents. Furthermore, it is difficult to conduct toxicity tests for MPs while maintaining stable concentrations of MPs in the test solution. As a result, the toxic effects reported in most studies have been calculated based on nominal MPs concentrations. These factors have been considered likely to lead to inaccurate evaluations of the effects of MPs themselves. Therefore, the aim of this study is to evaluate the impact on aquatic organisms in order to support the risk assessment of MPs.

Additive-free low-density polyethylene particles of 10, 30, and 100 μm in size were used for the toxicity tests. These MPs were produced by mechanical crushing and subsequently aged by ultraviolet irradiation to better simulate MPs present in natural environments. In addition, a method for maintaining stable MP concentrations in the test solution during exposure was experimentally verified. For the test organisms, three marine algal species and three crustacean species were selected.

NOEC values based on concentrations predicted using μFT-IR were ≥6 mg/L for the two algal species, Dunaliella primolecta and Phaeodactylum tricornutum. In Cyanobium sp., the NOEC was 0.33 mg/L, suggesting that the effects of MPs on algae may be relatively strong in cyanobacteria.

In the two crustacean species, Americamysis bahia and Tigriopus japonicus, the NOEC values were ≥4 mg/L across all tested particle sizes. The NOEC for lethality in another crustacean species Acartia sinjiensis was 0.18 mg/L in the 100 μm MP treatment, suggesting stronger effects of larger MP particles in this species. In contrast, developmental effects were found regardless of particle size and concentrations.

Through this study, we concluded that more accurate toxicity values than those reported in previous studies can be obtained by conducting toxicity tests that consider several important factors relevant to MP exposure. Overall, the observed toxicities in this study were lower than those reported previously. This may be primarily attributable to the use of MPs without plastic additives and improved MP dispersion conditions in the test water.

1.04.P–We010 Enhanced growth and transcriptomic responses in amphipods exposed to aged and fragmented polyethylene microplastics in sediment

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Public and regulatory concerns regarding microplastic (MP) risks in benthic ecosystems have increased, yet most toxicity data still rely on pristine and spherical particles. Because environmental MPs undergo weathering and differ in shape, size, and polymer type, findings based on pristine spheres may not extrapolate to aged, irregular MPs. Many studies also report either phenotypic endpoints or molecular responses, whereas few link these levels mechanistically. To address these gaps, we conducted sediment toxicity tests using the estuarine amphipod Grandidierella japonica and artificially aged and fragmented polyethylene microplastics (afPE-MPs), integrating growth endpoints with de novo transcriptomics.

We prepared afPE-MPs by crushing PE pellets, classifying particles with an ultrafine precision classifier, and UV-irradiating them in organic solvent. In a preliminary 10-day exposure, amphipods received supplemental food and were exposed to 1% w/w afPE-MPs of three size classes (10, 30, and 100 μm). No significant mortality was observed, whereas dry body weight increased significantly in all afPE-MP treatments.

A follow-up 10-day exposure was performed using 0.1% and 1% w/w of 30 μm afPE-MPs. Surviving amphipods were dissected, and total RNA was extracted separately from head and body tissues. This test again showed enhanced body length, confirming reproducible growth stimulation. Gene set enrichment analysis revealed down-regulated enrichment of translation, peptide biosynthesis, ribosome biogenesis, RNA processing, DNA replication, and cell-cycle processes. In contrast, up-regulated gene sets were enriched for vesicle organization, Golgi vesicle transport, ER-to-Golgi transport, endosomal/lysosomal transport, and protein ubiquitination. These results indicate that the growth enhancement in response to afPE-MPs was unlikely driven by broad activation of canonical biosynthetic pathways. Instead, growth stimulation coincided with cellular resource reallocation, intracellular trafficking, and cellular remodeling. Because food was supplied, enhanced growth is unlikely to be explained solely by microplastic-associated biofilm nutrition. Overall, our findings suggest an adaptive response to afPE-MPs exposure and show the value of linking organism-level endpoints with transcriptomics to interpret MP

effects.

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1.05.P - Environmental Omics in Ecotoxicology and Eco-Surveillance

1.05.P–Tu008 Dose–Response Metabolomic Analysis Identifies Candidate Biomarkers of Palladium (Pd) Exposure in Earthworms (Eisenia fetida)

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Palladium (Pd), a key component of automotive catalytic converters, has been increasingly detected in terrestrial environments, particularly in roadside soils, due to the abrasion of converters during vehicle activity. Despite increasing evidence of Pd contamination in soil, its sublethal effects at the metabolomic level and their implications for ecological risk assessment remain largely unexplored. Therefore, this study aims to examine the sublethal effects of Pd on earthworms (Eisenia fetida) through metabolomic analysis and dose-response modeling. Earthworms were exposed to Pd-spiked soils across a concentration gradient for 7 days to assess sublethal metabolic responses. No significant survival and growth effects were observed during the exposure period. Untargeted metabolomic profiling was performed using GC-MS/MS. Metabolite selection was driven by dose–response modeling to identify concentration-dependent changes, supported by ANOVA and PLS-DA for statistical significance and group discrimination. Benchmark dose (BMD) analysis was further applied to identify toxicologically sensitive biomarkers based on their low BMD values. Our analysis identified a total of 170 metabolites, of which 50 were determined to be significantly affected and concentration-dependent. Disturbed metabolites were mainly involved in amino acid metabolism, energy metabolism, and detoxification pathways. Notably, alanine, asparagine, and aspartic acid have high toxicological sensitivity reflected by the lowest BMD. These candidate biomarkers require further validation for ecological risk assessment. These findings highlight the potential of metabolomic responses as early biomarkers for detecting sublethal Pd toxicity and supporting ecological risk assessment.

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1.05.P–Tu009 Toxic Responses and Transcriptomic Analysis of Coho Salmon Exposed to 6PPD-Quinone

In recent years, growing attention has been paid to traffic-derived chemicals as emerging contaminants in aquatic ecosystems, due to their potential to enter surface waters and impact aquatic organisms. Particularly, 6PPD, which is extensively used in tire manufacturing, is transformed into 6PPD-quinone (6PPD-Q) by ozonation. Concerns have been raised about its release into aquatic environments via tire and road wear particles (TRWPs). Previous studies have demonstrated that 6PPD-Q causes acute lethal toxicity in a range of aquatic organisms, with salmonid species showing particularly high sensitivity. Among them, coho salmon (Oncorhynchus kisutch) has been identified as one of the most sensitive species to 6PPD-Q exposure. Although the toxicity of 6PPD-Q has been evaluated in many studies using conventional mortality-based endpoints, mechanistic understanding based on molecular-level responses remains limited. Omics-based approaches, such as RNA sequencing (RNA-seq), provide an effective

approach for examining physiological responses to environmental stressors. In this study, we aimed to re-evaluate the toxic responses of coho salmon exposed to multiple concentrations of 6PPD-Q and to explore associated physiological responses using comprehensive gene expression analyses (RNA-seq) of the brain, gills, and liver. We estimated the LC50, ILC50, and LT50 values for 6PPD-Q exposure. The 96-h LC_{50} was estimated to be 48.7 ng/L, consistent with previous studies and confirming the extreme sensitivity of coho salmon to 6PPD-Q. ILC50 values in the liver, brain, and gill are 0.221, 1.53, and 6.99 μg/kg wet weight, respectively. Exposure to 250, 500, 1,000, 2,000, and 4,000 ng/L 6PPD-Q resulted in LT50 values of 4.98, 4.31, 3.59, 2.88, and 2.10 h, respectively, indicating a concentration-dependent decrease in LT50. Notably, a small number of coho salmon survived exposure to a lethal concentration (200 ng/L), indicating the presence of individuals with elevated tolerance ("super coho salmon"). Gene expression patterns were clearly differentiated among the liver, brain, and gill samples. However, differences in gene expression between super coho salmon and normal coho salmon were not clearly detected under the present experimental conditions. In the presentation, we will further discuss the more detailed physiological responses revealed by the comprehensive gene expression analysis.

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1.05.P–Tu010 Mechanistic Insights into Oxidative Stress and Inflammation–Associated Metabolic Pathway Perturbations in Garlic Farmers Exposed to Mixed Fungicides

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Mixed fungicide exposure in garlic farmers has been associated with adverse health effects; however, the underlying biological mechanisms need to be characterized at the metabolic level. This study aimed to characterize blood metabolic alterations and identify metabolic pathways associated with fungicide exposure. Blood samples were collected at pre-exposure and during exposure from a control group (N = 62) and a fungicide-exposed group (N = 130). Metabolic profiling was performed using proton nuclear magnetic resonance (^{1}H-NMR) spectroscopy, and multivariate analysis was conducted using MetaboAnalyst 6.0. Sleep maintenance insomnia was more prevalent among exposed farmers (OR = 2.656, 95% CI: 1.291–5.464), indicating a potential link between fungicide exposure and sleep disturbances. Significant separation of metabolomic profiles was observed according to exposure status (PERMANOVA F = 47.762, R^2 = 0.30084, p = 0.001), indicating a clear exposure-associated metabolic shift. Pathway analysis revealed perturbations in neurotransmitter-related (tryptophan and tyrosine) and redox-related (glutathione and cysteine–methionine) metabolic pathways, together with dysregulated inflammatory biomarkers (e.g., IL-6 and TNF-α). Inflammation may be associated with alterations in tryptophan metabolism, potentially shifting serotonin–melatonin balance and contributing to sleep disturbances. Changes in tyrosine and redox-related pathways further suggest altered catecholamine biosynthesis and oxidative stress responses. Oxidative stress and inflammatory biomarkers indicated redox imbalance and dysregulated immune responses during exposure, supporting coordinated metabolic, oxidative, and immune alterations. These findings suggest that mixed fungicide exposure induces neurotransmitter-related, redox, and immune dysregulation in garlic farmers, potentially contributing to neurotoxicity and sleep-related disturbances.

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1.05.P–Tu011 Exploratory Serum Proteomic Alterations Associated with PM2.5 Exposure among Healthy Young Adults in Thailand

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Ambient fine particulate matter (PM2.5) exposure is an important environmental risk factor associated with cardiovascular and metabolic diseases. Increasing evidence suggests that chronic PM2.5 exposure may induce early vascular and cardiometabolic alterations even in apparently healthy individuals; however, the molecular mechanisms underlying long-term environmental exposure remain poorly characterized. This study investigated serum proteomic alterations among healthy young adults residing in regions with contrasting ambient PM2.5 levels in Thailand.

Serum samples from healthy adults aged 20–40 years residing in Chiang Mai (n = 51), a region with relatively high ambient PM2.5 levels, and Songkhla (n = 52), a region with lower PM2.5 levels, were subjected to exploratory proteomic analysis using liquid chromatography–tandem mass spectrometry. Differentially expressed proteins were identified using fold change and adjusted p-value criteria, followed by Gene Ontology functional enrichment analysis. A total of 17 differentially expressed proteins were identified between the two groups, including 13 upregulated and 4 downregulated proteins in the Chiang Mai group. Proteins potentially related to endothelial dysfunction, coagulation, extracellular matrix remodeling, and cardiometabolic regulation were prominently altered. Notably, fibronectin, von Willebrand factor, kininogen-1, and protein Z-dependent protease inhibitor were upregulated in the high-exposure group, whereas cholesteryl ester transfer protein and properdin were downregulated. Functional enrichment analysis demonstrated involvement in biological processes related to stress response, cellular regulation, metabolic processes, and signal transduction, with enrichment of proteins localized to the extracellular region and extracellular space.

These findings suggest that chronic PM2.5 exposure may be associated with serum proteomic alterations potentially linked to endothelial dysfunction, coagulation imbalance, extracellular matrix remodeling, and cardiometabolic risk, even among apparently healthy young adults. This exploratory study provides mechanistic insight into the potential cardiovascular effects of long-term ambient PM2.5 exposure and supports future validation studies in larger populations.

Keywords: PM2.5; Proteomics; Environmental Exposure; Cardiometabolic Risk; Endothelial Dysfunction

1.05.P–Tu012 Assessing the Association between Pesticide Concentrations and Microbial Community Diversity in Mokpo Wetland

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Agricultural pesticide runoff can influence wetland ecosystems by affecting water quality, aquatic organisms, and microbial communities involved in key biogeochemical processes. Microbial communities contribute to nutrient cycling, organic matter decomposition, and ecosystem stability; therefore, shifts in their diversity and composition can provide important information on wetland responses to chemical stressors. However, field-based evidence linking pesticide exposure to microbial community variation in Korean wetlands remains limited, especially in systems influenced by agricultural inflow. To address this gap, we investigated Mokpo Wetland, an inflow-connected part of the Ramsar-designated Upo Wetland complex in the Republic of Korea, where surrounding agricultural land may contribute to pesticide input through runoff. Pesticide concentrations were measured across inflow, upstream, and downstream sites, and microbial communities were analyzed using 16S and 18S rRNA

gene amplicon sequencing. Pesticide burdens were generally elevated at the inflow sites, and microbial community profiles showed site-specific variation along the hydrological flow path. Alpha diversity showed a decreasing tendency at sites closer to the inflow area. Community composition analysis revealed distinct assemblage patterns at the inflow sites, where Patescibacteria accounted for a relatively high proportion among bacterial phyla, Flavobacterium among bacterial genera, Ochrophyta among eukaryotic phyla, and Diatomea among eukaryotic genera. These findings suggest that spatial variation in microbial communities within Mokpo Wetland may be associated with site-specific differences in pesticide exposure. To our knowledge, this study provides the first in situ investigation of microbial community variation along the hydrological flow path in relation to pesticide exposure within Mokpo Wetland. These findings provide a basis for better understanding how agricultural runoff may influence wetland microbial ecosystems and support future assessments of chemical stressors in freshwater wetlands.

1.05.P–Tu013 Effects of Tire Wear Particles on Survival, Growth, and Reproduction of Eisenia fetida: A DEB Modeling Approach

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Tire wear particles (TWPs) and microplastic (MP) fibers are pervasive co-contaminants in agricultural soils, yet their combined ecotoxicological effects on soil organisms remain largely uncharacterized. This study investigated individual and combined effects of TWPs and PET MP fibers on the earthworm Eisenia fetida over a 7-day soil exposure, assessing body weight change and oxidative stress biomarkers, including hydrogen peroxide (H_2O_2), malondialdehyde (MDA), superoxide dismutase (SOD), glutathione (GSH), and total antioxidant capacity (TOAC), and metabolic changes.
Four treatment groups were established: clean soil control, TWP only (0.5 g/kg), MP fiber only (0.5 g/kg), and combined TWP + MP (0.25 g/kg each; total particulate load 0.5 g/kg). Each treatment was replicated three times with ten adult earthworms per replicate, maintained at 20 ± 1 °C under a 16:8 h light: dark photoperiod.
After 7 days, body weight loss was greatest in the combined TWP + MP group (−0.19 g per individual), substantially exceeding the control (−0.06 g) and either single-contaminant treatment (−0.02 g each). H_2O_2 was highest under TWP-alone exposure (~16.8 μmol/g), while the combined treatment yielded significantly lower H_2O_2 (~4.6 μmol/g; p < 0.05) than even the control (~9.8 μmol/g). MDA followed a consistent pattern, lowest in the combined group (~2.28 nmol/g) versus TWP alone (~3.97 nmol/g), though differences were not statistically significant. The 28-day biomarker panel (H_2O_2, SOD, MDA, GSH, TOAC) and metabolic analysis are ongoing and will be presented at the conference.
These findings reveal that co-exposure produces greater organismal harm than either contaminant alone, yet paradoxically reduces oxidative stress markers — suggesting contaminant interactions alter toxicity pathways beyond simple additivity. Single-contaminant risk frameworks may therefore underestimate ecological hazard in co-contaminated soils.

1.05.P–Tu014 Toxic Chemical Contamination and Effects on endogenous metabolites in the Mexican Morelet's Crocodile (Crocodylus moreletii)

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Persistent organic pollutants (POPs), characterized by high environmental persistence and bioaccumulation potential, pose a global threat to wildlife health. Crocodilians, as long-lived apex predators in aquatic ecosystems, are particularly vulnerable to the chronic effects of these contaminants. A major spill of dichlorodiphenyltrichloroethane (DDT) into a lake inhabited by a closely related

crocodilian previously caused endocrine disruption and a severe population decline, highlighting the ecological risk of legacy organochlorine exposure. In Mexico's Yucatan Peninsula, historical DDT use raises concerns about the health of the Morelet's crocodile (Crocodylus moreletii), a conservation-relevant species regulated under CITES. However, detailed data on current contamination status and physiological responses remain limited. This study characterized POP accumulation profiles in the plasma of Morelet's crocodiles and explored their associations with steroid hormones and the plasma metabolome.
Plasma samples from approximately 50 wild and captive individuals were analyzed. Concentrations of POPs, including DDTs and polychlorinated biphenyls (PCBs), were quantified using GC-MS/MS. In parallel, non-target metabolome analysis was performed using LC-QToF-MS/MS. Multivariate analyses, including partial least squares (PLS) regression, were used to identify metabolic networks and pathways associated with contaminant exposure.
The results showed that p,p'-dichlorodiphenyldichloroethylene (p,p'-DDE), a persistent DDT metabolite, was the predominant contaminant, indicating that legacy DDT exposure remains a major concern in this region. Metabolome analysis identified 65 features significantly correlated with p,p'-DDE levels. Higher p,p'-DDE exposure was associated with suppression of the urea cycle and nitrogen metabolism. This metabolic shift suggests that p,p'-DDE may affect mitochondrial function through accumulation in mitochondrial membranes and inhibition of oxidative phosphorylation, thereby disrupting energy metabolism. In conclusion, Morelet's crocodiles appear to be chronically exposed to substantial p,p'-DDE levels, with possible impairment of key metabolic functions, including the urea cycle. Integration of contaminant and metabolome data with transcriptome profiles and non-invasive samples, such as scales and claws, may support high-precision, non-lethal monitoring strategies for the long-term conservation of this species.

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1.05.P–Tu015 Metabolomic and Lipidomic Impacts of Metformin to Zebrafish (Danio rerio) Embryos at Environmental Relevant Concentrations

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Metformin (MET) is one of the most widely prescribed anti-diabetic drugs globally, and a contaminant of emerging concern that has been detected in wastewater treatment plant effluents and surface waters at concentrations ranging from 0.008 to 41 µg/L. Because it targets the highly conserved AMP-activated protein kinase (AMPK) pathway, MET poses a risk of inducing sub-lethal biochemical effects in non-target aquatic organisms at environmentally relevant concentrations. However, few studies have characterised impacts on metabolic status of zebrafish, particularly during early embryonic development. In this study, zebrafish (Danio rerio) embryos were exposed to four concentrations of MET (0.5, 5, 50, and 100 µg/L) until 120 hours post-fertilization (hpf). Untargeted ^{1}H NMR-based metabolomics and lipidomics were applied to simultaneously characterize perturbations in polar metabolites and non-polar lipid species using a biphasic methanol/chloroform extraction protocol. Results shows limited impact on polar metabolites but clear dose-dependent effects on various lipid classes. These findings provide mechanistic insight into the toxicological mode of action of MET in embryonic fish and contribute to the refinement of ecological risk assessment frameworks for pharmaceutically active compounds in aquatic environments.

1.05.P–Tu016 Comparative effects of carrier solvents on polar and non-polar

metabolite profiles of zebrafish (Danio rerio) during embryonic development

Organic carrier solvents are commonly used to prepare concentrated stock solutions and for chemical dosing in ecotoxicology, with guidelines for their usage based on evidence of no or limited apical effects at low solvent concentrations. For many commonly used solvents, the Organisation for Economic Co-operation and Development (OECD) suggest concentrations below 0.01% (v/v) are safe for aquatic organisms. However, the implications for sensitive omics-based molecular techniques like metabolomics requires additional scrutiny, considering the known ability of many solvents to alter membrane permeability and denature proteins even at low concentrations. This study explored the effects of the solvents ethanol, acetone, methanol and dimethyl sulfoxide (DMSO) on the polar and non-polar metabolome of zebrafish (Danio rerio) embryos, following 7 days exposure to concentrations deemed safe based on apical endpoints. Results show altered metabolite profiles in embryos exposed to all solvents, with different responses observed between the four solvents. These findings hold important implications when designing controlled exposure studies using carrier solvents and highlight the importance of including appropriate vehicle and negative controls. Building from this, consideration is needed to evaluate the implications of solvent exposure as a factor that may modify molecular responses to chemical pollutants, to ensure that omics techniques enhance rather than obfuscate our knowledge of the molecular underpinnings of toxicity.

1.05.P–Tu017 Impact of Monsoon Variability on Plankton Stability: Implications for Trophic Transfer and Environmental Monitoring in Bivalve Habitat

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Plankton communities are important to coastal ecosystems and bivalve aquaculture especially ecotoxicology from shellfish toxins, yet the mechanisms by which monsoons affect to their structure and associated toxicological risks remain unclear. This study investigated seasonal dynamics from August to February by integrating 18S rRNA metabarcoding, microscopy, and physicochemical monitoring to assess how monsoon-driven variability shapes community stability. Results reveal a difference between the rainy (SE monsoon) and dry (NE monsoon) seasons. The rainy season showed high heterogeneity and a productivity-diversity paradox, while nutrient runoff and elevated temperatures boosted chlorophyll a, alpha diversity remained low. This suggests that high energy inputs trigger the dominance of a few opportunistic taxa, increasing the risk of Harmful Algal Blooms (HABs). From an environmental toxicology perspective, this dominance facilitates phycotoxin bioaccumulation in bivalves and alters the bioavailability of contaminants due to freshwater influx. Conversely, the dry season presented a stable, homogeneous state driven primarily by salinity, fostering higher diversity and balanced assemblages. Indicator species analysis and network modeling confirmed distinct seasonal changes, showing that bivalve food sources shift drastically in quality and safety. While the rainy season offers peak productivity, it introduces significant vulnerability to pollutants and toxicological stress. By combining molecular and morphological frameworks, this research demonstrates that monsoons reorganize the entire coastal food web. These findings provide a critical baseline for coastal management and bivalve aquaculture, offering predictive insights into how intensifying climate patterns may impact the long-term sustainability and safety of the seafood supply chain.

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1.05.T - Environmental Omics in Ecotoxicology and Eco-Surveillance

1.05.T01 Precision Environmental Health to Detect Real-World Chemical Exposure Hazards Using Sentinel Species

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Chemical pollution in aquatic environments occurs as complex mixtures of known and unknown compounds. This complexity presents a major challenge for ecotoxicology: targeted chemical monitoring can quantify selected substances, but often cannot determine which mixture components drive biological effects or whether exposures are likely to pose ecological hazards.

We present a Precision Environmental Health framework that links environmental chemical mixtures with biomolecular activity profiles in a sentinel species, with a Danube River case study. Water samples were collected from 12 mid- and downstream sites of Joint Danube Survey 3, extracted from large volumes (> 100 L), and reconstituted for 48-hour exposures of Daphnia magna at environmentally relevant and enriched concentrations. Bulk transcriptomics was conducted across five enrichment levels (1×–100×), while metabolomics was applied to two levels (1× and 10×). Targeted chemical analysis quantified 91 organic compounds. Multiblock correlation analysis linked chemical components with transcriptomic and metabolomic responses, enabling the identification of bioactivity signatures and prioritisation of potentially hazardous chemicals and sites.

Results showed that ten widely distributed analgesic and anti-epileptic pharmaceuticals, including carbamazepine, were associated with significant perturbations in neuroactive ligand–receptor interaction and lipid metabolism pathways. Only one site dominated by agricultural and industrial contaminants showed distinctive bioactivity profiles compared with the rest. Correlation analysis further estimated the relative contribution of candidate chemicals, supporting prioritisation of compounds most likely to drive mixture effects.

This study demonstrates how integrating sentinel species, chemical monitoring, and multi-omics analysis can generate biologically informed readouts of real-world mixture hazards. The resulting bioactivity profiles support ecotoxicity characterisation by distinguishing sites with similar or divergent biological effects, identifying pathways that respond consistently to mixture exposure, and generating hypotheses on the chemical drivers of toxicity. More broadly, this work advances omics-enabled environmental monitoring by shifting the focus from identifying which chemicals are present to understanding which biological processes are perturbed, supporting more predictive and prevention-oriented approaches to aquatic chemical risk assessment.

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1.05.T02 Integrated Exposure and Health Assessment of Nesting Green Turtles in a Remote Tropical Marine System

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Green turtles (Chelonia mydas) use a range of environments, yet little baseline data links chemical exposure, health, and reproduction at remote tropical rookeries. This Indigenous-led study, developed with Traditional Owners, recognises green turtles as culturally significant and an important food source. It provides a detailed health and exposure assessment of nesting green turtles in the southern Gulf of

Carpentaria, Australia, using samples from two consecutive nesting seasons at Mornington Island (October 2023) and Pisonia Island (October 2024). Surveys recorded 1,137 turtle emergence events over the two 10-day sampling events with 191 successfully completed nests observed. Adult females were sampled after egg laying alongside their eggs and nest sands (n = 45, Mornington; n = 46, Pisonia). Chemical analyses measured PFAS and trace metals in adult serum and eggs, supported by additional chemical suspect screening. Functional omics (metabolomics, lipidomics, proteomics) assessed biochemical health, while nest physical features and microbial communities provided environmental context. Measured PFAS burdens in serum were moderate and tightly distributed (ΣPFAS median 19.3 ng/mL [interquartile range 15.3–23.5; n = 45] at Mornington; 21.6 ng/mL [18.1–27.6; n = 46] at Pisonia; maxima <50 ng/mL). Trace metal exposure showed similar central tendencies between sites (ΣTrace metals medians 224 vs 227, n = 44 and 43), while specific elements (including aluminium, silicon, and uranium) were higher at Mornington. Only modest differences in overall exposure were found between islands. Egg contaminant profiles confirmed moderate maternal transfer of PFAS (medians 17.5 ng/mL at Mornington, 20.1 ng/mL at Pisonia), with trace metals lower in eggs than in serum. Mornington nests were shallower, with different sand grains and microbial/fungal profiles, and occasional pathogens affecting egg and hatchling health. Functional omics showed variation in energy metabolism, immune function, and stress pathways, but all within normal ranges for wild turtles. PFAS levels were linked to shifts in metabolism, indicating possible impacts on turtle energy use. The study establishes a quantitative baseline connecting chemical exposure, maternal transfer, health, and nesting environment, supporting future monitoring and management. The work also provides critical health and food safety data for Traditional Owners, strengthening community stewardship of this important resource.

1.05.T03 Integration of Metabolomics into Toxicity Identification Evaluation Using Chironomus riparius

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Toxicity Identification Evaluation (TIE) is a methodology used to identify causative toxicants in complex contaminated environments by exposing indicator organisms to environmental matrices such as water or sediment and evaluating their toxic responses. Although TIE is useful for identifying major toxic agents, conventional TIE has limited sensitivity for detecting subtle biochemical and physiological alterations that occur before visible toxic effects, often requiring weeks of exposure. To overcome this limitation, this study integrated metabolomics, a powerful tool for suggesting subtle toxicity and providing clues of its related mechanism, into the traditional TIE framework.

Chironomus riparius, a sediment-dwelling indicator species, was selected as the test organism to evaluate five major sediment pollutants: ammonia, copper, and three hydrophobic organic toxicants (acenaphthene, phenanthrene, and cyhalothrin). In parallel, metabolomic alterations in C. riparius were analyzed to identify metabolic signatures and to assess whether metabolomics could complement the limitations of conventional TIE.

In 10-day exposure experiments, mortality, the primary conventional TIE endpoint, showed significant changes only in high-concentration treatments for all five toxicants (p < 0.05). In contrast, metabolomic analysis after only 24 hours clearly distinguished control, low-concentration, and high-concentration groups for all toxicants through hierarchical clustering based on metabolomic composition and abundance. In addition, metabolites differentiating exposed and non-exposed groups, as well as dose-dependent metabolic responses, were identified at concentrations lower than the lethal concentrations. These results demonstrate that metabolomic alterations are more sensitive than mortality-based endpoints for detecting toxic responses and can reveal physiological and biochemical perturbations not captured by conventional assessments.

This study demonstrates that metabolomics can significantly enhance the sensitivity and quickness of

TIE. These findings support the development of a next-generation TIE framework integrating metabolomics-based biomarkers for sediment contamination assessment and ecological risk regulation.

1.05.T04 Scute Transcriptomics Reveals Field- and Site-Specific Stress Signatures in Morelet's Crocodiles

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Effect-based biomonitoring in protected wildlife requires non-lethal endpoints that capture biologically organized responses rather than isolated molecular changes. Morelet's crocodile (Crocodylus moreletii) is a long-lived apex predator inhabiting aquatic systems exposed to metals and persistent organic pollutants (POPs), yet molecular tools for assessing sublethal effects remain limited.
We assessed whether caudal scute transcriptomes provide interpretable stress-response signatures across heterogeneous field conditions. RNA sequencing was performed on non-lethal scute biopsies from 43 individuals, including six wild populations and a captive reference group. After read mapping and filtering, 30,170 genes were identified and 18,107 expressed genes were analyzed using principal component analysis (PCA), DESeq2, weighted gene co-expression network analysis (WGCNA), single-sample gene set enrichment analysis (ssGSEA), receiver operating characteristic analysis (ROC) and elastic-net modeling. PCA based on differentially expressed genes (DEGs) revealed a consistent axis separating captive individuals from wild populations, supporting structured biology rather than random variation. A conserved core of 85 DEGs shared across wild sites and a broader union set of 3,304 DEGs reflected shared and site-specific transcriptional responses. WGCNA showed that these responses were coordinated into modules associated with captive–wild status, including wild-enriched modules dominated by extracellular matrix remodeling, lipid metabolism and stress-related processes. ssGSEA resolved individual-level variation in oxidative stress and xenobiotic metabolism/detoxification pathways, indicating that scute transcriptomes capture shared field- and site-dependent stress signatures.
To translate this signal into field-compatible tools, we integrated module membership, expression strength, statistical support and discriminatory performance. This network-informed funnel prioritized 99 hub-like candidates and a final 10-gene biomarker panel from stress-associated modules. These results validate caudal scutes as responsive biological interfaces for non-lethal ecotoxicogenomics. By combining pathway scoring, co-expression networks and biomarker prioritization, this framework provides a practical basis for targeted molecular monitoring and for linking scute-derived responses with xenobiotic exposure, reactive oxygen species-related pathways and future adverse outcome pathway development.

1.05.T05 Bridging the Exposure Gap: Linking Contaminant Mixtures in Marine Sediment to Changes in Microbial Composition and Function using Multi Omics

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Marine coastal sediments are major sinks for metals and organic contaminants, which can accumulate and adversely impact organisms inhabiting these environments, including benthic microorganisms. Current sediment monitoring and regulatory frameworks largely rely on static measurements of a limited suite of contaminants based on macro-scale biological endpoints such as organism survival, and therefore fail to detect subtle, sublethal biological responses to complex, low-concentration contaminant mixtures. This

study investigated potential changes to microbial community composition and function in marine sediments exposed to in situ chemical mixtures. Marine sediments were collected from five sites in Moreton Bay, Queensland, Australia, where metals and per- and polyfluoroalkyl substances (PFAS) were quantified and integrated with analyses of benthic microbiome composition (16S rRNA gene sequencing) and function (metabolomics and lipidomics). Environmentally relevant mixtures of metals and PFAS altered both microbial community composition and core metabolic functions in marine sediments at concentrations detected well below current sediment quality guideline values. Metal concentrations differed significantly among sites, with consistently higher concentrations at the coastal locations closest to urban inputs. Microbial species richness differed with and a shift in community composition significantly differed among sites (p < 0.001). Integration of multi-omics profiling with contaminant chemistry identified perturbations to metabolic pathways and related biochemical processes correlating with PFAS. These findings demonstrate that contaminant mixtures can cause biological responses which may be missed by current monitoring, preventing remediation before irreversible changes occur. By utilising multi-omics to link contaminant chemistry to functional changes, this study highlights the capability of microbial markers to serve as early-warning indicators of environmentally realistic complex mixtures which could enhance future monitoring of marine ecosystems.

1.06.A.T - Exposure and Effects of Micro- and Nanoplastics in the Environment and Implications for Ecological Risk Assessment

1.06.A.T01 Plastic pollution and management to support sustainability: where are we now?

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Humanity is facing an unprecedented global plastic pollution crisis because of the dramatic increase in plastic use in the recent years and the mismanagement of plastic waste around the world. It has been estimated that annual global plastic production in the 1950s was around 1.7 million tons. The amount has increased to 299 million tons in 2013 and to over 367 million tons in 2020. In total, 8.1 billion tons of plastics have been produced since 1950. If the current rates of plastic production and use continue, annual global plastic production by 2050 will increase to 590 million tons. This will bring the total global plastic production to about 34 billion tons by 2050. Only 1/3 of plastics are recycled and reused, and 2/3 are discarded into the inland environment and later will find their way to aquatic ecosystems. Plastics tend to accumulate in the oceans due to their longevity and capabilities for long range transport. Moreover, the persistence of plastics in the environment, especially for petroleum-based plastics and after being fragmented into small particles at micrometer and nanometer in size (called microplastics and nanoplastics, respectively, hereafter called plastic particles) makes plastic pollution a greater concern compared to other man-made chemical pollution problems, such as dichloro-diphenyl-trichloroethane (DDT), polychlorinated biphenyls (PCBs), etc. This is because the lifetimes of chemical pollutants in the environment are often shorter than the lifetime of petroleum-based plastics, even for many persistent compounds. This poses potential exposures and risks to living organisms including humans and presents a warning to society. A question that can be asked is, “Where are we at the present time regarding research in support of ecological risk assessment, management, and regulation of plastic pollution to support sustainable development?” This presentation will discuss the science and regulatory status to date toward the global plastic pollution problems with a focus on micro- and nanoplastics and answer this question.

1.06.A.T02 Microplastics as Environmental Vectors Harboring Risks of Antimicrobial Resistance, Pathogens, and Trace Metals in Hanoi River Systems

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Antimicrobial resistance and plastic pollution represent threats to urban aquatic environments. While microplastics (MPs) are known to facilitate the formation of "plastispheres"—unique biofilms that harbor resistant bacteria—the potential for these particles to act as simultaneous transport media for both microbial and toxic risks is not yet fully understood.
This study investigated MPs as environmental vectors within Hanoi's rivers influenced by diverse wastewater sources: HN1 and HN2 (Kim Nguu River, near hospital wastewater), HN3 (Set River, pre-wastewater treatment), HN4 (Red River, before entering Hanoi), HN5 (Nhue River, after craft villages), and HN6 (Cau Den, Nhue River, domestic wastewater). Sediment, water, and MP samples were collected to quantify microbial density in colony-forming units (CFU), antibiotic resistance genes, including parE, rsmA, oprN, rpsJ, and mexF, via molecular techniques. Additionally, we analyzed the accumulation of trace metals and identified metal-resistance genes, including copA and dpsA, to evaluate the relationship between chemical and biological stressors.
MP concentrations exhibited distinct spatial variations, peaking in HN2 water (5,882 items/L) and HN4/HN5 sediments (50,000 items/kg wet weight). MPs significantly concentrated on trace metals (Lead > Cadmium > Nickel > Arsenic), with maximum lead accumulation at the hospital-influenced sites HN1 (55 x 10-3 µg/g) and HN2. Crucially, MPs acted as robust enrichment surfaces, supporting microbial densities (7.75 - 9.89 log CFU/g) approximately 100 times higher than surrounding sediments (6.20 - 6.99 log CFU/g). These "plastispheres" facilitated the intense colonization of pathogenic bacteria, notably Pseudomonas and Salmonella species. Furthermore, ARGs were highly concentrated on MPs; at sites impacted by medical wastewater, the parE and rsmA genes reached 6.03 and 6.38 log copies/g, respectively - roughly 1,000 times higher than in underlying sediments. Metal-resistance genes (copA, recG, dpsA) were also identified alongside lead- and cadmium-resistant bacteria).
MPs provide effective surfaces for robust microbial colonization, acting as potent hotspots for the rapid dissemination of pathogens, toxic trace metals, and ARGs in heavily urbanized aquatic environments. This empirical evidence underscores the urgent need for integrated pollution management strategies to mitigate the intersecting public health risks posed by plastic waste and biological contaminants.

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1.06.A.T03 Microplastics In The Organs Of Big Brown Bats (Eptesicus Fuscus) From North Carolina: Associations With County-Level Urbanization

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Plastic production has increased since the 1950s due to its low cost and versatility, raising concerns about environmental and health impacts. As plastics degrade, they form microplastics (MPs) that can be ingested or inhaled and subsequently accumulate in animal tissues. While the effects of MPs on marine organisms are relatively well studied, exposure pathways and impacts in terrestrial systems remain poorly understood.
Eptesicus fuscus (big brown bats) are widespread North American insectivores that can serve as bioindicators of MP exposure through airborne, aquatic, and insect-mediated pathways. In this study, we

evaluated 18 bats across six counties in North Carolina, USA. We assessed MP presence in the heart, lungs, liver, kidneys, and gastrointestinal tract and tested whether urbanization predicts MP burden. An urbanization index was developed using population density, impervious surface cover, and tree canopy metrics. Specimens were obtained opportunistically as a byproduct of the rabies testing.
We found MPs in every bat organ tested with the highest concentration of MPs in the gastrointestinal tract and lowest in the lungs. Total MP burden per individual bat was not correlated with urbanization levels; however, urbanization levels were positively correlated with MP counts within the gastrointestinal tract. These findings suggest that the primary mechanism of MP exposure in big brown bats is via ingestion. This study highlights the potential for widespread terrestrial exposure and underscores the need to better understand alternative pathways of microplastic uptake in insectivorous wildlife.

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1.06.A.T04 Preliminary Ecological Risk Assessment of Microplastic Particles in Tokyo Bay Sediments

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Tokyo Bay is a semi-enclosed coastal bay surrounded by a highly urbanized watershed, where microplastic particles (MPs) may accumulate in sediments. Because sediments act as both a sink for MPs and a long-term exposure pathway for benthic organisms, sediment data are essential for assessing ecological risks in coastal environments. In this study, we conducted a preliminary ecological risk assessment of MPs in Tokyo Bay sediments. Surface sediment samples collected from 36 stations during 2023–2025 were analyzed to determine MP concentrations, size distributions, morphologies, and polymer compositions. To account for particles smaller than the analytical detection limit, measured concentrations in the 20–5000 μm range were extrapolated to the 1–5000 μm range assuming a continuous power-law size distribution. Particle volume, surface area, and mass were also estimated from measured particle dimensions to support comparisons across different exposure metrics. Ecological risks were characterized by comparing the extrapolated sediment MP concentrations with species sensitivity distribution-based effect thresholds aligned to Tokyo Bay sediment particle conditions. The analysis focused mainly on food dilution, with particle volume used as the ecologically relevant metric, while tissue translocation and mass-based comparisons were considered as supplementary lines of evidence. This case study illustrates how field monitoring data can be linked with effect thresholds to evaluate sediment MP risks and highlights key uncertainties associated with small-particle extrapolation and toxicity data selection.

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1.06.B.T - Exposure and Effects of Micro- and Nanoplastics in the Environment and Implications for Ecological Risk Assessment

1.06.B.T01 Cross Method Imaging Validation of Neonatal Nanoplastic Brain Uptake and Long Term Behavioral Outcomes

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Nanoplastics (NPs) are increasingly recognized as emerging contaminants, yet their uptake during early life and the potential consequences for development and adult outcomes remain poorly understood. Our previous work demonstrated that 50 nm polystyrene NPs (PSNPs) can enter the neonatal mouse brain, with high accumulation in the thalamus visualized by whole organ light sheet imaging. Here, we extend this finding by confirming particle identity, visualizing their cellular localization using confocal and hyperspectral imaging, and assessing whether a single neonatal exposure produces measurable effects from early development through adulthood.

Neonatal mice received a single oral dose of fluorescently labeled 50 nm PSNPs at postnatal day (P)0. To characterize the signals detected by whole-brain light-sheet imaging, we examined tissue sections using higher resolution approaches. Confocal imaging provided intracellular visualization of PSNP-associated signals, while hyperspectral analysis verified NP-specific spectral signatures and enabled fluorescence-independent assessment. Together, these approaches support the interpretation of whole organ imaging and establish a workflow adaptable for screening brain infiltration by NPs of varying sizes and polymer chemistries.

Developmental outcomes were assessed using early life reflex tests (righting reflex and negative geotaxis, P4–10) and daily eye opening checks (P13–16). In adulthood, the same animals were evaluated in an IntelliCage system to measure behavioral flexibility in serial reversal learning. Adult females were then paired with males to assess mating success and litter production. These developmental, behavioral, and reproductive assessments are part of an ongoing effort to determine how early-life NP exposure may influence later outcomes and to identify exposure conditions that warrant deeper investigation.

These findings support cross-method validation of neonatal NP brain uptake and underscore the need for more prolonged, repeated, or sensitized exposure paradigms to determine whether early-life NP exposure produces subtle or context-dependent effects.

1.06.B.T02 A Radiotracer-Based Toxicokinetic Analysis of Micro- and Nanoplastics Across Inhalation, Oral, and Dermal Exposure Pathways

Micro- and nanoplastics (MNPs) raise critical concerns about their biological fate. Here, we establish a radiotracer-enabled framework integrating molecular imaging, quantitative biodistribution, and exposure–response modeling to systematically evaluate inhalation, oral, and dermal absorption pathways. We demonstrate that exposure route is the primary determinant of internal burden: inhalation drives dominant pulmonary retention, prolonged biological half-life, and systemic redistribution, whereas oral exposure results in rapid gastrointestinal transit with minimal systemic uptake. Dermal exposure, particularly under chronic or barrier-disrupted conditions, enables lymphatic transport and delayed systemic dissemination, highlighting a secondary but non-negligible pathway. Building on this route-centric framework, we further analyzed multiple polymer systems, including biodegradable PLA, PMMA, and polystyrene. Integration of in vivo exposure burden with cellular responses revealed that pulmonary exposure most strongly aligns with oxidative stress, mitochondrial injury, and cytotoxic thresholds. Human exposure modeling further supports that environmentally relevant inhalation scenarios can drive progressive internal accumulation within realistic timescales, whereas oral exposure contributes minimally. Collectively, this work defines exposure route as the primary organizing principle of microplastic

toxicokinetics and demonstrates that inhalation-driven accumulation is a generalizable phenomenon across diverse polymer types, with additional contributions from dermal exposure under chronic conditions.

1.06.B.T03 Lithium-Microplastic Composites Drive Germ Cell Pyroptosis via the ROS/NLRP3 Pathway

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Current risk assessments for the co-occurrence of lithium (Li) and microplastics (MPs) are largely based on simple binary mixture models, which may underestimate the distinct hazards posed by pollutant-loaded carrier particles in real plastisphere environments. In particular, it remains unclear whether Li adsorbed onto MPs behaves merely as a mixture component or as a new toxicologically relevant entity with its own biological effects.

To address this question, this study combined adsorption characterization, in vivo reproductive toxicity assays, and interaction-effect analysis to determine the role of Li–MP composites in male reproductive injury. Adsorption isotherm analysis showed that MPs had a considerable Li-loading capacity, with a maximum surface loading of 0.18 mg/g. Based on this, we compared the toxic effects of Li alone, simple co-exposure, and pre-adsorbed Li–MP composites.

The results demonstrated that the Li–MP composite acted as a distinct bioactive entity and caused more severe reproductive damage than Li alone. Specifically, exposure to the composite led to a markedly greater decline in sperm quality and a significant reduction in serum testosterone levels, which decreased by 30.74%, despite no further increase in Li bioaccumulation. Mechanistically, the aggravated toxicity was associated with enhanced oxidative stress, as reflected by increased ROS (1.36-fold) and MDA (1.59-fold) levels together with decreased SOD activity (0.83-fold). This was accompanied by elevated inflammatory responses, including increased IL-17A (2.79-fold) and IL-1β (1.71-fold), as well as activation of the NLRP3 inflammasome pathway, evidenced by upregulation of NLRP3 (1.98-fold), ASC (1.55-fold), and cleaved caspase-1 (1.81-fold). These alterations ultimately promoted germ cell pyroptosis and mitochondrial apoptosis.

Notably, whereas conventional binary mixture models predicted synergistic toxicity, the pre-adsorbed Li–MP composite behaved as a singular toxic unit with additive toxic effects. This discrepancy indicates that MPs do not simply function as passive carriers, but can amplify toxicity by transforming pollutants into novel composite entities after adsorption. This study therefore proposes the “pollutant composite,” rather than the binary mixture alone, as a more appropriate fundamental unit for risk assessment, thereby improving prediction of health outcomes associated with contaminant–plastic interactions in plastisphere environments.

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1.06.B.T04 Size-dependent pulmonary toxicity of inhaled micro- and nano-polystyrene and initial identification of microplastics in human lung cancer tissue

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Background: Airborne microplastics (MPs) are emerging environmental contaminants with potential implications for respiratory health, yet the biological consequences of chronic inhalation exposure remain poorly understood. This study investigated the size-dependent pulmonary toxicity of inhaled MPs associated with lung carcinogenesis.
Methods: Mice were exposed to aerosolized micro-polystyrene (mPS; 0.25μm) and nano-polystyrene (nPS; 20nm) for 12 weeks. Pulmonary effects were assessed using micro-CT imaging, exercise testing, histopathology, and transcriptomic profiling. Resected lung tumor tissues from patients with lung cancer were also analyzed for the presence of MPs.
Results: Repeated inhalation of environmentally relevant concentrations for up to 12 weeks produced significant pulmonary toxicity, with the most pronounced effects observed in the mPS-exposed group. Compared with nPS, mPS exposure resulted in greater reductions in lung volume, decreased exercise endurance, and more extensive histopathological alterations within lung tissue. Molecular analyses further revealed a marked increase in epidermal growth factor receptor (EGFR) expression following mPS/nPS exposure. Transcriptomic profiling identified Amphiregulin (AREG) and Mitogen-Activated Protein Kinase Kinase Kinase 13 (MAP3K13) as key regulators associated with EGFR-dependent MAPK signaling pathways, suggesting activation of molecular mechanisms linked to tumorigenesis. In addition to the experimental findings, MPs were detected in resected tumor tissues from patients with lung cancer, providing preliminary evidence that MPs can accumulate in human pulmonary tissue.
Conclusion: These findings demonstrate size-dependent pulmonary toxicity of inhaled MPs, with mPS exhibiting greater pathogenic potential than nPS, and suggest that MPs may promote inflammatory and oncogenic signaling pathways implicated in lung carcinogenesis.

1.06.B.T05 Polystyrene nanoplastics alter intracellular signaling modulating trophoblast differentiation

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Micro- and nanoplastics (MNPs) are widespread in the environment, and several studies have reported their presence in human placental tissues, raising concerns about potential risks to reproductive health. Proper placental development and function are essential for a successful pregnancy, as the placenta plays a critical role in nutrient exchange, hormone production, and maintenance of fetal growth. However, the impact of MNPs on placentation and placental function remains largely unknown. In this study, we examined the effects of nanoplastics on trophoblast syncytialization, a process essential for the formation of the syncytiotrophoblast layer and the maintenance of normal placental function, using the human choriocarcinoma cell line BeWo. We selected three types of polystyrene (PS) nanoparticles as model nanoplastics, unmodified PS, amino-modified PS (PS-NH_2), and sulfate-modified PS (PS-SO_4), all with a diameter of 200 nm, to investigate toxicity based on physicochemical properties.
First, a cell fusion assay using the NanoLuciferase-based HiBiT system was performed. Cells were

exposed to PS, PS-NH_2, and PS-SO_4 for 48 hours in the presence of forskolin to induce syncytialization. The results showed a reduction in luminescence in the PS and PS-NH_2 groups, whereas PS-SO_4 had no significant effect. Consistent with these findings, real-time RT-PCR analysis revealed that PS-NH_2 significantly decreased the expression of syncytialization markers, including CGB, ERVFRD-1, and SDC-1, along with a reduction in hCGβ production. Additionally, in the PS group, the expression of CGB and ERVFRD-1, as well as hCGβ production, were reduced at higher doses. Further mechanistic analysis revealed that both PS and PS-NH_2 significantly decreased intracellular cyclic AMP (cAMP) levels, indicating disruption of a central signaling pathway required for syncytialization and proper trophoblast differentiation. This disruption may lead to impaired placental development and function. Collectively, these findings suggest that nanoplastics, particularly PS-NH_2, impair trophoblast differentiation and disrupt placental function. Surface charge appears to be a critical determinant of nanoplastic-induced placental toxicity, with PS and PS-NH_2 inhibiting syncytialization, while PS-SO_4 exhibits minimal effects. Ongoing transcriptomic analyses aim to further elucidate the molecular mechanisms underlying these effects and their implications for pregnancy outcomes.

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1.06.P - Exposure and Effects of Micro- and Nanoplastics in the Environment and Implications for Ecological Risk Assessment

1.06.P–Tu018 Micro- and Nanoplastics in Injectable Local Anaesthetic Solutions: Detection and Quantification

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Microplastic and nanoplastic particles (MNPs) have been increasingly reported in environmental and human biological systems; however, their presence in injectable pharmaceuticals has received limited attention. Injectable local anaesthetics are routinely administered in clinical practice and may represent a direct pathway for MNP exposure, particularly given their contact with plastic-based packaging. In this preliminary analytical study, commonly used local anaesthetics including lidocaine, bupivacaine, and ropivacaine were analysed to assess potential MNP contamination. Samples from both plastic and glass vials were processed under contamination-controlled conditions and sequentially filtered to separate microplastic (>1 μm) and nanoplastic (0.3–1 μm) size ranges. To better reflect clinical practice, additional samples were prepared using standard plastic syringes. Polymer identification and quantification were performed using pyrolysis–gas chromatography–mass spectrometry (Py-GC-MS). Polyethylene terephthalate (PET) and polystyrene (PS) were detected across all anaesthetic types, with higher concentrations generally observed in samples packaged in plastic vials. Microplastic

concentrations were consistently higher than nanoplastic concentrations, with the highest PET and PS concentrations observed in lidocaine packaged in polyethylene vials (0.094 and 0.11 μg/mL, respectively). Polycarbonate (PC) was detected only in lidocaine samples, while polypropylene (PP) was observed in a single ropivacaine replicate. No additional MNP contribution was detected following preparation with plastic syringes. Notably, several expected polymers, including polyethylene (PE) and polymethyl methacrylate (PMMA), were not identified. These findings suggest that MNP contamination may occur upstream of final packaging and highlight injectable anaesthetics as a previously unrecognised exposure pathway. This work provides an initial analytical framework for investigating pharmaceutical contamination and supports the need for further studies to evaluate variability across products, manufacturing processes, and potential implications for human exposure.
Keywords: Clinical microplastic exposure, Injectable drug solutions, Micro- and nanoplastics, Py-GC-MS.

1.06.P–Tu019 Microplastics in a Southern Appalachian Forest: Assessing Connections Between Atmospheric Deposition and Terrestrial Food Chains

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Microplastics (MPs, <5mm) are ubiquitous global contaminants, yet there is little information about their fate through terrestrial food webs. In the Southern Appalachian Forest of the United States of America, the atmosphere is a major source of MP pollution for the area. We provide the first assessment of MPs in wild shrews (Sorex cinereus, Sorex fumeus, Blarina brevicauda) and earthworms (a common shrew food source) collected. Following dissection, we harvested shrews heart, lungs, liver, kidneys, gut, and brain to examine MP presence and composition among organs, while earthworms were sampled as a whole organism. Thirty earthworm and organs of 19 shrews were digested with hydrogen peroxide, filtered, and examined microscopically to assess MP count, type, and color. A subset of samples was analyzed via Raman Spectroscopy to identify the type of plastic. We found that shrews had 55% higher MP concentrations per gram of tissue than earthworms. We also found differences in MP concentration across shrew organs, with the highest mean concentration in the lungs (48.8 MP/g) and heart (20.4 MP/g) and the lowest in the gut (4.1 MP/g). Fibers were the most common plastic morphology found in the samples. Our results suggest possible biomagnification or trophic transfer of MPs in this terrestrial food chain. Furthermore, differences in MP concentrations among tissues could be attributed to differences in cellular turnover rates. Our results demonstrate the ability for MPs to be accumulated and transferred up trophic levels in terrestrial ecosystems.

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1.06.P–Tu020 Salt Marshes as Environmental Filters for Microplastics

Microplastic contamination in coastal environments has been widely reported; however, quantitative assessments across interconnected habitats such as tidal flats and salt marshes remain limited. In particular, the role of salt marshes as potential sinks or environmental filters for microplastics has not been systematically evaluated based on sediment concentration data.

In this study, we compiled published datasets of microplastic concentrations in coastal sediments and

compared them with preliminary results from Suncheon Bay, Korea, a representative salt marsh ecosystem. Global salt marsh data show considerable variability due to differences in sampling strategies, size thresholds, and analytical methods, making direct comparisons challenging. Nevertheless, existing studies consistently indicate that salt marsh sediments can accumulate substantial amounts of microplastics.

In Korea, reported concentrations in subtidal sediments range from 28–136 particles/kg d.w. along the South Sea coast and 240–656 particles/kg d.w. in Gwangyang Bay, while tidal flat sediments from the west coast range from approximately 400 to 6500 particles/kg d.w. In contrast, preliminary observations from Suncheon Bay show concentrations of 1530–6391 particles/kg d.w., with a mean of 3484 particles/kg d.w., exceeding those of typical subtidal sediments.

These results suggest that salt marshes, characterized by dense vegetation and cohesive sediment structures, may act as effective environmental filters that enhance the retention and accumulation of microplastics relative to adjacent coastal environments. However, standardized comparisons are needed to account for differences in size ranges and analytical methodologies. Future research should focus on controlled, habitat-based comparisons and unified protocols to better quantify the filtering capacity of salt marsh ecosystems.

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1.06.P–Tu021 Preparation of Surface-degraded Polyvinly Chloride Micro- and Nanoplastics for Environmentally Relevant Toxicity Assessment

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Microplastics (MPs), plastic particles <5 mm, and nanoplastics (NPs), plastic particles <1 μm are widespread in the environment. MPs and NPs (MNPs) have been observed in all components of the environment. Humans are estimated to be exposed to thousands to millions of MNPs annually or several milligrams daily through inhalation, ingestion, and skin contact. Consequently, MNPs have been detected in human tissues, and it has been reported that the presence of MNPs in humans is associated with serious health issues, including inflammatory bowel disease, cardiovascular disease, and various cancers. Although research on toxicological effects of MNPs has grown in recent years, the extent of their impact remains uncertain. Notably, environmental MNPs exhibit diverse physicochemical properties such as size, shape, and surface degradation. However, most experimental studies use pristine polymers that poorly represent real-world conditions. Currently, only a limited number of studies have focused on preparing environmentally relevant MNPs. Therefore, we have been developing environmentally relevant MNP preparation platform with various polymer types. Polyvinyl chloride (PVC), one of the most used polymers, was employed in this study as a model polymer due to its less attention in MNP research. We further characterized particle size and shape of prepared samples for comparison with real environmental samples and evaluated biological effects using broad-spectrum cell lines.

In this study, commercially available fragment shape PVC-MPs and laboratory prepared fragment and sphere shape PVC-NPs were utilized, and their size and shape analysis were performed. Surface degradation of MNPs was induced by exposing 172-nm vacuum ultraviolet radiation, which increased carbonyl formation as confirmed by ATR-FTIR. A strong positive correlation was observed between degradation time and the carbonyl index values, an indicator of oxidative degradation. The prepared PVC-MNPs were tested in human cell lines; A549, Caco-2, and THP1. Across all models, degraded PVC-MNPs induced stronger, dose-dependent cytotoxicity compared with non-degraded ones, and degraded NPs were consistently more cytotoxic than degraded MPs. These findings highlight the importance of considering environmentally relevant MNPs and their physicochemical characteristics into toxicity evaluation. Currently, the study is focusing on genotoxicity of prepared PVC-MNPs and those associated with additive chemicals.

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1.06.P–Tu022 Preparation and Cellular Assessment of Polypropylene Micro- and Nanoplastics Reflecting Real-World Environmental Properties

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Microplastics (MPs) and nanoplastics (NPs) have been detected in the environment and various human tissues, raising concerns about health impacts. Although environmental micro- and nanoplastics (MNPs) undergo morphological changes and surface oxidative degradation due to UV radiation and wave action, research remains heavily biased toward commercially available spherical polystyrene. Polypropylene (PP), the second most produced plastic, is severely understudied, and most studies ignore surface oxidative degradation. This study established a preparation platform for PP-MNPs reflecting real-world morphology and surface oxidative degradation, and systematically evaluated their cellular effects.
PP-MNPs were prepared by non-solvent induced phase separation: PP beads dissolved in xylene were re-precipitated by ethanol addition, with particle size controlled by varying addition rate. Surface oxidative degradation was induced by 172 nm vacuum UV irradiation. Characterization by SEM and ATR-FTIR, including carbonyl index (CI) calculation, confirmed that 0.3 mL/s ethanol addition yielded fragment-shaped MPs (approximately 3 μm) and 25 mL/s yielded imperfectly spherical NPs (approximately 250 nm), both resembling real environmental samples. No structural changes or impurities were detected, and post-degradation CI values matched those of environmental samples, confirming successful reproduction of real-world surface oxidative degradation.
Cytotoxicity was assessed using macrophage-like differentiated THP-1 cells, Caco-2 intestinal epithelial cells and A549 epithelial cells exposed to PP-MNPs for 24 hours (MTT assay). All cell lines showed concentration-dependent decreases in viability, with degraded PP-MNPs exhibiting significantly stronger cytotoxicity than non-degraded particles. Caco-2 cells were the most sensitive, and time-course analysis confirmed that stronger surface oxidative degradation correlated with stronger inhibition of cell proliferation.
These results demonstrate that surface oxidative degradation markedly enhances PP-MNPs cytotoxicity, underscoring the importance of environmentally realistic model particles in MNP health assessments. Future in vivo studies and evaluation of effects via intestinal immunity and gut microbiota are expected to advance health risk assessment of environmental MNPs.

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1.06.P–Tu023 Development of a Portable Hollow-Fiber System for Sampling and Quantifying Microplastics Larger Than 1 μm

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Microplastics (MPs) in treated drinking water have emerged as a regulatory concern, particularly in the European Union where routine monitoring is mandated, and in California where tap-water monitoring guidelines have recently been proposed. Although these frameworks outline recommended sampling and analytical approaches for both raw and treated water, their implementation remains impractical. Current protocols require prolonged sampling and the use of large, costly concentration systems capable of processing several hundred liters of water in situ, presenting significant technical and logistical barriers. Moreover, multiple studies suggest that MPs detected in tap water may originate from post-treatment contamination within distribution systems rather than from water purification facilities, underscoring the need for point-of-use measurements. To accurately evaluate human exposure and associated health risks, reliable and scalable methods are needed to quantify MPs—including their concentrations, size distributions, and polymer chemistries—directly at consumer endpoints.
Here, we present a newly developed portable hollow-fiber concentration system (Mitsubishi Chemical Cleansui Corporation) designed for rapid sampling of MPs >1 μm in tap water. The system is compact and installation requires only attachment to a standard faucet, comparable to operating a household shower head. Sampling several hundred liters of tap water can be completed within 30 minutes automatically, and MPs are retained within a dedicated concentration chamber integrated into the shower-head unit. The retained fraction is subsequently digested using 30% hydrogen peroxide and further concentrated onto a 1 μm silicon membrane filter. Identification and quantification are performed using micro-Raman spectroscopy coupled with imaging-based particle recognition.This presentation will demonstrate the system’s contamination control and will report an example of measured MP concentrations, size distributions, and polymer compositions from a faucet. The results highlight the capability of this field-deployable method to enable scalable, regulatory-relevant monitoring of microplastics in drinking water at the point of human exposure.

1.06.P–Tu024 Preparation of environmentally relevant polyethylene nanoplastics and evaluation of their cellular responses

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Recently, growing concerns have emerged regarding the adverse effects of plastic waste, particularly microplastics (MPs), defined as plastic particles smaller than 5 mm, and nanoplastics (NPs), which are less than 1 μm in size. Microplastics and nanoplastics (MNPs) have been detected not only in food and drinking water, but also in human lungs, blood, and placenta. Therefore, humans and other organisms cannot avoid exposure to MNPs. Furthermore, human epidemiological studies have indicated a relationship between MNPs and diseases, highlighting the growing importance of evaluating their biological effects. In addition, environmental MNPs comprise a wide variety of polymer types and exhibit diverse physicochemical properties. However, most laboratory studies rely on single-type model particles (e.g., spherical polystyrene), leading to a substantial gap between experimental systems and real-world environmental MNPs. In this study, we focused on polyethylene (PE), a material for which NPs are difficult to obtain and attempted to prepare reference samples and evaluate their cellular responses. We first established a preparation method for standard fragment shaped PE-NPs samples. Furthermore,

considering that surface modification (e.g., oxidative degradation) occurs in the environment due to factors such as ultraviolet radiation and wave action, we prepared degraded PE-NPs that reflect environmental conditions via 172 nm vacuum ultraviolet irradiation. The size, shape, and surface properties of the prepared PE-NPs were evaluated by SEM observation and ATR-IR spectroscopy. Comparative analyses with MNPs in the environment demonstrated that the prepared PE-NPs adequately reflect environmental conditions. Additionally, cytotoxicity assessments suggested that degradation treatment enhanced cytotoxicity. To evaluate cellular uptake, we also prepared labeled PE-NPs using Quantum dots, which are fluorescent nanoparticles containing metal atoms, enabling both qualitative assessment via fluorescence detection and quantitative assessment based on metal content. The physicochemical properties of labeled PE-NPs were also evaluated using SEM and ATR-IR. Evaluation of cellular uptake revealed that degradation treatment increased the cellular internalization of the particles. In the future, we aim to develop MNPs with diverse polymer types (PE, PP, PS, PVC, PET) and physicochemical properties (shape, size, surface properties) and assess their biological effects.

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1.06.P–Tu025 Adsorption of selected pharmaceuticals onto weathered and unweathered microplastics and optimisation of adsorption parameters.

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Pharmaceutical contaminants are classified as emerging pollutants, posing threats to many organisms due to their endocrine disruptive properties. Microplastics, a common global pollutant in many environments, may provide a suitable surface for pharmaceutical contaminants to adsorb onto. The aim of this study was to investigate the adsorption of selected pharmaceutical contaminants onto unweathered and weathered microplastics. The analytes of interest for this study were desogestrel, mestranol, norethindrone, flumequine, ofloxacin, and oxolinic acid. The study involved optimising the adsorption parameters, such as size and mass of the microplastic, pH, concentration, thermodynamic and kinetic studies. These parameters provided an improved understanding of the behaviour and fate of these pollutants and how they may interact in the environment. A comparison of the microplastic particle size showed that the smallest particle size studied, 300-600 μm, had the higher adsorption capacity range, 2.62 – 3.74 mg g-1 due to a greater surface area for adsorption. The adsorption capacity was determined using liquid chromatography with a PDA detector. A pH study was conducted by varying the solution pH between 2-10, with the highest adsorption capacity range, 2.03 – 3.07 mg g-1, at pH 8. There were notable differences in the adsorption between weathered and unweathered microplastic related to the pH, which could be attributed to the difference in the microplastic surface after weathering. The type of adsorption taking place between the microplastic and pharmaceutical pollutant, followed the pseudo second order model, that indicates chemisorption. The data obtained from the thermodynamic study fitted the Langmuir model showing that a monolayer adsorption takes place forming a homogenous surface. The microplastics were characterised using Fourier transform infrared spectroscopy (FT-IR) and Scanning electron microscope (SEM), before and after adsorption of the pharmaceutical contaminants. The outcomes from this study may be beneficial in improving pharmaceutical waste management, by understanding how these contaminants interact in the environment in the presence of microplastics. It may also assist to improve the removal efficiency of pharmaceutical contaminants at wastewater treatment plants as microplastics could potentially be utilised in a controlled manner to allow for the adsorption of pharmaceutical contaminants resulting in their removal from the wastewater.

1.06.P–Tu026 Microplastics Derived from UV-Weathered Biodegradable Mulch Films Induce Plant Stress and Rhizosphere Functional Shifts

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Biodegradable mulch films (BDMs) are promoted as alternatives to conventional polyethylene mulches, but weathering may generate residues with distinct ecological effects in agricultural soils. We compared microplastics derived from non-weathered and UVC-weathered commercial polylactic acid/polybutylene adipate-co-terephthalate (PLA/PBAT) BDMs in chili pepper (Capsicum annuum L.) and its rhizosphere. PLA/PBAT films were untreated or UVC-weathered for 28 days, then cryogenically milled, sieved, and incorporated into soil at 0.05% and 0.1% (w/w). At 56 days, material properties, plant stress responses, and microbial structure and function were assessed. UVC weathering roughened and oxidized surfaces, reduced thermal stability, and increased fragmentation susceptibility. Mean particle size decreased from 131.14 to 70.55 μm, surface O/C ratio increased from 0.11 to 0.24, and T5% decreased from 319.67 to 259.48 °C. Plant responses were most evident in the weathered 0.1% treatment, where shoot fresh weight and leaf number decreased from 4.29 to 3.28 g and from 17.78 to 11.33, respectively, relative to the control. Compared with the corresponding non-weathered treatment, maximum photosystem II efficiency decreased from 0.67 to 0.53, whereas energy dissipation per reaction center increased from 0.98 to 2.12, indicating a shift in photosystem II energy allocation. Weathered 0.1% BDM-MPs also increased malondialdehyde content and peroxidase and superoxide dismutase activities by 137%, 108%, and 72%, respectively, while catalase was not significantly affected. Respirometry showed greater O_2 consumption in UVC-weathered than non-weathered BDM-MP treatments, suggesting enhanced aerobic biodegradation potential. In contrast, Biolog EcoPlate AWCD was lowest in weathered treatments, indicating reduced utilization of common labile carbon substrates. Consistently, weathered BDM-MPs shifted bacterial composition and predicted aromatic compound transformation pathways without reducing alpha diversity. Together, these results suggest that UVC weathering did not elicit a uniform biological response, but rather shifted the effects of PLA/PBAT BDM-MPs across plant and rhizosphere compartments. These findings indicate that BDM residues should not be assumed environmentally benign solely because of their biodegradability; weathering status and particle properties should be considered in ecological risk assessment because responses may differ across the soil–plant–microbe continuum.

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1.07.P - Impact of Microplastics on Aquatic Organisms

1.07.P–Mo017 Ecotoxicity and Bioaccumulation of PET Microfibers of Different Sizes in the Freshwater Ostracod Cypridopsis vidua

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Microplastics represent one of the most relevant emerging contaminants worldwide due to their persistence and interaction with aquatic organisms. Microfibers derived from synthetic textiles, such as polyethylene terephthalate (PET), are among the most abundant fractions in continental water bodies. However, their ecotoxicological effects on detritivorous organisms such as freshwater ostracods remain poorly understood, particularly regarding the influence of particle size on ingestion, bioaccumulation, and toxicity. This study aimed to evaluate the concentrations at which PET microfibers of different sizes induce lethal effects in the freshwater ostracod Cypridopsis vidua, and to characterize their bioaccumulation and distribution in tissues and fecal pellets. It was hypothesized that toxicity depends on

microfiber size, with particles accumulating in the digestive tract and subsequently being excreted. Laboratory bioassays were conducted under controlled conditions, including acute (48 h) and chronic (21 days) exposures, using PET microfibers of three sizes (1, 10, and 50 μm) at concentrations ranging from 3 to 480 fibers/mL. The presence of microplastics in groundwater in Quintana Roo highlights the environmental relevance of this study. Organisms were cultured under standardized conditions (25 °C; 12:12 light–dark photoperiod). Mortality, population growth, and behavior were evaluated. Bioaccumulation was analyzed using ultraviolet (UV) fluorescence microscopy, allowing detection of microfibers in organisms and fecal pellets. Results showed bioaccumulation across all sizes, with active ingestion and fluorescence in the digestive tract, carapace valves, and other tissues. Acute bioassays showed a relationship between concentration and mortality, suggesting size-related toxic effects. Due to natural fluorescence in ostracods (pteridines), rhodamine B was used to stain PET microfibers and distinguish them from biological signals. This study improves the understanding of microplastic ostracod interactions. Cypridopsis vidua is proposed as a model organism and potential bioindicator for microplastic contamination in karst aquatic ecosystems of Quintana Roo, where these contaminants threaten water quality and biodiversity.

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1.07.P–Mo018 Development and Validation of a Direct Oral Administration Method for Microplastics for the Quantitative Assessment of In Vivo Kinetics and Vector Effects in Fish

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Microplastics (MPs) are frequently detected in the gastrointestinal tracts of fish collected from natural marine environments. Consequently, concerns have emerged regarding the potential translocation of ingested MPs into internal tissues and the transport of associated chemicals via so called vector effects. However, these processes remain poorly understood. Conventional laboratory exposure experiments typically rely on MP ingestion via waterborne routes; however, large interindividual variability in MP uptake makes it difficult to obtain highly reproducible data. To address this limitation, the present study developed a direct oral administration method to introduce MPs into the fish digestive tract together with feed. The effectiveness of this method was evaluated, and the vector effects of MPs were examined using polycyclic aromatic hydrocarbons (PAHs), a representative group of marine contaminants. Juvenile red sea bream (Pagrus major; body weight approximately 10–30 g) were used as test organisms. The administration apparatus was optimized to deliver MPs directly from the oral cavity to the stomach, and optimal feed viscosity and tolerable doses of feed and MPs for gastrointestinal administration were determined. To assess the reliability of the method, MPs with diameters of 250–300 μm were administered to juvenile fish (n = 3), and dosing accuracy was calculated as the ratio of the number of MPs excreted to the nominal number administered. Dosing accuracy consistently exceeded 95% in fish weighing approximately 10 g and 30 g, indicating that the developed method allows highly reproducible and accurate MP dosing. To assess vector effects, MPs (250–300 μm) were immersed for 48 h in seawater containing 16 PAHs at a concentration of 2 μg/L to allow PAH adsorption onto MP surfaces. These PAH adsorbed MPs were orally administered to juvenile fish ranges from one to three times. After a certain period, the fish were dissected, and PAH concentrations in the liver and muscle tissues were quantified using gas chromatography–mass spectrometry. The result indicated that no significant differences in PAH concentrations were observed between MP treated and MP-non-treated groups under any experimental conditions. These results suggest that, under the experimental conditions of this study, the vector effects of MPs for PAHs are limited.

1.07.P–Mo019 Assessing Factors Affecting Microplastic Toxicity on Aquatic Organisms Using Species Sensitivity Distribution

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Microplastic (MP) pollution has been shown to adversely affect aquatic organisms, causing physiological, reproductive, and behavioral alterations. Despite the rapid growth of research in this field, identifying the precise drivers of MP toxicity remains challenging due to the diversity of particle characteristics and variability in experimental methods. This study conducted a meta-analysis of existing MP exposure studies to identify key factors influencing toxicity, determine highly sensitive aquatic organisms, and effective testing methods. The findings aim to support improved impact assessment frameworks and serve as a guide for plastic-related thresholds.

A total of 3,997 articles related to MP and aquatic systems were retrieved from the Scopus database, of which 213 toxic values (76 species) met the selection criteria. Plastic characteristics, including size, polymer type, and shape, were gathered for analysis. Semi-chronic and chronic exposure data reporting lowest observed effect concentrations (LOECs) were used to construct species sensitivity distributions (SSDs) and estimate the fifth percentile hazard concentration (HC5). Analyses were conducted for individual characteristics along with their combinations.

The LOEC values ranged from 5.5 × 10-12 to 2.15 × 10^5 μg/L, with the lowest value observed in the fish Oryzias latipes. Toxicity varied across MP characteristics, with particle size often influencing sensitivity across both individual and combined analyses. Organisms exposed to smaller particles (0.001–1 μm, including nanoplastics) exhibited the lowest estimated HC5, at 1.24 × 10^{-6} μg/L (95% confidence level: 1.08 × 10^{-8} – 0.92 μg/L), more than 10,000-fold lower than that of the next size class (1-10 μm). Polystyrene particles appeared to induce toxicity at lower concentrations than polyethylene, as did spherical than fragment-shaped particles; however, these differences may be influenced by imbalanced data available. Variation of sensitivity across taxonomic groups was also revealed, where bivalves had the lowest HC5.

These findings highlight the importance of considering MP characteristics when evaluating effects on aquatic organisms. Future studies should further investigate the relationship between organism size and particle size to clarify exposure pathways. Additionally, the identification and validation of sensitive indicator species will be essential to improve assessment methods.

1.07.P–Mo020 Evaluating Crumb Rubber as a Proxy: A Comparison with Tire Wear Particle Effects in Tadpoles

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Tire wear particles (TWPs) are abundant yet understudied form of microplastic generated by tire abrasion on road surfaces. These particles vary in size, contain durability-enhancing chemical additives, and accumulate in aquatic systems like retention ponds during storm runoff. Frogs depend on these aquatic habitats for reproduction and early development, which may indirectly make them vulnerable to chronic TWP exposure. Within ecotoxicology studies, crumb rubber (CR) is commonly used as a proxy for TWPs in exposure, accumulation, and elimination assessments. However, few studies directly compare environmentally relevant TWPs with their proxies. This gap underscores the need to evaluate differences in ecological relevance and biological impacts between these two particle types. The primary objective of this project is to assess whether early stage amphibians accumulate TWPs and CR during a 96-hour exposure and whether these particles exhibit similar uptake and elimination patterns. Particle accumulation was measured every 24 hours in the gills, liver, and gastrointestinal (GI) tract and then tadpoles were transferred to particle-free water for an additional 96 hours to assess depuration at the same 24-hour intervals. CR exhibited higher accumulation in the gills (>10 particles/g tissue) and liver (>65 particles/g tissue), whereas TWPs showed greater accumulation in the GI tract (>0.002

particles g /g tissue). During depuration, CR was retained in the gills and liver to a greater extent than TWPs, although TWPs showed initial retention in both the liver and GI tract. Understanding the behavior of these particle types informs next steps focused on their sublethal effects and associated cellular responses. Aerobic organisms regulate reactive oxygen species (ROS) to maintain physiological balance. To evaluate stress responses, a static 96-hour exposure assay will be conducted using American bullfrog tadpoles (Gosner Stage 25). This approach will assess whether differences in TWP and CR exposure lead to distinct biological stress responses. Liver tissue will be analyzed for key oxidative stress biomarkers, including superoxide dismutase (SOD), catalase, and glutathione (GSH), which are synthesized and active in the liver. This work supports evaluating the physiological effects of TWP exposure and highlights key differences between CR and TWPs that are critical for interpreting laboratory toxicity studies and assessing real-world risks to developing amphibians.

1.07.P–Mo021 Increase in Microplastic Concentrations in Golden Clams (Corbicula fluminea) Between 2018 and 2025 in the Little Tennessee Watershed, North Carolina, USA

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Global plastic production continues to increase by ~8% annually despite growing concerns about its environmental and human health impacts. Recent studies have demonstrated that forested headwater streams in the Southern Appalachian Mountains of western North Carolina contain some of the highest concentrations of microplastics (MPs) ever recorded in freshwater systems; however, concentrations of MPs in rivers within this region and across different years have not been examined. We used Golden Clams (Corbicula fluminea) as biological indicators to assess changes in MP concentrations from 2018 to 2025 at six sites in the Little Tennessee River basin in western North Carolina, USA. For a more complete understanding of MPs in the whole freshwater system, atmospheric deposition and stream water samples were also collected and analyzed. Overall, from 2018 to 2025, we found a 54.5% increase in the mean number of MPs in our clam samples and a 73.9% increase in the mean MPs per gram of clam tissue, although those results varied among the six sites. Consistent with 2018 observations, fibers were the most prevalent type of MP, accounting for >90% of particles found in atmospheric samples, stream water samples, and clams. Our findings on counts and concentrations of MPs in Golden Clams are among the highest ever recorded from bivalves. We also found that MP counts and concentrations were high even in remote sections of the Little Tennessee River, which is considered a biodiversity hotspot for rare fish and freshwater mussels. Our findings support the need for further research into the pervasive nature and effects of MPs on freshwater systems and their influence on biodiversity, as native bivalve populations have experienced enigmatic declines in recent decades.

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1.07.P–Mo022 Toxicity of hexabromocyclododecane-enriched expanded polystyrene microplastics in black rockfish: Acute and sub-chronic oral exposure

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Hexabromocyclododecane (HBCD), a brominated flame retardant widely used in expanded polystyrene (EPS) production, is globally regulated as a hazardous substance owing to its high environmental persistence and bioaccumulation potential. Despite stringent regulatory measures, HBCD leachates and EPS microplastic (EPS-MPs) fragments legacy pollutants arising from manufacturing, disposal, and recycling remain ubiquitous in marine environments, posing threats to aquatic organisms via trophic transfer and associated toxicological effects. In this study, we investigated the toxicological impacts of EPS-MPs and their associated HBCD on adult black rockfish (Sebastes schlegelii), an ecologically and commercially important species along the South Korean coast. Fragmented EPS-MPs of two sizes (4.5 mm and 200 μm) were administered orally via gelatin capsules, with physiological evaluations performed on days 4 and 7 post-exposure. While no direct mortality or growth inhibition was observed over the 7 days sub-chronic exposure, a substantial proportion of EPS-MPs was retained within the gastrointestinal tract of high-dose individuals. Hepatic HBCD accumulation increased in a dose-dependent manner, concomitant with adverse systemic effects including decreased viability of leukocytes and splenocytes. Integrated multi-omics analysis of hepatic transcriptomes and metabolomes revealed size- and dose-dependent toxicological mechanisms, specifically a significant suppression of immune and inflammatory responses alongside a pronounced decline in metabolic activity. These findings demonstrate that while EPS-MPs may not trigger immediate lethality, they induce critical sub-lethal cellular responses characterized by transcriptional suppression and metabolic depression, with potential for significant ecological consequences under prolonged exposure.

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1.07.P–Mo023 Molecular Responses Across Generations to Ciprofloxacin and Polylactic Acid Microplastic Co-Exposure in Daphnia

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The presence of microplastics (MPs) in aquatic environments, together with coexisting micropollutants, raises concerns regarding long-term ecological effects arising from their potential interactive behaviors under simultaneous exposure conditions. In particular, biodegradable microplastics (BMPs), which are only partially degraded in freshwater systems, may function as carriers that modify the fate and toxicity of associated contaminants. Meanwhile, antibiotics introduced through anthropogenic activities such as excessive consumption and inadequate wastewater treatment have become widely distributed in freshwater environments at varying concentration levels. Despite this, the consequences of their combined exposure with BMPs over extended biological timescales remain largely unresolved.

To address this, the present study focused on Daphnia magna and examined multigenerational responses (F0–F3) following co-exposure to ciprofloxacin (CIP) and polylactic acid microplastics (PLA MPs). At the individual level, survival and cumulative offspring showed a decreasing trend in the combined

treatment in F0–F2, with partial recovery observed in F3. Although no significant differences in the time to first brood were observed in F0, significant reproductive delays emerged in F3, including prolonged time to first brood, extended interbrood intervals, and a reduced population growth rate.

At the molecular level, the parental generation (F0) exposed to CIP and PLA MPs for 21 days exhibited a significant 54.6% reduction in mitochondrial DNA copy number (mtDNAcn) relative to the control, whereas mtDNA integrity remained unchanged. Notably, the reduced mtDNAcn persisted across unexposed subsequent generations (F1–F3) in the CIP+PLA treatment group, demonstrating the long-term persistence of molecular alterations even after exposure cessation.

Overall, this study provides evidence that BMPs and antibiotics can induce transgenerational toxicity through mitochondrial genomic regulation.

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1.07.P–Mo025 Comprehensive Environmental Risk Assessment of Ship Paint-Derived Contaminants Released during Ship Hull In-Water Cleaning

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Ship antifouling coatings are increasingly recognized as a significant source of microplastics (MPs), metals, biocides, and organic matter released into the marine environment. These substances are primarily discharged during ship hull in-water cleaning (IWC), which has been identified by the International Maritime Organization (IMO) as a critical hotspot for the release of paint-derived pollutants. However, their integrated environmental risks remain insufficiently characterized due to the fragmented evaluation of individual contaminant groups in previous studies. To address this gap, the present study conducted a comprehensive assessment of multiple contaminant classes associated with antifouling paint emissions during IWC. Seawater samples were collected before and after cleaning operations, alongside IWC effluent samples obtained prior to and following onboard treatment processes. Target analytes included nano- and microplastics, metals, biocides, total suspended solids (TSS), and particulate and dissolved organic carbon (POC/DOC). Risk characterization was performed using multiple complementary approaches. For plastic particles, risk indices were derived based on polymer composition, hazard scores, and associated toxicity coefficients. For metals and biocides, predicted environmental concentrations (PECs) were compared against predicted no-effect concentrations (PNECs) to calculate risk quotients (RQs). TSS levels in wastewater were evaluated relative to background conditions and regulatory discharge thresholds. For POC and DOC, potential risk was evaluated considering the combined release of organic matter from both biofouling biomass and paint-derived sources. These results were then integrated to provide a holistic evaluation of the environmental risks associated with antifouling paint-derived contaminants released during IWC. The results demonstrate that IWC can act as a point source of multiple co-occurring hazardous substances, highlighting the importance of effective capture and treatment systems to mitigate environmental risk. This study supports the development of science-based management strategies and contributes to ongoing efforts to regulate IWC practices and minimize their environmental impact.

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1.07.T - Impact of Microplastics on Aquatic Organisms

1.07.T01 Effects of particle characteristics and chemical composition on microplastic toxicity in the marine rotifer: conventional microplastics and paint particles

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Microplastic (MP) pollution has become a global threat to marine ecosystems. The toxicity of MPs can vary depending on their physicochemical properties such as particle size, shape, and additives, suggesting that MPs should not be considered uniform contaminants in ecotoxicological assessments. Nevertheless, the relative contributions of particle properties and associated chemical components to MP toxicity remain poorly understood. Thus, in this study, we evaluated the particle-driven toxicity of pristine MPs (polypropylene and polyethylene) with different sizes and shapes and additionally investigated the toxicity of antifouling paint particles (APPs), which represent environmentally relevant and chemically complex MPs, to assess chemical-associated effects in the marine rotifer Brachionus koreanus. After exposure, the smaller MPs were more readily ingested than larger particles; however, ingestion rates were not directly associated with observed toxicity. In vivo toxicity tests showed that fragmented MPs more adversely affected survival and reproduction of rotifers than spherical MPs regardless of size. The toxicity of fragmented MPs increased with decreasing particle size but was reduced in the presence of food particles. These results suggest that particle shape plays a more critical role in determining MP toxicity than size, while environmental factors such as food availability can influence toxic responses. Multi-omics analyses consistently showed that fragmented MPs led to greater alterations in transcriptomic and metabolomic profiles than spherical MPs, with the strongest responses in smaller fragments. In particular, pathways associated with energy metabolism, particularly carbohydrate and lipid metabolism, were markedly affected by MP exposure. Furthermore, APPs and their leachates significantly altered survival, reproduction, transcriptomic and metabolomic profiles. Although whole APP suspension induced greater in vivo toxicity than leachates, ingestion of APP particles was not observed. Nevertheless, comparable transcriptomic and metabolomic responses were observed between whole APP suspension and leachate exposures, suggesting that associated chemicals play a major role in APP toxicity. Overall, our findings demonstrate that MP toxicity is influenced by both physical properties and chemical composition, highlighting the importance of considering multiple physicochemical properties to evaluate the ecological impacts of MPs in marine ecosystems.

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1.07.T02 Exposure to Nanoplastics Decreases Turbot (Scophthalmus Maximus) Survival to Infection by Tenacibaculum Maritimum

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Plastic pollution has resulted in the widespread accumulation of microplastics and nanoplastics (NPs) in marine environments, yet their impact on fish immune competence and disease susceptibility remains poorly understood. At the nanoscale, these particles can penetrate biological barriers, accumulate in

tissues, disrupt oxidative balance and interfere with immune signalling. This study investigated whether environmentally relevant concentrations of polystyrene NPs (PS-NPs; 100 µg/L) compromise immune defences in turbot (Scophthalmus maximus) juveniles and affect their vulnerability to bacterial infection. Fish were exposed to PS-NPs for 21 days and subsequently challenged with Tenacibaculum maritimum, a pathogen responsible for significant losses in marine aquaculture, via bath immersion. PS-NP exposure altered key haematological parameters, including elevated white blood cell counts and plasma peroxidase activity, alongside reduced plasma bactericidal capacity. Oxidative stress, measured as lipid peroxidation, was also significantly increased. Following bacterial challenge, PS-NP-pre-exposed fish exhibited markedly higher mortality (58%) compared to non-exposed infected controls (33%). These results demonstrate that environmentally relevant NP concentrations impair innate immune function in turbot, rendering them more susceptible to opportunistic infection. Taking turbot as a model for commercially valuable flatfish species, these findings carry direct relevance for both industry practices and regulatory frameworks governing marine pollution. These findings have direct implications for aquaculture biosecurity and underscore the need to incorporate sublethal pollutant effects into ecological risk assessments of plastic pollution in coastal marine systems.

1.07.T03 Integrating Physiology and Dynamic Energy Budget Modeling to Assess Food Chain-Level Effects of Microplastics and Tire Particles in Freshwater Ecosystem

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Microplastics (MPs) and tire particles (TPs) are recognized as pervasive contaminants in freshwater ecosystems due to their widespread occurrence, persistence, and potential ecological risks. Although the individual toxicity of MPs and TPs has been extensively investigated, their combined effects and trophic transfer within aquatic food chains remain insufficiently understood. Moreover, conventional toxicity assessments mainly focus on survival and growth endpoints, providing limited mechanistic understanding of how contaminant exposure alters organismal energy allocation and ecological functioning. To address these limitations, this study applied a Dynamic Energy Budget (DEB) theory-informed framework to evaluate the effects of MPs, TPs, and their mixture (MPsTPs) across a simplified freshwater food chain consisting of Chlorella vulgaris, Daphnia magna, and Danio rerio. Organisms were exposed to environmentally relevant concentrations (1 mg/L). Experimental endpoints, including growth, reproduction, feeding activity, and physiological stress indicators, were integrated with DEB-derived energy allocation proxies to assess changes in energy acquisition, maintenance, growth, and reproduction across trophic levels.

Results shows that contaminant exposure induced pronounced energetic disruption throughout the freshwater food chain. In Chlorella vulgaris, exposure elevated maintenance costs (p_M/p_A) while reducing growth allocation efficiency (p_G/p_A), indicating increased energetic demand for cellular maintenance at the expense of biomass production. In Daphnia magna, declines in reproductive efficiency (p_R/p_A) and energy availability were observed, particularly under MPsTPs exposure, suggesting a stress induced trade-off favoring survival over reproduction. At the secondary consumer, zebrafish exhibited elevated maintenance costs with reduced growth and reserve allocation, indicating chronic metabolic stress and constrained energy storage. MPsTPs exposure consistently produced stronger responses than individual exposures, highlighting potential additive or synergistic effects. These demonstrate that sublethal contaminant exposure can disrupt energy allocation across multiple trophic levels without necessarily affecting growth metrics. This study highlights the value of DEB-informed approaches for identifying hidden ecological impacts and provides mechanistic insight into how complex contaminant mixtures impair freshwater ecosystem functioning.

1.07.T04 Effect of Polyvinyl Chloride Microplastics on Copper Uptake and Neurotoxic Response on Dragonflies

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Dragonflies are regarded as good amphibiotic indicators of the health of freshwater ecosystems due to their sensitivity to changes in water quality. However, the toxicity of chemical contaminants is reported to be influenced by the presence of microplastics. Polyvinyl chloride (PVC) is among the commonly used plastics, and its microparticles are extensively recorded in freshwater ecosystems. Nevertheless, their interactions with chemical contaminants, such as metals, are poorly understood. The present study assessed the effect of polyvinyl chloride (PVC) microplastics on the uptake of copper (Cu) and the neurotoxic response in dragonflies. Neurotoxic response was assessed using the acetylcholinesterase activity. Dragonflies were collected from a pristine river and acclimatised for 72 hours before the experiment. During the experiment, dragonflies were exposed to distilled water (control), 0.5 mg/l Cu, 0.5 mg/l Cu + 2 mg/l PVC, and 0.5 mg/l Cu + 10 mg/l PVC treatments over 96 hours. The concentration of Cu was below the detection level in dragonflies from the control, with notable concentrations being observed for the three treatments. However, no significant difference was observed for Cu concentrations among the three treatments (p > 0.05). The control exhibited an AChE activity of 246.25 ± 48.10 U/ml, whereas a significant inhibition (112.25 ± 0.50 U/ml) was observed when exposed to 0.5 mg/l Cu. Nevertheless, an activity of 220.50 ± 30.93 U/ml was observed for 0.5 mg/l Cu + 10 mg/l PVC treatment. Moreover, no significant difference was observed for AChE activity between 0.5 mg/l Cu + 10 mg/l PVC and 0.5 mg/l Cu + 2 mg/l PVC (228.65 ± 19.13 U/ml) treatments (p > 0.05). Based on the current findings, treatments with PVC exhibited low inhibition of AChE relative to the 0.5 mg/l Cu treatment. These findings prompt the necessity to explore the long-term combined effect of metals and microplastics to elucidate the toxicity dynamics of these stressors.

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1.07.T05 Environmental Emissions of Antifouling Paint-Derived Microplastics from Ship Hull In-Water Cleaning and Hydroblasting

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Marine coatings, as polymer-based materials, are increasingly recognized as a significant source of microplastics (MPs) in the marine environment. Among these, antifouling (AF) paints have received particular attention due to their complex composition, which include polymeric binders, metals, and biocides, posing both physical and chemical risks upon release. Approximately 95% of AF paints are applied to submerged ship hull surfaces and may enter the marine environment throughout their life cycle, including application, operation, maintenance, and end-of-life processes. The International Maritime Organization (IMO) has identified ship maintenance activities, such as in-water cleaning (IWC) and hydroblasting, as key hotspots for microplastic release. This study quantified the abundance, mass concentration, and size distribution of AF paint-derived MPs generated during IWC and hydroblasting operations. Fourier transform infrared (FTIR) spectroscopy analysis indicated that paint particles (>20 μm) were predominantly composed of acrylic polymer, with >99% of particles smaller than 5 mm. Mass concentrations of AF-MPs were 24.7 mg/L for IWC and 1107.3 mg/L for hydroblasting, demonstrating substantially higher concentration in hydroblasting effluent. Mass-based emission factors (g/m2) were derived using total effluent volume and ship hull wetted surface area (WSA). Global annual emissions were estimated by combining emission factors with total WSA of the global fleet and hull

maintenance frequency. Estimated AF-MP emissions ranged from 87.0 to 1418.6 tons/year for IWC, decreasing to 11.7–190.0 tons/year with the application of particle treatment systems. In contrast, hydroblasting emissions were estimated at approximately 875.3 tons/year in the absence of treatment. Overall, ship hull maintenance activities were estimated to contribute approximately 8.5–20.4% of total marine paint-derived microplastic inputs. These results identify ship hull maintenance as a significant and well-defined sea-based point source of microplastic pollution. This study provides robust, empirically derived data to support science-based regulatory frameworks and management strategies aimed at mitigating marine microplastic pollution.

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1.08.P - Integrating Experimental and Modeling Approaches To Unravel the Mechanisms of Multiple Stressor Effects on Aquatic Ecosystems Under Climate Change

1.08.P–We018 Climate Warming Enhances the Toxicity of Chemical Mixtures: Implications for Genes Related to DNA Repair and Apoptosis in Freshwater Mollusks

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Chemical mixtures and rising temperatures are major drivers of molecular stress in aquatic organisms, yet their combined effects remain poorly understood. This study examined the impact of cadmium (Cd), bisphenol A (BPA), and endosulfan (End), individually and in mixtures, on DNA repair and apoptosis pathways in Physella acuta. Adults acclimated at 23°C were exposed to control conditions and a +2°C warming scenario (25°C) for 24 h, 7 d, and 21 d.

Organisms exhibited time-dependent transcriptional responses under both temperature conditions. An early stress response at 24 h involved modulation of DNA repair and apoptotic genes, followed by more treatment-specific patterns at 7 d and a general loss of transcriptional coherence at 21 d. However, warming altered these dynamics even more, resulting in less coordinated regulation of DNA repair pathways and more variable apoptotic responses over time.

Across temperatures, mixture exposures, especially Cd+End and ternary combinations, caused stronger and more persistent disruption of key DNA repair genes (XRCC3, Rad21, Rad50, PARP1) and apoptosis regulators (Casp3, AIF, NFkB p100) than single compounds. Overall, chemical mixtures induced greater molecular disruption, and moderate warming amplified these effects, highlighting the importance of considering multiple stressors under climate change scenarios.

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1.08.P–We019 Multistress at the Molecular Level: Analysis of Oxidative Stress Genes on Chironomus riparius Exposed to Chemical Mixtures and Different Temperatures

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There is a lack of knowledge about the mechanisms underlying responses to multistress in invertebrates. The gap is especially evident in aquatic invertebrates, which are essential in the food web of freshwater ecosystems. Oxidative stress is one of the most common effects of chemicals. To gain insight into how multistress can modulate oxidative stress-related genes, the effects of single, double, and triple mixtures of bisphenol A, cadmium, and endosulfan at four temperatures (18, 21.5, 23, and 25 ºC) have been studied. Three typical enzyme genes related to oxidative stress, Catalase, Superoxide dismutase Mn, and Superoxide dismutase Cu Zn, were selected to examine the impact of the three known toxicants (Bisphenol A, Cadmium, and Endosulfan). Fourth-instar larvae were exposed for 1, 2, and 4 days and then frozen individually. The RNA was extracted and retrotranscribed to analyze mRNA levels of the three selected genes by Real-Time PCR. As reference genes, actin and glyceraldehyde-3-phosphate dehydrogenase were used. The results show that time, temperature, and chemicals influence the response, opening new perspectives for mimicking the wild conditions. In addition, the complexity of result interpretation is highlighted by the number of variables implicated and the potential events that can occur in the cell during short-, medium-, and long-term molecular responses.

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1.08.P–We017 SEASON Project - How will climate change affect the risk associated with sediments contaminated with organic and inorganic pollutants?

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Climate change is driving significant alterations in aquatic systems through increased frequency of extreme weather events, shifts in physicochemical water parameters, and enhanced transport and remobilization of contaminants. These changes directly influence the fate, bioavailability, and toxicity of pollutants, particularly at the sediment–water interface, where sediments function as both sinks and secondary sources of contamination.

The SEASON project addresses these challenges through an integrated, interdisciplinary framework combining environmental toxicology, analytical chemistry, and hydrogeochemistry. The project focuses on temperature- and pH-driven processes that control contaminant speciation, mobility, and biological uptake. For example, increasing temperature can enhance diffusion, uptake rates, and bioaccumulation of pollutants, while pH shifts regulate metal release from sediments, potentially transforming them from stable reservoirs into active sources of exposure. Various investigations are conducted using sediment samples from impacted field sites, coupled with controlled laboratory and microcosm studies. Biological responses are assessed across multiple levels of organization, including molecular, cellular, and organismal endpoints, using model systems such as zebrafish. Complementary approaches include microbiome analyses, effect-directed analysis of complex mixtures, and advanced chemical characterization of metals and organic contaminants (e.g., PFAS). These datasets are integrated into mechanistic models describing pollutant partitioning, transport, and ecotoxicological effects. A central component of the project is the development of predictive modeling tools that link environmental drivers to contaminant dynamics and biological responses under climate change scenarios. Model outputs are validated against empirical data and used to identify key process-determining parameters governing environmental risk.

Therefore, the SEASON project aims to advance the mechanistic understanding and predictive capacity of pollutant behavior in aquatic systems under changing climatic conditions. The outcomes will support improved environmental risk assessment frameworks for contaminated sediments and contribute to evidence-based water resource management. In parallel, the project emphasizes stakeholder engagement, training, and dissemination to ensure effective translation of scientific findings into practice.

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1.08.P–We020 The Effects of Acute Temperature Changes on Oxidative Stress and Antioxidant Defense System in the Yesso Scallop Mizuhopecten yessoensis

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Over the last few decades, the global average sea surface temperature has risen rapidly due to global warming. In general, temperature is one of the most critical and dynamically fluctuating abiotic factors in aquatic environments, significantly affecting biological processes of marine organisms.This study investigated the effects of acute temperature changes on oxidative stress and stress-related responses in the Yesso scallop Mizuhopecten yessoensis. The intracellular reactive oxygen species (ROS), activities of antioxidant enzyme (e.g., glutathione S-transferase [GST], glutathione peroxidase [GPx], catalase [CAT], and superoxide dismutase [SOD]) and transcriptional expression of stress-related genes (e.g., GPx, CuZn/SOD, heat shock protein 70 [hsp70] and hsp90) were measured in response to acute temperature changes. At low temperature (12 °C), ROS level increased for up to 24 h and subsequently decreased, whereas at high temperature (28 °C), ROS levels slightly decreased after 24 and 48 h. Acute temperature stress significantly altered antioxidant enzymatic activities and stress-related genes expressions in M. yessoensis. Exposure to high temperature resulted in significant reductions in GPx and CAT activities, while GST and SOD activities increased after 72 and 48 h, respectively. In contrast, all stress-related genes were significantly downregulated in response to low temperature. Notably, hsp70 and hsp90 expression were significantly modulated by high temperature, suggesting their potential role in heat tolerance in M. yessoensis. In conclusion, high temperature led to an increase in the production of ROS and a corresponding change in the activity of antioxidant enzymes with the transcriptional expression of stress-related genes as the M. yessoensis attempts to mitigate the stress. Overall, these findings provide valuable information that acute water temperature changes induce ROS-mediated oxidative stress, resulting in cellular damage and the activation of antioxidant defense system in M. yessoensis.

1.08.P–We021 Assessment of synergistic effects of salinity and desalination chemical additives on coastal marine ecosystems

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Water resources in many regions of the world are facing critical challenges for facing the increasing demand of freshwater for multiple uses. Under this context, the development of seawater desalination has emerged as an alternative solution for producing high quality freshwater. However, this development introduces a significant amount of brine discharges into marine environments, highlighting an important global need to minimize their associated impacts on marine environment. Brine effluents from desalination plants are commonly discharged into the marine environment through submarine outfalls, resulting in a dense saline plume dispersion that affect marine environment. The high salinity and the presence of residual chemical additives in these effluents represent a primary environmental concern,

potentially affecting the sustainability of marine ecosystems and leading to potential seawater contamination. The general objective of this study is to assess the impacts of salinity and chemical additives associated with brine discharges on coastal marine ecosystems, by integrating oceanographic and physico-chemical characterization of saline plumes, and the evaluation of biochemical responses (oxidative and osmotic stress) in benthic communities under controlled laboratory bioassays. For that, we conducted controlled laboratory bioassays with the red macroalgae Rhodymenia corallina, a sensitive benthic bioindicator species previously used for brine discharge monitoring. Experiments evaluated: i) the effects of artificial brine exposure as the salinity factor; ii) artificial brine with antiscalant exposure as the combined salinity and chemical additive factor; iii) real brine exposure; and iv) the ecotoxicological effects of one conventional commercial additive vs one environmentally green alternative. Finally, the results obtained from the laboratory and literature-based evidence will be integrated to propose science-based thresholds and/or limits for excess salinity and desalination-derived chemical additives for a sustainable desalination development. The expected results will provide novel information on the combined effects of salinity and antiscalants, the comparative performance of green additive alternatives, and the suitability of benthic organisms as early-warning bioindicators.

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1.09.P - In Vitro, In Silico and Mechanistic Physiology for Understanding and Predicting In Vivo Toxicity and Endocrine Disruption

1.09.P–Tu027 Predicting Partition Ratios from MS/MS Spectra to Prioritize Structurally Unresolved Chemicals

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Non-targeted analysis (NTA) using high-resolution mass spectrometry detects large numbers of molecular features in environmental samples. Identifying and quantifying all detected chemicals is not feasible, so prioritization is necessary to focus effort on signals that may pose a higher risk to humans, wildlife, or ecosystems. While some prioritization approaches rely directly on observed signals, property-based approaches often require structural information or physicochemical descriptors that are unavailable for unresolved features.
This study investigates whether tandem mass spectrometry (MS/MS) data can be used to estimate partition ratios before full structural identification. Several in silico modeling strategies are being compared using cross-validation. Structure-agnostic approaches use latent representations learned directly from MS/MS spectra, while structure-informed approaches use molecular fingerprints, e.g. inferred from SIRIUS/CSI:FingerID. Prediction targets include partition ratios that govern phase distribution and are commonly used to assess environmental fate, transport, exposure potential, bioaccumulation, and internal exposure. Model performance, uncertainty, and applicability domains are compared across representation strategies and chemical classes.
This work aims to clarify when measurement-native approaches may provide useful early-stage prioritization for unresolved features and when explicit structural inference offers additional value. These predictive approaches may expand the information available for unidentified chemicals and support future hazard and risk assessment workflows using new approach methodologies (NAMs), especially for previously uncharacterized or difficult-to-test chemicals.

1.09.P–Tu028 Integrating In Vitro Bioluminescent Assays and Molecular Dynamics

to Assess Toxicity of Petroleum-Contaminated Soils

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Reliable assessment of petroleum-contaminated soils remains a major challenge in environmental toxicology, particularly due to discrepancies between chemical analyses and biological assays. Conventional solvent-based methods provide quantitative data but are incompatible with bioassays, while aqueous extracts often underestimate the toxicity of hydrophobic hydrocarbons.

This study proposes an integrated new approach methodology combining an enzymatic bioluminescent assay with molecular-level simulations to improve toxicity assessment of diesel-contaminated soils. Dimethyl sulfoxide (DMSO) was evaluated as a biocompatible extractant capable of solubilizing petroleum hydrocarbons while maintaining compatibility with a coupled enzymatic system consisting of NAD(P)H:FMN-oxidoreductase and bacterial luciferase.

Soil samples artificially contaminated with diesel fuel were extracted using aqueous DMSO and analyzed using a luminescence inhibition assay. Moderate DMSO concentrations preserved enzymatic activity, whereas higher concentrations caused partial inhibition. Diesel hydrocarbons dissolved in DMSO induced a clear concentration-dependent decrease in luminescence intensity. Soil extracts exhibited a strong dose–response relationship between contamination level and enzymatic inhibition, demonstrating that the proposed approach captures both contaminant presence and biologically relevant toxicity.

To provide mechanistic insight, molecular dynamics simulations were performed to evaluate the structural stability of the enzymatic system in different solvent environments. The simulations showed that DMSO and diesel components did not induce large-scale conformational changes but caused localized alterations in protein flexibility and hydration, providing a mechanistic basis for the observed inhibition effects.

Overall, the proposed approach integrates in vitro and in silico tools into a consistent framework for assessing petroleum-contaminated soils. This strategy enhances the reliability and ecological relevance of toxicity measurements and supports the development of new approach methodologies for environmental risk assessment of hydrophobic contaminants.

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1.09.P–Tu029 Deep Learning-Based Prioritisation of PFAS Risks Across Fish Ecotoxicity and Human Health Endpoints

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Per- and polyfluoroalkyl substances (PFAS) comprise a rapidly expanding group of highly persistent chemicals, yet toxicological evidence remains limited for most compounds. This creates a major challenge for risk assessment: the chemical space is expanding much faster than conventional testing can evaluate, while ecological and human health concerns continue to increase. Here, we present two complementary machine-learning studies designed to support large-scale PFAS toxicity prediction, mechanistic interpretation, and risk prioritisation from both ecological and human health perspectives. The first study focuses on fish ecotoxicity and establishes a predictive framework to estimate ecological safety thresholds across diverse PFAS structures and fish species. This framework enables systematic evaluation of toxicity variation, potential species sensitivity, and the role of chemical diversity in shaping

ecological risk. The second study focuses on human health relevance and develops a parallel predictive framework to assess PFAS-associated biological activity and toxicity thresholds across multiple health-related domains. Rather than relying on chemical-by-chemical evaluation alone, both studies use interpretable modelling strategies to identify broad patterns that may help explain why some PFAS are more likely to raise ecological or health concerns than others. Together, these studies provide a scalable predictive toxicology strategy for addressing PFAS data gaps, screening chemicals of potential concern, and supporting more targeted experimental testing. By integrating ecological and human health-oriented risk perspectives without directly extrapolating one to the other, this work offers a flexible framework for PFAS prioritisation, monitoring design, and proactive chemical regulation.

1.09.P–Tu030 Navigating In Vitro Testing Challenges for Complex Hydrocarbon Substances: Improving Dosing and Exposure Characterization

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High-throughput in vitro (eco-)toxicology is central to next-generation risk assessment, yet substances with poor water solubility remain difficult to test reliably. Hydrophobic chemicals, including polycyclic aromatic hydrocarbons (PAHs) and complex hydrocarbon mixtures, may partition to media constituents and plastics, causing unstable exposure concentrations. This undermines conventional dose-response analyses based on nominal concentrations and complicates in vitro-to-in vivo extrapolation (IVIVE). This work addresses the challenge of achieving reproducible and well-characterized exposures for hydrophobic substances in in vitro test systems that cannot be achieved/maintained using common media-miscible solvents such as DMSO. The influence of dosing strategies on bioactivity outcomes for PAHs tested individually and within a complex hydrocarbon substance was evaluated, by combining in vitro bioassays with partitioning modeling and analytical chemistry. The work showed that standard dosing techniques employed here often fail to maintain steady exposure, leading to variability and underestimation of bioactivity. Results demonstrate that conventional in vitro dosing approaches are inadequate for complex hydrocarbon substances with difficult to test properties. We identified opportunities for methodological refinement to stabilize exposure and accurately quantify bioavailable concentrations.
By improving dosing and exposure characterization, this work advances testing strategies for hydrophobic substances. These findings support more reliable hazard identification and strengthen IVIVE, with implications for regulatory assessments and broader application to difficult-to-test chemicals in environmental toxicology.

1.09.P–Tu032 Mechanism-Informed Classification of Per- and Polyfluoroalkyl Substances Using the Adverse Outcome Pathway-Based Explainable Artificial Intelligence Platform, ToxBAI

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Per- and polyfluoroalkyl substances (PFAS) are increasingly detected in consumer products and related exposure sources, with growing evidence of potential human toxicity. However, the mechanistic pathways linking consumer product-associated PFAS to toxicity remain insufficiently understood. Given the thousands of PFAS requiring evaluation, conventional toxicity testing alone is not feasible. Therefore, new approach methodologies (NAMs)-based prioritization frameworks are needed to consider both exposure relevance and toxicity potential. In this study, we constructed a consumer product-associated PFAS inventory and developed a mechanism-informed classification framework using ToxBAI, an adverse outcome pathway (AOP)-based explainable artificial intelligence (AI) platform.

The PFAS inventory was built by integrating chemical databases, product-use information, literature, and corporate reports, and was organized by product-use type and expected exposure route. Curated substances were screened using ToxBAI, our in-house platform that predicts PFAS toxicity potential using models trained on ToxCast and Organisation for Economic Co-operation and Development Test Guideline (OECD TG)-based toxicity data. Model outputs were interpreted with AOP-informed features to classify substances by predicted toxicity and biological interpretability.
To support evidence-based prioritization, AI-derived classifications were compared with toxicity evidence from ToxCast, ToxRef, literature, and regulatory reports. These sources were used to evaluate whether predicted high-concern substances were supported by experimental, mechanistic, or regulatory evidence, while identifying data-poor substances with limited toxicological characterization. Overall, the framework integrates product-use relevance, expected exposure route, predicted toxicity, and mechanism-informed explainability.
This study demonstrates the utility of ToxBAI as a prioritization tool for PFAS used or detected in actual consumer products in the context of next-generation risk assessment. Rather than uniformly screening all structurally defined PFAS, this approach focuses on PFAS with product-use or detection evidence and classifies their toxicity potential in a mechanistically interpretable manner. It can support selection of data-poor consumer product-associated PFAS for follow-up testing and evidence integration, while linking human exposure potential with predicted toxicity.

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1.09.P–Tu033 A Framework to Characterize Uncertainty in Dose Extrapolation from In Vitro Bioassays

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Thousands of chemicals require regulatory evaluation, yet in vivo toxicity data remain limited. New approach methods (NAMs), particularly in vitro bioassays, are increasingly being considered to support chemical risk assessment; however, there is a need to foster confidence in their ability to reliably translate in vitro bioactivity into biologically relevant in vivo dose metrics and to determine if the responses are adequate for chemical evaluations. Quantitative in vitro–in vivo extrapolation (Q-IVIVE) provides a method for using the in vitro dose and response information for comparisons with in vivo toxicity data and exposure data for risk-based evaluations. This study presents a structured framework to systematically characterize and quantify key sources of uncertainty in Q-IVIVE dose extrapolation. The proposed approach integrates uncertainty analysis directly into the Q-IVIVE workflow through four steps: (1) defining mechanistic processes governing dose extrapolation, (2) identifying key sources of uncertainty, (3) quantifying uncertainty in critical parameters and models, and (4) propagating uncertainty to derive confidence bounds around administered equivalent doses (AEDs). The framework explicitly accounts for chemical disposition in in vitro systems, including volatility, solubility, and sorption to plastic, which influence free concentrations and may lead to substantial bias when nominal concentrations are used. The framework also emphasizes the importance of accurately characterizing in vivo TK parameters, such as biotransformation rates which are often dominant contributors to uncertainty and variability. In addition to improving transparency and confidence in Q-IVIVE, the approach facilitates identification of key drivers of uncertainty, thereby informing targeted data generation and Q-IVIVE method refinement through Integrated Approaches to Testing and Assessment (IATA). This proposed framework provides a practical foundation for integrating uncertainty of NAM data into risk-based

evaluations and advancing the application of NAMs to support decision-making.

1.09.P–Tu034 Evaluation of Metabolic Capacity and Drug-Metabolizing Enzymes of Azole Antifungal Agents Using In Vitro Drug Metabolism Assays with Red-Crowned Crane Liver Microsomes

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Avian aspergillosis is a fungal disease primarily affecting the respiratory system, with increased risk in immunocompromised individuals. Voriconazole (VRCZ), an azole antifungal agent, is a first-line treatment due to its potent antifungal activity against Aspergillus species; however, its narrow therapeutic window and substantial large interspecies variability in metabolism pose a challenge to maintaining therapeutic plasma concentrations. The red-crowned crane (Grus japonensis), classified as Vulnerable, cannot be used for in vivo pharmacokinetic studies for ethical reasons. This study therefore aimed to evaluate VRCZ metabolic capacity and identify the enzymes involved using hepatic microsomes derived from an individual that died in an accident. Hepatic microsomes were incubated with VRCZ in the presence of an NADPH-regenerating system. Metabolites were comprehensively screened using LC-QToF-MS and structurally characterized. VRCZ and two identified metabolites were quantified by LC-MS/MS. The disappearance of VRCZ and the formation rates of metabolites were calculated, and kinetic parameters (Km, Vmax) were estimated using the Michaelis–Menten model. Intrinsic clearance (CLint, in vitro) was calculated as the Vmax/Km ratio. Enzyme involvement was evaluated using ketoconazole (CYP3A4 inhibitor) and omeprazole (CYP2C19 inhibitor). Two metabolites were identified: VRCZ N-oxide and a hydroxylated form. The N-oxide metabolite exhibited higher Vmax (85 pmol/min/mg) and Km (13 μM), indicating a low-affinity, high-capacity pathway. The hydroxylated metabolite showed lower Vmax (3.2 pmol/min/mg) and Km (1.4 μM), suggesting a high-affinity, low-capacity pathway. CLint was higher for the N-oxide pathway, indicating its dominance in overall metabolism. The scaled in vivo hepatic clearance (CLH) was intermediate among avian species and comparable to in vivo values reported for the red-tailed hawk. Ketoconazole strongly inhibited VRCZ metabolism (IC50: 4.8 μM), with particularly potent inhibition of hydroxylation (IC50: 1.5 μM) and weaker inhibition of N-oxide formation (IC50: 32 μM), indicating predominant CYP3A involvement in hydroxylation and partial contribution to N-oxide formation. Omeprazole also reduced VRCZ clearance (IC50: 96 μM), supporting a major role of CYP3A in hydroxylation, whereas N-oxide formation involves both CYP3A and CYP2C subfamily enzymes.

1.09.P–Tu035 Machine Learning Classification of Algal Toxicity Based on Infrared Spectral Data: A Fast, Animal-Free Screening Strategy

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Regulatory frameworks such as Registration, Evaluation, Authorisation and Restriction of Chemicals mandate comprehensive ecotoxicological hazard assessment, but traditional in vivo studies often involve labor-intensive and resource-intensive experimental procedures. Algae, as primary producers, are key sentinels in aquatic ecosystems, their 96-h EC50 remains a traditional metric in ecotoxicology. In this study, we propose a novel approach using machine learning and infrared (IR) spectroscopy methods for efficient and accurate EC50 prediction. EC50 data (96 h, algae) were curated from the open EcoTOX database, SMILES strings were retrieved via CirPy, and a binary toxicity label was assigned at a threshold of 100 mg L^{-1}. The initial dataset contained 218 toxic and 34 non-toxic compounds; class

imbalance was corrected using Synthetic Minority Over-sampling Technique (SMOTE), yielding 436 balanced instances. A set of 67 binary IR bond features was reduced by removing invariant and highly correlated predictors (r > 0.75). Four machine learning algorithms—Random Forest, Support Vector Classifier, k-Nearest Neighbors, and Extreme Gradient Boosting (XGBoost)—were optimized through RandomizedSearchCV with 5-fold cross-validation. Model stability and predictive power were assessed over 15 randomized train/test splits using F1-score and recall.
Tree-based ensemble models demonstrated more stable results. XGBoost achieved an F1-score of 0.90 ± 0.02 and a recall of 0.95 ± 0.01, while Random Forest reached an F1-score of 0.89 ± 0.03, demonstrating high reliability in detecting toxic compounds. SHapley Additive exPlanations (SHAP) analysis revealed that the C–H stretch at 2890 cm^{-1} (mean SHAP 0.07) and the O–H stretch in the 3500–3560 cm-1 region (SHAP 0.06) were the most influential spectral signatures, while 45 additional bond features together accumulated a sizeable SHAP of 0.21, underscoring the multivariate nature of aquatic toxicity. These interpretable, high-recall models provide a rapid, cost-effective prescreening tool aligned with the 3R principles, capable of prioritizing chemicals for further in vitro testing.

1.09.P–Tu036 Japanese Program on Endocrine Disruption: EXTEND 2022

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Ministry of the Environment, Japan (MOEJ) has been conducting testing and assessment of endocrine disrupting effects of chemicals under the program “EXTEND 2022” (Extended Tasks on Endocrine Disruption) since October 2022, developed based on the preceding programs EXTEND 2010 and 2016. Two-tiered framework for testing and assessment of endocrine disrupting effects of substances was established in EXTEND 2010 and test methods have been developed aiming at establishment of standard test protocols using fish, amphibians, and invertebrates. For substances selected referring to their existence in the ambient aquatic environment in Japan and potential endocrine properties obtained through literature survey, candidate chemicals for testing have been identified and relevant in vitro and in vivo tests have been conducted. Medaka Extended One Generation Reproduction Test (MEOGRT) has been conducted for some of the substances as a Tier 2 definitive test.
Referring to the WHO/IPCS definition on endocrine disruptors and the OECD Conceptual Framework for Endocrine Disruptor Testing and Assessment (EDTA), risk-based approach to endocrine disrupting effects has been adopted. MEOGRT study for nonylphenol conducted in EXTEND 2010 was referred to in environmental risk assessment of nonylphenol ethoxylates under Chemical Substances Control Law, which led to designation of the substances as Class II Specified Chemical Substances.
Outlines and present states of EXTEND 2022 as well as results and outcomes of the preceding programs will be discussed.

1.09.T - In Vitro, In Silico and Mechanistic Physiology for Understanding and Predicting In Vivo Toxicity and Endocrine Disruption

1.09.T01 Comparative Characterization of Cytochrome P450-mediated Xenobiotic Metabolism in Elephants using In Silico Phylogenetic Analysis, Transcriptomics, and In Vitro Metabolic Assays

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Elephants are increasingly exposed to persistent environmental contaminants, including heavy metals, pesticides, pharmaceuticals, plastics, and natural toxins, particularly as habitat loss brings them closer to agricultural and human-impacted areas. Reported mortality events in Asia and Africa highlight their potential vulnerability to these toxicants. However, the mechanisms underlying elephant-specific sensitivity remain poorly understood, limiting the ability to predict in vivo toxicity and underscoring the need for integrated in silico and in vitro approaches. In this study, we integrated in silico phylogenetic analysis, transcriptomic profiling, and in vitro metabolic assays to characterize cytochrome P450-mediated Phase I metabolism in elephants. CYP gene repertoires were compared with mammalian genomes, including those of the Asian elephant, African elephant, human, mouse, and other representative species. RNA-seq analysis was performed using Asian elephant tissues, including liver, kidney, and intestine. Functional metabolic capacity was further evaluated using Asian elephant liver microsomes with selected neonicotinoid insecticides for CYP and chlorzoxazone, a typical CYP2E probe substrate. Phylogenetic analysis revealed elephant-specific features in CYP gene repertoires. CYP2E- and CYP4A genes in both Asian and African elephants showed signatures of pseudogenization. Transcriptomic analysis showed tissue-specific expression of multiple CYP genes, with several CYP families expressed in the liver. In contrast, functional full-length transcripts of CYP2E and CYP4A were not clearly detected. Finally, in vitro assays showed that selected neonicotinoid insecticides were metabolized by elephant liver microsomes; however, their metabolism did not appear to be predominantly mediated by CYP-dependent pathways. Additionally, CYP2E-associated chlorzoxazone metabolism was very low or undetectable. Together, these findings indicate that elephants have distinct CYP-mediated xenobiotic metabolic profiles that may influence their susceptibility to chemicals that require CYP-dependent detoxification or bioactivation. This integrated in silico and in vitro framework supports the prediction of elephant-specific in vivo chemical susceptibility and highlights the need for species-specific toxicological assessment in wildlife.

1.09.T02 Molecular Mechanisms of 2,3,7,8-Tetrachlorodibenzo-p-Dioxin Toxicity in Rough-Toothed Dolphin Fibroblasts: Insights from Transcriptomics

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Marine mammals are susceptible to long-term exposure to persistent organic pollutants (POPs) because they are apex predators with long lifespans. Through trophic transfer and biomagnification, these contaminants may accumulate in tissues and cause chronic toxic effects. 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) is one of the most widely studied dioxin-like compounds and is widely used to study aryl hydrocarbon receptor (AhR)-mediated toxicity. However, the dose-dependent effects of TCDD on transcriptional regulatory networks and downstream biological functions in cetacean cells remain poorly

characterized, and the extent to which these responses depend on AhR signaling is not fully understood. In this study, to investigate these underlying transcriptomic mechanisms, fibroblasts of rough-toothed dolphins (Steno bredanensis) were used as an in vitro model and combined TCDD exposure with AhR inhibition.
Total RNA was extracted from fibroblasts derived from rough-toothed dolphins stranded in 2017 in Tanegashima, Japan, and subjected to RNA sequencing, followed by comparative transcriptomic analyses across treatment groups. Selected gene expression changes were validated by qPCR. Global expression patterns were primarily influenced by interindividual variation, whereas differentially expressed genes (DEGs) exhibited clustering patterns associated with TCDD concentration. Low- and high-concentration TCDD exposures (1 and 50 nM, respectively) induced partially overlapping but largely distinct transcriptional responses. Under low-concentration exposure, 86% of DEGs were classified as AhR-dependent, including canonical AhR-responsive genes such as CYP1A1, AHRR, and TIPARP. In contrast, this pattern was less consistent at high concentrations, suggesting the involvement of additional regulation mechanisms beyond canonical AhR signaling. High-concentration exposure elicited a broader response, with 83% of DEGs categorized as AhR-independent. These AhR-independent genes were significantly enriched in pathways related to ribosomal function, oxidative phosphorylation, and lipid metabolism.
These results demonstrate a concentration-dependent shift from AhR-mediated responses at low TCDD exposure to broader AhR-independent cellular perturbations at higher exposure levels. This study provides a framework for understanding the molecular basis of dioxin-like toxicity and for identifying biomarkers and regulatory pathways relevant to contaminant exposure in marine mammals.

1.09.T03 Evaluation of Thyroid Hormone System Disruption in Early Life Stages of Japanese Medaka

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Endocrine-disrupting chemicals (EDCs) are major focus of aquatic ecotoxicology and chemical regulation. Under the current framework for testing and assessment of EDCs in Japan (EXTEND 2022), amphibians (Xenopus laevis) are used to detect thyroid hormone system disruption (THSD), whereas fish (Japanese medaka, Oryzias latipes) are used to detect estrogenic, androgenic, and steroidogenic effects. However, recent studies have proposed zebrafish (Danio rerio) as an alternative model for detecting THSD, raising the possibility of fish-based THSD assays. Although several thyroid hormone (TH)-related endpoints (e.g., swim blader inflation, eye development, TH levels, and thyroid morphology) have been shown to be effective in zebrafish, it remains unclear whether these endpoints are applicable to Japanese medaka, a key model species EXTEND 2022. In this study, we examined THSD in early life stages toxicity test (OECD TG 210) using Japanese medaka.
Japanese medaka were exposed separately to three chemicals from fertilization to 30 days post-hatch in accordance with OECD TG 210. Well-characterized THSD chemicals (THSDCs) with distinct MOAs were selected as reference substances: ampicillin as an inert substance; propylthiouracil (PTU), a thyroid peroxidase (TPO) inhibitor; T4, a thyroid hormone. After exposure, triiodothyronine (T3) and thyroxin (T4) levels, as well as survival rate and growth, were assessed.
As an inert substance, ampicillin had no effect on any of the assessed endpoints. PTU decreased survival rate and T3 and T4 levels in a concentration-dependent manner, suggesting TH-antagonistic effects in medaka. T4 slightly decreased survival rate at the highest concentration and increased T3 and T4 levels in a concentration-dependent manner. Results for the additional substances, including iopanoic acid, an iodothyronine deiodinase 2 (Dio2) inhibitor; perchloric acid, a sodium iodide symporter inhibitor; and methimazole, a TPO inhibitor, together with the TH-system-related endpoints including thyroid follicle and eye morphological analyses, will be presented. So far, the results are consistent with the expected

MOAs of the tested substances, supporting the potential applicability of this method for detecting THSD in early life stages of Japanese medaka.

1.09.T04 KCC-Informed AOP Interpretation of CMIT/MIT-Induced Inflammatory Signaling, DNA Damage Response, and Apoptosis in Human Cell Models

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Chloromethylisothiazolinone/methylisothiazolinone (CMIT/MIT) is a biocidal mixture associated with severe respiratory and systemic health outcomes following South Korea's humidifier disinfectant disaster. However, the mechanistic linkage between early molecular perturbations and disease-relevant pathological outcomes remains poorly understood. This study integrated two complementary approaches to characterize CMIT/MIT toxicity. First, toxicological evidence was organized using the IARC key characteristics of carcinogens (KCCs) as an evidence-organization framework, identifying electrophilic/thiol-reactive chemistry, oxidative stress, genotoxicity, and altered cell-fate regulation as major mechanistic axes. Based on these findings, a draft adverse outcome pathway (AOP) was constructed by integrating KCC-informed upstream events with downstream disease endpoints derived from AOP 272 and AOP 296. Second, four human-derived cell models; pulmonary (BEAS-2B), hepatic (HepG2), neuronal (SH-SY5Y), and immune (Jurkat T) were exposed to CMIT/MIT at equitoxic concentrations (EC1, EC20) for 24 h. Cytotoxicity, oxidative DNA damage (8-OHdG), DNA damage response proteins, apoptosis-related markers, and a 46-cytokine multiplex panel were evaluated. CMIT/MIT induced concentration-dependent cytotoxicity and ROS elevation across all cell lines, accompanied by cell type-specific alterations in DNA damage response and apoptosis pathways. Cytokine profiling revealed coordinated inflammatory reorganization rather than isolated marker changes, with distinct response signatures across cell types. Mapping these signatures onto CTD and AOP-Wiki suggested mechanistic associations with pulmonary fibrosis, hepatocellular carcinoma, and hepatic encephalopathy. Together, these findings demonstrate that integrating KCC-based evidence organization with multi-endpoint in vitro profiling provides a mechanistically grounded strategy for CMIT/MIT hazard characterization.

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1.09.T05 Validation and Application of an Extended in-vitro Yeast Bioassay to Detect Antifungal Compounds in Water Samples

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Antifungal compounds are widely detected in aquatic ecosystems because of their extensive use in agriculture and human and veterinary medicine. Although adverse ecological impacts have been observed, antifungal compounds remain underrepresented in ecotoxicological testing, and there is a dire need for bioanalytical methods to assess antifungal toxicity in the aquatic environment. The current study aims to validate a yeast toxicity assay to specifically detect antifungal compounds by using an extended exposure time. A high-throughput microplate-based resazurin assay was optimised using Saccharomyces cerevisiae to evaluate cytotoxicity after acute (4 h) and extended (24 h) exposure. Twenty chemicals, including ten antifungal and ten non-antifungal compounds, were individually tested to determine assay sensitivity and specificity. The findings indicate clear time-dependent anti-fungal activity, which was not observed for the non-antifungal compounds. The ratio of the 50% inhibition (IC50) values at 4 h and 24 h

was used as a diagnostic toxicity metric. Non-antifungal chemicals consistently exhibited 4 to 24 h IC50 ratios below 10, whereas all antifungal compounds showed ratios greater than 10, reflecting specific time-dependent effects on yeast and improved assay specificity towards antifungal compounds. Moreover, this toxicity assay was also applied to wastewater effluent and surface water extracts, determining the applicability of this approach to better comprehend toxicity drivers in the real water samples. Overall, this study demonstrates the potential of an extended yeast assay to distinguish the toxicological impacts of antifungal compounds from non-antifungal compounds. This validated assay provides a rapid, sensitive, and scalable bioanalytical tool for detecting antifungal activity in aquatic matrices, which provides a foundation for future application in environmental toxicology, early-tier ecological risk assessment, and integration into effect-directed analysis.

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1.10.B.T - Environmental and Human Toxicology and Ecology: Linking Contaminants, Wildlife Sentinels, and Ecological Risk Assessment

1.10.B.T01 Exposure to the Synthetic Estrogen 17α-Ethinylestradiol Alters Courtship Behaviour but Not Sperm Traits in a Freshwater Fish

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Pharmaceutical contaminants are increasingly detected in aquatic environments as a result of wastewater discharge. One compound of particular concern is the synthetic estrogen 17α-ethinylestradiol (EE2), a key component of human oral contraceptives that can disrupt endocrine signalling in exposed wildlife. Although estrogenic contaminants are known to influence reproductive physiology and behaviour, their effects across multiple reproductive traits are rarely examined. We investigated whether exposure to environmentally relevant concentrations of EE2 alters reproductive behaviour and sperm traits in a freshwater fish, the pygmy halfbeak (Dermogenys collettei). Males were exposed to concentrations of EE2 (148–874 ng/L) prior to behavioural assays in which males encountered females either sequentially or simultaneously. During these trials we quantified courtship behaviour and latency to interact with females. We also measured multiple sperm traits including viability, morphology, and performance to assess potential effects on post-copulatory reproductive processes. Exposure to high EE2 consistently reduced male mating effort. Exposed males were slower to initiate interactions with females and displayed reduced courtship behaviour across both mating contexts. In contrast, EE2 exposure had no detectable effects on sperm traits, and male preferences for female traits were unaffected. These findings demonstrate that estrogenic contaminants can disproportionately alter behavioural components of reproduction while leaving post-copulatory traits unchanged. Integrating behavioural and physiological endpoints provides a more comprehensive understanding of how endocrine disrupting contaminants may influence reproductive processes and population dynamics in aquatic organisms.

1.10.B.T02 Stimulus-Specific Escape Behavior in Medaka Fish under Different Predator-Like Conditions

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The presence of pharmaceuticals and personal care products (PPCPs) in aquatic environments is an

increasing concern, as many of these substances can alter fish behavior, particularly escape behavior. Previous studies have shown the significant difference in escape behavior among medaka inbred strain. However, it remains unclear how different response is triggered by different stimuli in fish. This study conducted two predator-like stimuli test (the “Ball-Drop” test and the “Peek-A-Boo” test) and compared the different response in Japanese medaka (Oryzias latipes) between distinct behavior tests.
In the “Ball-Drop” test, an overhead ball was released after 8 min-adaption period to simulate aerial predation. And a predator image was presented after 5 min-adaption period to simulate lateral predation in the “Peek-A-Boo” test. The swimming behavior was recorded during the test and analyzed by UMATracker and DeepLabCut, and coordinate data was analyzed by Python. Besides, we conducted the exposure experiment of diazepam to explore the escape response of medaka under the stress of diazepam. The results show that the “Ball-Drop” stimulus lead to a suppression of locomotor activity compared with baseline (the mean value during the acclimation period), including the reduction of swimming velocity and significantly increase in freezing time after stimulus. In contrast, the “Peek-A-Boo” stimulus didn’t induce freezing but instead trigger an active avoidance response by maintained locomotion and reduced the time staying in the close area to a predator image. These findings demonstrated different responses to distinct predator-like stimuli. This study reveals stimuli-specific escape strategies and highlights the importance of stimulus selection for behavior test in neurotoxicity assessment. As detailed analyses of the diazepam exposure experiment are currently ongoing, the results will be addressed in the presentation.

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1.10.B.T03 PFAS Uptake and Sublethal Impacts in Barramundi: Insights for Guidelines

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Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants widely detected in aquatic environments and biota. Differences in chain length and functional group can strongly influence uptake, creating uncertainty in ecological risk assessment—particularly for tropical species. We quantified bioaccumulation and linked internal burdens to organism-level responses in barramundi (Lates calcarifer), a key Indo-Pacific aquaculture and wild fishery species for which PFAS data are limited. Fingerlings were exposed in the laboratory to seven PFAS (perfluoroalkyl carboxylic acids, PFCAs; and sulfonic acids, PFSAs) at concentrations spanning environmentally relevant to upper-bound scenarios, using a semi-static renewal design for 7 or 28 days. Whole-body PFAS concentrations were used to estimate bioconcentration factors (BCFs) and track compound-specific uptake over time; survival, weight, and length were measured to assess mortality and growth. Bioaccumulation followed clear physicochemical patterns: longer-chain PFAS accumulated more than shorter-chain analogues, and PFSAs differed from PFCAs, indicating functional-group effects. Most compounds approached a partial steady state by day 28, whereas PFHxS continued to increase. Uptake increased with chain length, with 28-day BCFs of 0.55, 21 and 63 L/kg ww for PFBS, PFHxS and PFOS, respectively; overall, BCFs ranked PFDA > PFOS > PFHxS > PFOA > PFBS ~ PFHxA ~ PFBA. Biological responses were subtle and did not consistently track accumulation. Mortality remained low, indicating limited acute toxicity at the tested concentrations. Growth was more sensitive: exposed fish had reduced weight and total length relative to controls, with longer-chain PFAS producing stronger and more consistent inhibition after 28 days, while shorter-chain PFAS caused weaker, less concentration-dependent effects. Integrating exposure, internal dose, and organismal responses in a tropical marine fish strengthens ecological benchmarks and seafood safety assessments. This is particularly relevant in Australia, where freshwater guideline values for PFOS and PFOA are often applied to marine species.

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1.10.B.T04 Neuroactive pollution disrupts cognition in fish by causing sex-specific effects on spatial learning

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Cognition underpins how animals perceive, navigate, and respond to their environment, yet these fundamental processes are increasingly threatened by environmental pollutants. Neuroactive pharmaceuticals are now routinely detected in aquatic ecosystems, raising concern about their potential to disrupt key cognitive functions in wildlife. Here, we tested whether exposure to the antidepressant amitriptyline, a widespread pharmaceutical pollutant, impairs spatial learning in wild-caught guppies (Poecilia reticulata). Using a repeated-trial maze assay, we quantified learning performance across 12 trials following an 11-d exposure to either a freshwater control (0 ng/L) or ecologically relevant low (52 ng/L) or high (496 ng/L) concentrations of amitriptyline. We found strong evidence of spatial learning across all treatment groups, with maze solve times and navigational errors declining over trials. However, males exposed to low and high concentrations of amitriptyline made 26% and 34% more errors, respectively, compared to control males. Female learning, by contrast, was unaffected by amitriptyline exposure, revealing sex-specific cognitive effects. Control males were more accurate than females, yet this advantage was lost under exposure and ultimately reversed at high concentrations, where males performed worse than females. These results emphasise the need to consider sex differences in cognitive responses when assessing the ecological impacts of environmental contaminants.

1.10.B.T05 Short-Term Reproductive Toxicity of Orysastrobin in Danio rerio

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Orysastrobin(OST) is a pesticide developed to reduce the environmental residue and toxicity associated with existing strobilurin fungicides and to provide disease control tailored to the agricultural environment of Asia. Although it has been detected in Korean water systems at levels of 0.218–0.41 μg/L (2023, detection rate 100%), ecotoxicological studies on this compound are limited. In this study, a reproductive toxicity assessment (OECD TG 229) was conducted using Danio rerio. The reproductive toxicity test was performed using a continuous flow-through exposure system; after a 7-day pre-incubation in culture medium, D. rerio were exposed to OST for 21 days, and the egg production was assessed. Additionally, gene expression profiles were analyzed to identify the mechanism of toxicity. The results showed that while no significant effects on the egg production of D. rerio were observed before or after OST exposure, OST exposure caused changes in the expression of genes related to reproduction (cyp19b, esr1, ghrh, vtg1, ghra, ghrb, fshr, lhr, cyp11a) in the tissues of both female and male D. rerio. In other words, while no effects were observed at the individual level, changes were confirmed at the gene level in genes related to endocrine disruption, oxidative stress, and cell death. This study examines the effects of orysastrobin, a novel trace contaminant, on aquatic ecosystems and can serve as scientific evidence for the future management of trace contaminants.

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1.10.C.T - Environmental and Human Toxicology and Ecology: Linking Contaminants, Wildlife Sentinels, and Ecological Risk Assessment

1.10.C.T01 Herbicide Contamination and Health Effects in Rice Frogs (Fejervarya limnocharis) from Agricultural Paddy Fields in Thailand

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Intensive herbicide use in Thai agriculture poses potential risks to ecosystem and human health. Building on previous monitoring (2010–2011) using rice frogs as sentinel species, this study examined herbicide contamination levels (atrazine, glyphosate, and paraquat) and assessed their effects on Fejervarya limnocharis health at organismal (liver and body weight) and population (growth patterns and size-frequency distribution) levels. Rice frogs were sampled from two paddy fields with contrasting herbicide application intensities in Nan Province, Thailand, between July 2020 and February 2021. Residues of all three herbicides were detected in water and frog tissues at both sites, with significantly higher paraquat concentrations at the intensive-use site. Liver weights exhibited significant site-related differences in February 2021, suggesting xenobiotic exposure effects. Body weights differed significantly between sites in July 2020. Growth patterns and size-frequency distributions showed significant site-related differences and disproportionate distributions, indicating population-level impacts. These findings demonstrate that herbicide contamination in paddy field ecosystems can bioaccumulate in amphibian sentinel species and cause adverse health effects at multiple biological levels, potentially leading to subtle but persistent changes in paddy field ecosystem structure and function. This study supports the use of amphibian biomonitoring for assessing agrochemical impacts in Asian rice agroecosystems.

1.10.C.T02 Effects of Bushfire Fighting Chemicals on Frog Development and Disease Susceptibility

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Climate-driven fires are becoming more frequent and severe, leading to a widespread increase in the use of bushfire fighting chemicals. These formulations are often applied in landscapes containing freshwater habitats, yet their effects on amphibians, particularly across sensitive life stages and in the context of disease, remain poorly understood. Australian frogs are already highly threatened by the fungal disease chytridiomycosis, and additional chemical stressors may further increase the vulnerability of disease-threatened populations. We investigated the effects of several commonly used firefighting chemical formulations, including BlazeTamer 380, Phos-Chek LC95W, Phos-Chek WD881, Forexpan S and Solberg Fire-Brake 3150A, using a combination of in vivo and in vitro exposure experiments. Experiments were conducted on striped marsh frog (Limnodynastes peronii) and tusked frog (Adelotus brevis) tadpoles, amphibian kidney cells (Xenopus laevis A6 cell line), and cultures of the fungal pathogen Batrachochytrium dendrobatidis (Bd). Endpoints included tadpole survival, growth, development, pigmentation, Bd zoospore and sporangial growth and host cell viability, growth and susceptibility to infection. We compared the sensitivity of tadpoles across two life stages and found that early larval stages were generally more sensitive than late larval stages. Exposure to several formulations impaired tadpole growth and delayed development, while the Phos-Chek LC95W formulation also caused pronounced darkening of tadpole colouration (increased pigment cover) even at low concentrations (0.02

g/L). The foam and water enhancer formulations caused comparatively less severe sublethal effects. In vitro assays showed that both Fire-Brake 3150A and Phos-Chek LC95W reduced Bd sporangial growth, and while Fire-Brake was comparatively more toxic to Bd, Phos-Chek LC95W was more toxic to the amphibian cells. Our findings demonstrate that bushfire fighting chemicals can have significant adverse consequences on developing frogs and alter host–pathogen interactions. These results highlight the need for a more comprehensive assessment of the ecological impacts of the broad range of chemicals used to control and suppress bushfires.

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1.10.C.T03 Combined Climate Change and Pollutants Disrupt Physiology and Reproduction in a Red Seaweed

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Seaweeds are keystone species with high environmental and economic value. The red alga Palmaria palmata plays an important role in structuring subtidal habitats in the North Atlantic and is increasingly harvested and cultivated for its food and nutraceutical applications. However, its reproductive cycle is driven by poorly understood environmental cues that synchronise life stages, resulting in potential disruptions due to anthropogenic global change. This study aims to assess how short-term extreme climate events and effluent pollution affect reproductive patterns in this species.
Sporulating seaweed fragments were exposed to marine heatwaves (MHW) and environmentally relevant concentrations of wastewater treatment plant effluent (EFF) for 10 days, followed by 10 days of recovery. The growth and photosynthetic efficiency were monitored every 5 days to assess the effects of exposure on the thalli's physiological health, and samples were removed after exposure and after recovery for transcriptomics. Spore release was induced from fragments, and the spore release time, number of spores released, and early male gametophyte growth were recorded to represent treatment effects on sporulation success.
Thalli exposed to EFF grew 26% less in fresh weight than controls, while those exposed to MHW and combined MHW+EFF grew ~10% less; however, the latter grew 18% more in surface area than controls. EFF exposures increased the quantum yield of photosystem II (Fv/Fm, 19%), and decreased total photosynthetic efficiency (ETRmax, 31%). Other treatments led to decreases in Fv/Fm, and showed no differences after recovery, while MHW+EFF led to increased ETRmax by the end of the experiment compared to controls (32%). Thalli exposed to EFF released spores faster (2-5 days in release conditions) and in higher concentrations (up to 540,000 spores/g tissue) than controls (1-3 weeks, ~100,000 spores/g). Other exposures did not yield meaningful spore release. Molecular analyses and early gametophyte growth measurements are in progress.
These results suggest strong, but complex effects of anthropogenic perturbations on spore release in this species. Routinely released wastewater treatment plant EFF increases the speed and efficiency of spore release, potentially leading to disruption in reproductive timing synchrony compared to more gradual releases. On the other hand, heatwaves could present even larger threats, nullifying entire reproductive events.

1.10.C.T04 Dual Bioassay Endpoints Reveal Structure-Driven PFAS Toxicity Patterns in a Freshwater Diatom

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Per- and polyfluoroalkyl substances (PFAS) are persistent, structurally diverse contaminants for which ecological risk assessment at the primary producer level remains limited, particularly under chronic exposure conditions where conventional single-endpoint assays often fail to capture the full progression of sublethal physiological responses. Here, we present a 7-day multigenerational bioassay using the freshwater diatom Cyclotella meneghiniana, integrating chlorophyll fluorescence and Nile Red-based lipid accumulation to resolve early photochemical disruption and subsequent metabolic responses across ten PFAS spanning carbon chain lengths C4–C11 and two functional groups (carboxylates and sulfonates). Structure-driven toxicity patterns were consistently observed: long-chain perfluoroalkyl carboxylic acids produced the strongest effects across both endpoints, short-chain compounds showed no measurable responses, and sulfonated PFAS primarily disrupted photochemical processes with limited downstream metabolic consequences. Chlorophyll fluorescence provided higher sensitivity and reproducibility across compounds, while lipid accumulation captured additional compound-specific metabolic responses not reflected in fluorescence alone. Species sensitivity distributions constructed from our data and published microalgal datasets further indicated compound-specific differences in ecological relevance. These findings demonstrate that the two endpoints together — rather than either alone — more fully resolve the structure-dependent progression of PFAS toxicity in primary producers, offering a practical framework for more ecologically relevant and structure-aware risk assessment.

1.10.C.T05 Validation of ecotoxicological assessment methods for soil algae regarding soluble pollutants

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Soil is a key environmental medium that provides the basis for material cycling and biological habitats in terrestrial ecosystems. Water-soluble pollutants are a critical point in ecotoxicity assessments because they are highly likely to be directly exposed to organisms within soil pore water. Soil algae can respond to pollutants as primary producers in the soil environment. However, existing soil ecotoxicological assessment methods have primarily focused on plants and earthworms. There is a relative lack of verification regarding the applicability and reliability of assessment methods for water-soluble pollutants using soil algae. This study aims to examine the validity of an ecotoxicological assessment method for water-soluble pollutants using soil algae and to verify the repeatability and reproducibility of the assessment results across different experimental conditions. To this end, a representative soil alga Chlorococcum infusionum was selected as the test organism and the biomass of soil algae grown in heavy metal-contaminated soil were evaluated under various laboratory conditions. The results showed that soil algae exhibited biomass inhibition in a concentration-dependent manner and repeatability and reproducibility were confirmed regardless of the test environment. This suggests that the soil algae ecotoxicity assessment method is a useful technique for evaluating the ecotoxicological effects of water-soluble pollutants.

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1.10.P - Environmental and Human Toxicology and Ecology: Linking Contaminants, Wildlife Sentinels, and Ecological Risk Assessment

1.10.P–Mo026 Effects of environmentally relevant pharmaceuticals and their mixtures on early life stages of marine invertebrates

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Coastal ecosystems worldwide are increasingly exposed to complex mixtures of pharmaceutically active compounds (PhACs) originating from wastewater effluents, raising concerns about their ecological and potential human health implications. Despite growing detection of these contaminants, their combined effects on early life stages of marine invertebrates, key drivers of population dynamics and ecosystem stability, remain poorly understood. This study aimed to evaluate the individual and mixture toxicity of three widely detected pharmaceuticals: carbamazepine (CBZ), diclofenac (DCF), and sulfamethoxazole (SMX), at environmentally relevant concentrations.

Early life stages of the sea urchin Paracentrotus lividus and the ascidian Herdmania momus were exposed to single compounds and their mixtures. Fertilization success and larval development were quantified and analyzed using binomial generalized linear models, and mixture effects were compared to predictions based on response addition.

Responses were compound-, endpoint-, and species-specific. In P. lividus, larval development was more sensitive than fertilization, with DCF and mixture treatments significantly impairing normal pluteus formation across all concentrations. Mixture exposures consistently produced stronger and more predictable effects than several single-compound treatments. For larval development, low-concentration mixtures exceeded additive expectations, while medium and high concentrations were approximately additive or less-than-additive, indicating concentration-dependent interaction patterns. Fertilization responses in both species were largely less-than-additive. Cross-species analyses revealed similar concentration–response slopes for fertilization, suggesting comparable relative sensitivity across phylogenetically distant taxa.

These results demonstrate that environmentally relevant pharmaceutical mixtures can disrupt critical developmental processes in marine invertebrates. Incorporating mixture toxicity and multiple early life-stage endpoints into environmental risk assessment frameworks will enhance the ecological relevance and predictive power of both ecological and human health hazard evaluations.

1.10.P–Mo027 Bioavailability and Toxicity of PFAS and Metals in Contaminated Sediments: A Multiscale Zebrafish-Based Approach

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Sediments can act both as sinks and sources of pollutants. Therefore, studying the fate, availability and toxicity of pollutants in realistic scenarios is key to understanding the potential effects that these contaminants could pose to the environment and its wildlife. Persistent organic pollutants (POPs), particularly per- and polyfluoroalkyl substances (PFAS), are of significant concern due to their wide distribution, resistance to degradation, and bioaccumulative properties. Similarly, metals are also non-degradable and can bioaccumulate through trophic levels, posing long-term ecological risks. However, ecosystems are most commonly contaminated with a mixture of different compounds, and their bioavailability might be affected by the sediment properties and environmental conditions. Thus, the importance to test sediment toxicity through direct exposure.

Our aim is to determine the toxicity of sediments using zebrafish as a model organism, focusing on endpoints such as teratogenicity, behavior, gene expression and cell morphology. To achieve this, over sixty sediment samples from different locations of interest in Sweden were collected. All samples were analyzed for PFAS and metal content, and six samples with different profiles were selected to assess their toxicity through in vivo and in vitro tests. Zebrafish embryos were exposed to contaminated sediments through a sediment-contact assay. Embryos were assessed through a Fish Embryo Toxicity (FET)-based test after being exposed for five days to different amounts of the selected sediment samples. Subsequently, one amount for each sediment was selected for conducting behavioral and gene expression assays. Additionally, extracts from the sediment samples mainly contaminated with PFAS, were used to expose zebrafish embryos and zebrafish liver cells. Toxicity of extracts was assessed by exposing zebrafish embryos through a 5-day long FET-based test, followed by behavior and gene expression assays at selected concentrations. Furthermore, cell-painting based phenomics was applied on zebrafish liver (ZFL) cells, investigating large-scale changes in cell morphological phenotypes after exposure to the sediment extracts.
In addition, sediment toxicity may be influenced by climate change due to changes in environmental parameters like temperature, pH or frequency of remobilization events. Therefore, future investigations will focus on studying sediment toxicity under varying conditions simulating climate change.

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1.10.P–Mo028 Nationwide Occurrence and Spatial Distribution of Liquid Crystal Monomers in Freshwater and Coastal Sediments of South Korea

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Introduction: Liquid crystal monomers (LCMs), components of liquid crystal display devices, have recently attracted attention as a class of emerging organic contaminants due to their persistence, bioaccumulation potential, and possible toxicity (1–3). The rapid increase in electronic waste and related industrial activities has raised concerns regarding the release of LCMs into the environment (3,4). However, information on their occurrence and distribution in sediments in South Korea remains limited. This study evaluates the occurrence, spatial distribution, compositional characteristics, and preliminary ecological risks of LCMs in freshwater and coastal sediments in South Korea.
Materials and Methods: The concentrations of 32 LCMs, including 17 fluorinated (F-LCMs) and 15 non-fluorinated compounds (nonF-LCMs), were determined in 78 surface sediment samples collected from major river basins and coastal regions across South Korea. Sediment samples were extracted using ultrasonic extraction, followed by clean-up with column chromatography, and analyzed using gas chromatography-tandem mass spectrometry (GC-MS/MS) in the MRM mode.
Results and Discussion: Among the 32 target compounds, 29 LCMs were detected in at least one sample. NonF-LCMs exhibited higher detection frequencies (7.69–50%) than F-LCMs (2.56–26.92%). Total LCMs concentrations ranged from not detected to 128 ng/g dry weight (dw), with a mean value of 6.47 ng/g dw. Freshwater sediments showed significantly higher contamination levels than coastal sediments, with mean concentrations of 14.0 and 2.25 ng/g dw, respectively. Non-fluorinated LCMs predominated in both freshwater (85.6% of total LCMs) and coastal sediments (72.2%). Spatial distribution patterns indicated elevated concentrations in areas influenced by urban and industrial activities. Preliminary ecological risk assessment showed that most sites posed low risk; however, several freshwater sites exhibited elevated risk levels with risk quotient values exceeding 1 (RQ > 1).
Conclusion: This study provides the first systematic evidence of LCM occurrence and distribution in sediments in South Korea, demonstrating higher accumulation in freshwater environments compared to coastal areas. Although overall ecological risks remain low, localized contamination hotspots highlight

the need for continued monitoring and further investigation into the environmental behavior and impacts of these emerging contaminants

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1.10.P–Mo029 Effects of Acute Ibuprofen Exposure on Lithium-Induced Reproductive Toxicity in Mice

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With the increasing use of lithium in medicine and energy storage, its environmental presence and associated health risks have raised significant concerns. While lithium exposure is known to induce reproductive toxicity, its interaction with widespread pharmaceuticals remains underexplored. Ibuprofen, a common nonsteroidal anti-inflammatory drug, can reduce renal lithium clearance; however, whether its acute use exacerbates lithium-induced male reproductive toxicity is unclear. This study established a mouse model to investigate the combined effects of lithium and ibuprofen on the male reproductive system. To simulate an existing lithium burden, mice were exposed to lithium via gavage for 35 days, while ibuprofen was administered by oral gavage during the final four days at a clinically relevant dose. Following exposure, systemic retention and reproductive organ accumulation were assessed via lithium concentrations in the blood and testes. Following exposure, systemic retention and reproductive organ accumulation were assessed via lithium concentrations in the blood and testes. Results demonstrated that compared to the lithium-only group, co-exposure significantly elevated lithium concentrations in both blood and testes, indicating enhanced retention and testicular accumulation. Furthermore, the combined exposure group exhibited more severe testicular histopathological injuries, including disordered spermatogenic cells, vacuolation, and compromised spermatogenic epithelial integrity, accompanied by a further reduction in serum testosterone levels. Mechanistically, co-exposure exacerbated testicular oxidative stress, evidenced by significantly increased reactive oxygen species (ROS) and malondialdehyde (MDA) levels, along with decreased superoxide dismutase (SOD) activity. These findings indicate that acute ibuprofen exposure exacerbates lithium-induced male reproductive toxicity by promoting testicular lithium accumulation, impairing structural integrity, and aggravating oxidative stress, providing crucial evidence for the health risk assessment of lithium under realistic co-exposure scenarios.

1.10.P–Mo030 Ecotoxicological Assessment of Pharmaceuticals in Ceriodaphnia silvestrii and Daphnia similis

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Pharmaceutical residues have already been detected in aquatic environments, as conventional wastewater treatment plants may not completely remove these compounds. Once released into surface waters, they pose risks to aquatic organisms, including sensitive microcrustaceans. This study assessed the ecotoxicity of eight compounds, including acetaminophen, atenolol, carbamazepine, diclofenac, ibuprofen, naproxen, propranolol, and triclosan, to Ceriodaphnia silvestrii and Daphnia similis. The Effect Concentrations (EC50) were determined for each compound through acute toxicity bioassays (48 h), allowing the comparison of species sensitivity and identification of those posing the greatest ecological risks. Overall, EC50 values for both species were similar, with notable differences only for acetaminophen. The variability in sensitivity among pharmaceuticals reflects differences in chemical structure and mode of action. Propranolol produced a low EC50 in C. silvestrii (2.07 mg/L), indicating high sensitivity, while D. similis required a slightly higher concentration (4.96 mg/L). Triclosan was the most toxic compound,

showing very low EC50 values for both C. silvestrii (0.18 mg/L) and D. similis (0.16 mg/L). Given its widespread use in personal care products, these results suggest that even relatively low concentrations of triclosan may adversely affect aquatic microcrustaceans. Although effect concentrations ranged from µg to mg/L, they were substantially higher than levels typically detected in surface waters and municipal effluents (ng to µg/L). Nonetheless, the compounds identified as highly toxic should be prioritized in water quality monitoring programs. The strong correlation in sensitivity between the two species supports their applicability in ecotoxicity testing, with C. silvestrii offering advantages for future chronic assays due to shorter test duration and native ecological relevance. Regulatory gaps in micropollutant monitoring provide a basis for future research on sublethal effects, bioaccumulation, and behavioral responses to strengthen environmental risk assessment protocols.

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1.10.P–Mo031 Ecotoxicity of the Veterinary Antibiotic Tylosin and Its Degradation Products in Agricultural Sod-Podzolic Soil and Chernozem

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This study investigates changes in the ecological status of tylosin-contaminated soils typical for agricultural regions in the European part of Russia. Two soil types — agricultural sod-podzolic soil (Albic Glossic Retisol) and chernozem — were used to simulate contamination. Tylosin was applied at concentrations of 100, 300, and 600 mg/kg, and samples were collected 1, 7, and 30 days after application.

Toxicity was assessed via bioassays, including phytotesting and analysis of soil microbiota structure and function (e.g., substrate consumption by microorganisms). Ecological status was evaluated using integrated indices based on the Triad approach. Residual tylosin and its metabolites were quantified by HPLC.

Results showed that integrated indices of ecological status increased with stress level during the first observation period in both soils, with the most pronounced differences observed on day 7. Biotic indicators revealed a stronger dose-response relationship in sod-podzolic soil compared to chernozem. Tylosin disrupted the ecological state of soils, shifting them into the “disturbed” category, and in some sod-podzolic variants — into “highly disturbed”.

HPLC analysis confirmed that tylosin fate depends on soil type and initial concentration. The dominant degradation pathway is the formation of tylosin B (desmycosin), indicating that the key inactivation step is the cleavage of the terminal mycarose sugar. In sod-podzolic soil, tylosin B accumulated and persisted, likely due to lower microbial activity, posing an environmental risk even after 30 days. In contrast, chernozem showed higher capacity for complete mineralization of both tylosin and its primary metabolites, with rapid decline of tylosin B concentrations, indicating lower risk of persistent product accumulation.

A promising direction for further research is to determine the conditions and duration of preservation of toxic metabolites and their accumulation in agricultural plants.

1.10.P–Mo032 The Role of Brain Morphology in Mediating the Cognitive and Behavioural Effects of a Neuroactive Pollutant

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Cognition allows animals to acquire, process and integrate information to navigate their environment and adjust behaviour accordingly. While this is critical for fitness and survival, particularly in ecosystems impacted by rapid anthropogenic change, these processes are increasingly threatened by environmental pollution. Neuroactive pollutants, such as pharmaceuticals, have become ubiquitous in aquatic systems worldwide. However, it is unclear how the neurochemical effects of these contaminants on the brains of exposed wildlife translate into disruptions to cognition and, ultimately, fitness-related behaviour. The executive functions are a set of control processes that regulate cognition to allow flexible, goal-directed behaviour, and are linked to the telencephalon, an area of the forebrain, in fish. We used female guppies (Poecilia reticulata) from two artificial selection lines, each with substantial divergences in either relative brain or telencephalon size, to explore how variation in brain morphology, at a global or region-specific level, may interact with the effects of a neuroactive pollutant on cognition and behaviour. The fish were exposed to either a freshwater control (0 ng/L) or environmentally realistic low (28 ng/L) or high (105 ng/L) concentrations of amitriptyline, an antidepressant and widespread pollutant. Following this, we used the Free Movement Pattern Y-maze to quantify executive functioning across two domains: working memory and cognitive flexibility. These findings will provide the first insight into how selective investment into functional cognitive capacity, including executive functioning specifically, may mediate the effects of a neuroactive pollutant on cognition, and how this may dictate fitness-related behaviour in exposed wildlife.

1.10.P–Mo033 Comparative effects of PFAS with different carbon chain lengths on fetal development in mice

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PFAS have been widely used in consumer and industrial products for their water- and oil-repellent properties, but their persistence in the environment and human body has raised concerns about reproductive and developmental toxicity. PFAS have a variety of chemical structures, among which carbon chain length is known to influence their pharmacokinetics, but few studies have investigated how carbon chain length affects reproductive and developmental toxicity. Not only legacy PFAS - characterized by a carbon chain length of eight (C8) – but also other PFAS with varying carbon chain lengths have been increasingly detected in human samples, highlighting that assessing the risks to pregnant women and fetuses. In this study, we aim to collect knowledge on the effects of PFAS carbon chain length on reproductive toxicity, particularly focusing on fetal growth. Pregnant ICR mice were administered with PFAS with carbon chain lengths of 4, 6, 8, and 10 (PFBA, PFHxA, PFOA, and PFDA, respectively) or the alternative compound GenX, once daily by forced oral gavage from gestational day (GD) 10 to GD17. On GD18, the mice were dissected under isoflurane inhalation anesthesia. First, based on epidemiological evidence of reduced birth weight, we evaluated fetal weight. The results showed that fetal weight was significantly reduced in PFOA- and PFDA-treated group. During this period, no deaths of dams were observed, and there were no changes of dam body weight or food intake in each PFAS-treated group. On the other hand, maternal liver weight was increased in PFOA-, PFDA-, and GenX-treated group whereas markers of liver damage were increased only in PFOA- and PFDA-treated group. These results indicate no overt maternal toxicity that compromises vital functions; however, potential impacts of PFOA and PFDA on liver function remain a possibility. Next, we evaluated the effects on the

placenta, which has an important function in maintenance of pregnancy and fetal development. Placental weight was increased significantly in GenX-treated group and tended to be increased in PFOA-treated group, suggesting a possible effect on placental toxicity. Collectively, long-chain PFAS may impair fetal and placental development and maternal liver function, while GenX may also impair placental development. In the future, we aim to investigate the effects of PFAS carbon chain length on placental function and to examine the relationship between placenta toxicity and reduced fetal weight.

1.10.P–Mo034 NMR-based metabolomic profiling of PM2.5-associated amino acid–derived methylated metabolites in blood: Implications for DNA methylation

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Air pollution, particularly PM2.5, is a major concern in Northern Thailand due to frequent seasonal haze exposure. PM2.5 has been linked to oxidative stress and inflammation, which may disrupt one-carbon metabolism and methylation-related pathways. However, metabolic signatures of these alterations in human biofluids remain under-explored. This study aimed to investigate alterations in methylation-related metabolites associated with prolonged PM2.5 exposure. Blood samples were collected from healthy participants residing in high- and low-PM2.5 exposure areas over a 15-year period, and metabolomic profiling was performed using ^{1}H-NMR spectroscopy. Multivariate and univariate analyses were applied to identify significantly altered metabolites, with Partial Least Squares Discriminant Analysis (PLS-DA) for R^2 and Q^2 accuracy indicating a distinct separation between exposure groups. Integrated analysis revealed significant increases in 7-methylguanine and N2-methylguanine, alongside decreases in N(4)-methylcytosine, 6-methyluracil, and dihydroxyacetone phosphate in the high-exposure group. These metabolites are involved in DNA/RNA metabolism, methylation processes, nucleotide balance, and energy metabolism. Long-term PM2.5 exposure was associated with perturbations in methylation-related pathways, potentially reflecting oxidative stress–induced DNA damage and repair processes. These findings suggest perturbation of one-carbon metabolism related to methylation capacity under chronic PM2.5 exposure and highlight candidate metabolites as potential biomarkers linking environmental exposure to metabolic and epigenetic alterations.

1.10.P–Mo036 Neurotoxic Effects of Strobilurin Fungicides in Caenorhabditis elegans

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Strobilurin fungicides are widely used agrochemicals that inhibit mitochondrial complex III. While their developmental toxicity has been documented, their potential neurotoxic effects on non-target organisms remain poorly characterized. This study evaluated the neurotoxicity of representative strobilurin fungicides (azoxystrobin, trifloxystrobin, pyraclostrobin, and kresoxim-methyl) using Caenorhabditis elegans as a model organism

Exposure concentrations were set at the half-maximal effective concentration (EC50) for developmental toxicity for each compound. Strobilurin exposure increased reactive oxygen species (ROS) levels and induced morphological alterations in dopaminergic neurons, suggesting sub-lethal neuronal stress rather than overt neurodegeneration. Behavioral assessments and molecular analyses are currently underway to further characterize the underlying mechanisms.

These findings suggest that strobilurin fungicides pose neurotoxic risks to non-target invertebrates, with implications for ecological risk assessment of agricultural fungicides.

1.10.P–Mo038 Challenging the Endpoint Hierarchy Assumption in Chronic Daphnia magna Toxicity Assessment

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Chronic ecotoxicity assessments have long operated under the implicit assumption that sublethal endpoints precede lethal effects in a predictable, hierarchical progression. Here, we challenge this assumption using a standardized multi-endpoint framework for Daphnia magna that integrates mortality, growth inhibition, morphological deformities, cardiac disturbance index (CDI), and heart rate within a single experimental design.

Using arsenic as a model toxicant, endpoint sensitivity did not conform to a fixed hierarchy under chronic exposure. Mortality emerged as the most sensitive endpoint (EC50 = 0.0009 mg/L), occurring at concentrations comparable to or lower than morphological deformities (EC50 = 0.00093–0.00188 mg/L) and growth inhibition (EC50 = 0.00175 mg/L). CDI showed lower sensitivity (EC50 = 0.00334 mg/L), while heart rate did not reach a 50% effect within the tested range. Rather than representing a linear progression, these endpoints reflect mechanistically distinct layers of biological disruption that respond independently to contaminant exposure.

These findings directly challenge prevailing assumptions about endpoint hierarchy in chronic toxicity testing and highlight the risk of underestimating toxicity when assessments rely on a single sublethal endpoint. The proposed framework provides a biologically grounded, multi-dimensional approach to chronic toxicity assessment in Daphnia magna, with implications for how chronic test batteries are designed and interpreted in regulatory contexts.

1.10.P–Mo040 Climate change-related environmental conditions alter perfluorobutane sulfonamide (FBSA) toxicity in Caenorhabditis elegans

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Climate change-associated environmental factors, including elevated temperature and salinity, are increasingly recognized for their potential to modify the toxicity and ecological risks of emerging contaminants. Perfluorobutane sulfonamide (FBSA), a novel C4 sulfonamido derivative widely used in the semiconductor industry, has raised concerns due to its environmental distribution and potential biological effects. In the present study, the interactive effects of temperature and salinity on FBSA-induced toxicity were evaluated using the nematode model Caenorhabditis elegans. Nematodes were exposed to varying temperature or salinity conditions in the absence or presence of FBSA, followed by assessment of survival and behavioral endpoints, including head thrashes, body bends, and pharyngeal pumping. Elevated temperature alone significantly reduced survival and increased head thrashes, while no significant effect was observed on body bends. Increased salinity independently impaired survival, head thrashes, and body bends. Under co-exposure conditions, elevated temperature did not further enhance FBSA-induced mortality but significantly potentiated FBSA-induced impairment of pharyngeal pumping. In contrast, increased salinity enhanced FBSA-induced toxicity on survival, body bends, and pharyngeal pumping, although no synergistic effect was observed on head thrashes. These findings indicate that climate-related environmental factors can differentially modulate FBSA toxicity and suggest that salinity may play a critical role in aggravating the neurobehavioral and physiological toxicity of emerging PFAS alternatives. This study highlights the importance of incorporating climate-associated environmental variables into ecological risk assessment frameworks for emerging per- and polyfluorinated alkyl substances (PFAS) contaminants.

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1.10.P–Mo041 Chronic Copper–Zinc Toxicity to Freshwater Mussel Glochidia Is Strongly Modified by Plant Derived Dissolved Organic Matter

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Urban waterways frequently receive copper (Cu) and zinc (Zn) from infrastructure runoff (e.g. roofs, tyres, and brake pads) at concentrations that exceed ecological guideline values. These metals pose a particular risk to sensitive early life stages of freshwater invertebrates, including mussel larvae (glochidia). Dissolved organic matter (DOM) can reduce metal bioavailability through complexation; however, the effectiveness of DOM mediated mitigation is highly dependent on DOM source, composition, and metal mixture context. Understanding these interactions is essential for assessing risks to culturally and ecologically important freshwater mussels and for designing effective nature based mitigation strategies.

We have investigated the influence of native plant derived DOM on chronic Cu, Zn, and Cu–Zn mixture toxicity (1:6 ratio) to glochidia of the New Zealand endemic freshwater mussel Echyridella menziesii. Leaf leachates were prepared from four native species—Kōwhai (Sophora molloyi), Mānuka (Leptospermum scoparium), Kānuka (Kunzea robusta), and Pōhutukawa (Metrosideros excelsa)—and assessed across a gradient of DOM concentrations. Glochidia survival and viability responses were measured under chronic exposure conditions and compared with metal only controls.

DOM significantly modified chronic metal toxicity; however, the magnitude and direction of effects varied among plant species, metal type, and exposure concentration. In contrast to responses observed in other native taxa within the same programme, Kōwhai sourced DOM increased glochidia sensitivity at higher DOM concentration. Observations indicate that DOM composition, rather than bulk DOM concentration alone, is a key driver of chronic toxicity outcomes.

These findings highlight the importance of explicitly incorporating sensitive life stages and metal mixtures into DOM based mitigation assessments. While plant derived DOM can reduce metal toxicity in some taxa, it may increase risk for glochidia, with important implications for freshwater mussel conservation and restoration. Results are being integrated with complementary chemical characterisation and bioavailability modelling to improve prediction of mixture toxicity and support species specific risk assessment. Collectively, these data support a more cautious and targeted application of native vegetation in urban stormwater and riparian designs where protection of native taonga, including freshwater mussels, is an objective.

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1.10.P–Mo042 Practical Application of Data Quality Evaluation Method for Ecological Hazard Assessment: A Case Study

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In Japan, regulatory ecological hazard assessment places strong emphasis on data quality evaluation

based on standardized ecotoxicity test guidelines with recommended species, ensuring transparency and reliability. As a result, assessments often rely on a limited number of highly reliable and information-rich datasets. When acceptable data are scarce, however, uncertainty may increase. Under such circumstances, there is growing demand for an approach, termed the WoE (Weight of Evidence) approach, which enables more comprehensive judgment through maximum use of available data. To meet this need, a data quality evaluation method that can be applied to diverse studies, including scientific literature, without relying on guideline compliance, is essential.

Our previous study proposed a transparent method for systematically evaluating ecotoxicity data of varying quality and completeness. It incorporates structured evaluation criteria and criterion-specific decision guidance, informed by prior expert evaluations, to support consistent judgments across diverse data sources, including non-guideline studies. Building on this, the present study focuses on its practical application in ecological hazard assessment.

In this study, we are conducting case studies in which the proposed method is applied to the ecological hazard assessment of selected chemical substances and compared with conventional guideline-based approaches. Attention is given to situations where conventional assessments rely on limited evidence. In such cases, application of the method is expected to facilitate the structured and transparent incorporation of literature-derived data that are often excluded or underutilized, thereby broadening the available evidence base. The explicit evaluation of reliability and relevance in the method is expected to facilitate the clarification of key issues, thereby contributing to enhanced transparency in expert judgment.

Through this comparative analysis, the study explores how the method may support more comprehensive hazard characterization and provide a clearer and more explicit basis for data selection and weighting.

1.10.P–Mo043 Approach to “One Substance, One Assessment” via the “Data Quality Evaluation Method for Ecological Hazard Assessment”

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Environmental risk assessment (ERA) of chemicals has been carried out for various regulatory objectives. Concrete approaches to risk assessment differ depending on respective objectives and targets to be evaluated.
Evaluation of the quality of the knowledge on chemicals’ effects to organisms has played a significant role for such ERA practices. Respective systems for such evaluation have been developed and implemented in accordance with relevant regulatory objectives with experts’ participation. There are differences in target species, acceptance of knowledge on non-standardized organisms, rigorousness of reliability evaluation, and acceptance of knowledge with limited reliability. Not much attention has been paid to harmonization among systems and common use of evaluated knowledge.
Based on Klimisch’s concept of reliability evaluation of toxicity data, it would be practical to standardize scientific reliability evaluation to share the results, and to determine adoption/rejection of knowledge based on the methods defined for respective evaluation systems.

The "Data Quality Evaluation Method for Ecological Hazard Assessment," developed in the project of the Ministry of the Environment with substantive contribution by National Institute for Environmental Studies, has adopted the two-axis evaluation of reliability and relevance, and has systematized the quality evaluation to refer to wider range of knowledge.
- Regarding reliability, the system aiming at uniform evaluation not restricted to standardized test species by materializing the detailed items has been developed, which will contribute to objectify, formulate and

increase transparency of the expert judgement.
- Regarding relevance, the evaluation system to itemize the judgment for a certain regulatory objective is being developed. It would be modified for application to different objectives.
Under this new system, it is expected that results of reliability evaluation will be shared among different objectives, and it could greatly contribute to improve efficiency and consistency of evaluation work under the idea of “One Substance, One Assessment”.

Objectifying the perspective of evaluating the quality of hazard data as mentioned above should also be effective for application of weight-of-evidence approach to wider range of knowledge to improve the evaluation systems.

1.10.P–Mo044 An AI-Based Study on Water Toxicity Using Behavioral Analysis of Endemic Daphnia

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Aquatic environments are increasingly affected by heavy metal contamination originating from industrialdischarge, agricultural runoff, and urban wastewater. Among these pollutants, copper is one of the mostcommonly detected metals in freshwater systems and is known to induce physiological stress and behavioral alterations in aquatic organisms. Behavioral responses, such as changes in swimming activity and movement patterns, are considered sensitive indicators of sublethal toxicity and may provide earlier signals than conventional toxicity endpoints such as mortality. However, continuous and quantitative behavioral monitoring remains challenging using traditional observation methods.In this study, an AI-based behavioral analysis framework was developed to evaluate water toxicity using Daphnia species as bioindicators. A video monitoring system consisting of multiple observation chambers and a camera-based recording device was established to continuously record Daphnia movement under controlled laboratory conditions. Four Daphnia species were considered in this study, including Daphnia magna, Moina, Daphnia pulex, and Simocephalus similoides, with current experiments primarily focusing on D. magna and Moina.Baseline behavioral observations were first conducted under normal culture conditions to establish reference data for movement and activity patterns. Preliminary copper exposure experiments were then designed using environmentally relevant concentrations of copper(II) chloride dihydrate. Recorded videos wereconverted into image frames, and representative frames were manually labeled to train an AI-based object detection model. The trained model successfully generated tracked videos with automatic identification and bounding-box labeling of individual organisms, enabling continuous observation of movement andspatial distribution.This study aims to establish a baseline platform for AI-assisted behavioral toxicity assessment and to explore the potential of automated behavioral analysis for future water toxicity monitoring and ecotoxicological research.

1.10.P–Mo045 Otolith Microchemistry of Red Finfold Barb, Hypsibarbus vernayi, From Nan Province, Northern Thailand

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Metal contamination remains a significant concern in freshwater ecosystems, where fish may accumulate elements through water, sediment, and diet. Recent reports of metal contamination in freshwater systems in Nan Province provide important regional context for this study. Otoliths are calcified structures in the inner ear of fish that may retain chemical information over time, but their use in freshwater contamination

studies remains less developed than in marine systems. This study examined otolith chemistry in red finfold barb, Hypsibarbus vernayi, from Nan Province, Thailand, to evaluate whether elemental patterns in otoliths may provide useful information on environmental exposure. Fish were collected from four locations in Nan Province: Thung Chang, Tha Wang Pha, Bo Kluea, and Wiang Sa. Otoliths were removed, cleaned, embedded in resin, polished to expose the sectioned surface, and analysed using an electron probe microanalyser (EPMA). Elemental concentrations were compared between otolith regions, including core and edge, within each location and among locations. Otoliths were dominated by Ca, with additional elemental signals detected at lower concentrations. Differences between core and edge were limited and location-specific. Significant core-edge differences were detected for Mn in Thung Chang and for As, K, and Zn in Wiang Sa ($p<0.05$). Differences among locations were more evident than differences between otolith regions. Significant differences among locations were detected at the edge for K, Hg, and Cd ($p<0.05$), and at the core for K, Hg, Cd, and Zn ($p<0.05$). Post hoc analyses showed that K provided the most consistent spatial separation among locations, whereas Hg and Zn showed more limited pairwise differences. Although Cd showed a significant overall location effect at the core, no pairwise comparison remained significant after post hoc adjustment. These findings indicate that otolith microchemistry in this freshwater fish contains both within-structure and among-location signals, although the response was strongly element-specific. EPMA was useful for spatially resolved screening of elemental patterns in otoliths, but interpretation should remain cautious because elemental incorporation may also be influenced by physiology and biomineralisation. Future work should integrate water, sediment, and soft-tissue measurements to strengthen ecotoxicological interpretation.

1.10.P–Mo046 Testicular Oocytes in Rice Frogs Fejervarya limnocharis: Natural Variation or Endocrine Disruption? Implications for Biomonitoring in Asia-Pacific Ecosystems

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Gonadal intersex conditions, particularly testicular ovarian follicles (TOFs), are widely used as biomarkers of endocrine-disrupting chemical (EDC) exposure in amphibians. However, baseline intersex prevalence data from reference populations are essential for accurate interpretation. This study investigated TOF occurrence in rice frogs (Fejervarya limnocharis), a common sentinel species in Asian agricultural ecosystems, to evaluate its utility as an EDC biomarker. Three populations were sampled from pristine habitats with no known contamination history across Thailand (2011–2023): northern (Nan Province), central (Saraburi Province), and southern (Yao Yai Island, Phang Nga Province) regions. Whole-organ histological examination was performed on adult male gonads to assess TOF prevalence and characteristics. TOFs were detected at unexpectedly high prevalence across all reference sites: Nan (25/56 males, 44.6%), Saraburi (46/50 males, 92%), and Phang Nga (24/46 males, 52.2%). TOFs appeared as round previtellogenic oocytes with central spherical nuclei; some showed signs of atresia. Notably, normal spermatogenesis occurred in affected individuals, with all developmental stages of male germ cells present and spermatozoa evident in efferent ducts, suggesting functional reproductive capacity was maintained. These findings indicate that TOF occurrence in F. limnocharis may represent a natural characteristic associated with the undifferentiated type of gonadal sex differentiation reported in some anuran species, rather than EDC-induced pathology. The high baseline prevalence across geographically isolated, uncontaminated sites suggests these structures may be remnants of the gonadal differentiation process. Caution is therefore warranted when interpreting TOF presence as evidence of EDC exposure in species with undifferentiated gonadal development. Species-specific baseline data from reference

populations are critical for effective amphibian biomonitoring programs in the Asia-Pacific region.

1.10.P–Mo047 Comparative Sensitivity of Congeneric Cladocerans to Imidacloprid and Implications for Ecological Risk Assessment

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Emerging contaminants have become an important environmental issue due to their widespread detection in several environmental compartments. Among these compounds, pesticides are of particular concern because of their potential impacts on aquatic organisms. Imidacloprid, a neonicotinoid insecticide extensively used worldwide, has been frequently reported in freshwater environments. In this context, the present study investigated the ecotoxicological effects of imidacloprid on congeneric cladoceran species commonly employed in toxicity testing, focusing on survival, reproduction, and feeding activity (algal ingestion rate) under controlled laboratory conditions. Acute toxicity assays were performed using the exotic species Daphnia similis, Daphnia magna, and Ceriodaphnia dubia, as well as the native species Ceriodaphnia silvestrii, exposed respectively to concentration ranges of 1–8 mg/L, 1–5 mg/L, and 4–64 mg/L. Chronic exposure tests assessed reproductive performance in daphniids (D. similis and D. magna) at concentrations of 0.025, 0.05, 0.1, and 0.2 mg/L. Feeding experiments compared ingestion rates among the four species exposed to 0.05, 0.1, and 0.2 mg/L. Furthermore, species sensitivity distribution (SSD) models were generated, and ecological risks to freshwater communities were estimated using the MEC/PNEC risk quotient approach. The findings demonstrated clear interspecific differences in sensitivity to imidacloprid, with acute toxicity ranking as follows: C. silvestrii > C. dubia > D. similis > D. magna. Chronic exposure significantly reduced neonate production after 15 and 21 days, with effects already observed at the lowest tested concentration (0.025 mg/L) for both Daphnia species. In feeding assays, C. silvestrii was the most sensitive species, exhibiting reduced algal ingestion at 0.1 mg/L, whereas no significant feeding impairment was detected in the other cladocerans. Overall, the study highlights the relevance of interspecific variability in ecotoxicological responses and emphasizes the importance of incorporating native species into pesticide environmental risk assessments.

1.10.P–Mo048 Ecotoxicological Profiling of Antimicrobials in Relation to Application, Exposure, Mitigation of Antimicrobial Resistance (AMR), and Potentially Sensitive Organisms

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Antimicrobial resistance (AMR) in pathogenic microorganisms associated with the use of antimicrobials has become a growing concern in medicine and public health. At the same time, antimicrobial agents exert harmful effects on aquatic organisms and are therefore recognized as a class of emerging contaminants. Comprehensive ecotoxicity data and exposure monitoring should be required for supporting the environmental risk assessment of antimicrobials in contributing to a One Health approach. This study aimed to achieve a more refined ecological risk assessment of antimicrobials by addressing existing gaps in ecotoxicity data. To this end, we compiled ecotoxicity data on antimicrobials, considering applications and usage patterns, environmental detection concentrations and frequencies, and relevance to

antimicrobial resistance (AMR) mitigation, including data for potential target organisms such as protozoa and prokaryotes (bacteria and cyanobacteria).
Given the current limitations in available test data, this study examined a broad range of antimicrobial modes of action, including inhibitors of cell envelope synthesis, protein synthesis, DNA and/or RNA synthesis, and folic acid synthesis. Ecotoxicity tests were conducted using three standard aquatic species (i.e., algae, daphnids, and fish), as well as the ciliate Tetrahymena sp., the luminescent bacterium Allivibrio fischeri, and multiple cyanobacterial genera, such as Synechococcus and Cyanobium. For the luminescent bacterium, both standard acute toxicity tests (30 min) and extended chronic exposure tests (24 h) were conducted.
The combined analysis of literature and experimental data suggests that key data vary depending on the combination of test species and antimicrobial mode of action. For example, cell envelope synthesis inhibitors tend to show lower sensitivity in standard test species (e.g., algae, daphnids, and fish), whereas higher sensitivity is often observed in prokaryotes. This indicates that reliance solely on standard species may overlook sensitive taxa, highlighting the need for broader taxonomic coverage in antimicrobial risk assessment.

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1.10.P–Mo049 Acute toxicity of azoxystrobin and difenoconazole to the crustacean Dugastella valentina (Ferrer Galdiano, 1924)

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<p>The extensive rice paddies cultivated in the Mediterranean region contribute significantly to the input of pesticides into adjacent aquatic ecosystems. The excessive use of these substances currently poses a risk to the health of aquatic biota, since different pesticides inevitably end up reaching these environments. Therefore, this study aims to evaluate the acute effects of the fungicides azoxystrobin (AZ) and difenoconazole (DF) on the native shrimp species Dugastella valentina. Individuals of D. valentina were collected from a preserved water spring and transported to the laboratory. Subsequently, the organisms were acclimatized for 24 hours in 30L aquaria containing 20L of water from the collection site. The experiments were carried out at 20 ± 1°C with a 16/8 photoperiod. Each pesticide had 10 replicates per concentration, with one individual per replicate, and a duration of 96 hours. For the experiments, the analytical standard of each pesticide was used for the exposures. The concentration ranges used in the tests were: 0, 20, 60, 180, 540, and 1620 µg L^{-1} for AZ, and 0, 40, 120, 360, 1080, and 3240 µg L^{-1} for DF. After the exposure period, dead organisms were counted, and the LC50/96h values were determined using the MOSAIC software. Regarding toxicity, it was observed that the least toxic compound was DF, with a LC50/96h of 1050 (IC: 701 – 1590) µg L^{-1}, while AZ was the most toxic, with a LC50/96h of 567 (IC: 299 – 1240) µg L^{-1}. This difference in toxicity may be associated with the mode of action of the pesticides. Azoxystrobin is a strobilurin that inhibits complex III of the mitochondrial electron transport chain, blocking ATP production and causing cell death due to cessation of energy respiration. On the other hand, DF is a triazole that inhibits the enzyme C14-α-demethylase (CYP51), interfering with ergosterol biosynthesis and compromising fungal cell membrane integrity. Thus, the results indicate that

AZ affects shrimp more, as it acts on mitochondrial respiration, a universal and essential process for aerobic organisms, leading to rapid death even at low concentrations (20–540 μg L^{-1}). Therefore, knowledge of the acute toxicity of locally relevant pesticides is essential in order to deeply understand the ecotoxicological effects caused by these substances and, thereby, establish environmental strategies for greater protection of aquatic ecosystems.</p>

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1.10.P–Mo035 Beyond Chemicals: Integrating Personality, Social Context, and Environment in Behavioral Ecotoxicology

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Behavioral ecotoxicology measures the observable responses of individuals or populations to chemical stressors. Behavioral studies are often characterized by large inter-individual variability in response and conflicting results between studies. One reason is that behavior arises from a complex interplay between intrinsic individual traits, such as personality and activity level, and extrinsic environmental and social context. Traditional ecotoxicology frameworks often emphasize toxicant concentration or exposure duration while neglecting elements such as experimental venue and intrinsic behavioral traits that can significantly influence outcomes. We propose that fish personality and social context should be considered when designing behavioral experiments. Therefore, this paper reviews our research on the effects of fish personality and social context on the responses of Danio rerio and male Aphaniops stoliczkanus to environmentally relevant concentrations of sertraline. We highlight how interactions can lead to different responses for different personality types and different experimental venues. We found that D. rerio personality traits significantly modulate responses to sertraline, where low-boldness females exhibited stronger anxiety response than high individuals, while effect on sociability varied by personality type. Similarly, when different sized shoals of the killifish A. stoliczkanus was exposed to sertraline and predators there were significant interactions between the two factors. We recommend that studies on fish behavior, particularly those which investigate neuroactive pollutants such as sertraline, pre-screen each fish for personality type, and include this a factor in analysis. Further, we recommend that fish behavior is assessed using shoal numbers that permit the display of natural responses. Single fish tests should be avoided for naturally social species. Implying personality and social context while designing ecotoxicological studies improve its contribution to environmental risk assessment and regulatory decision-making.

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1.10.P–Mo037 Is The Emerging Insecticide Chlorantraniliprole Toxic To Freshwater Biota?

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Recently, chlorantraniliprole, an anthranilic diamide insecticide, has increasingly been detected in waterways around Melbourne. This raises concerns about whether it is present at concentrations that are toxic to aquatic life. There is some information in the international literature on the impacts of chlorantraniliprole on non-target organisms, but its effects on Australian aquatic organisms remain

unknown. The aim of this study was to determine the toxicity of chlorantraniliprole on a range of Australian aquatic macroinvertebrates and plants. Acute (short-term exposure) and chronic (long-term exposure) water-only toxicity tests were conducted on the non-biting midge Chironomus tepperi, the amphipod Austrochiltonia subtenuis, the water flea Daphnia carinata, the backswimmer Anisops doris and duckweed Spirodela polyrhiza. Chlorantraniliprole concentrations were measured in the exposure solutions. Four of these species were affected by chlorantraniliprole; in particular, nominal concentrations as low as 0.001 mg/L resulted in no emergence of C. tepperi larvae into adults, 0.1 mg/L reduced the survival of D. carinata, and 0.25 mg/L reduced the survival of A. subtenuis. However, at a significantly high concentration (10 mg/L), chlorantraniliprole exposure resulted in a 50% reduction in S. polyrhiza growth compared to the control. Anisops doris were not affected following exposure to up to 1.0 mg/L for 14 days. Of all the species tested, C. tepperi was the most sensitive taxon. This may be due to the mode of action of chlorantraniliprole, which targets ryanodine receptors that regulate calcium channels involved in physiological functions such as movement, growth, and metamorphosis. Backswimmers were not affected by chlorantraniliprole, likely because they breathe through air bubbles collected from the water's surface, which they store in their abdomen, trapped by hydrophobic hairs that prevent them from exposure to contaminants through respiration. Furthermore, chlorantraniliprole concentrations of 0.0026 mg/L and 0.0013 mg/L were measured at two sites in Melbourne, which, based on our laboratory data, may pose a high risk to the emergence of C. tepperi larvae into adults. The findings of this research help us understand the risks of chlorantraniliprole on local species and, from there, whether management actions are required to prevent detrimental consequences to local aquatic ecosystems.

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1.10.P–Mo039 Marine Gas Oil Triggers Metamorphosis in Sea Urchin Larvae

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Metamorphosis is a critical process in the life cycle of most marine benthic invertebrates, determining settlement success, recruitment, and ultimately population dynamics and coastal marine biodiversity. Marine Gas Oil (MGO), a low-sulphur distillate fuel increasingly used in coastal and emission-control zones, is generally regarded as a cleaner alternative to heavy fuel oils. However, the ecological risks associated with MGO spills remain poorly understood. In this study, we investigated the acute effects of MGO on the metamorphosis of the sea urchin Paracentrotus lividus, a keystone species of Atlantic and Mediterranean rocky shores. We also evaluated whether the presence of bacterioplankton and biofilms influences the effect of MGO on larval metamorphosis. Competent larvae were exposed under controlled laboratory conditions to a range of MGO concentrations (1–250 µL L^{-1}). When larvae were exposed only to MGO in bacteria-free seawater (UV-sterilized, double-filtered seawater; 0.1 µm), MGO induced low levels of metamorphosis (<15%) after 24 h, increasing to 35% at the highest exposure concentration after 72 h. In contrast, the inductive effect of MGO on P. lividus metamorphosis increased notably in the presence of either bacterioplankton or biofilms, reaching up to 86% within 24 h. These results suggest that the rapid and pronounced metamorphic response observed in the presence of MGO may be mediated by shifts in microbial communities rather than by a direct effect of the fuel itself. Our findings indicate that MGO pollution in coastal waters may alter larval settlement success by short-circuiting adaptive metamorphic delay, with potentially important consequences for the structure and functioning of marine benthic ecosystems. Further research is needed to elucidate how MGO-induced changes in microbial communities influence metamorphosis in marine invertebrates. In the context of increasing coastal pollution and the fundamental role of larval metamorphosis in maintaining marine biodiversity, the

development and adoption of safer alternatives to petroleum-based fuels are essential to reduce the environmental impacts of maritime transport.

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2. Environmental Chemistry and Exposure Assessment

2.01.A.T - Advances in Bioaccumulation Assessment: From Models to Field Data

2.01.A.T01 Tiered and Integrated Methods for Bioaccumulation Assessment

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Bioaccumulation (B) assessment can be challenging due to empirical data gaps and limitations in existing metrics and methods. A weight-of-evidence (WoE) approach that guides problem formulation (data relevance), and the collection, generation, reliability evaluation, and integration of multiple lines of evidence in a consistent and transparent framework was developed to aid decision-making. The method follows Organisation for Economic Cooperation and Development (OECD) guidance for a WoE approach and was operationalized in the Bioaccumulation Assessment Tool (BAT). An OECD Integrated Approach to Testing and Assessment (IATA) for B assessment (2023) applies the methods to help evaluators navigate assessment challenges. The WoE approach within the BAT is intended for relatively data-rich chemicals (with multiple lines of empirical evidence) and includes bioaccumulation and food web models for representative aquatic and air-breathing species. For relatively data poor chemicals, even where only chemical structure (i.e., SMILES notation) is known, the Bioaccumulation Estimation Tool (BET; in the Exposure And Safety Estimation (EAS-E) Suite on-line platform), enables screening-level B assessment. The BET includes the same B models that are within the BAT, for consistency across concepts, models, and metrics. The B models can integrate in vivo, in vitro and in silico toxicokinetics data, e.g., on biopartitioning and biotransformation, for neutral and ionizable organic chemicals (IOCs), to calculate: laboratory bioconcentration factors (BCFs) and biomagnification factors (BMFs) in fish; field bioaccumulation factors (BAFs) and BMFs in aquatic species (algae, invertebrates, fish); and BMFs and total elimination half-lives in air-breathing laboratory and ecological species (mammals and birds). EAS-E Suite has been updated with measurements and new models for calculating chemical partitioning and biopartitioning to refine estimates, enabling consideration of the best available science in decision-making. Case studies showing BET hypothesis generation and testing with measured in vivo B metrics will be presented, including for chemicals of concern (e.g., per- and poly-fluorinated alkyl substances). Applications of the BAT for legacy pollutants (e.g., organochlorines) and chemicals of concern (e.g., PAHs, siloxanes) will be summarized. Collectively, the tiered methods support B assessment decision-making while reducing the need for unnecessary animal testing.

2.01.A.T02 Trophic Dilution of Cyclic Volatile Methylsiloxanes (D4–D6): Monitoring Evidence from Tokyo Bay and Lake Kasumigaura, Japan

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Cyclic volatile methylsiloxanes (cVMS), including octamethylcyclotetrasiloxane (D4), decamethylcyclopentasiloxane (D5), and dodecamethylcyclohexasiloxane (D6), are widely used in

consumer and industrial products and are frequently detected in aquatic environments. However, their bioaccumulation behavior remains uncertain, particularly across different aquatic systems. This study evaluates the trophic transfer behavior of cVMS based on environmental monitoring data from both a marine and a freshwater ecosystem in Japan. Surface sediments and aquatic biota were collected from Tokyo Bay, a highly urbanized coastal embayment, and Lake Kasumigaura, a shallow eutrophic freshwater lake. Monitoring in Tokyo Bay has been conducted continuously at fixed sites since 2012, allowing assessment of long-term spatial and temporal trends, while samples from Lake Kasumigaura were collected in 2023 across multiple locations and species. Concentrations of D4, D5, and D6 were quantified by GC/MS, and trophic levels of organisms from Lake Kasumigaura were determined using compound-specific nitrogen stable isotope analysis of amino acids. cVMS were consistently detected in sediments and biota from both systems, with D5 showing the highest concentrations. Overall concentrations in fish from Tokyo Bay were higher than those from Lake Kasumigaura. Trophic magnification factor analysis based on monitoring data yielded TMF values below unity for all cVMS, indicating trophic dilution rather than biomagnification. These results provide empirical evidence that cVMS do not biomagnify in aquatic food webs across contrasting environmental settings.

2.01.A.T03 Trophic Dilution of Cyclic Volatile Methylsiloxanes in Two Japanese Field Food Webs

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Bioaccumulation can be evaluated using several metrics, including the trophic magnification factor (TMF), which is a field-based measure particularly relevant for hydrophobic, lipophilic compounds where dietary uptake is the primary route of chemical exposure in aquatic organisms. Reported field TMFs of cyclic volatile methylsiloxanes (cVMS), however, vary widely (D4: 0.081-1.4, D5: 0.1-3.1, D6: 0.04-2.7), largely due to spatial exposure gradients from point sources and sampling bias. Because these ranges span the criterion value of 1, field studies have yielded mixed conclusions, indicating both trophic dilution (TMF 1).

This study evaluated TMFs of cVMS at two Japanese sites with minimal exposure gradients: the Yugawara coast and Lake Kasumigaura. Concentrations of D4, D5, D6, and two reference polychlorinated biphenyls (PCB-153 and PCB-180 which are non-metabolizable compounds) were measured in biota and sediments to determine field TMFs. In parallel, the Multibox AQUAWEB model was employed to predict biota concentrations and TMFs for the food webs in the study locations.

The Yugawara coast was divided into two sub areas (rocky and sandy), each represented by an independent marine food web and characterized by negligible exposure gradients due to their small, open configurations. Both measured and modeled TMFs of cVMS were consistently below 1, with strong ($p < 0.05$) or moderate ($p = 0.05–0.10$) statistical significance, indicating trophic dilution. In contrast, measured and modeled TMFs for PCBs exceeded 1 with strong statistical significance, confirming trophic magnification.

For Lake Kasumigaura, a mild exposure gradient was explicitly incorporated into the model to improve predictions of biota concentrations and TMFs. Model predicted concentrations closely matched measured values for D4, D5, D6, and PCB-180, with model biases near unity, demonstrating good model performance. All three cVMS exhibited trophic dilution (TMF 1).

Overall, this study provides additional evidence that cVMS undergo trophic dilution in both marine and freshwater food webs under conditions of no or mild exposure gradients, likely reflecting greater metabolic transformation compared with non-metabolizable reference compounds.

2.01.A.T04 Assessment of Bioaccumulation of 31 Legacy and Currently Used Pesticides in Freshwater Systems in South Korea

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Currently used pesticides (CUPs) are widely used as alternatives to legacy pesticides. However, as these CUPs are frequently detected in aquatic environments, a comprehensive assessment of their potential environmental impact is required. Especially in regions dominated by rice paddy cultivation, the risk of pesticide runoff into freshwater is elevated, yet field-based studies investigating the bioaccumulation potential of these CUPs in aquatic organisms remain insufficient. Therefore, this study investigated the contamination levels and distribution patterns of legacy and currently used pesticides in Korean freshwater systems, including freshwater, sediments, and crucian carp tissues (muscle, liver, gill, egg/gonad, blood, and brain), to assess bioaccumulation potential and ecological hazards. Of the 31 target pesticides, 21 were widely detected in freshwater, with total concentrations ranging from 131 to 2,941 ng/L, reflecting heavy application during the rice-farming season. In fish muscle, 13 pesticides were identified, with total concentrations ranging from 1.72 to 107 ng/g wet weight (ww). In contrast, only four pesticides were detected in the sediment, indicating low sediment affinity, with total concentrations ranging from non-detected (ND) to 7.30 ng/g dry weight (dw). The pesticides predominantly detected in freshwater and fish muscle were widely used compounds, including bromobutide, diphenylamine, thifluzamide, alachlor, and metolachlor; however, they exhibited low bioaccumulation potential in all fish tissues (Log BAF < 3). Pendimethalin, although rarely detected in freshwater and sediment, was frequently detected in fish muscle at relatively higher concentrations. The concentration of pendimethalin in muscle also exhibited a significant positive correlation with fish size ($p < 0.01$, Spearman) and a high bioaccumulation potential (Log BAF > 3) in most fish tissues, including muscle. Ecological risk assessment revealed high risks (RQ > 1) for bromobutide (3.03), thifluzamide (2.07), and chlorpyrifos (2.06), indicating potential adverse effects on aquatic organisms. These results highlight the importance of evaluating both exposure and bioaccumulation in monitoring programs and the need for continued monitoring and management of key pesticides that pose ecological risk, such as bromobutide, thifluzamide, chlorpyrifos, and pendimethalin.

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2.01.A.T05 Rapid migration and accumulation of Hg(II) in zebrafish brain

Traditional analytical techniques (such as ICP-MS and isotope tracing) cannot capture the real-time spatiotemporal changes of pollutants in vivo. Limitation of various detection methods often underestimate the ability of inorganic mercury (Hg^{2+}) to penetrate the biological barriers, thus most studies focused on its highly toxic form: methylmercury (MeHg). In this study, a highly selective near-infrared dual-zone AIE Hg(II) probe was synthesized by taking advantage of strong photostability of aggregation-induced luminescence (AIE) technology in complex biological matrix. Deep tissue imaging and real-time dynamic tracking of Hg(II) were then conducted in zebrafish in vivo. The results showed that Hg^{2+} rapidly entered

the bloodstream through the intestine and cross the blood-brain barrier, exhibiting a lasting accumulation effect in the brain. These results were in strong contrast to traditional viewpoint that Hg(II) has limited effects on the central nervous system. Further, real-time imaging data were transformed into quantitative analytical data, which showed that the neurotoxicity and environmental health risks of Hg(II) cannot be underestimated. This study provides a new quantifiable criterion for the evaluation of Hg toxicity, and demonstrates the potential and significance of AIE technology in solving complex environmental problems.

2.01.B.T - Advances in Bioaccumulation Assessment: From Models to Field Data

2.01.B.T01 Occurrence and trophic transfer of legacy and emerging PFAS in european freshwaters

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Per and polyfluoroalkyl substances (PFAS) are a large and structurally diverse group of persistent chemicals that are now ubiquitously present in aquatic environments. Due to their resistance to degradation, potential toxicity, and ability to bioaccumulate, PFAS pose a significant concern for ecosystem health and food web integrity. Despite growing attention, the mechanisms governing their trophic transfer and accumulation across different organism groups remain insufficiently characterized. In this contribution, we present a comprehensive assessment of legacy and emerging PFAS across freshwater food webs at multiple European sites. The study integrates data from organisms representing several trophic levels, including aquatic invertebrates, fish species, and higher predators such as piscivorous birds and mammals, enabling evaluation of contaminant dynamics across ecological gradients. A sensitive and selective LC MS/MS method was developed and validated for the simultaneous determination of a broad spectrum of PFAS in diverse biological matrices. The analytical workflow incorporates optimized extraction procedures, isotope dilution quantification, and matrix specific calibration, ensuring accurate and reproducible measurements in tissues such as muscle, liver, and reproductive organs. Our results demonstrate that PFAS behavior in food webs is strongly influenced by molecular structure. Long chain compounds show clear bioaccumulation and biomagnification trends, particularly in higher trophic levels, whereas short chain and emerging PFAS display more variable and compound specific patterns. Species traits and tissue characteristics further contribute to the observed variability. This study provides new insights into PFAS distribution and trophic transfer in aquatic ecosystems and highlights the importance of multi trophic monitoring approaches. The findings are relevant for improving environmental risk assessment and informing regulatory strategies, with implications extending beyond Europe to global freshwater systems.

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2.01.B.T02 Monsoon-Driven Dynamics and Trophic Magnification of PFAS in Diked and Undiked Estuaries

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Per- and polyfluoroalkyl substances (PFASs), characterized by their amphiphilic nature with hydrophobic tails and hydrophilic heads, have been widely utilized in diverse industrial applications. Once introduced,

PFASs widely distributed throughout aquatic ecosystems, where they partition and accumulate in biota, posing potential ecological risks through food webs. This study investigated the dynamics and trophic magnification of PFASs under monsoon-driven seasonal variation (pre- and post-monsoon; May and August, 2023) in a diked estuary (the Geum River estuary) and an undiked, free-flowing estuarine system (the Seomjin River, upper and lower sites). Bulk carbon stable isotope ratios and compound-specific stable isotope analysis of amino acids (CSIA-AA) for both carbon and nitrogen isotopes were applied to identify basal food sources, estimate trophic position (TP), and characterize food-web structure. Trophic magnification factors (TMF) were evaluated based on the relationships between concentrations and TP. Average total PFAS concentrations in biota were highest in the Geum River estuary across both season. Seasonal transition from pre- to post-monsoon, the proportion of long-chain perfluoroalkyl carboxylic acids (PFCAs; ≥C8) decreased, whereas long-chain perfluoroalkyl sulfonates (PFSAs; ≥C6) increased. F-53B was detected in all biota samples during the pre-monsoon period. TMFs based on the CSIA exhibited clear spatial and seasonal variability. Notably, PFNA (C9) showed biodilution trend at the upper site of the Seomjin River during the premonsoon period,whereas PFOS (C8) exhibited a biomagnification trend during the post-monsoon period at the Geum River estuary. These results indicate that site- and season-specific environmental conditions, together with differences in food web structure, strongly influence PFAS bioaccumulation and trophic magnification. This study underscores the importance of integrating hydrological variability and food web dynamics to better understand the mechanisms driving spatiotemporal variations in PFAS behavior in estuarine ecosystems. This would improve comprehensive understanding of TMF patterns under hydrologically variable estuarine conditions.

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2.01.B.T03 Dietary Uptake and Depuration Kinetics of Per- and Polyfluoroalkyl Substances (PFAS) in the Polychaeta Perinereis wilsoni

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Experimental data on the bioaccumulation kinetics of PFAS in invertebrates like polychaetes, particularly by food exposure, remain limited. This study investigates the dietary uptake and depuration kinetics of perfluoroalkyl acids (PFAAs) and their alternatives in the polychaete, Perinereis wilsoni through a controlled feeding experiment. P. wilsoni is an ecologically important species, serving as a key prey item for fish, crabs, and shellfish, and is also widely used as fishing bait. P. wilsoni were fed spiked food pellets and the number of pellets ingested by individuals was recorded. This was followed by a 28-day depuration phase during which they were provided with unspiked food pellets three times per week. The food pellets were spiked with a mixture of perfluoroalkyl carboxylic acids (PFCAs; C3–C17), perfluoroalkyl sulfonates (PFSAs; C4–C12), and five alternative PFAS. Two polychlorobiphenyl compounds were also spiked as reference compounds. PFAS concentrations in food, sandworm and water samples were analyzed using liquid chromatography–tandem mass spectrometry. Uptake and depuration rate constants were estimated using first-order kinetics based on whole-body burden. Gut uptake efficiency (α) of PFCAs ranged from 110 % for PFBA to 40% for PFOcDA. The α decreased from PFBA to PFHxA, remained relatively constant (with RSD < 10%) from PFHxA to PFTeDA, and decreased again from PFTeDA to PFOcDA. Among PFSAs, α was similar for PFBS, PFPeS, and PFHxS (with RSD < 4%), decreased for PFHpS, and remained stable up to PFDoDS (RSD < 2%). Among alternative PFAS, ADONA showed the highest α (96%), while 11Cl-PF3OUdS showed the lowest (38%). Depuration half-lives of both PFCAs and PFSAs did not increase monotonically with chain length. In

PFCAs, mid-chain compounds (PFHxA to PFNA) as well as PFTrDA and PFTeDA exhibited longer depuration half-lives (>100 days) than PFDA, PFUnDA, PFDoDA, PFHxDA, and PFOcDA (18–59 days). Similarly, in PFSAs, PFBS to PFHpS showed longer depuration half-lives (>100 days) compared to PFOS–PFDS (8.0–32 days). The pattern of longer depuration half-lives for mid-chain compounds was consistent with observations from our seawater exposure experiments. The present study demonstrated that the bioaccumulation kinetics in this polychaete species were different from that in fish, suggesting the need for further research into the bioaccumulation kinetics of other aquatic invertebrates.

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2.01.B.T04 Terrestrial Bioaccumulation in Insects: Assessing the Dominant Pesticide Exposure Route with Ladybugs.

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The first Tier of the pesticide environmental risk assessment for non-target terrestrial arthropods (NTAs) has a data requirement on effect studies with two standard test species involved in pest control, using contact exposure to dried spray residues on glass plates. The glass plate residue is considered a worst-case exposure scenario compared to the exposure that NTA experience after a downward spray event in the field via contact with residues on (3D-structured) natural substrates, such as plant leaves and soil. This exposure scenario may still underestimate the dietary intake from food residues (e.g., prey material for predaceous NTA), as well as direct exposure to the spray droplets during PPP-application (and spray drift). As it is often the internal dose that drives pesticides above a toxic threshold, we studied the pesticide accumulation in NTA over a 1 week period using different exposure routes. A single (non-toxic) spray dose was applied using a Potter tower spray system to expose ladybugs via (i) topical overspray, (ii) a dried residue on natural substrate surface (leaf or soil), (iii) dietary intake of oversprayed food items. Two binary mixtures of two active substances were tested on larvae and adult ladybugs (Coccinella septempunctata). After topical overspray, all four chemicals decreased from the exterior residues of larvae and adults to <20% within one day, and the volatile chemicals showed faster disappearance from the exterior residue. Internal residues were highest at the first samping point of 2 h, and after that more slowly decreased from tissue. For ladybird larvae intake via contaminated food items was the dominant exposure route in the next five days studied, for ladybird adults the leaf residue contact and soil residue contact was the long term dominant exposure route. For both tested species residues for several exposure routes were above the 90-percentile Residue Unit Dose values measured in field trials with pesticides. Topical overspray exposure results in a short term peak, and other exposure routes dominate the exposure profile depending on NTA species/lifestage/chemical. Based on these findings we suggest to take additional exposure routes into account in NTA risk assessment, while differentiating between organism groups.

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2.01.B.T05 Extreme variability in trace element bioaccumulation across marine species: what roles for differences in diet and physiology vs environment?

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This study assessed levels of potentially toxic trace elements including Hg, Cd, As and Pb, in a variety of

marine shellfish and finfish species in the Bay of Plenty, New Zealand, to understand the influence of emissions from local volcanoes and the potential safety of locally harvested seafood. While geothermal contributions to some elements were apparent, the variability in trace element total burdens was far greater between species. In some species, the contribution of a specialized diet seems apparent such as high levels of vanadium in zooplanktivores feeding on salps. In rock lobsters, extremely high levels of total arsenic seem more related to the physiology of arsenic metabolism in this group which is still poorly understood. Mercury in this study was strongly influenced by geothermal sources, although the extreme variability in mercury bioaccumulation was dominated by elemental rather than organic mercury. Related but ecologically differing species accumulated lead, which suggests some physiological influence on lead uptake in this group of fish. Associations between elements were apparent such as the influence of selenium on mercury, and correlations between zinc and cadmium. However, clearly there is still much that we do not understand about the key determinants of trace element bioaccumulation in marine biota and there is still a need for fundamental studies on diet, physiology and environmental determinants of elemental uptake.

2.01.P - Advances in Bioaccumulation Assessment: From Models to Field Data

2.01.P–Mo051 Exposure to Persistent Organic Pollutants in Australian Waterbirds

There is growing worldwide recognition of the threat posed by persistent organic pollutants (POPs) to wildlife
populations. We aimed to measure exposure levels to POPs in a Southern Hemisphere aquatic waterbird species, the
nomadic gray teal (Anas gracilis), which is found across Australia. We collected wings from 39 ducks harvested by recreational
hunters at two sites (one coastal, one inland) in Victoria, southeastern Australia, in 2021. We examined three groups of POPs:
nine congeners of polychlorinated biphenyls (PCBs), 13 organochlorine pesticides (OCPs), and 12 polycyclic aromatic hydrocarbons
(PAHs). The PCBs, OCPs, and PAHs were detected at quantifiable levels in 13%, 72%, and 100% of birds,
respectively. Of the congeners we tested for in PCBs, OCPs, and PAHs, 33%, 38%, and 100% were detected at quantifiable
levels, respectively. The highest levels of exposure to POPs that we found were to the PAH benzo[b]fluoranthene, occurring
at a concentration range of 1.78 to 161.05 ng/g wet weight. There were some trends detected relating to differences
between geographical sites, with higher levels of several PAHs at the coastal versus inland site. There were several strong,
positive associations among PAHs found. We discuss potential sources for the POPs detected, including industrial and
agricultural sources, and the likely role of large-scale forest fires in PAH levels. Our results confirm that while Australian
waterbirds are exposed to a variety of POPs, exposure levels are currently relatively low. Additional future investigations are
required to further characterize POPs within Australian waterbird species.

2.01.P–Mo052 Temporal Dynamics of Molecular Biomarkers and Tissue-Level PAHs

Localization in the Green Mussel Perna viridis: An Integrated Approach for Coastal Environmental Monitoring

Surapa Chinplikanon[1], Tongchai Thitiphuree[1] and Noppadon Kitana[1] (1)Chulalongkorn University

Polycyclic aromatic hydrocarbons (PAHs) are persistent organic pollutants that pose significant risks to marine ecosystems. This study utilizes the green mussel Perna viridis as a tropical sentinel species to evaluate the relationship between molecular stress responses and the spatial accumulation of PAHs in tissues. Mussel samples were collected monthly over a seven-month period (August 2023 to February 2024) to determine seasonal variation in gene expression across several functional pathways. These findings were integrated with immunohistochemistry assays using the 2G8 monoclonal antibody to visualize tissue-specific PAHs accumulation. The molecular data revealed three distinct functional gene clusters. Metabolic and detoxification pathway showed increased activity in the later study months. Glutathione s-transferase and p-glycoprotein peaked in January, while cytochrome P450 exhibited a substantial surge in February. Stress response and transcriptional regulation pathway including heat shock protein, CCAAT/enhancer-binding protein gamma, estrogen-related receptor and dopamine receptor showed a synchronized bimodal pattern with significant peaks in September and November. Growth and reproduction pathway: Integrin remained at baseline before peaking in February, while ring finger protein reached its maximum in January. A strong positive correlation was observed between glutathione s-transferase and cytochrome P450, heat shock protein and CCAAT/enhancer-binding protein gamma. The correlation found relating positively with shell width and body weight, displaying significant sex-specific divergence with higher expression in males than females. The integration of IHC for PAHs localization with these diverse biomarkers provides a detailed framework for interpreting contaminant responses. These findings offer an improved strategy for environmental monitoring and the interpretation of physiological stress in coastal sentinel organisms.

2.01.P–Mo053 A Machine Learning-Assisted Toxicokinetic Model for Predicting Uptake and Elimination of Organic Compounds in Freshwater Crustaceans

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Ecological risk assessment is increasingly constrained by the limited availability of toxicokinetic (TK) data required to characterize internal exposure dynamics across diverse environmental chemicals and conditions. Because toxic effects are governed by internal concentrations, the inability to estimate time-resolved exposure profiles remains a major bottleneck for screening-level assessment. Here, we present a machine learning (ML)-assisted TK framework to predict uptake and elimination rate constants and reconstruct internal concentration–time profiles for freshwater crustaceans. Multiple models were benchmarked on a curated TK dataset integrating molecular, biological, and environmental descriptors. The multi-task neural network outperformed all benchmark models (Random Forest, Support Vector Regression, XGBoost, and single-task neural network) in predicting elimination rate constant, achieving the lowest RMSE of 0.317 and the highest R^2 of 0.648 on original scale test set. Integration of predicted rate constants into a one-compartment TK model yielded reconstructed profiles in good agreement with experimental observations (NRMSE = 0.053), with 66.79% of predictions within three-fold of observed values. Feature importance analysis identified life stage as the dominant predictor of TK rate constants, with exposure duration, and organic matter–related variables also contributing substantially. This proposed framework enables structure-informed and context-aware prediction of internal exposure dynamics for data-poor chemicals, supporting screening-level ecological risk assessment and prioritization of contaminants of concern in aquatic ecosystems.

2.01.P–Mo054 Structural and Physicochemical Characteristics of Outliers in BCF

Prediction Models

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Bioconcentration factor (BCF) is widely used in ecological risk assessment to evaluate chemical accumulation in aquatic organisms. Although QSAR and machine learning models have been applied to BCF prediction, chemicals showing large prediction errors remain poorly characterized. In this study, we investigated structural and physicochemical characteristics associated with discrepancies between predicted and measured BCF values.

Measured BCF data were obtained from the NITE database. BCF prediction models were constructed using molecular descriptors calculated by AlvaDesc. Based on prediction errors, chemicals with predicted BCF values less than one-fifth of the measured values were defined as “underestimated,” whereas those with predicted values more than five times the measured values were defined as “overestimated.” XGBoost classification models were then constructed to identify structural characteristics associated with underestimated and overestimated compounds.

The BCF prediction model constructed using 1,332 compounds achieved an R^2 value of 0.587. For underestimated group, a 10-feature model achieved a Macro-F1 score of 0.478 ± 0.019, and important descriptors were related to molecular planarity and hydrophobicity.

In contrast, for overestimated compounds, a 10-feature model achieved a Macro-F1 score of 0.583 ± 0.083, and important descriptors were related to oxygen-containing substructures, carbon-related structures, and electronic properties.

The identified descriptors provide insight into structural characteristics associated with large prediction errors in BCF prediction models. In addition, in vitro metabolic rates of selected compounds were evaluated using S9 metabolism assays. Ongoing molecular docking analyses with metabolism-related enzymes may further clarify the role of metabolic interactions in BCF prediction errors.

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2.01.P–Mo055 Machine Learning Prediction of Pharmaceutical Breakthrough in Biochar Columns

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Performing biochar column experiments is often a long and costly process. Characterizing pharmaceutical adsorption patterns is essential for optimizing biochar as a sustainable adsorbent for wastewater remediation. However, predicting pharmaceutical breakthrough is complex because adsorption strongly depends on both biochar and pharmaceutical properties. In this study, a large breakthrough dataset containing 37 pharmaceuticals and 2 biochar materials was used to train machine learning models: Random Forest, XGBoost, and CatBoost. To assess data quality, analytical models such as the Yoon–Nelson model were applied, and the fitting quality was used to evaluate how data quality affects ML prediction. Two scenarios were considered: (i) point-wise selection, predicting missing points within the breakthrough curve and (ii) Leave-One-Compound-Out, predicting a complete unseen breakthrough

curve. Results show that point-wise prediction achieved the highest performance for Random Forest and CatBoost, with improved results when models were trained on higher-quality data. Prediction of a full breakthrough curve led to lower overall performance for all three models, and the effect of data quality was less pronounced in this scenario. Feature importance analysis identified bed volume as the dominant predictor, highlighting the influence of biochar-dependent breakthrough behaviour. Interestingly, distinct pharmaceutical breakthrough curves were still observed despite physicochemical properties showing limited relative importance. Overall, these results demonstrate the potential of machine learning models to reduce extensive analytical work by accurately completing or predicting full biochar breakthrough curves.

2.01.P–Mo056 Bioaccumulation Assessment of New Chemical Substances under Japan's Chemical Substances Control Law Using Read-Across and QSAR

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The safety assessment of industrial chemical substances in Japan is conducted based on the Chemical Substances Control Law (CSCL). Manufacturers and importers of new chemical substances are required to notify the authorities of the safety assessment results, such as biodegradation, bioaccumulation potential and 28-day repeated-dose toxicity. To evaluate the persistence of a new chemical substance, a biodegradation test (OECD Test Guideline 301C or 301F) is first conducted. The purpose of the test is to investigate the persistence of the new chemical substance in the environment, as well as the presence of its biodegradation products that may be released in addition to the parent chemical. If the substance is judged "not readily degradable" from the test result (BOD < 60% and more than 1% of biodegradation product) under the CSCL, the bioaccumulation potential (B, "Not highly bioaccumulative" as BCF less than 5,000) and the toxicity of the new chemical and its biodegradation products are assessed. From the perspectives of testing costs and animal welfare, the use of read-across based on expert judgment using test data from chemical substances with similar structures and physicochemical properties and Quantitative Structure-Activity Relationship (QSAR) approaches are considered acceptable for the B assessment of new chemical substances under the CSCL.
In this poster, we present case studies on the B assessment of chemical substances under the CSCL using read-across and QSAR approaches.

2.02.A.T - Advances in Environmental Chemistry for Quantitative Exposure Assessment and Risk-Informed Management of PFAS and Emerging Contaminants

2.02.A.T01 Target and non-target analysis of volatile and non-volatile PFAS in air

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Per- and polyfluoroalkyl substances (PFAS) are subjects of global concern for the last 26 years. Not only use for industrial and consumer products, PFAS in food and drinking water are strictly regulated and Japanese water supply law enforced measurement of PFAS and PFOA in every three months in Japan. However, potential exposure of PFAS to humans through ambient air is rarely investigated even though precipitation was known as one of significant sources of PFAS pollution on the global scale.
We have developed several research tools including cryogenic air sampler, NS20, FM4, GAIAC, Triporous rice husk activated carbon etc. for the last ten years. Both gas and particle sampler were first reported in 2021 by Wu, continue with mass balance analysis of PFAS in air by Lin (2020) and recent nationwide monitoring by Asakawa (2025).
Here we report recent results of air pollution of PFAS in Osaka metropolitan city and Ogasawara Islands

using updated method of target and non-target analysis.
Air samples were collected by using particle and gas sampler (NS20; Sibata Scientific Technology Co., Ltd., Japan). The air samples were collected from Osaka during February 2025, April 2025, and March 2026. Whereas the samples from Ogasawara were collected in November 2024, respectively. The air sampler was assembled with a four-stage cascade impactor equipped with quartz fiber filters to collect particulate matter, followed by an adsorbent cartridge containing one polyurethane foam (PUF) and several new material adsorbents to collect the gaseous phase.
In this report, we successfully measured forty-one volatile PFAS using GC-Orbitrap HRMS and fifty-six semi-/non-volatile PFAS using LCMSMS in ambient air samples. There were remarkable differences of concentrations and compositions of PFAS between remote Islands of Ogasawara and populated city of Osaka. Characteristic analysis revealed an interactive mechanism between long-range transportation and discharge into local environment.
Interestingly, some of brominated PFAS and iodide PFAS were detected in not only Osaka but also remote Island. Medical use of these chemicals in Japan may have a reason for the detection of these chemicals mostly in Japan. The integrated approach of the target quantification (including volatile, semi and non-volatile) and non-target screening of PFAS enables valuable insights on PFAS pollution complexity, source related identification and possible risks due to combined exposure of PFAS mixtures.

2.02.A.T02 Advancing Atmospheric PFAS Monitoring: Optimization of Sampling and Total Fluorine Analysis

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The occurrence and environmental fate of PFAS in the atmosphere remain poorly understood, primarily due to limitations in current sampling and analytical methods. Many volatile fluorinated compounds exhibit low sorption efficiency on conventional adsorbents, demanding an improved sampling strategy to effectively capture and extract volatile fluorinated substances. Although several analytical methods have been developed for PFAS detection across various matrices, few are suitable gaseous samples.

Given the structural diversity of PFAS and the presence of numerous unidentified compounds, conventional target analysis is unlikely to provide a comprehensive assessment of atmospheric PFAS exposure. To address this limitation, broader analytical approaches such as suspect screening and measurements of total and extractable organofluorine have been introduced. The total fluorine approach quantifies all fluorine present in a sample, including both inorganic and organic fractions. Incorporating an additional extraction step enables isolation of the organofluorine fraction, typically considered anthropogenic and largely associated with PFAS.

This study systematically evaluates different sorbent materials (XAD-2, GAIAC and PUF) for the collection of volatile fluorinated compounds under controlled laboratory conditions. In parallel, extraction solvents and protocols were optimized to improve recovery and representativeness of the collected fluorinated fraction. In addition, the NS20 air sampler configuration was further evaluated both in laboratory and field settings to identify an optimal sample train setup.

Results demonstrated differences in sorption capacity and selectivity between the tested materials, affecting both target PFAS capture and total fluorine measurements. The combined optimization of sampling and extraction conditions enabled a more robust assessment of volatile fluorinated compounds, including both known PFAS and unidentified organofluorine fractions. This project provides an improved analytical framework for characterizing atmospheric fluorinated compounds and supports more reliable assessment of PFAS occurrence in air.

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2.02.A.T03 Optimization of Stable Carbon Isotope Ratios of PFOA and PFOS Using High-Resolution Mass Spectrometry

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As concerns grow over the high environmental persistence and bioaccumulation potential of per- and polyfluoroalkyl substances (PFAS), tracing their emission and contamination sources has become increasingly important.

A carbon stable isotope analysis method using high-resolution mass spectrometer (Orbitrap) was applied to perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA), and measurement conditions were optimized. In addition, reagents from different manufacturers and production lots were analyzed, and spike experiments with three river water samples were performed to evaluate the applicability of this method to environmental samples.

All measurements were conducted using a Q Exactive Orbitrap mass spectrometer coupled to an UltiMate 3000 ultrahigh performance liquid chromatography system (Thermo Fisher Scientific). PFAS reagents were diluted to 1–50 μM with methanol (purity ≥99.8 %) and injected alternately in the sequence sample–reference–sample. For optimization of the analytical conditions, the effects of resolution (17,500–140,000), automatic gain control target (2×10^4–5×10^6), and analyte concentration (1–50 μM) were evaluated.

Using the optimized conditions, seven PFOA reagents and two PFOS reagents from different manufacturers and production lots were analyzed. The differences between elemental analysis−isotope ratio mass spectrometry (EA-IRMS) and Orbitrap measurements were within ±1.5 ‰, confirming the validity of the method. Two of the seven PFOA reagents exhibited highly depleted stable carbon isotope ratios (δ13C) values that ranged from −49.0 ‰ to −45.8 ‰, whereas the δ13C values of the remaining five were between −30.2 ‰ and −27.3 ‰. The implication was that the PFOA reagents could be categorized into two distinct groups based on the distributions of their δ13C values. It has been previously reported that PFOA can be divided into two groups based on δ13C values depending on the manufacturing process (electrochemical fluorination (ECF) vs. telomerization), and the results of this study are considered to reflect the same trend.

This study demonstrated that Orbitrap mass spectrometry enables highly precise measurements of PFOA and PFOS, which have been difficult to analyze using conventional IRMS techniques. These findings indicate that this method has strong potential as a useful tool for source identification of PFAS, discrimination of manufacturing processes, and investigation of environmental fate and transport.

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2.02.A.T04 PFAS testing outside drinking water: How is it done correctly?

PFAS testing has been done globally for the past decades from various sample types and regulations are set in drinking water in many parts of the world. From the exposure and toxicity standpoint, knowing the concentrations in other sample types can be a useful tool to understand how we and animals are exposed to PFAS.

From environmental testing standpoint, sample types may include soil, biosolids, ambient air, stack emission, wastewater, ground water, and so on. From biological sample testing, sample types can include

whole blood, plasma, serum, etc. Each sample type has unique challenges and overcoming those challenges to get reliable data is critical.
This presentation will be a review of PFAS measurements in various sample types and how they were prepared for consistent data collection for truly cross-industry perspective from environmental to clinical diagnostics and food safety and beyond.

2.02.P - Advances in Environmental Chemistry for Quantitative Exposure Assessment and Risk-Informed Management of PFAS and Emerging Contaminants

2.02.P–Tu051 Discovery of a Novel PFBS - specific ssDNA Aptamer for Short-Chain PFAS Monitoring

Kim Dongyun[1], Park Junyoung[2] and Jong Kwon Choe[1] (1)Seoul National University, (2)Yale University

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants of global concern due to their chemical stability, bioaccumulation potential, and adverse effects on human health and ecosystems. As regulatory restrictions on legacy long-chain PFAS, including perfluorooctane sulfonate (PFOS) and perfluorooctanoic acid (PFOA), intensify, short-chain PFAS are increasingly adopted as substitutes, with rising concentrations detected across aquatic environments. Their higher environmental mobility and lower hydrophobicity hinder both conventional treatment and reliable quantification, posing challenges for accurate exposure assessment. Among short-chain PFAS, perfluorobutane sulfonate (PFBS), a four-carbon sulfonate used as a substitute for PFOS, has shown the most pronounced increase in occurrence, making it a priority target for selective detection.
We developed a PFBS-specific ssDNA aptamer through 30 rounds of Systematic Evolution of Ligands by Exponential Enrichment (SELEX), incorporating PFOS and perfluoropentanoic acid (PFPeA) as counter-selection targets to eliminate cross-reactive sequences. Candidate aptamers identified by next-generation sequencing (NGS) were evaluated using three fluorescence-based platforms: FAM-quencher, Thioflavin T (ThT), and SYBR Green I assays. The dissociation constant (Kd) was determined to be 12.7 μM via the ThT assay. Among the three platforms, SYBR Green I yielded the most distinct fluorescence response. Circular dichroism (CD) spectroscopy revealed that PFBS binding reinforces the existing secondary structure without inducing conformational change, suggesting a pre-organized recognition mechanism. Isothermal titration calorimetry (ITC) confirmed both enthalpic and entropic contributions to binding, while molecular dynamics (MD) simulations showed that hydrophobic, electrostatic, hydrogen bonding, and dispersion interactions govern binding. Stronger binding to perfluoroalkyl sulfonates (PFSAs) over perfluoroalkyl carboxylates (PFCAs) underscores the critical role of the sulfonate head group in selectivity. An additional five targeted SELEX rounds further improved PFBS selectivity and binding affinity.
This study presents the first PFBS-specific ssDNA aptamer with a well-characterized binding mechanism, demonstrating its potential for integration into portable biosensor platforms for on-site quantification of short-chain PFAS and improved exposure assessment of emerging contaminants in aquatic systems.

2.02.P–Tu053 Enhanced performance for FOSA and FOSEs analysis with an ultra-sensitive PFAS-multiclass method in environmental samples

Ruth Marfil-Vega[1] (1)Shimadzu

With the increasing regulatory drivers and public pressure for managing PFAS in the environment, foods, and consumer and industrial products, laboratories are in need of efficient multiclass-PFAS methods that enable routine ultra-sensitive quantitation. As the classes of PFAS to be monitored expand the instrument performance may be compromised for specific compounds as their ionization efficiency changes based on

their physico-chemical properties. In this work we validated a LC-MS/MS method (LCMS-8065 XE, Shimadzu Corporation) for a multiclass-PFAS panel including PFCAs, PFSAs, FTSs, FOSAs, FOSAAs, FOSEs, FTCAS, PFESAs and PFECAs across matrices of environmental relevance (drinking water, wastewater, tissue…). Sample preparation varied depending on the matrix of interest: co-solvation and direct injection for drinking water, and pre-concentration (either Solid Phase Extraction or solvent extraction) for other sample types. Method Detection Limits (MDLs) were below 1 ng/L in drinking water for all targeted compounds. In solid samples, MDLs ranged from <0.05 to 0.2 ng/g for PFCAs, PFSAs, PFESAs and PFECAs, < 0.5 ng/g for FTSs and FTCAS, and < 0.6 ng/g for FOSAs, FOSAAs, and FOSEs. In this presentation we will share the detailed results of the method validation, with emphasis on classes of PFASs that are historically worse performers in multiclass-PFAS methods, such as FOSAs and FOSEs. We will also discuss relevance and impact of different sample preparation approaches on the instrumental method.

2.02.P–Tu054 Development of a Polar Organic Chemical Integrative Sampler with a Constant Sampling Rate

Kazushi Noro[1] (1)National Institute for Environmental Studies

The Polar Organic Chemical Integrative Sampler (POCIS) is a passive sampler that has been used to monitor hydrophilic organic contaminants in aquatic environments. To convert the amount of contaminants accumulated in POCIS into dissolved concentrations in water, compound-specific sampling rates are required. However, calibration experiments to determine these sampling rates are costly. Previous studies have attempted to develop simplified calibration methods and predictive models, but these approaches have not been successful.
In this study, we aimed to control the sampling rate and enable the quantification of all target compounds using a constant sampling rate. The properties of membranes and sorbents used in POCIS were evaluated, and an optimal combination suitable for achieving a constant sampling rate was determined. Calibration experiments were conducted for more than 70 compounds using this novel POCIS, and the variability in sampling rates among compounds was compared with that of conventional POCIS.

2.02.P–Tu057 Machine Learning-Assisted Aptamer Discovery and qPCR-Based Sensing Strategies for Monitoring PFAS Compounds in Water and Biological Systems

Jong Kwon Choe[1], Junyoung Park[1] and Donghyun Kim[1] (1)Seoul National University

Per- and polyfluoroalkyl substances (PFAS) are persistent emerging contaminants that pose increasing concerns due to their environmental stability, bioaccumulation potential, and adverse health effects. Rapid and selective monitoring technologies are therefore needed for both environmental surveillance and mechanistic toxicological investigations. This presentation introduces two complementary studies involving single-stranded DNA (ssDNA) aptamers targeting PFAS compounds.

The first part focuses on machine learning-assisted discovery of PFHxS-binding aptamers during the SELEX process. Multiple machine learning algorithms were evaluated to predict aptamer candidates with enhanced binding affinity and selectivity. Decision tree-based models, including Random Forest, LightGBM, and XGBoost, demonstrated superior predictive performance compared with neural network-based approaches. Using the XGBoost-guided workflow, a PFHxS-targeting aptamer exhibiting substantially improved binding affinity relative to conventionally selected sequences was identified while maintaining selectivity against structurally related PFAS analogues. In addition, the developed predictive framework was explored for investigating potential interactions between PFHxS and biologically relevant targets associated with cholesterol transport and genotoxic responses.

The second part presents a qPCR-amplified aptamer sensing platform for trace-level PFOS monitoring in aqueous environments. In this approach, PFOS-binding aptamers adsorbed onto gold nanoparticles undergo aggregation and precipitation upon interaction with PFOS, enabling quantification through qPCR amplification of aptamer-associated signals. The proposed sensing strategy successfully detected PFOS at ppt-level concentrations with minimal sample pretreatment and demonstrated applicability across diverse water matrices, including tap water, river water, and industrial wastewater. Mechanistic investigations further showed that aptamer loading and nanoparticle size significantly influenced sensing sensitivity and reproducibility.

Together, these studies demonstrate the potential of combining aptamer engineering, machine learning, and molecular amplification techniques to advance next-generation PFAS monitoring and assessment technologies.

2.02.P–Tu058 Utilising Cyclic Ion Mobility Mass Spectrometry to Assess Strategies to Reduce Environmental PFAS in Groundwater

Felicia Fredriksson[1], Ali Hussnain[1], Ingrid Ericson Jogsten[1], Sara Beverley[2] and Mike McCullagh[2]
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In Sweden, one of the main point sources of PFAS contamination is the historic use of aqueous film-forming foams (AFFF) at former and active firefighting training areas. Addressing PFAS leaching from AFFF-contaminated areas into groundwater has therefore become a critical environmental priority. Recent remediation initiatives have focused on innovative in situ barriers and on-site treatment systems, including activated carbon barriers designed to limit PFAS migration into groundwater. Accurate determination of PFAS in environmental samples is critical for assessing exposure and elucidating exposure pathways. However, reliable identification at trace levels (ng/L) and differentiation of PFAS isomers remains analytically challenging. This is of high relevance due to the reported differences in toxicity and environmental behaviour between branched and linear PFAS isomers.

A quadrupole-cyclic ion mobility-time-of-flight (cIM-ToF) mass spectrometer equipped with Wideband Enhancement was used to target characteristic PFAS drift time trendlines synchronized with the time-of-flight pusher This acquisition mode improves the ToF duty cycle and lowers detection limits. Analysis using a quadrupole-cIM-ToF mass spectrometer with Wideband Enhancement and UniSpray™ ionisation, provided enhanced selectivity, sensitivity, and collision cross section (CCS) measurements, which serve as complementary descriptors for PFAS identification.This analytical strategy has been applied to groundwater samples before and after the located activated carbon barrier to characterizer known, unknown, linear, and branched PFAS.

Groundwater samples contained a broad range of PFAS, including PFOA, PFOS, PFHxS, and PFNA. Typically, ΔCCS values below 1% has been observed compared to the PFAS library CCS values. Chromatographically coeluting linear and branched PFOS isomers in groundwater were successfully resolved using LC cIM at a resolving power, ≈ 160, enabling acquisition of isomer-specific product ion spectra. Multi-sequence functionality enabled resolution of homologous series constituents of linear and branched PFOS within a single analysis. Overall, the cyclic ion mobility mass spectrometry forms a valuable component of advanced PFAS characterization strategies, improving identification specificity for linear, branched, and unknown PFAS while enabling a more comprehensive assessment of the environmental impact and remediation performance of in situ barrier systems.

2.02.P–Tu060 Comparative Characterization of PFAS Mixture Profiles in

Commercial Ski Waxes

Eriko Yamazaki[1], Nobuyasu Hanari[1], Jin Hamaura[1], Keisuke Nakamura[1], Takamitsu Otake[1], Kazumi Inagaki[1], Yuichi Yoshida[2] and Makoto Watanabe[2] (1)National Institute of Advanced Industrial Science and Technology (AIST), (2)Shimadzu Corporation, Kyoto, Japan

Commercial ski waxes are consumer-related products of interest for per- and polyfluoroalkyl substances (PFAS), but product-level information on PFAS mixture patterns remains limited. They are relevant because ski waxes have been reported as PFAS-associated products and may show product-to-product differences in PFAS composition. Previous studies have mainly reported concentrations or compound-by-compound detection results, but fewer studies have compared the overall mixture profiles among products. The purpose of this study was to compare PFAS mixture profiles in commercial ski waxes using concentration data together with simple compositional descriptors.
PFAS in commercially available ski wax products were analyzed by liquid chromatography-tandem mass spectrometry. The analytical methods covered several PFAS classes. For the comparison of mixture patterns, we focused mainly on homologous perfluoroalkyl carboxylic acids, because they form a continuous compound series and are easier to interpret compositionally than a mixed list of unrelated PFAS classes. The product profiles were then compared from two viewpoints, measured concentrations and simple compositional features, such as whether one component dominated the profile or several components were distributed across the series.
The PFAS profiles varied among the ski wax products. In some products, the target PFAS were not detected or were detected only at limited levels. In other products, several PFAS were detected, and the relative contribution of each compound differed from product to product. For this reason, total concentration alone was not sufficient to describe the profiles. Comparing the compositional features helped show whether a profile was mainly controlled by one or a few components, or whether several homologues contributed to the profile.
Overall, the results show that ski wax products can differ not only in PFAS concentration but also in the distribution of individual PFAS within each product profile. Reporting these compositional features together with concentration data may help compare product-associated PFAS profiles, support screening of PFAS-associated products, and provide chemical context for future exposure and risk-related discussions.

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2.02.P–Tu063 A Preliminary Study on Fluorine Mass Balance and PFAS Contribution in Korean Environmental Samples

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<p>Organofluorine compounds are highly stable due to the strong C-F bond, and most detected in the environment are considered anthropogenic. Among them, per- and polyfluoroalkyl substances (PFAS) have been widely used since the 1940s, with at least 4,000 compounds estimated to exist. Since PFAS are highly persistent and frequently detected in wildlife and humans, several are regulated as persistent organic pollutants (POPs) under the Stockholm Convention. However, target analysis alone is insufficient to assess the overall organofluorine burden, and information on fluorine mass balance within environmental matrices remains limited. Therefore, in this study, total fluorine (TF) and extractable organic fluorine (EOF) were measured using combustion ion chromatography (CIC), and the contribution of target PFAS was evaluated in river water, tap water, and sludge samples. River water samples were collected from the upstream, midstream, and downstream regions of the Nakdong River, South Korea, in 2025, along with wastewater treatment plant (WWTP) effluent, downstream-derived tap water in 2026, and sludge collected in 2022 near the downstream region. A total of 46 PFAS were analyzed using liquid

chromatography-tandem mass spectrometry (LC-MS/MS). TF was measured by direct injection, whereas EOF was analyzed after pretreatment, using a Metrohm 930 Combustion Ion Chromatograph with CAR-PFAS verified. TF was detected in all water samples in the range of 183-272 ng F-/mL, while sludge samples exhibited significantly higher TF levels of 6,549,981 and 6,106,602 ng F-/g dry weight. EOF concentration ranged from 0.546 to 2.42 ng F-/mL, accounting for only 0.239-1.31% of TF, with notably higher levels observed at the midstream site and in WWTP effluent. Fluorine equivalents derived from target PFAS were substantially lower than EOF, indicating that target PFAS account for only a small fraction of the total organofluorine burden. These findings suggest that a substantial portion of organofluorine remained unidentified across all matrices and highlight the importance of combining TF, EOF, and target/suspect/nontarget PFAS analyses for fluorine mass-balance assessment. This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education(RS-2021-NR060122). Special thanks to Felicia Fredriksson, Welmoed Nauta, and Dipa Lalwani for their technical support and assistance.</p>

2.02.P–Tu065 An Analysis of the Functional Use Distribution of PFAS Intentionally Used in Commercial Products

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This study aims to systematically characterize the functional uses of per- and polyfluoroalkyl substances (PFAS) based on product-level data, with a focus on substances intentionally incorporated into commercial products. While PFAS are widely utilized due to their unique physicochemical properties, such as chemical stability and surface activity, there remains limited structured understanding of how individual substances are functionally applied across products.

In this study, publicly available product composition data provided by a manufacturer were compiled and curated. The dataset consists of product entries updated at irregular intervals, each containing up to seven PFAS substances, with concentration ranges (reported in six predefined percentage-based categories) and up to four non-exclusive functional use descriptors reported individually for each PFAS.

Although the dataset is partially structured, it presents several challenges, including inconsistencies in terminology, variation in descriptive granularity, and the use of semi-standardized functional labels. To address these issues, the dataset was harmonized through systematic data cleaning and normalization. The resulting curated dataset comprises approximately 100–150 distinct PFAS substances and approximately 50 consolidated functional use categories, enabling more consistent comparisons across product entries.

The harmonized data were further organized within a unified functional classification framework by integrating existing descriptors with additional categories introduced in this study. This framework supports analyses from multiple perspectives, including the occurrence of individual PFAS across products, their associations with functional use categories, and their distribution across reported concentration ranges. In addition, the dataset enables the examination of co-occurrence patterns of PFAS within products and their variation across application contexts.

While primarily descriptive, this study establishes a structured and harmonized dataset that facilitates systematic analysis of PFAS use in commercial products. The resulting framework provides a basis for identifying relationships between substances, functional roles, and product contexts, and supports future, more detailed analyses of PFAS usage patterns.

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2.02.P–Tu066 Comprehensive PFAS Screening in Textiles Using LC-MS/MS and GC-MS/MS

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Per- and polyfluoroalkyl substances (PFAS) are widely utilized in industrial applications for their unique stability and repellency. However, their persistence leads to environmental accumulation and human health risks. To mitigate them, the European Union Persistent Organic Pollutants (POPs) Regulation established strict concentration limits of 0.025 mg/kg (25 ppb) for compounds such as PFOA, PFOS, and PFHxS in textiles, a potentially significant source of exposure. The European standard EN 17681 provides the analytical framework, using LC-MS/MS for ionic PFAS (Part 1) and GC-MS for neutral volatile PFAS (Part 2).
This study developed analytical methods based on EN 17681-1/2 for 39 PFAS. For LC-MS/MS, 33 compounds were calibrated at 0.1–10 µg/L, with fluorotelomer alcohols (FTOHs) at 10–1000 µg/L . For GC-MS/MS, eight targets listed in the method plus four FTOHs were calibrated at 1–10 µg/L. The GC-MS/MS was equipped with a high-sensitivity ion source to ensure stable detection at trace levels; a preconcentration step can also be added to further enhance signals. Recovery tests were conducted by spiking textile samples below the current regulatory limit of 0.025 mg/kg . Furthermore, the study compared the previous EN 17681-1:2022 (methanol extraction) with the revised EN 17681-1:2025 (alkaline hydrolysis) using old ski-wear samples.
Results showed excellent linearity for all analytes (R > 0.998). Repeatability at the lowest calibration level was good, with %RSD (n=5) generally within 20%. Spike and recovery tests below the regulatory limit were successful, with recoveries between 70% and 130% and %RSD (n=3) within 11%. The high-sensitivity ion source on GC-MS/MS was critical for achieving stable responses at these trace levels without requiring additional preconcentration steps.
In the ski-wear analysis, the EN 17681 1:2025 alkaline hydrolysis pretreatment yielded significantly higher levels of NMeFOSE and 6:2, 8:2, and 10:2 FTOHs compared to the 2022 method. This confirms the effectiveness of the revised procedure in releasing bound or precursor PFAS.
The integrated use of LC-MS/MS and GC-MS/MS allows comprehensive PFAS screening below regulatory limits; targeting FTOHs in both LC-MS/MS and GC-MS/MS provides additional insights into the origin of FTOHs in the samples for better assessment of the exposure while using the products. By optimizing instrumental sensitivity, practical routine screening is possible without preconcentration.

2.02.P–Tu067 Insights into PFAS Uptake and Accumulation in Hydroponically and Pot-grown Kale Using Modified QuEChERS and SPE Coupled with LC-QTOF/MS

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Per- and polyfluoroalkyl substances (PFASs) are persistent contaminants widely used in consumer products, leading to their accumulation in the environment and food chains and raising concerns for ecological and human health. To effectively evaluate the risks of PFAS to the environment and living organisms, robust and reliable analytical methodologies are required. This study targeted eight legacy PFASs for analysis in soil, water, and plant samples. A modified QuEChERS (quick, easy, cheap, effective, rugged, and safe) was developed for the extraction of PFASs from solid samples, while solid-phase extraction (SPE) was applied for liquid samples. Following sample extraction, liquid chromatography quadrupole time-of-flight mass spectrometry (LC-QTOF/MS) was used for compound identification and quantification. Recoveries of the eight target PFASs across different matrices ranged from 72% to 125%, with the relative standard deviations below 20% (n=3). Following method validation, the established extraction procedures coupled with LC-QTOF/MS were applied to kale samples and their growing media. In hydroponic experiments, PFAS concentrations ranged from 27.58 to 1409.17 ng g^{-1} in

roots and from 15.21 to 267.87 ng g^{-1} in shoots. In pot experiments, on the other hand, PFAS concentrations ranged from 80.79 to 440.45 ng g^{-1} in roots and from 6.19 to 7407.09 ng g^{-1} in shoots. Among the PFASs taken up by kales, long-chain PFASs predominantly accumulated in the roots, whereas short-chain PFASs were more easily transported to and accumulated in shoots. These results demonstrate that the established methods are suitable for quantitative analysis of PFASs in environmental and plant samples and provide a scientific basis for research on plant uptake behavior and food safety risk assessment.

2.02.P–Tu068 Adsorption–Desorption Dynamics of Per- and Polyfluoroalkyl Substances (PFAS) in Plastic-Modified Cementitious Mortar and Corresponding Environmental Implications

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PFAS are persistent contaminants of growing environmental concern, and their interactions with porous construction materials may influence PFAS retention, transport, and release in built and aquatic environments, which remains poorly understood. This study examined the adsorption-desorption dynamics of 16 PFAS of different chain lengths and acid end groups in cement mortars containing microplastic aggregates (MPA) to determine how the cement matrix alters the potential for environmental adsorption and release of PFAS.

Mortar bars (MB) incorporating 50 volume% recycled polyethylene terephthalate (rPET) and high-density polyethylene (rHDPE) aggregates to replace sand were subjected to batch adsorption experiments at room temperature by immersing in a PFAS-fortified aqueous solution.

PFAS adsorption by MB containing MPA was enhanced for long-chain PFAS by up to 7.5 pg/g after 28 days, whereas differences in adsorption of short- and medium-chain PFAS were negligible. Total PFAS sorption capacity followed the trend MB < MB+rPET < MB+rHDPE, indicating that rHDPE provided a stronger nonpolar partitioning phase and potentially more stable retention sites within the cement pore network. Coupled hydrophobic interactions, pore entrapment, and increased contact area within the cementitious matrix governed PFAS adsorption, while inclusion of MPA modified these processes by increasing hydrophobic domains and pore connectivity.

Desorption assays at neutral (7.0) and acidic (3.0) pH showed partial PFAS release across all chain lengths, with notably higher leaching of short-chain PFAS; for example, PFBA reached 90.5 pg/g in both spiked and unexposed MB specimens. Enhanced release of PFBA from unexposed samples inferred that cement and MPA had an intrinsic PFAS reservoir. In contrast, MB containing MPA exhibited reduced susceptibility to leaching of short-chain PFAS, implying enhanced MPA retention, while the desorption behaviour of longer-chain PFAS remained largely unchanged. Furthermore, variation in media pH had no measurable effect on PFAS release.

These findings show that MPA-modified cement materials could act as both sinks and sources for PFAS and thus could impact the environmental performance of recycled MPA used in construction products, particularly in applications exposed to water infiltration. This work provides basic details necessary for improving risk assessment frameworks and guiding the sustainable design of next-generation construction materials.

2.02.P–Tu069 Restored saltmarshes as natural filters for Per- and Poly- fluoroalkyl substances (PFAS)

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Saltmarshes are critical coastal ecosystems that act as natural filters, trapping contaminants and reducing their transfer to adjacent marine environments. However, when degraded, these systems lose much of their capacity to retain pollutants. While restoration has been shown to enhance carbon sequestration, it remains unclear whether it also restores the capacity of saltmarshes to retain per- and polyfluoroalkyl substances (PFAS).
Our aim is to quantify PFAS concentrations in saltmarsh sediments and evaluate whether restoration condition, method, and age, influence contaminant retention. We collected 93 soil samples from 31 sites along the coastline of Victoria, Australia, spanning natural, degraded, and restored saltmarshes. Restored sites include two passive restoration methods, livestock exclusion (fencing) and tidal reinstatement through levee removal, and represent a gradient of restoration ages (0->50years). We sent the soil samples to ALS laboratory for identification and quantification of 30 PFAS analytes. We will assess differences among site conditions and restoration strategies using a space-for-time framework.
We hypothesize that restored saltmarshes will show increased PFAS retention compared to degraded systems, with retention capacity approaching that of natural reference sites over time, driven by increases in sediment organic matter that enhance PFAS sorption. Differences between restoration methods are also expected, with tidally restored sites likely showing higher trapping capacity than fenced sites due to greater sediment deposition and organic matter accumulation under increased tidal exchange. In addition, spatial variability in PFAS concentrations is expected across the Victorian coastline, reflecting differences in proximity to potential contamination sources, such as airports and areas with high use of firefighting foams.
This study will generate a regional-scale dataset of PFAS in saltmarsh soils in Victoria and provide novel insights into the role of restored coastal wetlands as contaminant sinks. By linking restoration to pollutant retention, this work positions coastal wetland restoration as a scalable, nature-based solution for managing PFAS contamination and informs chemical risk mitigation strategies globally.

2.02.P–Tu070 Assessment of Per- and Polyfluoroalkyl Substances (PFASs) in Japanese market Basket Study using Enhanced Matrix Removal (EMR) Cleanup

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Human exposure to per- and polyfluoroalkyl substances (PFASs) is a global concern due to their persistence and potential adverse health effects. Although diet is a major exposure pathway, comprehensive data on the occurrence across diverse food groups in Japan remain limited. This study addressed this gap by analysing 44 PFASs compounds across seventeen food groups categorised according to the 2023 Japanese National Health and Nutrition Survey. The complexity of food matrices poses a significant challenge for PFASs analysis, often leading to matrix interference and reduced sensitivity at trace levels. A Quick, Easy, Cheap, Effective, Rugged, and Safe (QuEChERS) based extraction method was optimised, and two cleanup approaches were evaluated: dispersive solid-phase extraction (dSPE) and Agilent Captiva Enhanced Matrix Removal (EMR) cartridges. The dSPE approach yielded a poor recovery rate (3.7-27.3%) across representative plant-based matrices, likely due to non-selective sorption and co-extraction interference. In contrast, EMR cleanup significantly improved recoveries (51.9-120.6%) and was subsequently applied to all food matrices using cartridge types to reduce the matrix interference. Among the analysed samples, Japanese horse mackerel exhibited the highest PFAS concentrations, including perfluorobutanoic acid (PFBA, 2,500 ng/kg wet weight (ww)),

perfluoroundecanoic acid (PFUnDA, 1,300 ng/kg ww), and perfluorooctane sulfonic acid (PFOS, 1,100 ng/kg ww). Short-chain perfluoroalkyl carboxylic acids (C4-C7) were generally more prevalent than sulfonic acids, whereas 6:2/8:2 diPAPs reached up to 5,000 ng/kg. The estimated total daily intake for a 50 kg individual was approximately 1,000 ng/day, based on the tolerable daily intake (TDI) values from the Food Safety Commission of Japan for PFOS and perfluorooctanoic acid (PFOA). Green tea was identified as a major contributor, primarily due to perfluorohexanoic acid (PFHxA) and perfluoropentanoic acid (PFPeA). Regional analysis in Okinawa revealed elevated PFPeA levels in sweet potato and lime juice, contributing up to 370 ng/day. These findings enhance the understanding of dietary PFASs exposure in Japan and highlight the need for targeted monitoring of staple and regional foods. EMR-based cleanup enables the reliable quantification of diverse PFASs in complex matrices, supporting future risk assessments and regulatory efforts.

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2.02.P–Tu071 Analysis of per- and polyfluoroalkyl substances in food contact materials

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Per- and polyfluoroalkyl substances (PFAS) are chemically stable organofluorine compounds characterized by their environmental persistence and potential for human exposure, leading to international regulatory restrictions. PFAS have been detected in food contact materials (FCMs) with water- and oil-repellent, and humans may be exposed to them through food consumption. However, information on PFAS occurrence in such products in Japan remains limited. This study aimed to comprehensively investigate PFAS concentrations in commercially available FCMs and cookware in Japan and to clarify how material composition and manufacturer affect PFAS profiles. Perfluoroalkyl carboxylic acids (PFCAs) were widely detected across the analyzed samples, with concentrations varying substantially by product type and manufacturer. The highest PFCA concentrations were observed in a paper lunch box made from bagasse pulp, indicating a strong influence of material composition. The total PFCA concentrations ranged from 0.38 to 46.2 μg kg−1. Perfluorooctanoic acid (PFOA) exhibited the highest concentration (26.4 μg kg−1) in a polytetrafluoroethylene-coated baking sheet. The detection of regulated PFAS, such as PFOA suggests possible unintentional contamination during manufacturing processes. As concentrations varied among products, manufacturing processes are considered to have a significant influence. Overall, PFAS contamination levels in this study were generally lower than those reported in previous investigations. These results demonstrate the widespread occurrence of PFCAs in commercially available FCMs and cookware and highlight material composition and manufacturing processes as key factors influencing PFAS profiles. This study provides important baseline data for assessing potential human exposure via food. Future work will expand the range of products and evaluate the migration of PFAS from FCMs into food to better understand exposure risks.

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2.02.P–Tu072 Concentration and Distribution of Per- and Polyfluoroalkyl Substances (PFAS) in a Tributary Stream (Jungnang Stream, South Korea)

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The concentrations and spatial distributions of 29 per- and polyfluoroalkyl substances (PFAS) in surface

water, sediment and the wastewater treatment effluent nearby Jungnang Stream (a tributary stream of the Han River in Seoul, South Korea) were investigated monthly from May to November 2025 using LC–MS/MS. The mean concentration of Σ29 PFAS was 69.75 ± 11.42 ng/L in surface water, 0.70 ± 0.40 ng/g (dw) in sediment. The mean concentration of Σ29 PFAS in the wastewater treatment effluent (49.05 ± 5.98 ng/L) were lower than those in adjacent surface waters, suggesting that WWTP discharge was not the primary point source of PFAS in the study area. This result highlights the limited contribution of WWTP effluent as a primary point source and emphasizes the importance of non-point sources in the Jungnang Stream watershed. Short-chain PFAS were dominant in water samples, whereas long-chain PFAS prevailed in sediments. Field-derived sediment-water distribution coefficients (log Kd) were calculated based on the measured concentrations. A linear increase in log Kd was observed with the number of carbon-fluorine (C-F) bonds, suggesting stronger sorption and higher environmental persistence of long-chain PFAS. This study provides insights into the multimedia distribution and environmental behavior of PFAS in an urban water system and offers a scientific basis for future environmental risk assessments and source management strategies.

2.02.P–Tu073 Occurrence and Characteristic Distribution patterns of Per- and Polyfluoroalkyl Substances in Road Dust from Southern Korea

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Per-and polyfluoroalkyl substances (PFAS) are a group of synthetic chemicals that have been widely used in manufacturing and consumer products since the 1940s. Due to their strong persistence and resistance to conventional environmental degradation processes, PFAS have become widespread environmental contaminants. In the environments, road dust serves as a major reservoir and transport vector for these chemicals, however its role in regional pollution characterization remains underexplored, particularly for ultrashort-chain compounds. In this study, we investigated the occurrence and distribution patterns of 51 PFAS, including ultrashort-chain PFAS, in road dust from 50 sites across industrial, urban and rural areas in southern Korea, with a particular emphasis on analyzing spatial distribution patterns across different land use categories. Samples were collected by sweeping various road surfaces and were extracted using USE (Ultrasonic Extraction), followed by a cleanup process using Envi-Carb and Oasis WAX cartridges. The final extracts were then analyzed via LC-MS/MS.
Out of 51 target compounds, 24 PFAS were detected. Total PFAS concentrations ranged from 0.84-93.9 ng/g, and PFAS levels in rural areas were significantly lower than those in urban and industrial areas (p < 0.0001). Trifluoroacetic acid (TFA), an ultrashort-chain PFAS, was detected in all samples and accounted for 27.5%–98.2% (median: 88.7%) of the total PFAS concentration, confirming its role as a ubiquitous background pollutant in the road dust network. Industrial complexes exhibited significantly higher PFOS levels (mean: 1.33 ng/g) compared to urban and rural area (p < 0.001), and PFMPA was detected in all industrial areas, reflecting the impact of localized industrial emission sources.
This study is among the first to characterize ultrashort-chain PFAS in Korean road dust and to link their compositional fingerprints to regional industrial structures and land use. The contrasting spatial behaviors of highly mobile ultrashort-chain PFAS and immobile long-chain PFAS provide a useful framework for using road dust as an integrated indicator of regional pollution characteristics.

2.02.P–Tu076 The role of GATA3 mediated IGF1 transcriptional inhibition in fetal liver developmental toxicity induced by 6PPDQ exposure during pregnancy

As a typical derivative of tire wear particles, N - (1,3-dimethylbutyl) - N '- phenyl-phenylenediamine quinone (6PPD-Q) has been frequently detected in road runoff, urban sewage, and atmospheric particulate matter in recent years. Although there have been reports suggesting its acute and chronic biological

toxicity, its effects on mammals, especially on maternal and fetal development during pregnancy, are still in the early stages of research. This study systematically revealed the molecular mechanism of 6PPD-Q-induced hepatic developmental toxicity in fetal mice by establishing a prenatal mouse exposure model. Research has found that exposure to 6PPD-Q during pregnancy can significantly cause pathological damage to the fetal liver, abnormal functional indicators, and inhibition of liver cell proliferation. In depth exploration at the mechanistic level indicates that 6PPD-Q can directly target the transcription factor GATA3, inhibit the transcriptional expression of the key growth factor insulin-like growth factor 1 (IGF1), thereby blocking the activation of the AKT signaling pathway and ultimately mediating fetal liver developmental toxicity. This study elucidates for the first time the core role of the regulatory axis "6PPD-Q-GATA3-IGF1-AKT" in fetal liver injury, providing a key theoretical basis for scientifically evaluating the health risks of tire derived pollutants, especially their potential harm to pregnancy and offspring development.

2.02.P–Tu077 Modeling the Behavior and Environmental Fate of Ionizable Pollutants: Sorption Dynamics under Variable Soil Chemistry

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A wide range of emerging environmental contaminants, including pesticides and industrial compounds, occur predominantly as charged species under environmental conditions. Among these, per- and polyfluoroalkyl substances (PFAS) represent a persistent and toxic subclass. Due to their widespread industrial use and environmental mobility, PFAS are now detected in soils, biota, and human biomonitoring studies. PFAS reach soils via emissions, biosolid application, and atmospheric deposition, accumulating especially near hotspots such as fire training zones and fluorochemical production sites.
The environmental fate of ionizable organic contaminants is complex. Unlike neutral compounds, whose soil sorption is often predicted using Koc and foc, the sorption of charged species like PFAS is influenced by pH, ionic strength, soil mineral composition, and competing ions such as phosphate. For example, ferrihydrite provides positively charged sorption sites for anionic PFAS, while phosphate competes for the same sites. Sorption is also affected by compound specific traits such as chain length and the fact that some PFAS are zwitterionic.
To accurately describe these processes, the SOILPROM project integrates ion exchange and speciation modules from ORCHESTRA, a tool for simulating chemical speciation and reactive transport processes, into the soil transport model PEARL. A key step is generating high quality sorption data using controlled soil column experiments.
A set of environmentally relevant ionizable PFAS will be examined using HPLC based column experiments. Columns will be packed with inert silicon carbide mixed with defined sorbents: organic matter (micronized peat), clay mineral (illite), and metal oxide (ferrihydrite). A SiC only column acts as a background control. Mobile phases will consist of dilute salt solutions covering a range of pH and ionic strengths, with or without the presence of phosphate. Low and constant flow rates ensure near equilibrium conditions, and retention times will be quantified via MS detection. Sorption coefficients will be calculated from elution data and normalized to dry sorbent mass.
These experiments will quantify how PFAS sorption is influenced by substrate type, ionic composition, and compound properties. The results will validate and parameterize mechanistic sorption models in ORCHESTRA and produce enhanced PFAS fate predictions in soils using PEARL.

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2.02.P–Tu078 Calculating Physico-Chemical Parameters of PFAS molecules using COSMOtherm: Distributions of pKa Values and Cell Membrane Binding Affinities

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The human and environmental concern for worldwide PFAS contamination requires accurate understanding of chemical fate assessment. Unfortunately, deriving accurate and meaningful physico-chemical parameters of PFAS chemicals presents several challenges. Firstly, the most abundantly studies PFAS chemicals are strongly ionizable acids in nature, and predominantly are present in their anionic form. This anionic form behaves very differently from the way chemical fate models are constructed in global risk assessment models. Whereas for neutral chemicals the octanol-water partition ratio (logP) is an adequate descriptor of the hydrophobic characteristic of micropollutants, and well predicts sorption to soil, sediment and tissue, this has been demonstrated to be an unreliable descriptor for anionic PFAS. Most experimental assays for logP are not designed to be applied with surface active agents such as PFAS anions, and most predictive computational tools have not been calibrated for such heavily fluorinated ionizable chemicals. A challenge for common PFAS chemicals such as PFOS and PFOA, is that the pKa cant be measured experimentally because it is well below pH 1.
This study set out to evaluate the software package COSMOtherm, which is able to perform molecular calculations with 3-dimensional conformers using high resolution of the atomistic distribution of surface charges. As a result, it can approximate the behaviour of both neutral and anionic forms in solvents, and thereby calculate distribution coefficients between environmental compartments and also pKa values. Furthermore, COSMOtherm can be used to directly calculate the binding affinity for phospholipid cell membranes for both the neutral and ionic form of PFAS molecules, circumventing the unreliable logP values to be used for chemical fate and toxicity assessment. The optimized conformer structures were created to be run with COSMOtherm calculation for set of 100 commonly studied PFAS structures, covering at least 13 different PFAS types. For each PFAS molecule, 50 different initiation runs were performed, to cover the conformer variability and evaluate the overall calculated phys-chem parameter distribution. The pKa values had a distribution of sometimes 2 pH units, indicating the importance of addressing the correct 3D-conformation structures. The cell-membrane binding coefficients were for a large set of PFAS compared to experimental data and to confirmed the accuracy of this computational approach.

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2.02.P–Tu079 Land Use and Soil Depth Govern Multi-Class Emerging Contaminant Signatures in Tropical Urban Soils

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Urban soils are increasingly recognized as reservoirs and potential secondary sources of emerging contaminants, yet depth-resolved information on multi-class contaminant mixtures remains limited. This study investigated the occurrence and vertical distribution of 48 per- and polyfluoroalkyl substances (PFAS), 3 quaternary ammonium compounds (QACs), bisphenol A (BPA), benzophenone-3 (BP-3), and N,N-diethyl-meta-toluamide (DEET) in soil profiles collected from 16 sites across agricultural soils, golf courses, urban parks, and forests in Singapore. Four depth intervals down to 40 cm were analyzed using solvent extraction coupled with LC–MS/MS.
PFAS concentrations showed clear land-use dependence, with mean levels of 66.14, 62.24, 52.48, and 22.19 ng/mL in urban parks, agricultural soils, golf courses, and forests, respectively. Elevated levels in urban parks likely reflected mixed urban inputs, including atmospheric deposition and stormwater runoff, while agricultural and golf course soils were influenced by irrigation water, fertilizers, agrochemicals and

turfgrass management. Forest soils showed the lowest PFAS concentrations, consistent with limited direct anthropogenic activity. Short-chain PFCAs, showed high detection frequencies across all land-use types, reflecting their high mobility, persistence, and widespread sources. Vertical profiles indicated greater PFAS migration in agricultural soils and golf courses, particularly for short-chain PFCAs detected at 30–40 cm, likely driven by irrigation-enhanced downward transport. In contrast, forest and urban park soils showed more limited vertical migration, with PFAS mainly retained in upper soil layers. Correlation analysis suggested common sources or similar behavior for legacy PFAS, whereas emerging PFAS showed more distinct source patterns.
Beyond PFAS, QACs, BPA, BP-3, and DEET were generally enriched in surface soils, indicating recent anthropogenic inputs and strong near-surface retention. Multivariate analysis differentiated contaminant profiles according to both land use and soil depth, highlighting the combined influence of urban land management, contaminant sources, and physicochemical properties on soil contamination patterns. Overall, this study demonstrates that tropical urban soils function as stratified archives of both persistent and usage-linked emerging contaminants, with implications for contaminant retention, leaching potential, and diffuse transport to the urban water cycle.

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2.02.P–Tu080 Monitoring Psychoactive Pharmaceutical Use in Japan During and After the COVID-19 Pandemic (2020-2023) Using Wastewater-Based Surveillance

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Psychoactive pharmaceutical use has increased globally, with additional shifts observed during the COVID-19 pandemic. In Japan, population-level consumption data remain scarce, hampered by cultural stigma and limited access to conventional data sources. Wastewater-based surveillance (WBS) is an objective approach for monitoring community-level pharmaceutical use but its use in Japan remains underexplored.
This study assessed the use of 11 psychoactive pharmaceuticals in Japan by analysing wastewater from two wastewater treatment plants (WWTPs). Influent samples from WWTP1, located in a town on Honshu Island (approximately 120,000 people), were collected biweekly from October 2020 to March 2023. Samples from WWTP2 in the Kanto region (about 1.8 million people) were collected daily during the 2-week lockdown and 2-week post-lockdown periods in 2021. Target compounds included selective serotonin reuptake inhibitors (SSRIs), serotonin-norepinephrine reuptake inhibitors, tricyclic antidepressants (TCAs), and other psychoactive agents, quantified using liquid chromatography-tandem mass spectrometry.
Ten of 14 biomarkers were detected at high frequency (≥97%). Venlafaxine metabolite, O-desmethylvenlafaxine showed the highest concentrations (16.6-226.8 ng/L), while nortriptyline metabolite, 10-hydroxynortriptyline (7.3-87.9 ng/L) was highest among TCAs. Among SSRIs, citalopram and sertraline were predominant whereas varenicline showed the lowest overall levels (mean <1 ng/L). There are notable differences between the two sites for several compounds. Sertraline was the most prominent in WWTP2 (80.8 mg/day/1000 people), significantly higher than at WWTP1 (7.3 mg/day/1000 people), suggesting catchment-level demographic or prescribing differences. Our analysis shows that COVID-19 restrictions had a minor influence on psychoactive pharmaceutical use patterns. Only

methylphenidate showed a significant difference between lockdown and post-lockdown periods (p = 0.001). Varenicline consumption varied significantly across years (p < 0.001), whereas other psychoactive pharmaceuticals showed no statistically significant temporal changes.
This study is the first WBS assessment of psychoactive pharmaceutical use in Japan, complementing traditional methods and advancing the utility of wastewater surveillance for monitoring mental health-related medication usage at the community level.

Disclaimer/Disclosure: The authors declare no conflicts of interest.

2.02.P–Tu081 Complementary DNA probe-guided truncation of aptamer for analytical performance enhancement in aptasensor for Nonlyphenol

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Endocrine disrupting chemicals (EDCs) are natural or man-made chemicals that may mimic or interfere with the body’s hormones, known as the endocrine system. Alkylphenols are frequently found in aquatic ecosystems, and they are known for their endocrine disrupting properties, which could have negative effects on humans even at low concentrations. Their ability to exert effects at very low concentrations makes their detection in environmental samples particularly important, indicating the need for further research. Alkylphenols contain nine subtypes, such as octylphenols (OPs) and nonylphenols (NPs), which are defined according to the number of carbon atoms in the alkyl chain. NPs exhibit estrogenic activity and are known to accumulate in aquatic organisms. NPs used in manufacturing are mixtures containing mostly NP. NP is widely used in the production of surfactants for consumer products, including detergents and cleaners. Aptamer-based biosensors, also known as aptasensors, are effective for detecting pollutants that are difficult to detect using conventional analytical methods, particularly those present in trace amounts in water. An aptamer is an artificially synthesized oligonucleotide sequence that can bind selectively to a target molecule. In this study, an aptasensor for NP detection was developed. A DNA probe and 7-Aminoactinomycin D (7-AAD) fluorophore were used to increase the resolution of the aptamer analysis. Five aptamers and three probes were first combined in pairs, respectively, and the fluorescence signal response of each complex was observed to determine the optimal pair for NP detection. As the concentration of NP increased, the fluorescence signal of the aptamer–probe complex increased accordingly. The selected aptamer–probe complex is expected to significantly enhance the fluorescence response toward NP, resulting in improved sensitivity and detection performance. This study may provide an effective sensing platform for rapid environmental monitoring of alkylphenols and broaden the application of aptasensor-based analysis for trace endocrine disruptors.

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2.02.P–Tu082 Nitrous Acid, Nitric Acid, Nicotine, Tobacco-Specific Nitrosamine, and Aldehyde Emissions from Heated Tobacco Products and Their Associated Health Risks

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Heated tobacco products (HTPs) have rapidly expanded in the tobacco market and are often promoted as reduced-risk alternatives to conventional cigarettes because they heat rather than combust tobacco. However, emissions of reactive nitrogen species and their potential health risks remain poorly

characterized. Here we quantified nicotine, tobacco-specific nitrosamines (TSNAs), aldehydes, nitric acid, and nitrous acid in mainstream aerosols from four commercially available HTP devices and conventional cigarettes, with aerosol collections performed in triplicate (n = 3) using the Health Canada Intense smoking regimen. Target compounds were analyzed by LC-MS/MS, HPLC, and ion chromatography. nitric acid concentrations in HTP aerosols ranged from 0.0296–153 μg/stick, and nitrous acid ranged from 0.00113–25.6 μg/stick, which were comparable to concentrations in cigarette smoke (0.663–715 μg/stick for nitric acid; 0.201–4.89 μg/stick for nitrous acid). Several aldehydes were not reduced in HTP aerosols; for example, acetaldehyde (0.0585–29.4 μg/stick) and acrolein (0.0400–10.2 μg/stick) were comparable to or higher than those in cigarettes. In contrast, nicotine (3.86–1,210 μg/stick) and TSNAs (0.0100–112 ng/stick) were substantially lower than those in cigarette smoke. Health risk assessment indicated elevated non-carcinogenic risks for aldehydes, with hazard quotient values reaching 2.2 for acetaldehyde and 4.7–230 for acrolein. The margin of exposure for nitrous acid ranged from 232–1,510, with some products below the reference value of 1,000. Carcinogenic risk estimates at the 90th percentile exposure exceeded the benchmark level of 1 × 10^6 for formaldehyde, acetaldehyde, NNN, and NNK, reaching up to 4.73 × 10^4. These results indicate that although HTPs reduce exposure to nicotine and TSNAs, emissions of aldehydes and nitrogen species may limit the overall reduction in health risks compared with conventional cigarettes.

2.02.P–Tu083 Development of a Sample Extraction Method for Target and Non-Target Screening of Contaminants of Emerging Concern in the Yamuna River

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The Contaminants of emerging concerns (CECs) present even at trace concentrations can pose a negative impact on both the ecosystem and human health, which necessitates the comprehensive environmental monitoring of CECs for their risk-based prioritization. The present study involves the development of an analytical method for Non-Target Screening (NTS) of CECs using Solid phase extraction (SPE) and Ultra-high performance liquid chromatography coupled with Quadrupole time-of-flight (UHPLC/QToF). The SPE method was optimized for different eluting solvents and cartridges (Bond Elut PPL and Bond Elut Plexa) across diverse sample matrices, such as river water, sewage treatment plant sample, and urine, validated with CECs standard, and isotopes identified that Bond Elut PPL cartridge performed better with isotopes recoveries ranging from 76 % to 91%. The developed method was applied to screen the emerging contaminants along a 22 km stretch of the River Yamuna in New Delhi, India. Sampling also included major drains discharging effluents from inefficient treatment plants, which significantly contribute to the pollution load. This comprehensive screening successfully detected various contaminant classes, including pharmaceutical (antibiotics, analgesics, lipid regulators etc), personal care products (UV filters, antimicrobials, parabens etc.) (PPCPs), pesticides (herbicides, fungicides, insecticides etc.), Per- and polyfluoroalkyl substances (PFAS) and industrial chemicals. Compound confirmation was achieved by analyzing adduct species and fragment ions with mass accuracy thresholds of ±10 ppm and ±30 ppm, respectively. A minimum of three fragments was matched against spectral libraries, including Agilent PCDL and AMOS (Analytical Methods & Open Spectra). These compounds were confirmed at concentrations extending down to the nanogram per liter (ng/L) level. This study will be beneficial to regulatory bodies in assessing risk and implementing guidelines and policies to curb the discharge of CECs into the River Yamuna.

2.02.P–Tu052 Electrochemical Detection of PFOA and PFOS Using a Biochar-Enhanced Cu-BTC Composite in Aqueous Media

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Per- and polyfluoroalkyl substances (PFAS), particularly perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS), are persistent organic pollutants that pose significant risks to aquatic environments and human health. However, current PFOA and PFOS monitoring largely relies on instrument-intensive methods, limiting rapid and on-site detection. Although electrochemical sensors offer a promising alternative for their monitoring, metal–organic frameworks (MOFs), despite their high surface area and strong affinity for organic contaminants, suffer from intrinsically low electrical conductivity, which limits their electrochemical sensing performance. To address this limitation, a composite electrochemical sensing platform was developed by integrating copper-based MOFs (Cu-BTC) with highly conductive biochar (BC) derived from waste tree branches. The Cu-BTC@BC composite was synthesized and modified onto a glassy carbon electrode, followed by structural and electrochemical characterization. The results confirmed the successful incorporation of Cu-BTC onto the biochar matrix, leading to enhanced surface characteristics and improved charge transport properties. Electrochemical measurements showed that the Cu-BTC@BC-modified electrode exhibited higher peak currents and reduced charge transfer resistance compared to pristine Cu-BTC or BC. In the presence of PFOA and PFOS, the sensor demonstrated a concentration-dependent electrochemical response in the nanomolar range, indicating improved electrochemical performance arising from the composite structure. By utilizing waste-derived materials, this low-cost sensing platform provides a practical approach for rapid, on-site screening of PFOA and PFOS in high-risk environmental matrices, such as industrial effluents and landfill leachates.

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2.02.P–Tu055 Simultaneous Determination of Atmospheric PFAS and Assessment of Indoor Air Pollution Based on Emission Behavior from Textile Products

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Per- and polyfluoroalkyl substances (PFAS) have been widely used in industrial applications because of their excellent performance such as water and oil repellency. However, certain PFAS have attracted attention due to their persistence, high accumulation, and toxicity. In particular, regulations regarding long-chain PFAS have been increasingly strengthened worldwide. Long-chain perfluorocarboxylic acids (LC-PFCA) were listed as Persistent Organic Pollutants (POPs) in 2025. Consequently, the use of alternative PFAS, including precursor PFAS and short-chain PFAS such as fluorotelomer alcohols (FTOHs), has increased. These compounds are commonly used in textile products for stain-resistant and water-repellent treatments. Previous studies have reported that the precursor and short-chain PFAS in textile products are emitted into the atmosphere and introduced to the body via inhalation. The concentrations of PFAS in indoor air are expected to be higher than those in outdoor air because the textile products containing precursor and short-chain PFAS are widely present in indoor environments. However, previous studies on PFAS have primarily focused on water and soil environments. Quantitative assessments of PFAS in the atmosphere remain limited, and insufficient information is available regarding the emission behavior of PFAS from textile products. The objectives of this study were to develop an analytical method for PFAS in the atmosphere, to quantitatively evaluate the emission behavior of PFAS from textile products, which are considered one of the primary sources of PFAS in indoor environments, and to investigate the indoor air pollution associated with PFAS in the textile

products. A highly sensitive and comprehensive analytical method for over 100 PFAS in the atmosphere was developed and applied to determine the PFAS concentrations in indoor air. The emission behavior of PFAS from textile products was evaluated by calculating emission rates using microchambers. The influence of textile products on PFAS concentrations in indoor air was assessed by integrating the measured emission rates with PFAS concentrations in indoor air. The analytical method for atmospheric PFAS developed in this study can be applied to other atmospheric environments (e.g., outdoor air and waste gas) and is expected to contribute to a comprehensive understanding of atmospheric PFAS pollution.

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2.02.P–Tu056 Development of a High-Temperature Combustion LC-IRMS Method for Carbon Isotope Analysis of Halogenated Organic Compounds

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Halogenated organic compounds, including disinfection by-products and per- and polyfluoroalkyl substances (PFAS), are of increasing environmental concern due to their persistence, mobility, and potential adverse effects. Compound-specific isotope analysis (CSIA) is a powerful tool for elucidating sources and transformation processes; however, accurate carbon isotope ratio (δ13C) measurements of difficult to decompose halogenated compounds remain challenging using conventional liquid chromatography–isotope ratio mass spectrometry (LC-IRMS).

In this study, we developed a high-temperature and high-pressure combustion interface for LC-IRMS to improve oxidation efficiency and enable reliable δ13C measurements of halogenated organic compounds. The system operates under high temperatures (200–600°C) and high-pressure conditions, promoting efficient conversion of organic carbon to CO2 without relying on highly concentrated oxidants.

The method was evaluated using 19 samples of 15 halogenated compounds, including chlorinated, brominated, and fluorinated species, and the obtained δ13C values were compared with those measured by elemental analyzer (EA)-IRMS. For chlorine- and bromine-based compounds, Δδ13C values (δ13C, LC-IRMS − δ13C, EA-IRMS) were within ±1‰ with recovery rates of 90–110%, indicating quantitative oxidation and high analytical accuracy. In addition, consistent results were obtained across different compounds, demonstrating good reproducibility of the method. In contrast, fluorinated compounds showed large isotope fractionation (−17 to 75‰) and low recovery (25–40%), indicating incomplete oxidation associated with strong C–F bonds.

These results demonstrate that the developed LC-IRMS method enables precise and accurate δ13C analysis of a wide range of halogenated organic compounds, particularly chlorinated and brominated species that are relevant environmental contaminants. This method expands the applicability of CSIA to water-soluble and non-volatile compounds and provides a valuable tool for source apportionment and environmental fate analysis. Furthermore, the observed limitations for fluorinated compounds highlight the need for further methodological improvements and provide insight into their environmental persistence and stability.

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2.02.P–Tu059 Advantage of fluorine free materials for measurement of PFAS Total

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"PFAS Total" is modern approach to understand inventories as groups with specific chemical structures, rather than individual analysis of PFAS, has advanced rapidly over the past 15 years and is part of the proposed ECHA regulations in 2023.
In fact, this idea is a derivative of the mass balance analysis technology invented by Japan in 2006. Mass balance analysis, which was developed as a research method for a comprehensive understanding of a wide variety of PFAS, has enabled scientific research and technological development based on the contribution ratio of individual PFAS to all fluorine compounds as the basis for understanding the phenomenon by combining the two approaches of bulk to specific and specific to bulk. This idea is not only used in PFAS, but also to prove the hypothesis of the natural generation of dioxins (Horii et al., 2008). However, the ultra-trace fluorine analysis technology is required to enable total PFAS measurement and mass balance analysis. This is difficult to spread in Europe and the United States, due to the low PFAS limit value (4 to 10 ng/L) in water samples, however in Japan, the environmental regulation value is 50 ng/L. Therefore, if the total PFAS measurement sensitivity required for mass balance analysis is 50 ng/L, the sensitivity required for fluorine measurement is about 34 ng/L. This is a sensitivity that can be sufficiently measured by commercially available Combustion Ion Chromatography.
In this report, we evaluated several materials for PFAS analysis, including PTFE, PEEK, activated charcoals and ion exchange adsorbents, their content of fluorine.
Tentative results of thirteen activated materials were reported recently, (Yamashita et al., 2024) and possible application for measuring adsorbable organically bound fluorine (AOF) by using ISO 18127 and USEPA Method 1621 were discussed. Above materials were applied to AQF2000H (Nittoseiko Analytech Co., Ltd) and
Metrohm 930 Combustion Ion Chromatograph to investigate the fluorine content.
As a result, Metrohm 930 Combustion Ion Chromatograph shown the lowest blank of fluorine after customized by "CAR-PFAS verified (chrome-extension://oemmndcbldboiebfnladdacbdfmadadm/https://staff.aist.go.jp/nob.yamashita/image/carpfasv1.pdf)". LOD of this instrument is 0.05 µg/L and significantly lower than ISO 18127 and USEPA Method 1621, where their LOD were 2.0 µg/L and 1.7 µg/L, respectively.

2.02.P–Tu062 EOF-CIC as a Proxy for PFAS Total in Drinking Water: Challenges, Uncertainty, and Improved Evaluation

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Per- and polyfluoroalkyl substances (PFAS) are widely detected in drinking water due to their extensive historical use and environmental persistence. Recent regulatory developments, including the EU Drinking Water Directive, introduce a "PFAS Total" parameter; however, no standardized analytical method exists for its determination. This study evaluates extractable organofluorine measured by combustion ion chromatography (EOF-CIC) as a proxy for PFAS Total in drinking water.

A key challenge is the incomplete recovery of highly polar PFAS, particularly trifluoroacetic acid (TFA), during EOF extraction, alongside uncertainty in converting fluorine measurements to mass-based regulatory values. To address this, we assess method performance across drinking water samples from multiple regions and examine the impact of fluorine mass fraction assumptions on PFAS Total estimation. An alternative workflow is proposed that separates TFA from EOF-based quantification and applies a structured approach for interpreting exceedances.

Results show that EOF-CIC provides broad screening capability but may both underestimate PFAS due to poor recovery of ultra-short-chain compounds and overestimate values due to contributions from non-PFAS organofluorine or inorganic fluorinated species. The choice of conversion factor significantly influences compliance assessment, with PFOA selected as a guideline-consistent reference compound. The proposed workflow reduces ambiguity and avoids inconclusive outcomes associated with current guidance.

Overall, EOF-CIC is best suited as a screening and compliance-support tool rather than a definitive quantitative method. The study highlights critical limitations and provides a practical framework for improving PFAS Total assessment under current regulatory requirements, contributing to more reliable monitoring and risk evaluation of drinking water quality.

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2.02.P–Tu064 An Operational Screening Framework for Fingerprints and Precursor Burdens of Per- and Polyfluoroalkyl Substances (PFASs) in Aqueous Film-Forming Foam (AFFF)-Impacted Waters and Sediments

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Per- and polyfluoroalkyl substances (PFAS) from aqueous film-forming foams (AFFFs) can persist in waters and sediments near firefighting training areas and air force bases. These sites are difficult to assess because legacy foam residues, replacement chemicals, unknown precursors, dilution, and stream mixing can occur together. Monitoring only a small number of target PFAS may underestimate the contamination burden.

This study investigated PFAS contamination in surface waters and sediments at three AFFF-impacted sites in South Korea, including one firefighting training facility and two air force bases. The objective was to develop a practical screening framework that can identify contamination hotspots, distinguish AFFF-related chemical signatures, and evaluate hidden precursor contributions. Fifty target PFAS were quantified using liquid chromatography coupled with tandem mass spectrometry. Additional PFAS-related compounds were screened using ion mobility spectrometry coupled with high resolution mass spectrometry, and the total oxidizable precursor (TOP) assay was applied to surface waters to estimate unknown oxidizable precursors. The results were interpreted using screening indicators based on PFAS composition, upstream-to-downstream changes, streamflow effects, and precursor formation. Surface waters contained total PFAS concentrations up to 7,940 ng/L. Perfluorooctane sulfonate and perfluorohexane sulfonate were major compounds at highly impacted sites, reaching 2,133 and 1,580 ng/L per liter, respectively. Sediments were mainly affected by long-chain perfluoroalkyl sulfonates, especially perfluorooctane sulfonate, which reached 3,570 ng/kg(dw). Suspect screening identified eight PFAS classes, including sulfonamide-based compounds related to electrochemical fluorination and a fluorotelomer betaine. The TOP assay showed that unknown oxidizable precursors ranged from 182 to 4,972 picomolar and accounted for 14 to 51 percent of total PFAS on a molar basis. Our combined approach identified outfall-adjacent hotspots, distinguished legacy electrochemical fluorination and fluorotelomer-related AFFF signatures, and clarified locations where dilution or stream mixing affected interpretation. This operational screening framework provides a practical tool for prioritizing follow-up investigation, treatment planning, and sediment management at AFFF-impacted sites.

2.02.P–Tu074 Integrated Assessment and Risk Prioritization of Legacy and Emerging Per- and Polyfluoroalkyl Substances in the Geum River Using High-

Resolution Mass Spectrometry

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Per- and polyfluoroalkyl substances (PFAS) are widely used synthetic chemicals characterized by high chemical stability and amphiphilic properties, but their environmental persistence, bioaccumulation potential, toxicity, and long-range transport raise concerns for ecological and human health risks. In Korea, PFAS studies have mainly focused on major river systems, and integrated assessments of both regulated and emerging PFAS in the Geum River basin remain limited. In this study, we investigated 39 legacy and emerging PFAS in the Geum River using targeted, suspect, and non-target analyses combined with QSAR-based predictions and ToxPi and Risk Index (RI) evaluations to assess their occurrence, hazard potential, and risk-based prioritization in the aquatic environment. Among the 39 PFAS investigated, 12 compounds were detected, with total concentrations ranging from 7.20 to 86.2 ng/L, and the average PFAS concentration in tributaries was approximately 1.61 times higher than that in the mainstream. Notably, perfluorobutanesulfonic acid (PFBS) was identified as the dominant compound at tributary T4, where its mass loading accounted for approximately 71% of the PFBS load observed at the most downstream mainstream site (M7), indicating that tributary inputs substantially contributed to downstream PFAS contamination. Suspect and non-target analyses further revealed the presence of a hydrogen-substituted analogue of PFBS (H-PFBS). QSAR- and ToxPi-based hazard assessments showed that long-chain PFAS (carbon chain length ≥ 8) exhibited relatively high persistence, bioaccumulation potential, and toxicity, whereas 6:2 fluorotelomer sulfonate (6:2 FTS) and H-PFBS displayed comparatively lower predicted hazard levels. In contrast, RI-based evaluation indicated that several PFAS with moderate intrinsic toxicological properties were identified as high-priority substances due to elevated environmental concentrations, highlighting a discrepancy between structure-based hazard potential and concentration-driven prioritization in the aquatic environment. Overall, this study presents an integrated PFAS assessment framework that combines chemical occurrence, structure-based toxicity prediction, and exposure-based risk prioritization, providing fundamental scientific information for establishing management priorities and supporting risk-based regulatory decision-making for PFAS.

2.02.P–Tu075 Occurrence, Behavior, and Mass Loading of Legacy and Emerging PFAS in Inflowing Rivers and the Coastal Waters of Osaka Bay

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Per- and polyfluoroalkyl substances (PFAS) are widely used in industrial and commercial applications, and some are highly persistent and bioaccumulative in the environment. Following the regulation of perfluorooctanesulfonic acid (PFOS), perfluorohexanesulfonic acid (PFHxS), perfluorooctanoic acid (PFOA), and long-chain perfluorocarboxylic acids (PFCA, C9–C21) as persistent organic pollutants (POPs), the use of alternative and emerging PFAS has increased. However, information on their environmental occurrence and behavior remains limited. The northern to eastern coastal region of Osaka Bay is a densely populated metropolitan and industrial area containing major chemical, steel, and shipbuilding industries. Rivers and coastal waters in this region are strongly affected by municipal and industrial wastewater discharges. In addition, because Osaka Bay is a highly enclosed coastal sea with limited water exchange, PFAS entering the bay are likely to remain in the eastern inner bay area and accumulate in sediments. This study investigated the occurrence and distribution of PFCAs and perfluoroalkane sulfonic acids (PFSAs), their precursors, and emerging PFAS, in surface river water (n = 53), and surface seawater (n = 11), and multi-depth seawater samples (n = 7) collected from Osaka Bay in September 2025. PFAS mass loading into Osaka Bay was also estimated using river concentrations and flow rates. Water samples were extracted using Oasis WAX cartridges, and analyzed by LC-MS/MS.

Relatively high concentrations of PFHxA, 7H-perfluoroheptanoic acid (7H-PFHpA), and emerging ether-linked PFAS, including hexafluoropropylene oxide trimer acid (HFPO-TA) and perfluoro-2-methoxypropionic acid (PF2MPA) were found. PFHxA and HFPO-TA, which are used as PFOA alternatives in fluoropolymer manufacturing, showed the highest concentrations at a site in the Ai River located immediately downstream of a wastewater treatment plant effluent discharge point, and their concentrations gradually decreased downstream. These results suggest that effluent from a wastewater treatment plant receiving industrial wastewater is a major source of these PFAS. In Osaka Bay seawater, elevated PFAS concentrations were observed in the eastern inner bay area. In addition, density stratification during summer suppressed vertical mixing, resulting in the retention of PFAS in the surface layer. The highest mass flux was observed in the Yodo River, followed by the Samondo River downstream of the Ai River.

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2.03.P - Advances in Exposure Modelling: Towards a Safe and Sustainable Tomorrow for Both Humans and the Environment

2.03.P–Mo057 Overview of Exposure Assessment Models Used in Chemical Risk Assessment under Japan's CSCL (Chemical Substances Control Law)

Shino Kuwa[1], Tomoko Aoyagi[1], Jun Nakamura[1], Akihiro Tamatsukuri[1] and Yuki Sakuratani[1] (1)National Institute of Technology and Evaluation (NITE)

This poster introduces exposure assessment models used in the risk assessment framework under Japan's Chemical Substances Control Law (CSCL). The CSCL adopts a tiered, stepwise approach to chemical risk assessment, incorporating conservative assessment at the initial stage while enabling more refined assessment where potential risks are identified. Within this framework, multiple exposure models are employed, each tailored to emission source, specific environmental media and for estimating environmental concentrations. This poster provides an overview of representative exposure models used under the CSCL, highlighting their methodological features and current limitations.

2.03.P–Mo058 Tiered Methods for Chemical Exposure and Risk Assessment within the EAS-E Suite Platform

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Thousands of chemicals in commerce require evaluation for human and ecological health risk, yet measured exposure data are limited. Mechanistic, high-throughput models are increasingly used to address these data gaps, but their utility depends on flexibility, transparency, and the ability to integrate higher-tiered information. The Exposure And Safety Estimation (EAS-E) Suite provides an integrated modeling platform that combines environmental fate, bioaccumulation, exposure, and risk assessment within a unified framework. Within EAS-E Suite, the PROduction-To-EXposure High-Throughput (PROTEX-HT) model links chemical production, life-cycle emissions, multimedia environmental fate, and aggregate human and ecological exposures. This work presents recent advancements in PROTEX-HT

and its implementation within EAS-E Suite. Key enhancements include: (i) explicit treatment of population and household scaling, (ii) inclusion of multiple human receptors (adult male, adult female, child) to capture variability in physiology and behavior, (iii) refined modeling of dermal exposure through application frequency and duration, and (iv) incorporation of down-the-drain emission pathways linking indoor chemical use to wastewater treatment and subsequent environmental releases. Model performance was evaluated against human biomonitoring data and available environmental monitoring data, demonstrating consistency with previous model versions and comparable predictive capability. Importantly, the EAS-E Suite framework supports a tiered approach to exposure assessment. At lower tiers, models can be parameterized using just chemical structure, production volume, and functional use information. At higher tiers, users can incorporate chemical-specific data, including environmental monitoring data, to refine model inputs, and reduce uncertainty. The integration of mechanistic modeling with higher-tier monitoring data within EAS-E Suite provides a flexible platform for chemical assessment. These advancements support next-generation risk assessment by improving transparency, enabling data integration, and enhancing confidence in exposure predictions for regulatory and sustainability applications.

2.03.P–Mo059 Introducing the Updated OECD POV and LRTP Screening Tool: Application for Recently Regulated POPs and Implications for LRTP Assessments

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The OECD POV and LRTP Screening Tool (The Tool) is a consensus-based multimedia fate model, developed by a group of scientists about 20 years ago, to assess the long-range environmental transport potential (LRTP) and overall persistence (POV) of organic chemicals. The Tool (Version 2.2), released in 2008, has found widespread use in variable regulatory contexts, including the Stockholm Convention (SC) on Persistent Organic Pollutants (POPs) for which it has been applied for Screening (Annex D) and in the Risk profile (Annex E) for 15 POPs. Here, we introduce an updated version of The Tool (Version 3.0) which features an updated parameterization of wet deposition and allows for consideration of transfer and accumulation of chemicals in a remote region following combined transport by air and water. In addition to these scientific improvements, software updates include improved results exporting, easier interface navigation, and a revised technical instruction manual. To offer scientific guidance on use, we exemplify the utility of the model by applying it to 20 neutral POPs that have been regulated under the SC after the previous version of The Tool was released. The updated version of The Tool increases its benefit to the scientific community, chemical industries, and regulatory agencies that are interested in LRTP assessments of organic chemicals in the context of the SC and beyond.

2.03.P–Mo060 Application of a screening level multimedia activity model for evaluating the fate of persistent mobile organic chemicals

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In recent years there has been increasing interest to screen and prioritize chemicals used in commerce with respect to their potential to contaminate drinking water sources. The German Environment Agency (Umweltbundesamt – UBA), for instance, has proposed screening criteria to identify chemicals that may pose hazards to drinking water. The hazard criteria aim to prioritize chemicals that are persistent, mobile and toxic (PMT) or very persistent and very mobile (vPvM). The development and application of exposure assessment tools would thus support prioritization activities. This study summarizes the development of a multimedia environmental fate and transport model, which supports the exposure

assessment of persistent mobile organic chemicals (PMOCs) under a variety of scenarios, including under steady-state, equilibrium and non-steady-state and non-equilibrium conditions. The developed model includes multilayer soil and aquifer compartments (unsaturated and saturated), which is used to enable a screening level estimate of exposure to PMOCs.

2.03.P–Mo061 Scenario-Based Modeling of Environmental Distribution and Human Exposure Pathways for PFAS Using PROTEX-HT

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Recent regulatory developments and growing scientific interest have highlighted the need to better understand the environmental behavior and human exposure of fluorinated substances. Regulatory frameworks for PFAS, fluorinated gases (F-gases), and related compounds are also expanding, reflecting a broadening scope driven by fluorine. Given the large number and diversity of fluorinated compounds, efficient approaches for organizing and interpreting their exposure characteristics are increasingly important. In this study, we evaluated the environmental distribution of PFAS and compared model-predicted differences in human exposure across substances and pathways, using the PROTEX-HT model implemented in the EAS-E Suite under a consistent scenario. This approach enabled us to quantify exposure and group substances based on similarities in their exposure profiles, particularly with respect to dominant exposure pathways and relative pathway contributions. In addition, we applied chemical space mapping to interpret variations in partitioning behavior and to investigate their underlying causes. Our analysis revealed that soil partitioning plays a dominant role in determining overall exposure levels for many PFAS under the evaluated scenario. We also identified clear distinctions in environmental fate and exposure pathways between different classes of compounds. For example, fluorinated gases and acidic PFAS such as perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) exhibited fundamentally different environmental partitioning behaviors, leading to different dominant exposure pathways to humans. These findings demonstrate that classification based on exposure characteristics is a useful strategy for interpreting complex PFAS datasets and distinguishing substance-specific behaviors within a collective assessment framework. Our results highlight the importance of explicitly accounting for differences in environmental distribution and exposure pathways when evaluating PFAS and suggest that model-based classification can support more refined PFAS management strategies. While these results demonstrate the utility of exposure-based, model-informed classification, the present analysis is limited to a single use scenario, and further evaluation incorporating realistic use patterns and emission quantities is necessary to better reflect real-world conditions.

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2.03.P–Mo062 Challenges in Understanding the Environmental Partitioning of Chemicals in the Environment: Limitations of the KOC Approach

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Several studies have applied screening level assessment approaches to identify substances that could potentially be mobile in the environment. Due to the lack of suitable alternative metrics, these prioritisation exercises have generally been based on the organic carbon normalised partition coefficient (KOC), considering it the principal indicator of substance mobility in the environment. However, concerns have been raised about the appropriateness of the KOC concept to indicate the potential for

substances to be mobile in the environment. The partitioning and binding of substances to components of soils and sediments is an important aspect of their environmental fate and can determine both their mobility and bioavailability. However, tests using defined natural soils do give variable results due to the extremely diverse nature of soil characteristics in terms of their contents of organic carbon, clay, and iron and aluminium (oxy)hydroxides, as well as their cation exchange capacity and pH. There are three principal mechanisms that contribute to the overall retention of substances in soils and other sub-surface media. These are phase partitioning, cation binding, and anion binding. There are several components of soils and other subsurface media that can be involved in one or more of these mechanisms; for example soil organic matter is important in phase partitioning for hydrophobic and nonpolar substances, but can also be important for the binding of cations. The extremely high variability of the overall distribution coefficient KD between different soils limits its usefulness as an inherent measure of the environmental fate of a substance. It may be possible to define partition coefficients for interaction mechanisms, such as cation or anion exchange (e.g., producing KCation and KAnion, respectively) that could then be applied collectively to consider all of the individual partitioning mechanisms, including the KOC value, to derive an overall partition coefficient. The need to include characteristics of the medium will improve the relevance of partitioning information for hazard and scenario-specific exposure assessment purposes, although it will also require that reference conditions are defined to allow comparisons to be made between different substances. Improved approaches are likely to need to take account of the local environmental conditions, and this will improve the relevance of the information especially for site-specific risk assessments.

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2.03.P–Mo063 Taking Account of Bioavailability in Assessing the Potential Risks Posed by Diclofenac in UK Surface Waters

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The nonsteroidal anti-inflammatory drug diclofenac has widespread use and can enter the environment via wastewaters. Diclofenac is a monocarboxylic acid with a pKa value of approximately 4, meaning that at pH 4 diclofenac will be present in approximately equal amounts in both ionised and unionised forms. At pH 6 approximately 99% of diclofenac will be present in the ionised form, and at pH 7 approximately 99.9% of diclofenac will be ionised. The physicochemical properties of diclofenac indicate that the substance is water soluble, ionised in aqueous environmental media, and unlikely to undergo significant environmental partitioning due to its presence in an anionic form in the environment. Diclofenac environmental behaviour is therefore typical of many other human pharmaceuticals. It readily ionises, is water soluble, and shows a limited tendency to partition to environmental matrices, which is unsurprising as these are often clinical design requirements for medicines. It has recently been proposed that Environmental Quality Standards (EQS) for diclofenac should take account of its ionisation and consider differences in the uptake and toxicity of the ionised and unionised forms. Normalisation of toxicity data for diclofenac based on pH has been reported to reduce heterogeneity in acute data and improve the Species Sensitivity Distribution (SSD) of chronic data. Bioavailability based approaches for EQS derivation are usually based on the normalisation of toxicity data to a consistent set of water chemistry conditions, and the calculation of a site-specific SSD. However, in cases where all species in the ecotoxicity database use the same bioavailability normalisation approach it may be possible to apply a bioavailability correction to an HC5 value derived from a bioavailability normalised SSD. Water chemistry conditions very widely across Europe, and EQS values that take account of this variation have been set within Europe for over a decade and are now widely implemented. This presentation considers the variation in local pH conditions of surface waters across Europe to identify differences in the relative sensitivity of areas to diclofenac toxicity.

2.03.P–Mo064 Refinement of Environmental Concentration Estimates Based on the Degradation Behavior of Household-Derived Chemical Substances - Focusing on Disappearance in Sewer Pipes

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Efforts have been made to elucidate the environmental behavior of chemical substances and to improve the accuracy of environmental concentration estimates. In risk assessments of priority assessment chemicals under Japan's Chemical Substances Control Law (CSCL), estimated environmental concentrations derived from exposure models have been compared with measured concentrations obtained from environmental monitoring. Substances for which large discrepancies between estimated and measured concentrations have been observed to date share a common characteristic: they are biodegradable chemicals used in large quantities in households. Household-derived chemical substances may be lost during transport through sewer pipes, removed at wastewater treatment plants (WWTPs), and further degraded in river waters after discharge into the receiving environment. Although degradation processes for some substances within sewer pipes have been reported, the available evidence remains limited compared with studies on fate in WWTPs and river waters. Therefore, to improve the accuracy of environmental concentration estimates and reduce the discrepancy between model estimates and monitoring data, we focused on losses within sewer pipes. In this study, we measured influent concentrations at three WWTPs for cocamidopropyl betaine (CAPB) and C12-amine oxide (AO), for which risk assessments have been conducted under the CSCL, to clarify actual loss patterns–particularly within sewer pipes–along the pathway from households to rivers via the sewer system.

The ratios of the quantities reaching WWTPs, based on measured influent concentrations, to the estimated quantities discharged from households for CAPB and C12-AO were approximately 13–46% and 17–21%, respectively. These results suggest that these ratios vary among substances. Substances with relatively low ratios may be more strongly affected by degradation and removal during transport through sewer pipes prior to reaching WWTPs. In addition, when ratios of 43.4% and 21.0% were applied to CAPB and C12-AO, respectively, in the estimation of river water concentrations, the estimated environmental concentrations decreased, and the discrepancy between measured and predicted concentrations was reduced. Further refinement of estimates is expected by considering substance behavior not only within sewer pipes but also in WWTPs and in river water.

2.03.P–Mo065 Precipitation-Driven Daily Variations in River Water Quality and Trace Metal Bioavailability Around the Ashio Copper Mine, Japan

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Trace metal contamination from abandoned mines poses significant risks to human health and river ecosystems. While river water quality, including trace metal concentrations, responds to precipitation, previous studies have primarily focused on variations associated with extreme rainfall events over seasonal timescales, such as differences between dry and wet seasons. Day-to-day variations remain poorly investigated. In addition, the bioavailability of trace metals is affected by water quality parameters other than trace metal concentrations, such as dissolved organic carbon (DOC) concentration, pH, and water temperature, and these parameters should also be influenced by daily precipitation. This study conducted a 27-day consecutive field survey of four rivers surrounding the Ashio Copper Mine in Japan to evaluate variations in trace metal concentrations and their bioavailability in response to daily precipitation. To evaluate the relationships between precipitation and time-series measurements of river water quality, a Bayesian state-space modeling approach was employed. Free ionic concentrations of five

trace metals (Cu, Zn, Cd, Pb, and Ni) were estimated using the Windermere Humic Aqueous Model, and the temporal changes in the ratios of free ionic to dissolved concentrations were quantified. Dissolved concentrations of several trace metals, particularly Cu, Zn, and Cd, exhibited site-specific temporal variation responses to daily precipitation. Furthermore, rainfall-induced fluctuations in trace metal concentrations resulted in downstream fluctuations. pH and dissolved concentrations of Ca and Mg generally declined following precipitation across most sites, whereas DOC concentrations generally increased after rainfall. These site- and parameter-specific differences in precipitation responses resulted in substantial spatiotemporal variability in free ionic to dissolved ratios of trace metals. At forest-dominated sites, even though dissolved concentrations of trace Cu and Cd were temporally stable, their free ionic concentrations fluctuated markedly, likely reflecting precipitation-driven variations in DOC. Our study provides empirical evidence that daily precipitation can significantly alter trace metal bioavailability across time and space.

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2.03.P–Mo066 Region-Specific Arc-Dependent Neuronal Activation Following Neonicotinoid Exposure in Transgenic Mice

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Among these insecticides, neonicotinoids (NNs) are extensively used in agriculture because of their relatively low toxicity to humans. Although NNs primarily target insect nicotinic acetylcholine receptors (nAChRs), they can also interact with mammalian nAChRs. Previous studies have reported NN-induced alterations in brain function, including anxiety-like behavior, locomotor dysfunction, and changes in neurotransmitter regulation. However, the neuronal activity patterns underlying these neurobehavioral effects remain largely unexplored.

Activity-regulated cytoskeleton-associated protein (Arc) is an immediate-early gene (IEG) widely used as a marker of neural activity and synaptic plasticity. In the present study, we investigated the effects of NN exposure on neural circuit activity in brain regions associated with emotional processing and motor regulation. To map activated neuronal populations, we used tdTomato expressing transgenic mice (Arc CreERT2 /R26Ai14), in which neurons undergoing Arc promoter activation are permanently labeled.

Following a 1 h exposure to clothianidin at the non-observed adverse effect level (NOAEL), significant increases in tdTomato-positive cells per mm² were observed in the granular layer of hippocampal dentate gyrus (GrDG), basolateral amygdala (BLA), and caudate putamen (CPu) compared with control animals. These findings indicated that acute clothianidin exposure induces region-specific alterations in Arc-dependent neuronal activity. The distribution of activated cells suggests preferential involvement of hippocampal-amygdalar-striatal circuits implicated in emotional processing, memory encoding, and locomotor regulation. In addition, our findings demonstrate that this transgenic mouse model may serve as a useful tool for assessing chemical-induced changes in brain-wide neuronal activity.

Overall, this study provides spatial evidence of NN-induced alterations in neural circuit activity and contributes to a better understanding of the mechanisms underlying pesticide-associated behavioral dysfunction in mammals. Further studies examining neurotransmitter alterations are currently

underway to clarify the neurochemical basis of these effects.

2.03.P–Mo067 From Wastewater Tracer to Predictive Indicator: Large-Scale Assessment of Sucralose and Water Quality Across Florida Aquatic Systems

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Wastewater influence is a major driver of water quality impairment in urbanized aquatic systems, yet rapid indicators of anthropogenic impact remain limited. Sucralose, an artificial sweetener resistant to environmental degradation and wastewater treatment, has emerged as a robust tracer of human wastewater influence in environmental waters. This study evaluates the occurrence, concentration distributions, and predictive relevance of sucralose using a long-term environmental dataset to develop concentration thresholds where sucralose transitions from a tracer into an indicator of water-quality impairment. Between 2014 and 2026, more than 5,000 environmental water samples submitted through analytical service projects were analyzed for sucralose using online solid-phase extraction HESI-HPLC-HRMS (Q Exactive orbitrap) operated in negative mode (MDL:11 ng/L). The historical dataset was used to evaluate concentration distributions and percentile ranges of occurrence (ND-110,000 ng/L), with concentrations above the 85th percentile interpreted as indicative of strong wastewater influence. Threshold development was evaluated using CuSum analysis on a subset of samples collected in the Biscayne Bay watershed, Tampa Bay, the Hillsborough River watershed, and Key Largo alongside nutrient and physicochemical measurements. Parameters included TP, TN, nitrate, nitrite, ammonia, silica, TOC, DOC, turbidity, dissolved oxygen (DO), chlorophyll, fDOM, and salinity. Results demonstrated distinct regional patterns in sucralose occurrence. Tampa Bay and the Hillsborough River watershed exhibited the highest concentration ranges (90-49,000 ng/L), reflecting wastewater treatment plant effluent and reclaimed water influence. Biscayne Bay and tributaries displayed intermediate concentrations associated with urban runoff and canal discharges (20-3,500 ng/L), while Key Largo exhibited the lowest ranges, with thresholds of 56 ng/L and 150 ng/L indicative of impairment. Elevated sucralose concentrations were associated with nutrient enrichment, higher turbidity and fDOM, and decreased DO. Statistical analyses identified concentration breakpoints indicative of measurable water quality decline, demonstrating that sucralose can function as a wastewater tracer and predictive indicator of ecosystem impairment. These findings support the application of sucralose as a management-relevant indicator for identifying anthropogenic influence and areas vulnerable to water quality degradation.

2.03.T - Advances in Exposure Modelling: Towards a Safe and Sustainable Tomorrow for Both Humans and the Environment

2.03.T01 A Stochastic Diffusion Model for Dynamic Internal Chemical Exposure Assessment

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In recent years, stochastic differential equations have been used to develop probabilistic exposure models that describe randomness in the accumulation of chemicals in organisms. These models can represent inter-individual differences in exposure levels through time-evolving probability distributions of internal chemical concentrations.

Existing stochastic exposure models can generate right-skewed, log-normal-like chemical concentration distributions, consistent with observed patterns in human bodies. However, they rely on a sink-dominating assumption and the obtained distribution represents only temporary exposure status. Over

time, the probability density of concentration distribution tends to become highly concentrated near a certain value, thereby failing to reflect empirical observations in human bodies.
To address this limitation, this study develops a positive stochastic exposure model based on a stochastic diffusion process. Its deterministic term represents changes in chemical concentration driven by input and first-order elimination, while its multiplicative stochastic term represents randomness in the accumulation.
The model will be derived, and its statistical characteristics will be examined. Monte Carlo simulation will generate paths of internal chemical concentrations and reconstruct their time-evolving distributions. Model behavior will be compared with existing stochastic exposure models. The resulting stationary distribution will also be fitted to biomonitoring data and compared with candidate distributions, including the log-normal distribution.
We hypothesize that the model can describe internal chemical concentration dynamics while producing a right-skewed inverse-gamma stationary distribution. This stationary distribution may fit well with the log-normal-like chemical concentration distributions observed in biomonitoring data, providing a link between theoretical exposure dynamics and empirical distributions.
The model-derived probability density function of internal chemical concentration can be used as a weight to calculate the expected value of species sensitivity, thereby enabling time-varying environmental risk estimation. This study is expected to support the interpretation of biomonitoring data and the development of dynamic environmental risk assessment methods.

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2.03.T02 Assessment of Time-Integrated Inhalation Cancer Risks of PAHs and Metals in an Industrial City via Machine Learning-Based Concentration Reconstruction

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Evaluating long-term exposure to hazardous air pollutants (HAPs) in industrial cities is challenging due to limited spatial and temporal coverage of routine monitoring. In this study, annual concentrations of 13 polycyclic aromatic hydrocarbons (PAHs) and 8 metals were reconstructed at 19 air quality monitoring stations in Ulsan, South Korea, from 2001 to 2023. Random Forest models were developed using criteria air pollutants, meteorological variables, temporal variables, and distances to major emission sources as predictors. Validation showed good agreement between measured and reconstructed concentrations, with R values of 0.85–0.86 for Σ7 PAHs and BaP toxicity equivalent concentrations (TEQBaP) and 0.66–0.80 for individual metals. Independent passive air sampling data also supported the reconstructed spatial patterns of PAHs. Positive Matrix Factorization identified traffic emissions, petrochemical activities, metal processing, and heavy manufacturing as major sources. The reconstructed concentrations showed distinct long-term trends for PAHs and metals. TEQBaP concentrations decreased across Ulsan after the early 2000s, whereas toxicity-weighted metal concentrations showed persistent spatial gradients near non-ferrous metal and heavy industrial areas. Year-specific reconstruction was compared with a conventional constant-concentration assumption using the 2023 annual mean. Under this assumption, long-term PAH exposure was underestimated by up to 14% in residential areas, whereas metal exposure was overestimated by up to 18% near industrial areas. Scenarios incorporating residence history further demonstrated that temporal changes in pollutant concentrations and residential location modified time-integrated exposure estimates. Year-specific inhalation cancer risks ranged from 2.92 × 10-8 to 4.52 × 10-8 for PAHs and from 4.48 × 10-6 to 5.73 × 10-6 for metals. These findings indicate that year-specific

concentration reconstruction provides a more reliable basis for long-term exposure and risk assessment in industrial cities. Consideration of both temporal variations in pollutant concentrations and residential mobility is therefore needed in epidemiological and regulatory applications.

2.03.T03 How Does Polymeric PFAS Degradation Influence Substance Flow Analysis of Non-Polymeric PFAS Contained in Outdoor Clothing?

Junichiro Koshiba[1], Akane Shimatani[2] and Yasuhiro Hirai[1] (1)Kyoto University, (2)Kyoto Universirty

It was reported that polymeric PFAS contained in outdoor clothing undergo degradation during the product lifetime. However, previous substance flow analysis (SFA) studies have not considered polymeric PFAS degradation during the product lifetime.
The objective of this study is to conduct an SFA of PFCAs (perfluoroalkyl carboxylic acids) and FTOHs (fluorotelomer alcohols), incorporating polymeric PFAS degradation, and to evaluate its influence on the stocks and emissions of PFCAs and FTOHs.
The target substances of this study were C6F13 side-chain fluorinated polymers (SCFPs), PFCAs (sum of PFBA to PFHpA), and FTOHs (sum of 4:2 and 6:2 FTOH). This study modeled polymeric PFAS degradation by considering (i) degradation of SCFPs into FTOHs, (ii) degradation of FTOHs into PFCAs, and (iii) the release of SCFPs, FTOHs, and PFCAs. The degradation rates were estimated based on observational data of FTOHs and PFCAs concentrations before and after weathering reported in previous studies. Because the estimated degradation rates varied depending on input parameters, SFA was conducted under five scenarios representing different degradation rates.
An SFA was conducted for outdoor clothing used in Japan from 1990 to 2040. In the SFA model, polymeric PFAS degradation was assumed to occur for 100 hours (typical outdoor exposure conditions) during the average lifetime of outdoor clothing in Japan (assumed to be 5.8 years). During the remaining lifetime, clothing was assumed to be stored indoors, and only the volatilization of FTOHs was considered. The initial concentrations of SCFPs, FTOHs, and PFCAs were assumed based on observational data reported in previous studies. Production volumes of outdoor clothing and disposal pathways were defined based on statistical data and interviews.
The results of four scenarios showed that the stocks of FTOHs and PFCAs derived from SCFPs were estimated to be 4–300 times higher than those initially present. However, one scenario suggested that the contribution of polymer-derived FTOHs and PFCAs was only 0.06 times the initially contained amounts. These results indicate that polymer-derived FTOHs and PFCAs may substantially contribute to the overall amounts of these substances in outdoor clothing. Such contributions may be overlooked if polymeric PFAS degradation is not considered in SFA studies. However, large uncertainties remain due to parameter assumptions, highlighting the need for further research on polymeric PFAS degradation.

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2.03.T04 Environmental Fate Modeling of Volatile Methylsiloxanes (D5 and D6) in Water and Sediments of Tokyo Bay Using the Multimedia Model G-CIEMS

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Methylsiloxanes are widely used in everyday consumer products, such as hair conditioners, as well as in various industrial applications. Some methylsiloxanes have been identified as substances of concern due to their high environmental persistence, bioaccumulation potential, and toxicity. Among them,

decamethylcyclopentasiloxane (D5) and dodecamethylcyclohexasiloxane (D6) are major compounds and are not currently listed under the Stockholm Convention on Persistent Organic Pollutants, although their potential listing has previously been considered. After being released into the environment, these substances are primarily distributed in the atmosphere and sediments. This environmental behavior differs from that of many other organic pollutants. Due to their strong partitioning to organic matter associated with suspended solids in surface waters, methylsiloxanes can be transported from freshwater systems to marine environments. Based on their high bioconcentration factors (BCFs), these substances may accumulate in higher trophic organisms, such as fish, potentially leading to human exposure.
In a previous study, we focused on D5 and D6 and conducted emission estimates and environmental fate simulations for the Tokyo Bay catchment area using the multimedia environmental fate model G-CIEMS. The Tokyo Bay catchment area was selected because of its high population density and large spatial area. Model performance was evaluated by comparing simulated concentrations with measured data for surface water, freshwater sediments, and the atmosphere. However, in the previous study, Tokyo Bay itself was not explicitly resolved because the model lacked high-resolution coastal compartments. In the present study, we developed dedicated coastal compartments for Tokyo Bay and simulated the environmental fate of D5 and D6 in both Tokyo Bay and its catchment area. Model reliability for Tokyo Bay was assessed by comparing modeled concentrations with measured data for marine water and marine sediments, demonstrating good agreement between the model predictions and observed values. This agreement suggests that the model can be used to evaluate environmental emissions of other substances with strong sorption behavior through comparison of modeled and observed concentrations.

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2.03.T05 One Health Chemical Assessment: Integrating Human and Ecological Exposure Modeling

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Humans and wildlife are exposed to a wide range of chemical substances released from multiple life-cycle sources into complex, multimedia environments through diverse exposure pathways. These exposures are often interconnected because humans and wildlife may share habitats, food webs, and ecosystem services. In the meantime, exposure levels and associated risks may differ substantially between humans and wildlife due to species-specific differences in exposure sources, pathways, behaviors, and susceptibilities. This interconnected and multidimensional nature of chemical exposure highlights the need for a systematic and mechanistic perspective in exposure modeling, as well as a holistic framework capable of tracking chemicals from production to their presence in both humans and ecological receptors. In this presentation, we introduce the state-of-the-science modeling framework PROduction-To-EXposure (PROTEX), which is designed to characterize the full continuum from chemical production and multi-source emissions, through multi-scale multimedia environmental fate and transport, to multi-pathway exposure and internal presence in humans and wildlife. PROTEX is grounded in theories of substance flow analysis, multimedia fate and transport, bioaccumulation, exposure science, and toxicokinetics. The framework integrates mechanistic descriptions of the physical, chemical, biological, and socioeconomic processes that influence human and ecological exposures. As an illustrative case study, we demonstrate the application of PROTEX to screen and rank chemicals commonly used in the United States, based on exposure rates and health risks for both humans and wildlife species. The rankings differ depending on the assessment goals and the receptor being protected. We discuss the connections and distinctions between chemical assessments aimed at protecting human health versus ecosystem integrity. We also explore how a holistic modeling framework such as PROTEX can support the integration of human and ecological health within the One Health paradigm.

2.04.P - Contaminants of the Offshore Energy Sector: Exposure, Effects and Risk Frameworks

2.04.P–Mo068 Derivation of tropical marine water quality guidelines for key produced water production chemicals

Diane Brinkman[1], Ross Jones[1], Rebecca Fisher[1], Constanza Buccella[1], Florita Flores[1], Kimberley Day[1], Winona Dougan[1], Madeline McKenzie[1] and Andrew Negri[1] (1)Australian Institute of Marine Science

Production chemicals are widely used in offshore oil and gas operations and may be discharged to the marine environment via produced water; however, robust marine water quality guideline values for many of these substances remain limited, particularly for tropical ecosystems. Here, new guideline values for three widely used production chemicals – monoethylene glycol (MEG), methyldiethanolamine (MDEA), and piperazine (Pz) – were derived using contemporary probabilistic frameworks and toxicity data predominantly from tropical marine species.

Chronic ecotoxicity testing was conducted across a broad taxonomic range, including microalgae, invertebrates, macroalgae, and echinoderms. Concentration–response relationships were modelled using Bayesian and model averaging approaches to derive negligible effect concentrations and 50% effect concentrations. Species sensitivity distributions (SSDs) were subsequently constructed to derive both chronic and acute guideline values.

For MDEA and Pz, additional mixture toxicity experiments were conducted to empirically evaluate assumptions of additive toxicity. Responses differed between species, with additive effects observed in a microalga and sub additive responses in an invertebrate, demonstrating that default assumptions of additivity may not be universally applicable.

These new guideline values fill critical gaps for commonly discharged production chemicals and highlight how regionally relevant, tropical marine datasets can produce guideline values that differ substantially from those derived using temperate, freshwater, or assessment factor approaches in other jurisdictions. The results support more transparent, consistent, and scientifically defensible chemical risk assessments for offshore produced water discharges.

2.04.P–Mo069 Assessing Produced Water Toxicity and Drivers Using Direct Bioassays and Mechanistic Modelling

Diane Brinkman[1], Rebecca Fisher[1], Constanza Buccella[1], Florita Flores[1], Heidi Luter[1], Winona Dougan[1], Maddi McKenzie[1], Ross Jones[1] and Andrew Negri[1] (1)Australian Institute of Marine Science

Environmental risk assessments for offshore produced water (PW) discharges are commonly based on predicted exposure scenarios and chemistry-derived toxicity estimates; however, uncertainties remain regarding the drivers of whole effluent toxicity and the reliability of modelling approaches for complex mixtures. This study presents an integrated assessment of PW toxicity from two Australian offshore oil and gas facilities representing contrasting discharge streams, combining whole effluent toxicity (WET) testing with mechanistic toxicity modelling.

At one facility, multi-year WET testing across tropical marine species was paired with detailed chemical characterisation to compare empirically derived toxicity units (TUwet) with chemistry-based predictions (TUchem). Monoethylene glycol contributed moderately despite high concentrations, whereas methyldiethanolamine and piperazine, although present at lower concentrations, contributed disproportionately to total predicted toxicity in some samples. Modelled toxicity was consistently underestimated observed toxicity, likely reflecting differences in species sensitivity, incomplete chemical characterisation, and potential non-additive interactions within the PW mixture.

At the second facility, long-term WET datasets (2006–2024) were re-analysed using Bayesian-derived negligible-effect thresholds and species sensitivity distributions, and coupled with mechanistic modelling

to identify toxicity drivers. Total recoverable hydrocarbon (TRH) fractions dominated predicted toxicity, with additional contributions from ammonia. Modelled toxicity generally exceeded overestimated toxicity, with larger discrepancies in older samples potentially reflecting contributions from uncharacterised production chemicals and analytical limitations. Agreement between TUchem and TUwet improved with refined analytical approaches, although modelling remained conservative.
Overall, the results demonstrate that mechanistic toxicity models are valuable tools for interpreting complex mixture toxicity, but their application requires careful consideration of analytical inputs and validation against WET data to avoid systematic over- or underestimation of environmental risk.

2.04.T - Contaminants of the Offshore Energy Sector: Exposure, Effects and Risk Frameworks

2.04.T01 Using Whole Effluent Toxicity testing to inform Produced Water risk assessment and adaptive management

Rebecca Fisher[1], Diane Brinkman[1], Constanza Buccella[1], Florita Flores[1], Heidi Luter[1], Winona Dougan[1], Madeline McKenzie[2], Ross Jones[1] and Andrew Negri[1] (1)Australian Institute of Marine Science, (2)James Cook University

Whole Effluent Toxicity (WET) testing has become a central tool in risk-based management of offshore produced water (PW) discharges, providing an empirical measure of whole-mixture toxicity that captures interactions among constituents not readily resolved through chemical analyses alone. Within Australian regulatory frameworks, WET testing is used both to support ecological risk assessment and to inform adaptive management of ongoing discharges; however, these applications differ fundamentally in their objectives, statistical requirements, and interpretation. Here we synthesise multi-year WET datasets from two Australian offshore oil and gas facilities representing contrasting discharge types and operational contexts to, to evaluate how WET testing can best support these distinct management objectives.
Species sensitivity distributions (SSDs) derived from multi-species chronic toxicity data provide a robust basis for ecological risk characterisation, but are sensitive to species composition and are poorly suited to detecting temporal trends. In contrast, repeated testing of a smaller, consistent subset of species supports species-level analyses using negligible-effect and effect-concentration metrics that are more powerful for detecting change and supporting adaptive management responses. We propose a dual-framework approach in which periodic multi-species SSDs are used for risk assessment, while more frequent reduced-species WET testing is used to support adaptive management and operational decision-making.

2.04.T02 Realised Environmental Risk from Offshore Produced Water Discharges: Evidence from In Field Water Quality Monitoring and Field Derived Dilution Estimates at a Floating LNG Facility

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Environmental risk assessments for offshore produced water discharges are commonly based on predicted exposure scenarios; however, field studies that directly characterise realised exposure and risk in the receiving environment under operational conditions remain limited. This study presents an in field assessment of produced water (PW) discharges from a floating liquefied natural gas (FLNG) facility, focusing on water quality monitoring and field derived dilution behaviour to evaluate environmental exposure and risk.
Seawater samples were collected across multiple tidal conditions at locations proximal to the PW discharge point, along the vessel hull, and at increasing distances astern. Samples were analysed for a broad suite of organic and inorganic constituents associated with produced and cooling waters. Empirical

dilution-distance relationships were derived from field observations of a dye release and used to interpret contaminant attenuation with distance from the discharge point. Concentrations of PW constituents were generally low and rapidly attenuated with distance. Only a limited number of analytes, principally phenols and selected metals, were detected above analytical reporting limits in near field samples, with concentrations declining to background levels within short distances from the discharge location. Evidence of persistent co mingling between PW and cooling water plumes was limited.
Realised ecological risk was assessed using mixture toxicity modelling based on measured seawater chemistry. Predicted toxicity from measured seawater concentrations was well below thresholds associated with adverse effects, and substantially lower than those implied by toxicity predictions of the source produced water at equivalent dilutions. The results demonstrate that in field monitoring and empirically derived dilution estimates provide a robust basis for characterising realised environmental risk from offshore PW discharges and validates the conservatism of source-based risk assessments.

2.04.T03 Sublethal Effects of Synthetic Fluids from Offshore Wind Turbines on Atlantic Haddock (Melanogrammus aeglefinus) Embryos.

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Offshore wind energy is rapidly expanding. While effects related to construction and mechanical disturbances have received increased attention, a knowledge gap persists regarding the release and effects of compounds during the operational phase. Especially, ecotoxicological data of the synthetic oils using relevant exposure scenarios and marine species is lacking.
This study evaluated the ecotoxicity of a synthetic coolant and a lubricant oil commonly used in offshore wind turbines (OWTs) on embryos of the economically relevant marine species Atlantic haddock (Melanogrammus aeglefinus). The exposure was conducted using an oil droplet exposure system designed to generate oil dispersions that mimic environmentally realistic scenarios.
Sublethal effects, including morphological alterations, body burden, benchmark dose (BMD) analysis, and gene expression, were assessed using the oil droplet exposure system. Embryos were exposed for 9 days to four sublethal nominal concentrations: control (0 µg/L), low (15 µg/L), medium (50 µg/L), and high (150 µg/L), from epiboly 50% to prehatching stages. Morphological observations suggest that both fluids induce oxidative stress in Atlantic haddock embryos, with more pronounced effects in lubricant-exposed individuals. The increased toxicity observed with the lubricant is most likely due to the accumulation of oil droplets on the egg chorion, which elevates local concentrations and enhances the bioavailability of compounds beyond those present in the water-soluble fraction, including larger molecules that are potentially more toxic and transferable to the embryo.
Acute lethality was assessed using the water-accommodated fraction, comparing zebrafish (Danio rerio) and Atlantic haddock. EC50 values were 2 and 44 mL/L (zebrafish) and 4 and 14 mL/L (Atlantic haddock) for coolant and lubricant, respectively. Despite similar EC50 values, mortality patterns differed between species: zebrafish embryos died predominantly in early development (before completion of organogenesis), while Atlantic haddock showed mortality in the later stages (closer to hatching).
The use of two species and two exposure systems provided complementary ecotoxicological data for difficult to test substances, such as the high-performance synthetic fluids used in OWTs. This research contributes to a more complete characterization, strengthening the environmental risk assessment of the offshore wind energy industry.

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2.04.T04 Ecotoxicological Consequences of Chronic Ionising Radiation Exposure in Marine Ecosystems

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Marine ecosystems are exposed to ionising radiation from a range of anthropogenic sources, including nuclear power production, fuel reprocessing, legacy weapons testing, accidental releases, and naturally occurring radioactive materials (NORM) associated with industrial activities such as offshore oil and gas. Despite this, the ecological consequences of chronic low-dose radiation exposure in marine environments remains poorly understood. In this study, we conducted a literature review to evaluate the current state of marine radiotoxicological data and determine whether chronic exposures to environmentally relevant radiation dose rates pose an ecological risk in marine environments. To do this, publicly available articles were screened using predefined inclusion criteria adapted from the Australian New Zealand Governments (ANZG) Water Quality Guidelines Initiative, focusing on chronic exposure scenarios, environmentally relevant endpoints, and marine or ecologically comparable taxa. A total of four studies met these criteria for taxa including molluscs, polychaetes, microalgae and macroalgae. Data of acceptable quality were collated to evaluate the dose–response relationships, sensitivities across taxa, and the applicability of existing radiological protection frameworks to marine systems. The literature indicates that there is a substantial lack of chronic toxicity data at low dose rate exposures, particularly for tropical species. Additionally, inconsistencies in experimental design, dosimetry, and endpoint selection limited data quality and comparability across many studies. This review identified critical knowledge gaps in the understanding of chronic radiation effects in marine environments and highlights the need for targeted experimental studies using representative species and realistic exposure scenarios. Addressing these gaps will strengthen environmental risk assessments and support evidence-based decision-making for nuclear and NORM-producing industries in marine ecosystems globally by supporting more robust, evidence-based management of radioactive contaminants in marine ecosystems.

2.04.T05 Effects of Low Dose Ionising Radiation on Reproduction in the Australian Estuarine Amphipod Melita plumulosa

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Potential contaminants associated with the decommissioning of offshore oil and gas infrastructure are an emerging environmental challenge, particularly if subsea infrastructure such as pipelines that possibly contain Naturally Occurring Radioactive Materials (NORM) are left in situ. While these structures may increase biodiversity by providing artificial reef habitat, the ecological implications of chronic low-dose ionising radiation exposure from NORM to marine organisms remain poorly understood due to the paucity of marine radiotoxicological data. Consequently, there is a high level of uncertainty in environmental risk assessments for radiation contamination in marine ecosystems, and it is uncertain whether current radiation protection standards are relevant. The aim of this project was to quantify the effects of radiation exposure on reproduction in the Australian estuarine amphipod Melita plumulosa. Controlled laboratory experiments were conducted using a sealed Caesium-137 source to deliver a gradient of environmentally relevant low dose rates, ranging from 30 – 8,000 µGy/h. After 10-day exposure periods, the number of juveniles and embryos per adult female were compared to the controls (i.e., adult M. plumulosa exposed to the same conditions but without radiation), and the dose-response relationships were modelled using Bayesian statistics to identify ecotoxicological thresholds. Such data

will contribute to improving the scientific basis for environmental radiological risk assessments in marine ecosystems and contribute to evidence-based decision-making regarding the ecological risks associated with NORM-contaminated offshore infrastructure.

2.05.P - Cross-System Mercury Cycling in Asia and the Pacific: Linking Atmosphere, Land, Oceans, and Biota

2.05.P–Tu084 Meltwater-driven Mercury Bioavailability and Trophic Transfer in Antarctic Coastal Food Webs

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Mercury (Hg) cycling in polar coastal ecosystems is gaining increasing attention as climate-driven glacial retreat intensifies meltwater discharge and alters marine productivity. Along the Western Antarctic Peninsula, summer meltwater modifies water column stratification, organic matter inputs, and primary productivity, potentially enhancing the retention, transformation, and trophic transfer of total mercury (THg) and methylmercury (MeHg), its most bioaccumulative and toxic form. Yet how these environmental drivers jointly regulate MeHg bioavailability and trophic transfer across coastal food webs remains poorly understood. Antarctica's relative isolation from direct anthropogenic pressures and its short trophic webs make it an exceptional natural laboratory to examine mercury processes with reduced confounding variables. This study investigates how seasonal meltwater inputs and phytoplankton productivity pulses regulate THg and MeHg bioavailability, bioaccumulation and biomagnification across a simplified coastal food web. Sea surface temperature, sea surface salinity and chlorophyll-a time series will be used as proxies of meltwater influence, stratification and productivity. During austral summer campaigns in 2025 and 2026, surface water, sediments, phytoplankton/particulate organic matter, Antarctic krill, and humpback whale biopsies were collected. THg and MeHg will be quantified across compartments, while δ13C, δ15N and δ34S will define carbon sources, trophic position and food web structure. Biomagnification will be assessed through BMFs, trophic magnification slopes, and trophic magnification factors. Preliminary results suggest that meltwater-associated particulate organic matter acts as a key vector for Hg delivery to coastal waters, and that productivity blooms influence MeHg formation and trophic uptake efficiency. We hypothesize that high-melt periods increase THg loads while episodic productivity pulses enhance MeHg incorporation into the base of the food web, with amplified biomagnification signals at upper trophic levels. These findings advance our mechanistic understanding of how climate-sensitive hydrological and biological processes jointly control mercury bioavailability in polar systems. Given that Antarctica serves as a sentinel ecosystem for global environmental change, this work provides critical baseline data applicable to mercury risk assessments in other climate-sensitive coastal regions across the Asia-Pacific and beyond.

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2.05.T - Cross-System Mercury Cycling in Asia and the Pacific: Linking Atmosphere, Land, Oceans, and Biota

2.05.T01 International Proficiency Testing Program for Mercury Analysis:

Framework, Item Preparation, and Result Analysis

Mercury pollution is a very complex issue. Mercury easily volatizes into the air, travels on a global scale, and affects environments and people far from the source of emission. Therefore, to address mercury pollution, global monitoring of various media with high accuracy is necessary. Monitoring data obtained by a number of laboratories must be compiled for global-scale analysis; data comparability is essential. Under the co-organization of the United Nations Environment Programme (UNEP) and the National Institute for Minamata Disease (NIMD), proficiency testing (PT) for mercury analysis was organized. Four rounds of PT have been conducted since 2021. The target media for the PT changes with each round. PT1: Human hair from the general population. PT2: Freeze-dried yellowfin tuna. PT3: Dry powdered estuary sediment. PT4: Freeze-dried human urine from the general population. In each round, the PT item was completely homogenized and treated to maintain stability throughout the PT period. Homogeneity and stability were confirmed to ensure they did not affect the primary cause of the PT performance evaluation.
The performance of the PT participants was evaluated using robust analysis. The participants' z-scores were evaluated based on the median and the normalized interquartile range (NIQR) of the participants' reported values. The NIQR-to-median ratio for each PT was as follows: PT1 (hair): total mercury, 8.4%; PT2 (fish): total mercury, 6.8%; methylmercury, 9.4%; PT3 (sediment): total mercury, 8.8%; PT4 (urine): total mercury, 23%. This PT program provided important information for the quality management of participating laboratories and the comparability of monitoring data for mercury assessments on a global scale.

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2.05.T02 Historical mining as the primary source of mercury in a mixed industrial river system: evidence from isotope analyses

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Australia’s long history of mining has left a persistent environmental legacy. In the Latrobe Valley, Australia, coal-fired power generation and legacy mining districts coexist within a connected river system that ultimately drains into the ecologically significant Gippsland Lakes. While emissions from power stations have been relatively well characterised, the contribution of historical mining to ongoing metal contamination remains poorly constrained.
This study investigates the sources, spatial distribution, and environmental fate of mercury (Hg) within the Latrobe-Thomson river system, with a focus on distinguishing between mining- and power station-derived inputs. Sediment samples were collected downstream of legacy mining sites in the Thomson River and Stringers Creek, as well as downstream of coal-fired power stations in the Latrobe River and Traralgon Creek. Concentrations of Hg were analysed alongside total organic carbon and lithogenic proxies. Mercury isotopic compositions were used to further resolve contaminant sources and transport pathways.
Results show substantially higher Hg concentrations in sediments influenced by legacy mining ($\bar{x}$ = 1106.6 ± 1868.1 ng g^{-1}) compared to those influenced by power stations ($\bar{x}$ = 129.0 ± 72.3 ng g^{-1}), with intermediate levels observed at river confluences ($\bar{x}$ = 448.2 ± 290.8 ng g^{-1}). Mercury isotope signatures provide clear source discrimination: sediments downstream of mining areas exhibit near-zero Δ^{199}Hg and δ^{202}Hg values consistent with direct mining inputs, while coal combustion residues display negative values. Downstream sediments closely match mining signatures, indicating a dominant and persistent influence of legacy mining on Hg transport. Sediments downstream of power stations display isotope

signatures that differ markedly from those of coal-derived materials, indicating minimal incorporation of atmospheric emissions into fluvial sediments.
These findings demonstrate that historical mining remains the primary driver of Hg contamination in the Latrobe Valley river system, despite decades of regulated industrial activity. The results highlight the importance of accounting for legacy sources in catchment management and provide critical context for assessing contamination risks in the Gippsland Lakes. This work advances understanding of metal transport in complex industrial landscapes and supports informed strategies for monitoring and remediation in similar river-lake systems globally.

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2.05.T03 Bridging Research and Policy for Mercury Management in Australia: Outcomes from the 2025 Mercury Australia Network Workshop

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Robust science is important to develop and inform policy for the protection of the environment. However, there are not always clear communication pathways between research academics and those in government to inform and strengthen national policy on environmental protection. In November 2025, the Mercury Australia Network hosted a workshop of twenty-six representatives from the research, policy, and regulatory communities across Australian Federal and State/Territory Governments. The workshop focussed on four key themes related to mercury (Hg) with links back to the Minamata Convention on Mercury:
1) Hg waste management, including for the emerging field of offshore oil and gas infrastructure;
2) Hg releases and contaminated sites in Australia, including historical contamination;
3) Hg exposure, pathways, and risks to human health;
4) Challenges for effectiveness evaluation (data gaps and lag times, i.e. between policy decisions and implementation, and between emission reduction and effects due to natural processes).
The Workshop also surveyed participants using an online interactive platform and the results were discussed in real-time. Survey questions included “What is the number one priority for mercury management in Australia?” and “How should the Australian research community and Government work together on managing mercury issues?”. Responses to the latter included improved data sharing & transparency (addressing confidentiality and public scrutiny issues), establishment and improvement of communication platforms, policy integration (i.e., linking research to regulation), improving national and international collaboration, improved resourcing via pooled expertise and shared fellowships, and focussing on multidisciplinary, applied and community-inclusive research, especially in collaboration with Indigenous peoples.
This presentation will summarise the key research insights and policy considerations discussed at the Workshop for each of the above themes, and will highlight the value of bringing together researchers, regulators, and policymakers for the improvement of environmental protection from mercury.

2.05.T04 Global patterns of seafood-mediated methylmercury exposure compared with persistent organic pollutants using a unified modeling framework

Seafood consumption is a major exposure pathway for both mercury and persistent organic pollutants, yet comparative understanding of their global exposure patterns remains limited. While these substances

share key characteristics, including long-range transport and bioaccumulation, it remains unclear how common exposure structures and substance-specific properties jointly shape national dietary exposure.
In this study, we applied global multimedia models for mercury and persistent organic pollutants developed within a consistent modeling framework to estimate seafood-mediated dietary exposure to methylmercury (MMHg), polychlorinated biphenyls (PCBs), and polybrominated diphenyl ethers (PBDEs). The models share common representations of atmospheric and oceanic transport, as well as input fields derived from CMIP6 Earth system models and global fisheries statistics used for exposure estimation. Differences are limited to substance-specific processes, emissions, and parameters, enabling direct comparison of inter-substance behavior. Concentrations in marine particulate organic matter were simulated by the models and used to estimate seafood concentrations. National dietary intake was estimated using global food balance statistics for marine products, and normalized by the global mean to facilitate inter-substance comparison.
Rank correlations of national dietary intake indicate a strong common structural basis across substances, suggesting that seafood dependence is a primary driver of global exposure. However, systematic deviations are observed across geographic settings. In island and Small Island Developing States, MMHg exposure remains elevated while persistent organic pollutants are comparatively reduced, whereas in some coastal regions exposure to persistent organic pollutants exceeds that of MMHg. These patterns reflect differences in controlling processes, with MMHg influenced by ocean biogeochemical cycling and persistent organic pollutants more strongly dependent on emission distributions. The divergence is further enhanced for PBDEs, consistent with their more limited long-range transport and stronger confinement to coastal regions. These findings indicate that global dietary exposure patterns are shaped by both shared structural drivers and substance-specific processes, providing a robust basis for inter-substance comparison and improved understanding of mechanisms controlling global contaminant exposure.

2.06.P - Emerging Contaminants in Agriculture and Food: Sources, Transport and Exposure Risks

2.06.P–We022 Comparative developmental toxicity of the herbicide imazapyr in Takifugu obscurus and Danio rerio: antioxidant imbalance, apoptosis, and immune-related transcriptional responses

Imazapyr (IMA) is a broad-spectrum imidazolinone herbicide increasingly applied in coastal wetlands and other aquatic-adjacent systems, raising concerns about its risks to non-target aquatic organisms. This study evaluated the developmental toxicity of IMA and the associated biochemical and molecular responses in Takifugu obscurus (a brackish-water model) and Danio rerio (a freshwater model). Fertilized embryos were exposed throughout embryogenesis to a gradient of nominal IMA concentrations (0-10 mg/L for pufferfish; 0-1 mg/L for zebrafish), encompassing environmentally relevant levels to stress-inducing levels. Survival, hatching, body length, cardiac function, and locomotor behavior were assessed during early development. Oxidative status was evaluated by measuring antioxidant defenses: superoxide dismutase (SOD), catalase (CAT), total anti-oxidant capacity (T-AOC); reactive oxygen species indicators: hydrogen peroxide (H2O2), superoxide anion (·O2-), hydroxyl radical (·OH); oxidative damage: malondialdehyde (MDA), while acetylcholinesterase (AChE) activity was measured as a neurotoxicity-related biomarker. Biochemical biomarkers were further integrated using the integrated biomarker response v2 (IBRv2) approach. The results showed that IMA delayed early hatching and altered locomotor behavior in both species, with species-specific sensitivities in survival and body length, and non-monotonic response patterns at low doses. Biochemical assays and apoptosis staining indicated that IMA disrupted redox homeostasis, promoting oxidative damage and apoptotic responses. Immune- and stress-related transcripts were also perturbed, albeit in species- and dose-dependent manners. Overall, these findings indicate that IMA can induce developmental and sublethal toxicity in early-life-stages fish

via oxidative stress-associated pathways, highlighting the need to consider both water-column exposures and localized hotspot scenarios in ecological risk assessment.

2.06.P–We024 From Soil to Predators: Bioavailability and Trophic Transfer of Heavy Metals in a Mustard–Aphid–Ladybird Food Chain

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The use of sewage sludge in agriculture raises concerns over the accumulation and transfer of toxic trace elements through terrestrial food chains. This study examines the bioavailability and trophic transfer of cadmium (Cd), lead (Pb), and zinc (Zn) in a mustard (Brassica juncea)–aphid (Lipaphis erysimi)–ladybird (Coccinella septempunctata) food chain, using soil amended with sewage sludge at 0%, 5%, 10%, 20%, and 40% (w/w). Results revealed that metal uptake by mustard roots increased with sludge concentration, although root-to-shoot translocation remained limited. Cd exhibited biomagnification from plant shoots to aphids, but not to ladybirds. Zn showed consistent biomagnification across all trophic levels, while Pb displayed limited transfer at both trophic transitions. Aphids efficiently eliminated Cd through honeydew excretion, and metal sequestration occurred during ladybird metamorphosis. Notably, biomass and predation rates of ladybirds were statistically unaffected (p > 0.05) across treatments, indicating no lethal or sub-lethal effects. These findings highlight the complex dynamics of trace metal movement in soil–plant–insect systems and provide insight into ecological risks associated with sludge application.

2.06.P–We025 Preliminary Study on Transfer Kinetics of Per- and Polyfluoroalkyl Substances from Food Contact Materials into Foods

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Per- and polyfluoroalkyl substances (PFAS) are used in food contact materials (FCMs) due to their water and oil repellency and thermal stability. Although PFAS have been detected in paper-based FCMs, PFAS transfer kinetics from FCMs into food remain unclear. This study aimed to characterize PFAS transfer from FCMs into food via extraction tests.

FCMs were selected based on our preliminary screening. Glass fiber and paper-based products were immersed in n-heptane and ultrapure water at 25°C and 60°C for up to 7 days. PFCA concentrations in the solutions were quantified by liquid chromatography-tandem mass spectrometry. We evaluated equilibrium levels, transfer rate constants, and estimated daily intakes (DI).

Transfer behavior differed among FCM material types. For instance, PFHxA in paper-based products showed higher transfer rate constants (1.79 /day) and equilibrium fractions (36%) than those in glass fiber products, for which the transfer rate constants and equilibrium fractions were 0.59 /day and 3 %, respectively. Furthermore, the estimated DI of PFOA, assuming consumption of a meal using the tested product, was up to 0.023 ng/(kg day), corresponding to 3–35% of the reported DI in Japan. These findings suggest that the transfer may occur under realistic usage conditions and contribute to human exposure via FCMs.

This study provides important baseline data for assessing potential human exposure to PFAS derived from FCM contamination. Future studies should expand the range of target products, compounds, and extraction conditions to clarify the conditions that promote the transfer.

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2.06.P–We026 Development of a Screening Test for the Mobility of Polar and Ionisable Substances in the Environment

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The partitioning of chemicals to components of soils and sediments is an important aspect of their environmental fate and mobility. Screening level assessment approaches to identify potentially mobile substances have generally been based on KOC, because organic matter plays a dominant role in the adsorption of many substances to surface soils. However, there are concerns about the usefulness of the KOC concept to indicate the potential mobility of ionisable substances, principally because: (1) adsorption to organic matter is less important for some ionisable substances; and (2) levels of organic matter in subsurface soils are much lower than in surface soils, so other interactions may be more dominant in those media. Currently, there is a lack of suitable alternative metrics by which the other interactions between substances and components of soils and sediments can be measured.
The OECD TG 121 screening method for the measurement of KOC on an HPLC system is often carried out as a simple, quick and cheap method that provides consistent results. The cyanopropyl stationary phase allows for the interaction of polar and non-polar groups of a chemical, but it does not include other interactions that may be influential in determining the adsorption properties of more polar and ionisable substances, including ion exchange interactions and some polar interactions.
It may be possible to extend the general concept of the OECD TG 121 screening test to consider additional interactions that occur in soils and other subsurface media, which are especially relevant for polar and ionisable substances. This work investigates whether state-of-the-art mixed mode stationary phases might have the potential to act as surrogates for surfaces where adsorption occurs in soils or sediments reflecting such interactions.
The most promising HPLC solid phases for the intended purpose were identified, and tests were performed with more than 50 substances using strong cation exchange (SCX) and weak cation exchange (WCX) columns, both combined with reversed phase material. The results obtained for cationic test substances present a promising basis for the development of an extension of the OECD TG 121 method. The results of this study are intended to provide a possible solution to better understanding the potential mobility of ionisable chemicals in the environment and improve the mobility assessment of polar and ionic substances in low organic carbon soils and subsurface media.

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2.06.P–We027 Insights Into the Distribution and Accumulation of PFAS in the Soil-crop Continuum Using a Mass Balance Analysis Strategy

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Per- and polyfluoroalkyl substances (PFAS) have been widely detected not only in wastewater, but also in surface water, reclaimed water, and drinking water. Among PFAS, perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) have been classified by the International Agency for Research on Cancer (IARC) as Group 1 and Group 2B carcinogens, respectively. The widespread occurrence of PFAS in the environment has therefore raised increasing concerns regarding their accumulation in food crops and subsequent human exposure through the food chain. Irrigation using reclaimed water or PFAS-contaminated surface water is considered a major pathway for PFAS entry into agroecosystems. Previous studies have shown that long-chain PFAS tend to be retained in soils, whereas short-chain PFAS exhibit

greater mobility and accumulation in the aerial tissues of crops. However, the complex interactions among soil properties, plant physiology, PFAS characteristics, and environmental conditions that collectively govern PFAS accumulation within the soil-crop continuum remain poorly understood. Therefore, this study aimed to investigate the distribution and accumulation of six legacy PFAS in lettuce (Lactuca sativa), using a soil pot experiment designed to simulate field conditions with a total PFAS concentration of 10 ng L^{-1}. Concentrations of PFAS in soils, pore water, roots, and shoots were quantified using LC-QTOF/MS, followed by mass balance analysis to evaluate PFAS partitioning and transport within the soil-crop system. Results showed that most PFAS were retained in soils and soil pore water, while only a small fraction accumulated in shoots, particularly for short-chain PFAS. In addition, PFAS exposure affected root development, suggesting adverse effects on plant growth and the potential for reduced crop yield. Findings from this study provide important insights into the environmental fate of PFAS in agricultural systems and may support future prediction of PFAS residues in leafy vegetables, as well as the development of mitigation strategies to reduce PFAS contamination in soils and minimize human dietary exposure.

2.06.P–We028 Quantification and Characterisation of Microplastics in Retail Mussels: is There Cause for Concern?

Microplastics (MPs) are ubiquitous contaminants in marine ecosystems and an emerging concern for seafood safety and human exposure. Filter-feeding bivalves, such as mussels, readily accumulate MPs and are consumed whole, making them effective bioindicators and direct vectors of dietary exposure. This study quantified and characterised MPs in retail mussels purchased from five major supermarkets in Cape Town, South Africa, encompassing locally produced and imported products. Four commercially important species were analysed (Choromytilus meridionalis, Mytilus galloprovincialis, M. edulis and M. chilensis), representing frozen whole and half-shell mussels, mussel meat, and canned mussels.
A total of 240 individual mussels (80 composite samples) were digested using potassium hydroxide, filtered, and visually analysed under stereomicroscopy with stringent contamination control and blank correction. MPs were identified and classified by abundance, size, shape, and colour following established guidelines. Microplastics were detected in 86% of individual mussels, with 967 particles recorded overall. Mean abundance was 3.58 ± 0.15 MPs per individual and 2.30 ± 0.18 MPs g^{-1} wet tissue. Although MP abundance per gram did not differ significantly among retailers, mussel product type had a significant effect, with canned mussels containing higher MP concentrations than frozen mussels and mussel meat.
Fibres dominated the MP assemblage (~45%), followed by fragments (~25%), with most particles < 2 mm in size and predominantly transparent or dark-coloured. MP abundance per individual increased with tissue mass, while MP concentration per gram decreased with increasing mussel size. The widespread occurrence of MPs across retailers, species, and product types suggests contamination at multiple stages, including environmental exposure, harvesting, processing, and packaging.
These findings provide baseline data on MP contamination in retail seafood from southern Africa and indicate that mussel consumption represents a measurable route of human MP exposure. Routine monitoring of MPs in commercially important bivalves, alongside improved aquaculture and processing practices, is recommended to support seafood safety assessments and evidence-based management.

2.06.P–We029 Assessment of Acetamiprid Toxicity in TM3 Leydig Cell Spheroids In Vitro

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Several scientific studies have confirmed the increasing presence of various agrochemicals in the

environment in the last decade. Their accumulation in air, soil or water, their long-term persistence and slow degradation in the ecosystem can have adverse effects on human health and wildlife. Currently, particular attention is paid to a relatively new class of agrochemicals called neonicotinoids (NEOs). Among the NEOs is the widely used acetamiprid, which is highly effective against pests at low doses. Acetamiprid (N-[(6-chloropyridin-3-yl)methyl]-N'-cyano-N-methylethanimidamide) is designed to target nicotinic acetylcholine receptors in insects, but its widespread use has resulted in negative effects on non-target animals such as mammals. Therefore, the determination of risks associated with negative consequences on the central nervous system, endocrine system or reproductive functions is highly relevant. Numerous experimental studies have suggested that acetamiprid negatively affects the male reproductive system, leading to decreased serum testosterone levels, altered cellular metabolic activity, and morphological changes in the testes. In the present in vitro study, we investigated the effects of acetamiprid on murine TM3 Leydig cells cultured as three-dimensional spheroids. TM3 cell spheroids were exposed to various concentrations of acetamiprid ranging from 4 μM to 500 μM for up to 7 days. Subsequently, spheroid size, shape, solidity and viability were continuously monitored and evaluated. Using a Zeiss Z1 Observer automated inverted microscope and TissueFAXS software, the development of spheroids was monitored. In case of viability, alamarBlue assay was used. The obtained results did not reveal significant changes (P > 0.05) in spheroid area (μm²), used as a size parameter, across the tested concentration range. Similarly, shape-related parameters, including roundness and spheroid firmness, remained unaffected (P > 0.05) following exposure to acetamiprid at concentrations between 4 μM and 500 μM. A slight reduction in spheroid viability was observed only at the highest tested concentrations (350 μM and 500 μM). Although these pilot findings did not demonstrate substantial alterations in the evaluated parameters of TM3 spheroids, further studies are required to elucidate the potential mechanisms underlying the effects of acetamiprid on Leydig cells and male reproductive health.

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2.06.P–We030 From Land to Sea: Environmental Drivers and Transformation Pathways of Glyphosate and Glufosinate in Tropical Coastal Waters

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This study presents the first large-scale dataset of glyphosate (GLYP), glufosinate (GLUF), and their respective metabolites, aminomethylphosphonic acid (AMPA) and 3-(methylphosphinico)-propionic acid (MPPA), based on 73 seawater samples collected along the Vietnamese coastline between May and July 2024, aboard the French research vessel ANTEA. The sampling covered a gradient from estuarine to offshore waters under contrasting hydrological conditions. AMPA (8.4-291.4 ng L-1) and GLYP (3.7-34.9 ng L-1) dominated and exhibited clear decreasing trends with salinity (Spearman R = −0.49 to −0.55, p < 0.001), indicating strong terrestrial inputs. In contrast, GLUF (10.8-35.5 ng L-1) and MPPA (10.8-49.2 ng L-1) showed lower detection frequencies and weaker spatial gradients. The integrated metric (∑Herb&Meta) was significantly correlated with dissolved silica (SiO_2; R ≈ 0.55-0.60, p < 0.001), dissolved organic carbon (DOC; R ≈ 0.45-0.52), the absorption coefficient at 254 nm (a254; R ≈ 0.40-0.48), and nitrates plus nitrites ($NO3^- + NO2^-$; R ≈ 0.30-0.40), while exhibiting negative relationships with salinity and the spectral slope S275–295 (R ≈ −0.40), highlighting co-transport with riverine organic matter and nutrients and dilution along the salinity gradient. Fluorescence-based dissolved organic matter

(DOM) indicators further revealed significant associations. The humification index (HIX) and humic-like components were positively correlated with herbicide concentrations, suggesting a preferential linkage with terrestrially derived, aromatic DOM pools. Metabolite-to-parent ratios (AMPA/GLYP) indicate that transformation predominantly occurs upstream or within river systems prior to coastal transport, with limited in situ degradation in marine waters. GLYP and GLUF exhibited distinct environmental behaviors, likely reflecting differences in usage patterns and transformation pathways. Multivariate analyses (PCA) and machine learning models (Random Forest and Elastic Net) identified SiO_2, DOC, a254, and salinity as key predictors ($R^2 \approx 0.25$-0.45), confirming dominant terrestrial control but only moderate predictive performance due to environmental complexity. Overall, this study demonstrates that herbicide transport in coastal waters is tightly coupled with DOM composition and agricultural runoff, providing new insights into the processes governing the transport and environmental exposure of emerging contaminants in large tropical coastal systems.

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2.06.P–We031 Transport of Coated-Fertilizer-Derived Microplastics and Polylactic Acid in Paddy Watershed Rivers Using Micro-Fourier Transform Infrared Spectroscopy

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Controlled-release fertilizers are widely used in paddy fields because they reduce fertilization labor and regulate nutrient release. However, after nutrient release, plastic coatings can remain in fields and drainage channels and be transported to rivers and coastal waters. Information is still limited for small coated-fertilizer-derived particles and biodegradable alternatives, such as polylactic acid, in agricultural watersheds.

This study investigated microplastics larger than 20 micrometres in the Kumaki and Otsu Rivers, which drain paddy watersheds into Nanao West Bay, Japan. Surface water was sampled in September 2025, during drainage before rice harvest, and in January 2026, during the non-cultivation period. Thirteen river and bay-water samples were collected. Water volumes of 120–400 litres were concentrated using a 10 micrometre plankton net. Samples were processed by hydrogen peroxide oxidation and sodium iodide density separation, filtered onto silicon membranes, and analyzed using micro-Fourier transform infrared imaging. Particles were identified using spectral library matching, band confirmation, optical image checking, and reference spectra. River discharge and instantaneous transport were estimated from measured width, depth and velocity.

Coated-fertilizer-derived particles were detected at all Kumaki River sites, with concentrations of 80–2940 particles per cubic metre and contributions of up to 62.9% of total microplastics. Their median long-axis length was 35.7–73.8 micrometres, indicating dominance of particles smaller than 100 micrometres. Larger particles were observed near the Kumaki River mouth during pre-harvest drainage, suggesting flushing of particles retained on paddy soils or around drainage channels. The maximum instantaneous transport at the river mouth was estimated at 2865 particles per second. Polylactic acid was detected in the lower Otsu River at 1240 particles per cubic metre in September and 100 particles per cubic metre in January, with an estimated September transport of 227 particles per second.

These results suggest that paddy watershed rivers can act as continuous pathways for small agricultural microplastics, not only during cultivation but also after field operations have ended. Micro-Fourier

transform infrared imaging was useful for tracing small source-specific particles, and the transport estimates provide a basis for linking watershed inputs with accumulation in semi-enclosed coastal waters.

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2.06.P–We032 Role of the Transpiration Stream in the Uptake and Transport of Legacy PFAS in Leafy Vegetables

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Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants that have been shown to accumulate in crops, raising concerns about potential risks to human health. Consequently, numerous studies have sought to elucidate the mechanisms governing PFAS uptake in plants to support the development of effective mitigation strategies. Current understanding primarily attributes PFAS uptake to compound-specific properties, such as chain length, and plant physiological characteristics, with mass flow via the transpiration stream often considered a key transport pathway. However, systematic investigations into how transpiration influences the transport of PFAS with varying chain lengths remain limited, constraining our ability to predict PFAS accumulation in crops under different environmental conditions. This study investigated the uptake and translocation of six legacy PFAS in hydroponically grown lettuce and spinach under varying transpiration regimes. Plants were exposed to target PFAS at 5 ng L^{-1}, and three photoperiod treatments were applied to modulate transpiration rates. Concentrations of PFAS in nutrient solutions, roots, and shoots were quantified using LC-QTOF/MS. Mass balance analysis indicated that PFAS accumulation in shoots decreased with increasing chain length. Furthermore, correlation analysis revealed a positive relationship between transpiration and shoot accumulation for PFAS with higher mobility, suggesting that transpiration-driven mass flow plays a critical role in their upward transport. These findings provide new insights into the interplay between environmental and physiological factors governing PFAS behavior in crops and contribute to improved assessment of food safety risks associated with PFAS contamination across diverse growing conditions.

2.07.P - Environmental Exposure, Effects, and Risks of Organophosphate Esters and Plasticizers

2.07.P–Tu085 Systematic Evaluation of the Carcinogenic Potential of Di-isononyl Phthalate in Humans

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Di-isononyl phthalate (DINP) is a high–molecular weight phthalate widely used in polyvinyl chloride (PVC) and other commercial products. This assessment systematically evaluates human, animal, and mechanistic evidence to determine the carcinogenic potential of DINP in humans. Peer-reviewed studies were identified through systematic PubMed and Embase searches, supplemented by regulatory reviews to capture relevant GLP and guideline-compliant studies. Mechanistic evidence was organized using the key

characteristics of carcinogens (KCCs). All evidence was critically appraised and integrated following WHO IPCS principles for cancer hazard evaluation. Four epidemiological studies assessed DINP exposure using specific metabolites. Three reported no statistically significant associations with breast cancer incidence or mortality. One small case–control study reported a statistically significant but imprecise association with prostate cancer, limited by small sample size and inadequate control for confounding. Overall, human data do not support an association between DINP and cancer. Four rodent cancer bioassays (three in rats, one in mice) identified inconsistent increases in liver, kidney, and mononuclear cell leukemia tumors. Liver tumors were observed in multiple studies and are explained by a peroxisome proliferator–activated receptor alpha (PPARα) mode of action considered not relevant to humans. Kidney tumors and mononuclear cell leukemia occurred only in specific rat strains and are attributed to rodent-specific mechanisms. These findings indicate DINP is unlikely to pose a human cancer hazard. Mechanistic evidence from 127 studies showed inconsistent or absent activity across most KCCs. DINP was not genotoxic or immunosuppressive, and observed effects on cell proliferation were consistent with rodent-specific tumor mechanisms. Epidemiological evidence does not support a link between DINP exposure and cancer in humans. Although tumors occur in rodents, their modes of action are not relevant to humans. Collectively, the evidence indicates that DINP is unlikely to be carcinogenic to humans.

2.07.P–Tu086 Distribution, Environmental Fate, and Risk Assessment of Microplastics and Organophosphate Flame Retardants in Agricultural Soils

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Agricultural soils are increasingly recognized as a major sink for plastic-derived contaminants, yet baseline data for Taiwan remain scarce. This study presents the first systematic, region-wide investigation of microplastics (MPs) and organophosphate esters (OPEs) in Taiwanese farmland soils, addressing the co-occurrence, sources, and ecological/health risks of these two co-emerging contaminant classes. Forty topsoil samples (0–10 cm) were collected from northern (n = 20) and southern (n = 20) Taiwan, covering three land-use types: open farmland, screen-houses, and greenhouses. MPs were isolated by NaCl density separation with H_2O_2 digestion, enumerated by stereomicroscopy, and identified by micro-Fourier transform infrared spectroscopy (micro-FTIR). Seventeen OPEs were extracted by ultrasonication with hexane–dichloromethane–acetone, cleaned up by Florisil solid-phase extraction, and quantified by gas chromatography–tandem mass spectrometry (GC-MS/MS). MP abundance ranged from 2.8 to 44.36 items/g (mean 10.22 items/g, south) and 4.40 to 34.38 items/g (mean 13.88 items/g, north), with particles of 25–100 μm dominating and polypropylene and high-density polyethylene as the most frequently identified polymers, consistent with mulch films, weed barriers, and packaging materials. All 17 OPEs were detected at every site, with mean ΣOPEs of 13.01 ng/g; tris(2-isopropylphenyl) phosphate, triphenyl phosphate, and tris(2-butoxyethyl) phosphate were the dominant congeners, indicating contributions from building materials, plasticizers, and agricultural inputs. Northern soils showed higher OPE burdens than southern soils. Principal component analysis and positive matrix factorization apportioned sources to plastic additives, flame retardants in building materials and foams, and urban/industrial deposition. Ecological risk quotients were generally <0.01, although tris(2-ethylhexyl) phosphate reached moderate risk in northern samples. Non-carcinogenic hazard indices for adults and children were 10^{-3}–10^{-7}, well below unity. Polymer hazard indices were highest in open farmland (340.4 south; 298.4 north). These findings establish the first baseline of MP–OPE co-contamination in Taiwanese agricultural soils, identify open farmland as a priority management target, and provide a scientific basis for source-reduction strategies and regulatory benchmarks for the Asia-Pacific region.

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2.07.P–Tu087 Mode of Action and Human Relevance Assessment for Diisononyl Phthalate (DINP)-Induced Liver Tumors in Rodents

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Di-isononyl phthalate (DINP) is a high-molecular-weight plasticizer widely used in flexible PVC products. Chronic rodent tests have shown that DINP induces liver tumors in mice and rats, which are hypothesized to occur via a rodent-specific peroxisome proliferator-activated receptor alpha (PPARα) mode of action (MOA). While PPARα activation occurs across species, the downstream biological events leading to tumor formation are generally considered unique to rodents and not relevant to humans. To evaluate whether DINP-induced rodent liver tumors occur through this PPARα MOA, a comprehensive weight-of-evidence (WoE) assessment was performed using a published MOA framework for PPARα activator-induced liver tumors. This framework includes four key events (KEs): (1) PPARα activation, (2) alteration of cell growth pathways, (3) perturbation of cell growth and survival, and (4) clonal expansion, leading to liver tumors as the adverse outcome. Animal and human data for DINP and its metabolites were systematically evaluated using modified Bradford Hill considerations, including assessment of data gaps and uncertainties. Evidence was drawn from peer-reviewed literature and unpublished laboratory studies identified through authoritative assessments and targeted PubMed searches. The WoE strongly supports KEs 1 and 3 and the adverse outcome for DINP, with KEs 2 and 4 reasonably inferred based on the overall evidence. Alternative MOAs, including genotoxicity and aryl hydrocarbon receptor activation, were not supported, while activation of PPARγ or CAR/PXR was weakly supported and based on limited in vitro data. Evidence of cytotoxicity occurred only at higher doses and later time points than those inducing PPARα activation, indicating a secondary role.
Comparative data demonstrate reduced sensitivity to DINP and its metabolite MINP in humans and non-rodent species relative to rodents. Limited human and primate data indicate no perturbation of cell growth and survival, and no evidence links DINP exposure to liver cancer in humans. Overall, the WoE indicates that DINP-induced rodent liver tumors occur via a rodent-specific PPARα MOA and are unlikely to be relevant to humans.

2.07.T - Environmental Exposure, Effects, and Risks of Organophosphate Esters and Plasticizers

2.07.T01 Silicone Wristbands Reveal Ubiquitous Human Exposure to Ortho-Phthalates and Non-Ortho-Phthalate Plasticizers in Southern California

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In the United States and abroad, ortho-phthalates and non-ortho-phthalate plasticizers continue to be used within a diverse array of consumer products. Prior California-specific biomonitoring programs for ortho-phthalates have focused on rural, agricultural communities and, to our knowledge, these programs have not measured the potential for exposure to non-ortho-phthalate plasticizers. Therefore, the potential for human exposure to ortho-phthalates and non-ortho-phthalate plasticizers have not been adequately addressed in regions of California that have higher population density. Since there are numerous sources of ortho-phthalates and non-ortho-phthalate plasticizers in population-dense, urban regions, the objective

of this study was to leverage silicone wristbands to quantify aggregate ortho-phthalate and non-ortho-phthalate plasticizer exposure over a 5-day period across two different cohorts (2019 and 2020) of undergraduate students at the University of California, Riverside (UCR) that commute from all over Southern California. Based on 5 d of aggregate exposure across two different cohorts, total ortho-phthalate plus non-ortho-phthalate plasticizer concentrations ranged, on average, from ~100,000-1,000,000 ng/g. Based on the distribution of individual ortho-phthalate and non-ortho-phthalate plasticizer concentrations, the concentrations of di-isononyl phthalate (DiNP, a high molecular weight ortho-phthalate), di(2-ethylhexyl) phthalate (DEHP, a high molecular weight ortho-phthalate), and di-2-ethylhexyl terephthalate (DEHT, a non-ortho-phthalate plasticizer) detected within wristbands were higher than the remaining seven ortho-phthalates and non-ortho-phthalate plasticizers measured, accounting for approximately 94-97% of the total mass depending on the cohort. Overall, our findings raise concerns about chronic DiNP, DEHP, and DEHT exposure in urban, population-dense regions throughout California.

2.07.T02 Spatiotemporal Distribution, Source Apportionment, and Health Risk Assessment of Atmospheric Organophosphate Esters in an E-Waste Recycling Facility

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Organophosphate esters (OPEs) are widely used as flame retardants and plasticizers, including as substitutes for restricted brominated flame retardants, and can be released from electronic waste during dismantling and recycling. This study investigated the atmospheric occurrence, gas-particle distribution, source contributions, and human health risks of OPEs at an electronic waste dismantling and recycling plant in Guanyin District, Taoyuan, Taiwan. Indoor and outdoor air samples were collected monthly from May 2023 to April 2024 at four sites in two plant areas, and 17 target OPEs were quantified using gas chromatography tandem mass spectrometry. Principal component analysis, positive matrix factorization, and 120 h backward trajectory analysis were applied to evaluate potential sources and transport pathways; exposure and risk were assessed using estimated daily intake, hazard quotient, and cancer risk calculations for adults and toddlers. Ten OPEs were detected in all samples. Chlorinated OPEs dominated the atmospheric profile. Outdoors, tris(2-chloroisopropyl) phosphate, tris(1,3-dichloro-2-propyl) phosphate, triphenyl phosphate, and tributyl phosphate were the major compounds, with concentration ranges of 0.14-6.53, 0.003-3.63, 0.01-1.41, and 0.02-1.21 ng/m3, respectively. Indoors, tris(2-chloroisopropyl) phosphate, tris(1,3-dichloro-2-propyl) phosphate, and tris(2-chloroethyl) phosphate were dominant, ranging from 0.21-9.87, 0.007-3.44, and 0.07-5.13 ng/m3. Gas-phase concentrations generally exceeded particle-phase concentrations, while alkyl OPEs showed stronger particle-phase association. Source analyses indicated contributions from plastic products, electrical and electronic materials, building materials, furniture, hydraulic oils, and lubricants, with possible influence from long-range transport from northern and eastern China during certain months. Exposure assessment showed dust ingestion as the primary pathway, followed by dermal absorption, whereas air inhalation contributed minimally. Hazard quotient values were below 1 for adults and toddlers, suggesting low non-carcinogenic risk. However, tris(2-butoxyethyl) phosphate showed potential cancer risk in both indoor and outdoor scenarios, indicating the need for exposure control and further carcinogenic risk assessment. These results provide field-based evidence for managing emerging flame retardants in circular economy facilities in the Asia-Pacific region.

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2.07.T03 Occurrence, Source Apportionment, and Health Implication of PM2.5-Bound Organophosphate Esters in Malaysia

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Particle-bound organophosphate esters (OPEs) in tropical Southeast Asia remain poorly characterized, despite rapid urban expansion, diverse emission sources, and the strong influence of the monsoon season, which may affect their distribution and transport. As a result, inhalation exposure to particulate OPEs in this region remains insufficiently understood. This study aimed to investigate the concentration of PM2.5-bound OPEs in 14 diverse microenvironments across Peninsular Malaysia, encompassing high-density urban, industrial, semi-urban/agricultural, and regional background sites. A total of 168 samples PM2.5 were collected from January 2023 to December 2023 using a High-Volume Air Sampler. OPEs collected on filters were extracted and quantitatively analyzed using GC-MS/MS. The result showed that from Σ17OPEs, the highest mean concentration was observed approximately 6.54 ± 2.59 ng/m3 at the industrial site of Gelang Patah. Across the peninsular, the chemical profile was dominated by chlorinated OPEs, with tris(1,3-dichloro-2-propyl) phosphate (TDCPP) emerging as the most abundant and frequently detected congener, followed by triphenyl phosphate (TPhP) and tris(1-chloro-2-propyl) phosphate (TCIPP). Principal component analysis and positive matrix factorization indicated that construction materials, polymer-related emissions, and flame retardant applications were the dominant sources of $PM_{2.5}$-bound OPEs, while seasonal variation was strongly influenced by the Northeast Monsoon. Risk assessment revealed that children consistently exhibited higher inhalation exposure than adults at all sites. However, all HQ and CR values remained below the risk threshold, indicating that the non-carcinogenic and carcinogenic risks were low.

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2.07.T04 Global Surface Water Occurrence of Organophosphate Esters from the AQUA-GAPS/MONET Passive Sampling Network

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Organophosphate esters (OPEs) are high-production-volume chemicals that are used as flame retardants and plasticizers in a wide variety of consumer and industrial products. Unlike legacy pollutants such as polybrominated diphenyl ethers (PBDEs), which are regulated under the Stockholm Convention, there is no coordinated global monitoring of OPEs, limiting our ability to assess their spatial distribution and the drivers of exposure on a global scale. The Aquatic Global Passive Sampling Network AQUA-GAPS/MONET was established to support the global monitoring of legacy compounds in water but can equally be applied for monitoring of emerging contaminants such as OPEs. In this study, we aimed to determine background dissolved concentrations of 14 OPEs in global surface waters and assess their relationship with latitude, population density, and potential ecological risk. To address this, we deployed silicone rubber passive samplers at over 30 freshwater and marine sites, resulting in 53 deployments worldwide including locations across the Asia-Pacific region. Of the 14 target OPEs, 13 were detected above the limit of quantification (LOQ) in at least one sample, while tripropyl phosphate (TPP) was below the LOQ in all samples. Tris(2-butoxyethyl) phosphate (TBOEP) and tributyl phosphate (TNBP) were the most ubiquitous compounds, detected at 96% of samples. The chlorinated OPEs tris(1-chloro-2-

propyl) phosphate (TCIPP) and tris(2-chloroethyl) phosphate (TCEP), and the alkyl OPE triethyl phosphate (TEP) showed the highest median dissolved concentrations (363, 142, and 355 pg/L, respectively) detected at 60, 68, and 38% of samples. Dissolved OPE concentrations spanned several orders of magnitude, from 0.004 pg/L for isopropyl triphenyl phosphate (ip-TPP) up to 5,300 pg/L for TCEP, highlighting the wide range of OPE concentrations across diverse aquatic environments. Measured concentrations were well below available aquatic predicted no-effect concentrations (PNECs, µg/L range), suggesting negligible ecological risk at background locations. These findings provide the first globally comparable passive sampling data for OPEs in surface waters and highlight the value of existing monitoring networks such as AQUA-GAPS/MONET for tracking emerging contaminants at a global scale.

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2.08.P - Innovations in Understanding the Chemical Fate and Exposure of Plastics in the Environment

2.08.P–Mo070 Study on Phenolic Endocrine-Disrupting Chemicals in Leachate from Landfill Sites in Tropical Asia

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Landfill leachate is generated when rainwater and moisture contained in waste pass through landfill waste layers, and it can act as a transport medium for chemicals derived from plastic products and other waste components. In tropical Asia, where landfill disposal remains a major waste management option and rainfall is high, understanding leachate-mediated chemical contamination is important. Phenolic endocrine-disrupting chemicals, including bisphenol A (BPA) and nonylphenol (NP), have been detected leachate from landfill in this region. However, long-term changes within the same landfill and their relationship with landfill closure remain insufficiently understood.

This study evaluated the occurrence, characteristics, and long-term trends of phenolic endocrine-disrupting chemicals in leachate from municipal solid waste landfill sites in Manila, Jakarta, Malaysia, and India from 2002 to 2025. Leachate samples were treated with solid-phase extraction and then analyzed using gas chromatography–mass spectrometry. In addition to concentration data, the concentration ratio of BPA to NP (BPA/NP ratio) was used as a compositional indicator to reduce the influence of rainfall-driven dilution and changes in leachate volume.

BPA/NP ratio showed increasing trends at closed landfill sites in Manila, Malaysia, and India, whereas no clear increase was observed at the active landfill site in Jakarta. This pattern suggests that the relative increase in BPA at closed sites cannot be explained solely by hydrological dilution. Instead, closure-related changes in internal landfill conditions may influence the behavior of phenolic contaminants and may be associated with the secondary generation or release of BPA from polymer-containing waste, including polycarbonate and BPA-based epoxy resin.

These findings indicate that phenolic endocrine-disrupting chemicals are present in landfill leachate from tropical Asia and that their composition can vary depending on landfill management stage. BPA/NP ratio may be a useful indicator for evaluating long-term changes in leachate contamination under conditions strongly affected by rainfall and dilution. This study provides field-based evidence that landfill closure can influence the environmental behavior of plastic-derived contaminants in tropical Asian landfill systems.

2.08.P–Mo071 Polymer-Specific Density Distributions of Microplastic Aggregates Reveal Their Differential Settling Behaviors in Tokyo Bay Seawater

Yutaka Kameda[1] and Emiko Fujita[1] (1)Chiba Institute of Technology

Understanding the fate of microplastics (MPs) in marine environments remains challenging, particularly due to the limited availability of long-term, high-resolution observational datasets. A persistent discrepancy exists between global MP load estimates and concentrations reported by field monitoring programs. In particular, in situ quantification of settling fluxes and deposition velocities is technically difficult, as sediment-trap deployments require substantial cost, labor, and long-term maintenance. Consequently, many previous studies have relied on theoretical sedimentation models—most commonly Stokes-type equations—to infer MP depositional dynamics. However, these models require accurate measurements of particle size and effective density in situ, and such datasets are scarce, especially for MP-containing aggregates in coastal seawater.

In this study, we present the first monitoring results characterizing both size distributions and in situ density spectra of MP-bearing aggregates (>20 μm) in the seawater of Tokyo Bay. Aggregates were collected using a 10-μm plankton net and subsequently fractionated into discrete density classes via cascade density separation using sodium iodide solution. Each density fraction was digested using a modified Fenton reaction, and MPs >20 μm were identified, quantified, and polymer-typed using imaging micro-Fourier transform infrared spectroscopy. Microscopic imaging prior to digestion enabled direct measurement of aggregate dimensions, providing pair-matched datasets of size, density, and polymer composition. Using these empirically derived values, polymer-specific deposition velocities were estimated based on theoretical settling models. The resulting deposition patterns were further compared with polymer compositions of MPs in seabed sediment samples from Tokyo Bay to evaluate consistency between predicted and observed depositional signatures. This integrated monitoring and analytical framework provides rare observational evidence for polymer-dependent settling behavior of MP-containing aggregates in a semi-enclosed coastal system and offers a methodological pathway to reduce uncertainty in global MP fate modeling.

2.08.P–Mo072 Assessment of Polymer-Specific Deposition Dynamics of Microplastics (>20 μm) Using Sediment Traps in a Eutrophic Lake

Yutaka Kameda[1] and Emiko Fujita[1] (1)Chiba Institute of Technology

The vertical transport and deposition dynamics of microplastics (MPs) represent a critical yet insufficiently resolved component of their environmental fate in aquatic ecosystems. Understanding when, how, and which polymers transition from the water column to benthic environments is essential for predicting long-term accumulation, ecological exposure, and biogeochemical implications. Although most synthetic polymers—particularly polyolefins—exhibit densities comparable to or lower than freshwater and seawater, numerous studies now suggest that aggregation processes can facilitate particle settling. Interactions with suspended inorganic minerals, microbial biofilms, phytoplankton, and extracellular polymeric substances can modify the physicochemical properties of MPs, effectively increasing particle density, hydrodynamic drag, and settling efficiency. However, key knowledge gaps remain regarding the polymer-specific characteristics of MP aggregates—including their size distributions, composite densities, and morphological features—that govern deposition rates and fluxes across diverse aquatic settings. Despite growing concern, empirical field observations of MPs >20 μm settling in natural waters remain limited, particularly in eutrophic lake systems where elevated primary productivity and high organic matter concentrations may accelerate aggregation and deposition relative to marine systems. Eutrophic lakes therefore represent ideal natural laboratories to assess polymer-dependent sedimentation behavior under biologically enhanced particle collision environments.

In this study, we present results from a field monitoring program designed to quantify the deposition

behavior of MPs larger than 20 μm in one of Japan's most eutrophic freshwater lakes. Sediment traps were deployed at 1.0, 2.5, and 4.5 m depths and retrieved at two-month intervals to capture temporal variation in deposition fluxes. Retrieved particles were analyzed using micro-Fourier transform infrared imaging, enabling polymer-specific identification of 16 different materials. In addition to polymer classification, the workflow allowed measurement of size distributions of MP-containing aggregates and characterization of polymer-dependent deposition patterns.

2.08.P–Mo074 Development of a High-Resolution Analytical Method for Detecting Biodegradable Microplastics (>20 μm) in Surface Waters and Sediments Using Micro-FTIR Imaging

Yutaka Kameda[1] and Emiko Fujita[1] (1)Chiba Institute of Technology

Production and commercial use of biodegradable plastics—including polylactic acid (PLA), polyhydroxybutyrate (PHB), polybutylene adipate terephthalate (PBAT), and polybutylene terephthalate (PBT)—have expanded rapidly as policy-driven substitutes for traditional polyolefins. In Japan, for example, agricultural films, seedling pods, and protective field materials are increasingly manufactured from these polymers, and governmental guidelines explicitly encourage their adoption to mitigate polyolefin-derived MP emissions to marine ecosystems. Biodegradable polymers are commonly assumed to mineralize into carbon dioxide and water via hydrolysis and microbial activity within soil or compost environments over timescales ranging from months to several years. However, emerging evidence suggests that their degradability in aquatic environments—including surface waters, sediments, and low-nutrient marine systems—may be substantially reduced. Several recent experimental and field studies indicate that these materials may persist for extended periods, and in some cases fragment into microplastic forms more rapidly than conventional polymers. This raises the possibility that biodegradable MPs may exhibit higher environmental mobility, broader dispersal potential, and distinct exposure-based ecological risks compared with traditional microplastics. Despite these concerns, virtually no systematic monitoring data exist regarding the environmental occurrence, distribution, or physicochemical characteristics of biodegradable polymer-derived MPs in aquatic systems. To address this critical gap, this study proposes and validates a high-resolution analytical workflow capable of detecting and identifying biodegradable MPs ≥20 μm in both surface water and sediment samples. The method integrates automated particle isolation with micro-Fourier transform infrared imaging, enabling polymer-specific mapping, size determination, and compositional classification of PLA, PHB, PBAT, and PBT particles with high reproducibility and spectral accuracy.
This presentation describes the development, optimization, and application of this analytical approach and discusses its potential for establishing baseline occurrence datasets and supporting future environmental risk assessments of biodegradable microplastics in freshwater and marine ecosystems.

2.08.P–Mo075 Longitudinal Distribution and Estimated Marine Export of Microplastics Larger Than 20 μm in the Klang River, Malaysia

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Urbanized rivers are important pathways for microplastic transfer from land to coastal seas, but source contributions and transport loads remain uncertain, especially for small particles. The Klang River flows through the Kuala Lumpur metropolitan region and discharges to the Strait of Malacca. This study evaluated the longitudinal distribution, polymer composition and marine discharge of microplastics larger than 20 micrometres in this urbanized tropical river.

Sampling was conducted during the dry season from 15 to 19 June 2025. Surface water was collected at 16 river sites from upstream reaches to the estuary, together with one wastewater treatment effluent and one residential drainage sample. Water volumes of 10–50 litres were concentrated in the field using a 10

micrometre plankton net. Samples were treated by oxidation and density separation, filtered onto silicon membranes, and analyzed by micro-Fourier transform infrared imaging. Microplastics were identified, counted and measured. Transport loads were calculated at 13 sites where river width, depth and velocity could be measured.

Microplastic concentrations in river water and drainage samples ranged from 12 to 271 particles per litre. Concentrations were generally lower upstream, higher in the middle reaches, and lower near the estuary, where dilution and dispersion by seawater may have affected concentrations. The mean of site-level median particle sizes was 66.5 ± 19.0 micrometres, showing that fine particles dominated. Principal component analysis of polymer composition separated the sites into groups interpreted as domestic and sewage influence, industrial influence, and riverbank retention or accumulation hotspots. The residential drainage and wastewater treatment effluent were classified with the domestic and sewage group, suggesting a broad contribution from wastewater-related sources. Sites with a higher proportion of industrial land use showed a marked increase in transport load.

The estimated microplastic discharge to the coastal sea reached approximately 2.3 × 10^7 particles per second under the observed dry-season conditions. These findings indicate that combining polymer composition, land-use information and field-based discharge measurements can help identify widespread domestic inputs and localized industrial contributions. The approach provides evidence for prioritizing monitoring and mitigation in rapidly urbanizing watersheds.

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2.08.P–Mo076 Microfragmentation of Biodegradable Plastics Driven by Biological Weathering in Freshwater

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Biodegradable plastics have gained attention as alternatives to conventional petroleum-based plastics; however, under incomplete degradation conditions in freshwater environments, they may undergo fragmentation and generate microplastics (MPs). Nevertheless, microfragmentation processes driven by biological weathering and the quantitative assessment of the resulting MPs remain poorly understood. In this study, polystyrene (PS) as a representative petroleum-based plastic and polylactic acid (PLA) and poly(butylene adipate-co-terephthalate) (PBAT) as biodegradable plastics were selected to comparatively investigate their microfragmentation behavior driven by biological weathering in freshwater environments. In particular, this study aimed to comprehensively evaluate the effects of biofilm formation and structural deterioration on the generation of MPs. To this end, biofilm formation and microbial community composition on film surfaces were analyzed, and structural changes were assessed using SEM, FT-IR, and GPC. Additionally, film-derived MPs were quantitatively determined on a mass basis using pyrolysis GC/MS. The hypotheses of this study were as follows: (1) biodegradable plastics (PLA and PBAT) exhibit higher biological weathering intensity than PS, and (2) these differences in weathering intensity determine microfragmentation patterns and the generation of MPs. This study is expected to elucidate the link between biological weathering and microfragmentation of plastics in freshwater environments, and contribute to understanding the environmental fate and potential exposure pathways of biodegradable plastics.

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2.08.P–Mo077 Status Quo in Prediction of Diffusion Coefficients of Additives in Polymers

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Predictive modeling of additive diffusion in polymers has transitioned from scientific research to a regulatory tool for materials science and environmental toxicology. Government agencies, European Food Safety Authority (EFSA), U.S. Food and Drug Administration (FDA), accept validated models to demonstrate compliance with regulations for food-contact materials. This approach significantly reduces reliance on costly and time-consuming experimental migration testing. For human health and the environment protection, chemical regulations require that these models provide a “reasoned overestimation” of real-world migration. The current status quo is shifting from semi-empirical “worst-case” correlations to advanced mechanistic frameworks. Key research trends include using molecular dynamics to investigate microscopic transport mechanisms and integrating machine leaning with molecular descriptors for rapid, data-driven property predictions. Additionally, predictive modeling is expanding its applications to sustainable materials like bio-based polylactic acid, recycled plastics, etc. However, substantial challenges remain. Standardized parameters for glassy polymers like polystyrene are often inadequate, leading to systematic underestimation of diffusion coefficients requiring urgent refinement. Furthermore, accurately predicting the effects of plasticization, polymer swelling, and environmental weathering on diffusion coefficients remains complex. Resolving these gaps is essential for robust chemical exposure assessments. This study examines the current state and challenges in predicting diffusion coefficients of additives within polymers.

Key-words: diffusion coefficient; polymer; additive; predictive model; machine learning

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2.08.P–Mo078 Standing Stock and Source Attribution of Microplastics in the Tsurumi River Estuarine Ecosystem, Japan

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Thompson et al. (2004) identified a discrepancy between the cumulative production of plastics and the amounts observed in the environment, suggesting the existence of microplastics as a previously overlooked fraction. Over the past two decades, in addition to this discrepancy, extensive research has been conducted worldwide to characterize the environmental occurrence of microplastics, driven by concerns regarding ecological and human health risks. However, microplastic distribution within ecosystems and the pathways through which they are transferred across food webs to organisms remain poorly understood.
This study aims to quantify the standing stock of microplastics and elucidate their dynamics and sources within the Tsurumi River estuarine ecosystem, Japan, a system known for relatively high microplastic contamination. To address this challenge, we integrated ecosystem modeling with field observations of microplastics.
Our results indicate that microplastics with particle sizes of 20 to 5,000 μm are present at approximately 9 g m^{-2} within the estuarine ecosystem. Of this total, 93.5% was associated with sediments, 1.0% with river water, and 5.4% entangled with algae, while less than 0.1% was present in animal biomass. These findings suggest that sediments act as the primary sink for microplastics in tidal flat environments. Source apportionment analysis identified several dominant pathways through which microplastics are transferred to organisms within the ecosystem.

Overall, this study provides a quantitative framework for linking environmental distribution, trophic transfer, and source attribution of microplastics, thereby advancing ecosystem-based risk assessment and informing effective management strategies.

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2.08.P–Mo079 Plastics Driven Endocrine Disrupting Phthalates Found in Particulate Matters of Northeast Asia Air Samples

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Phthalates are commonly used as a plastic plasticizer in various fields, including cosmetics and medical devices. Due to their widespread use, phthalates can be found in water, atmosphere, and soil. They are known as endocrine disruptors and are regulated accordingly. However, they continue to be widely used due to the lack of adequate substitutes. While phthalates are designated and monitored as water pollutants, there are no current regulations in the air, leaving them in the regulatory blind spot. Particulate-bound phthalates (PBPs) refer to phthalates that are adsorbed to PM2.5 in the atmosphere. Although PBPs are present in the air with gaseous phthalates. However, they are known to have longer persistence and are more difficult to degrade than gaseous state. PBPs can enter into the human body through inhalation, and as a particulate matter, they may remain for a long time. This is significant because long term exposure to PBPs can be harmful to health. PBPs are often regarded as proportional to PM2.5 concentration because they are adsorbed to PM2.5. To confirm this relationship, we aimed to investigate the correlation between PBPs and PM2.5 across four countries in Northeast Asia. PBPs and PM2.5 concentrations were analyzed for one month in five cities in Northeast Asia, Beijing, Seoul, Seosan, Ulaanbaatar, and Noto. The correlation between total PBPs and PM2.5 concentration in five cities was weak ($R2 = 0.220$), but rather, there was a strong correlation between plastic waste and total PBPs ($R2 = 0.951$). Even at the same PM2.5 concentration, regions with large plastic waste emissions will have a significant impact on PBP concentration, while regions with small plastic waste emissions can expect relatively little impact on PBP concentration. PBP cannot be predicted properly with air quality prediction using PM2.5. This suggests that PBP is a blind spot pollutant whose exposure can be misguided due to the presence of overall PM2.5.

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2.08.P–Mo080 Comprehensive Analysis of Additives in Recycled Pellets Using Pyrolysis GC-MS

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Toward the establishment of a circular economy, plastic recycling is being promoted globally. To reduce potential chemical exposure through recycled plastics and to ensure the safety of recycled plastic materials and products placed on the market, there is an urgent need to establish analytical methods capable of comprehensively identifying chemicals contained in plastics.
In this study, a screening approach using pyrolysis gas chromatography–mass spectrometry (Py-GC/MS) was employed to develop a simple and comprehensive analytical method. The objectives were (i) to identify organic compounds in recycled pellets, and (ii) to evaluate the validity of the proposed method. A total of 28 recycled pellet samples were analyzed. Each sample was cut into approximately 0.5 mg pieces and directly introduced into the Py-GC/MS without pretreatment, and semi-volatile components in the samples were thermally desorbed and analyzed. Among the detected compounds, those with a mass

spectral match of 70% or higher and a retention index deviation within ±20 were selected as candidate identifications.
From 28 recycled pellet samples, 10 ultraviolet (UV) absorbers, 9 antioxidants and their degradation products, 15 plasticizers, 8 fragrance compounds, and 13 other substances were detected. These results indicate that recycled pellets contain a wide variety of chemicals with diverse functions. In addition, target analysis was performed on the same samples for 13 UV absorbers (10 benzotriazole and 3 benzophenone UV absorbers) for which reference standards were available, and the results were compared with those obtained in this study. The proposed method was able to detect compounds present at medium to high concentrations (approximately ≥2 ng/g). These results demonstrate that the proposed method is effective as a simple and comprehensive qualitative approach for identifying chemical substances in recycled plastics.
Furthermore, its applicability to recycled pellet samples with complex compositions suggests that the method can be extended to a wide range of plastic materials. This approach may contribute to the development of practically applicable comprehensive analytical methods in industrial settings. In addition, it has potential applications in the assessment of chemical exposure risks associated with recycled plastics and in the safety evaluation of recycled plastic products.

2.08.P-Mo108 Airborne Microplastic Dynamics During Extreme Weather Events in Taiwan: Transport Mechanisms, Particle Characteristics, and Exposure Risks

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Airborne microplastics are emerging atmospheric contaminants that may affect human health and ecosystems. In Taiwan, extreme weather events such as typhoons, transboundary haze, and hailstorms occur frequently, but their role in controlling airborne microplastic transport, redistribution, and risk remains poorly understood. This study evaluated how contrasting weather events influence airborne microplastic concentrations, physical characteristics, polymer composition, transport pathways, and ecological risk. Thirty-one air samples were collected during two typhoons, one haze event, and one hailstorm, covering periods before, during, and after documented events. Samples were analyzed microscopically for particle shape, color, and size, while polymer types were identified using micro-Fourier transform infrared spectroscopy. Multivariate analysis was performed by applying Principal Component Analysis to identify the main factors influencing variation and simplify the data structure. Hierarchical Cluster Analysis was used to group microplastics with similar features and examine similarities and differences among these groups. Five-day backward air-mass (120 hours) trajectories were also used to assess potential long-range transport sources. The results showed clear event-dependent variation in airborne microplastic concentrations. During Typhoon 1, intense rainfall reaching 130 mm coincided with a decrease in microplastic concentration to approximately 40 items/m³, suggesting rainfall-driven dilution and wet removal. In contrast, Typhoon 2 had much lower rainfall, with a peak of only 10 mm, but showed substantially higher concentrations, reaching approximately 200 items/m³, indicating that limited rainfall combined with wind activity may promote particle suspension and accumulation. Backward trajectory analysis further indicated that incoming air masses may contribute to microplastic deposition through regional transport. Ecological risk remained persistently “Very High” across five of six sampling periods, with index values exceeding 9,000. These findings suggest that extreme weather events influence airborne microplastics through interacting mechanisms, including resuspension, long-range transport, accumulation, dilution, atmospheric degradation, and wet deposition. This study advances understanding of atmospheric plastic pollution under climate-related weather disturbances in a subtropical island environment.

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2.08.P–Mo073 Ecotoxicological Evaluation of Microplastics with Different Particle Sizes

Microplastics (MPs), generated from the fragmentation of plastic products as well as from cosmetics and synthetic fibers, have become a global environmental concern due to their widespread presence in aquatic systems, the atmosphere, and biota. However, conventional ecotoxicity tests have primarily been developed for water-soluble chemicals and are therefore limited in their ability to assess particle-specific physical effects, such as adhesion to organism surfaces, interactions with the digestive tract, and competition with food particles.
In this study, we developed a novel test system to evaluate the physical effects specific to MPs using Daphnia magna as a model organism. To ensure reproducibility and precise particle size control, commercially available spherical polystyrene (PS) particles (1, 3, 10.5, and 31.4 μm) were used. To eliminate potential interference from dispersant additives, PS suspensions were pretreated by centrifugation to separate supernatant and particle fractions, which were subsequently tested independently.
An extended acute immobilization test was employed, consisting of the standard 48-h OECD TG202 test followed by continued observation up to 96 h under feeding conditions. This approach enabled the evaluation of MP effects on feeding behavior and nutrient uptake.
The results showed no apparent adverse effects for larger particles (31.4 and 10.5 μm), whereas smaller particles (3 and 1 μm) significantly increased mortality even after the initiation of feeding. Microscopic observations confirmed particle accumulation in the digestive tract, while excretion was not completely inhibited, suggesting that mortality was not caused by intestinal blockage but by reduced nutrient uptake due to interference with feeding. In addition, 1 μm particles adhered to the gill region and body surface, indicating that physical interactions contributed to early acute effects. Furthermore, strong toxicity was observed in the supernatant fraction, indicating that additives in the dispersant, rather than the particles themselves, were responsible for the observed toxicity.
These findings highlight the importance of distinguishing particle-specific physical effects from those of dispersants and additives in MP ecotoxicity assessments and suggest that MP toxicity should be reconsidered from the perspective of feeding interference and impaired nutrient uptake.

2.08.P–Mo081 Occurrence of Plastic Additives in Microplastics from Sediments of Tokyo Bay and Their Contribution to Sediment Contamination

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Microplastics (MPs) are widely distributed in marine environments and accumulate in sediments, a major environmental sink for plastic debris. Plastics contain various additives and can sorb organic contaminants, suggesting that MPs may act as carriers of chemical substances. Although the occurrence of MPs in marine sediments has been widely reported, their contribution to chemical contamination in sediments remains poorly quantified. This study investigated the occurrence of additives in MPs isolated from coastal sediments and evaluated their contribution to additive concentrations in sediments.
MPs isolated from Tokyo Bay sediments in a previous survey were analyzed. The particles ranged from 315 μm-1 mm and 1-5 mm, and consisted mainly of polypropylene, polyethylene, and polyethylene–polypropylene mixtures. Corresponding sediment samples from the same locations were also examined. Target compounds included bisphenols, alkylphenols, benzotriazole ultraviolet stabilizers (UV-326, UV-327 and 8 compounds), brominated flame retardants (decabromodiphenylether: BDE209, decabromodiphenylethane: DBDPE), oxidation product of Irgafos168 (TDTBPP), polychlorinated biphenyls and triclosan. After extraction and purification, compounds were identified and quantified

using gas chromatography-electron capture detector and gas chromatography-mass spectrometer. Several additives, including nonylphenol, UV-326, UV-327, BDE209, DBDPE, TDTBPP and triclosan, were detected in MPs. Large MPs (>1 mm) tended to retain higher concentrations of hydrophobic additives, suggesting enhanced release from smaller particles due to their larger specific surface area. Despite their presence, contributions to total sediment concentrations were below 0.1% even at maximum values, except for TDTBPP, which reached up to approximately 1%. Less hydrophobic compounds such as nonylphenol and triclosan showed indications of relationships between concentrations in MPs and sediments, whereas highly hydrophobic brominated flame retardants did not.
MPs in Tokyo Bay sediments were associated with various plastic additives, though their direct role in sediment contamination seemed limited. The results indicate that additive behavior in MPs varies depending on particle size and chemical hydrophobicity, suggesting that MPs do not function as a uniform carrier phase for contaminants. Nevertheless, MPs containing additives may still act as vectors for contaminant transport if sediments are disturbed.

2.08.P–Mo082 Pyrolysis Gas Chromatography-Mass Spectrometry Method Development to Detect Halogenated Polymer Polychlorotrifluoroethylene

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Polychlorotrifluoroethylene (PCTFE), is a halogenated high-performance fluoropolymer widely used in medical and aerospace packaging. PCTFE is synthesised from the homopolymerisation of chlorotrifluoroethylene (CTFE). The fluorine (F) and chlorine (Cl) in its structure are densely arranged, providing excellent chemical corrosion resistance and inertness. However, its manufacturing, use, and transformation via physical, chemical, and photochemical pathways release halogenated micro- and nanoplastics (MNPs), leading to potential human and environmental risks. Currently, the information on the occurrence, fate and exposure pathways is inadequate due to the lack of available analytical methods for environmental monitoring.
This study aimed to develop a Pyrolysis Gas Chromatography Mass Spectrometry (Py-GC-MS) analysis method to accurately quantify PCTFE in a range of matrices. The single-shot mode of a multi-shot micro-furnace pyrolyser-PY-3030D (Frontier Lab Ltd., Fukushima, Japan), coupled with a GC-MS - GC2030 (Shimadzu Corporation, Japan), was used to develop methods to identify and quantify key pyrolytic markers. Three homologous series of markers containing Cl and F, ranging from dimers to hexamers, were tentatively identified (listed as A, B, and C series).
When pyrolysed with polyvinylchloride (PVC) to simulate common blister pack formulations, the B series markers suffered extreme suppression theorised to be due to pyrolytic reactions with HCl radicals from the PVC. Meanwhile, series C oligomers showed both enhancement and suppression. Series A showed minimal interference and was reproducible throughout the experiment. These findings suggest that PVC and environmental matrices can influence the formation of the PCTFE pyrolysis products, affecting quantification that signify the importance of selecting appropriate pyrolytic markers. The reproducible and systematic response of series A in polymer mixtures emphasizes its robustness and suitability for accurate quantification of PCTFE in complex environmental matrices. The next steps in the research will be to test complex environmental matrices (e.g. soil) through spike and recovery tests, on the formation of the PCTFE pyrolytic markers.

2.08.P–Mo083 Mechanistic Insights into Polyvinyl Alcohol Biodegradation: Integration of Single-Strain Experiments and AI-Based Enzyme Structure Modeling

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Polyvinyl alcohol (PVA) is a water-soluble polymer widely used in applications such as unit-dose

detergent packaging. After use, dissolved PVA enters municipal wastewater systems and is biodegraded into carbon dioxide and water by activated sludge under aerobic conditions, as demonstrated by standardized tests such as OECD Test Guideline 301B. We have shown that PVA degradation in activated sludge is mediated by intracellular enzymes of Gram-negative bacteria, including Sphingopyxis species isolated from wastewater treatment plants, and identified polyvinyl alcohol dehydrogenase (PVADH) as a key enzyme initiating PVA degradation via oxidation of hydroxyl groups on the PVA backbone.

In this study, we investigated the biodegradation behavior of water-dissolved PVA under conditions relevant to wastewater treatment by combining single-strain biodegradation tests with biomolecular structure prediction. A PVA-degrading Sphingopyxis strain, detected in wastewater systems and capable of using PVA as the sole carbon source, degraded more than 90% of PVA within 48 hours, and the degradation rate indicator showed good correlation with activated sludge test results. Biodegradation tests were also conducted for PVA materials with different degrees of saponification. Partially saponified PVAs were biodegraded, and their degradation rate indicators correlated well with results from activated sludge tests, indicating that such PVAs can be efficiently degraded by PVA-degrading microorganisms of natural origin.

To gain molecular-level insight, we analyzed the interaction between PVADH and PVA using Boltz-2, an AI-based biomolecular structure prediction model. The three-dimensional structure of PVADH predicted from its amino acid sequence showed similarity to cytochrome-c–pyrroloquinoline quinone (PQQ)-dependent alcohol dehydrogenases. Docking simulations suggested that PVA binds within the enzyme pocket in proximity to the PQQ coenzyme. These results support a degradation mechanism in which PVADH oxidizes hydroxyl groups on the PVA chain via a PQQ-mediated reaction. Similar analyses of partially saponified PVAs with different degrees of saponification also indicated stable binding within the PVADH pocket. Overall, the structural analysis results are consistent with the biodegradation behaviors observed in activated sludge and single-strain tests and support the proposed microbial degradation mechanism of PVA under aerobic wastewater treatment conditions.

2.08.P–Mo084 Rapid Mass Conversion and Ecological Risk-Oriented Quantification of Environmental Microplastics across Diverse Shapes

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<p>Microplastics monitoring has been fundamentally constrained by a critical inconsistency: field investigations predominantly report particle number concentrations, whereas environmental risk assessment and flux estimation rely primarily on mass-based metrics. This disconnect introduces substantial uncertainty in evaluating environmental loads, transport fluxes, and ecological risks. Here, we present a rapid and accurate framework for mass conversion of environmental microplastics across diverse particle shapes by integrating shape-aware modeling with AI-assisted image analysis. Based on a large environmental dataset, microplastics were automatically classified into fibers, fragments, and pellets using a deep neural network (ResNet50), achieving high classification accuracy (>92%). To overcome limitations associated with conventional two-dimensional imaging, we incorporated thickness estimation and introduced morphology descriptors (e.g., circularity) to better characterize irregular particle geometries, particularly pellet-like particles. Building upon these parameters, we established a suite of shape-specific mass conversion models that enable robust estimation of particle mass directly from imaging-derived features. Compared with conventional empirical approaches, the proposed framework substantially reduced estimation bias (up to ~7-fold improvement) while markedly improving computational efficiency (saving approximately 2 hours per 100 particles). In addition, we highlight emerging AI-assisted image correction strategies that mitigate aggregation artifacts and segmentation discontinuities in instrument-based imaging, further enhancing the reliability and consistency of

microplastic quantification. Importantly, converting particle number into environmentally relevant mass metrics enables improved linkage between monitoring data and ecological risk assessment, pollutant flux estimation, and exposure-response analyses. Overall, this work bridges the long-standing gap between number-based observations and mass-based environmental assessment, providing a scalable, field-compatible, and high-throughput solution for next-generation microplastics monitoring. The proposed framework also demonstrates strong potential for future standardization and integration into environmental regulatory and risk assessment frameworks.</p>

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2.08.P–Mo085 Biodegradable Mulch Film: A Hidden Source of Ultraviolet Absorbers and Microplastics in Agricultural Environments

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In recent years, the market of biodegradable mulch films has grown rapidly, raising concerns about plastic pollution and environmental safety of their organic additives, particularly ultraviolet absorbers (UVAs) with persistence and highly toxicity. In this study, a one-year field mulching experiment was conducted to systematically investigate the occurrence, release behavior, and crop uptake risks of UVAs under real agricultural conditions. Microplastics began to generated at the fourth month after mulching, after one year, the abundances of biodegradable film derived- microplastics in the soils were 250– 483 items/kg. Biodegradable mulch films contain extremely high concentrations of UVAs (Σ22UVAs: 92.5–1604.9 μg/g), which was 1.6–27.7 times than conventional polyethylene film (Σ22UVAs: 58.0 μg/g). Analysis of residual films collected at different time points over one year showed that after one year of mulching, the release rates of UVAs from biodegradable films reached 50.4% to 99.2%. The release behavior was closely linked to the physicochemical properties of the film components. Over time, the UVAs level in the soil gradually increased. Additionally, in the three biodegradable films-mulched areas, UVAs were detected in tomato fruits (568.1–1019.8 ng/g), suggesting that long-term consumption of tomatoes grown under biodegradable mulch may pose potential exposure risks. Furthermore, agricultural workers face occupational exposure risks, as the concentration of UVAs adsorbed on silicone wristbands worn by farmers was significantly higher than that in the general population. It is estimated that the total annual release of UVAs from biodegradable mulch films globally ranges from 9.2 to 168.7 tonnes, urgent attention and regulation are needed regarding the production and application of biodegradable mulch films.

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2.08.P–Mo086 Using Solid-Phase Microextraction (SPME) for in situ detection of plastic-derived additives in marine invertebrates

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Plastic-derived additives, including phthalates and phenolic compounds, are increasingly recognized as dynamic contaminants in marine systems, with complex exposure pathways and evolving bioavailability. However, monitoring these compounds in marine organisms remains challenging, as conventional approaches rely on destructive sampling and provide only limited temporal and spatial resolution.
This study develops and applies a non-lethal, in situ analytical approach for detecting plastic-derived

additives in marine invertebrates using Solid-Phase Microextraction (SPME). We establish and optimize a SPME-based protocol to quantify a suite of common additives: dimethyl phthalate (DMP), dibutyl phthalate (DBP), di(2-ethylhexyl) phthalate (DEHP), bisphenol A (BPA), and 4-nonylphenol, directly from living organisms. The method is evaluated in sessile filter feeders, including ascidians (Microcosmus exasperatus, Polycarpa mytiligera) and the giant clam Tridacna gigas, selected for their ecological relevance and potential as bioindicators of contaminant exposure.
Field sampling is conducted in situ across seven sites spanning two contrasting marine regions: the eastern Mediterranean Sea and the Red Sea, encompassing both temperate and tropical reef environments. This design enables comparison of contamination patterns across distinct environmental regimes while preserving organism integrity. The non-lethal approach further allows repeated sampling of the same individuals, improving resolution of temporal variability and organism-level exposure.
The developed method provides a sensitive and minimally invasive tool for detecting plastic-derived contaminants in marine biota under environmentally realistic conditions. By integrating cross-regional comparisons with repeatable, non-destructive sampling, this work advances current monitoring capabilities and contributes to improved assessment of contaminant fate, bioavailability, and biological exposure pathways of plastic-associated chemicals across diverse marine ecosystems.

2.08.P–Mo087 Microplastics–Heavy Metal Co-Contamination in Soil–Plant Systems Near E-Waste Sites: Evidence of Nanoplastic Formation and Human Health Implications

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Informal e-waste dismantling is becoming a major contributor to microplastics (MPs), nanoplastics (NPs), and heavy metal contamination in the terrestrial environment. Nevertheless, their overall effects on soil-plant interactions are poorly known. This study explores the prevalence, nature, and possible hazards of MPs, NPs, and related metals in the soils and plants of informal e-waste dismantling sites.

The levels of microplastic in soils were found between 400 and 8820 Mps kg -1 with the highest concentration was detected at active dismantling sites which proves informal e-waste processing to be a significant contributor to MP pollution. Plant analysis showed that there were significant amounts of MP in both edible vegetables and shrubs with roots having the highest concentrations over above ground tissues, with some of the highest concentrations of up to 31,600 MPs kg -1, especially in root vegetables. The majority of detected MPs were small (<300 μm) and very weathered, which means that they were highly fragmented and were found to form NPs.

The characterization of polymers by μ-FTIR revealed a wide variety of materials, both traditional plastics and e-waste-specific polymers, such as PVC, ABS, styrene copolymers, and electronic resins. FESEM-EDX analysis also indicated that MPs are often adsorbing toxic metals, Pb, Cd, Cu, and Hg, and it may be important to note that they are vectors and enable the transport and bioavailability of metals. Higher bioconcentration and translocation factors are evidence of the movement of MPs and NPs in the soil to plants.

The exposure assessment indicates that there are significant daily and annual intakes of MPs in the form of vegetables, and children were found to be the most vulnerable population. All in all, the results highlight the problems of environmental and human health risks of informal e-waste dismantling, which highlights the necessity of better waste management practices and stronger food safety laws.

2.09.P - Integrative Analytical and Toxicological Approaches to Understanding

Plastics as Environmental Contaminants and Contaminant Vectors

2.09.P–We051 Screening for Potentially Hazardous Additives in Bioplastic Bags

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The use of biobased and biodegradable plastics is growing rapidly, however the potential toxicities of additive chemicals specific to these alternative materials remain unclear. This study used a panel of chemically activated luciferase gene expression (CALUX) assays to evaluated the nuclear receptors-mediated activities of biobased and biodegradable plastic bag samples collected from four Asian countries. AhR agonistic activities were detected in most of the plastic extracts obtained using a dichloromethane (DCM)/hexane mixture (1:3 v/v) as extraction solvent, and the activity levels were the strongest in biobased polyethylene (BioPE) samples from Japan and oxo-degradable PE (OxoPE) samples from Indonesia, Myanmar and Thailand. Weak ERα agonistic, AR antagonistic and PPARγ2 antagonistic activities were observed in only one butenediyl/terephthalic copolymer sample. Preliminary identification of potential AhR agonists in representative plastic extracts was attempted by combining fractionation with deactivated silica-gel and non-target analysis with two-dimensional gas chromatography–time-of-flight mass spectrometry (GC×GC–ToFMS). Compounds that could be identified in major AhR agonistic fractions included the antioxidant butylated hydroxytoluene (BHT) and a BHT derivative, the flame retardant synergist dicumene, substituted thiophenes, several plant-synthesized hydrocarbons, adipate and citrate plasticizers, and an unknown nitrogen-containing compound. The occurrence of these compounds in other bioplastic samples and their AhR agonistic potential remain to be determined.

2.09.P–We052 Evaluation of the Contribution of Resuspended Microplastics in Sediments to the Bioaccumulation of Hydrophobic Organic Pollutants in Bivalves

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Surface sediments act as a secondary source of contamination for hydrophobic compounds such as polychlorinated biphenyls (PCBs), which were used in the past but are now regulated. The phenomenon whereby chemicals continue to cause contamination even after they have been regulated is defined as legacy contamination. One factor contributing to the persistence of contamination is suspected to be the presence of microplastics in sediments, which adsorb hydrophobic contaminants and are easily suspended in water bodies. Therefore, the objective of this study was to evaluate the contribution of microplastics in sediments to the prolonged legacy contamination of PCBs.

An exposure experiment was conducted using polyethylene (PE) particles adsorbed with PCBs, which were added to the sediment and exposed to the blue mussels (Mytilus galloprovincialis). Four treatment groups were designed: the control group (CTL), the sediment group (SED: exposing only sediment), the MP feeding group (MP-I: exposing sediment and PE particles), and the MP leaching group (MP-L: exposing sediment and PE particles, but considering only the leaching of PCBs derived from PE particles). The absolute amount of CB105 (one of PCB congeners) in each treatment group was adjusted to be equal. Exposure was conducted by removing the blue mussels from the water along with their nets, stirring the sediment once a day using a magnetic stirrer, and returning them to the water after 60 minutes. After the 5-day exposure period, the gonads of four individuals from each treatment group were analyzed.

The results of the exposure experiment showed that the median CB105 concentration was 7.5 ng/g-lipid in SED, 22 ng/g-lipid in MP-I, and 7.4 ng/g-lipid in MP-L. MP-I exhibited a concentration approximately three times higher than that in SED and MP-L. Therefore, it was considered that the presence of PE particles—which tend to form suspensions during stirring in MP-I—made it easier for the blue mussel to ingest them, allowing CB105 to migrate via the digestive organs to the gonads in significant amounts. Consequently, this suggests that when microplastics that are more easily suspended

than sediment particles are present in the sediment, aquatic organisms have more opportunities to ingest microplastics that have adsorbed chemicals, making it easier for the chemicals to transfer into biological tissues.

2.09.P–We053 Evaluating microplastic particles as vectors of exposure for plastic additive chemicals using a food web model

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Microplastic particles (MPs) represent potential hazards for humans and wildlife, including as vectors for chemical exposure (e.g. plastic additives and pollutants sorbed from the surrounding environment). The leaching of chemicals from MPs has been identified as a potential exposure pathway but the relative magnitude of this pathway under environmentally relevant conditions remains unclear. Here, we describe a modification of the ACC-HUMANSTEADY bioaccumulation model to include dietary exposure to MPs containing either accumulated chemicals from the surrounding environment or embedded plastic additive chemicals (PACs). Chemical transfer to humans and wildlife is described using two-film resistance concepts assuming spheroidal or cylindrical particles of different sizes. The relative contribution of MPs and environmental media to the estimated daily chemical intake in humans was assessed in various exposure scenarios, for a range of hypothetical chemicals with varying octanol-water and air-water partition coefficients (KOW and KAW, respectively; i.e. 0 10 mg d-1, and the concentration of hydrophobic plastic additive is >5% wt wt-1. The contribution made by MPs as vectors of exposure decreased with increasing particle size and decreasing ingestion rates of MPs. Human health risks were evaluated for four specific PACs to illustrate the application of the model for risk assessment. Risks were negligible when the ingestion rate of MPs was <100 μg d-1. Uncertainties are high regarding the characterization and quantification of ingestion of MPs by humans and wildlife, including particle sizes and polymer composition, as well as on the presence of PACs in MPs. These data gaps need to be addressed if the issue of MPs as vectors of chemical exposure is to be fully understood. The work illustrates that mechanistic models, which account for all major exposure pathways, can be used to identify the importance of different exposure pathways, help prioritize research needs and support decision making.

2.09.P–We054 Development of Simultaneous Analysis method of microplastic and tire-wear particles by Py-GC/MS

IN WOO CHOI[1] (1)Korea University

Microplastics (MPs) and tire-wear particles (TWPs) are major urban contaminants that enter aquatic and atmospheric environments via road dust. Many studies have adapted the use of Py-GC/MS for individual analysis of either thermoplastics or tire elastomers, but methods that quantify both materials simultaneously within a single run remain scarce. This separation limits direct comparison of MP and TWP loadings across studies and increases the analytical burden of environmental monitoring. The objective of this work is to develop and validate a simultaneous Py-GC/MS method for routine quantification of common thermoplastic MPs together with the principal tire elastomers in complex environmental matrixes, such as road dust. Reference standards for targeted polymers were established using the Frontier Microplastics Calibration Standard (MPs-SiO2, Frontier Laboratories, Japan), which is widely adopted as reference standard for microplastic quantification in environmental matrixes. Natural rubber (NR) and styrene-butadiene rubber (SBR) reference standards were prepared by dissolving in tetrahydrofuran. For pyrolysis, curie-point pyrolyzer was optimized at 650℃ for 15 seconds. Quantification used selected-ion-monitoring (SIM) mode for SBR and butadiene rubber (4-vinylcyclohexene, m/z 54), PE (m/z 55), PET (m/z 105), and PS (m/z 91), with PP monitored in scan mode. GC condition was optimized with 1:50 slit, showing high intensity against target ions while preven

column contamination. Calibration was linear across all analytes (R^2 > 0.99) with limits of detection of 0.23–1.23 µg/g. By integrating two contaminant classes within one workflow, this method enables direct comparison of MP-to-TWP ratios across urban environments and supports more efficient source apportionment and management of traffic-related particulate pollution.

2.09.T - Integrative Analytical and Toxicological Approaches to Understanding Plastics as Environmental Contaminants and Contaminant Vectors

2.09.T01 Tracing micro and nanoplastics in food: the role of packaging and food contact materials

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Micro- and nanoplastics (MNPs) have been detected in a wide range of foods and beverages, contributing to widespread human exposure and raising concerns about potential health effects. While environmental contamination is often considered the dominant source, the contribution of food contact materials (FCMs), such as packaging, storage, and processing items, remains insufficiently understood. This limits the development of effective mitigation strategies. Here, we investigated the release of MNPs from commonly used FCMs under realistic conditions of use. Tested materials included polypropylene kettles, plastic drinking water bottles, single-use paper cups lined with polyethylene or polylactic acid, plastic food storage containers, reusable cups, recycled plastic containers, ziplock bags, and baby feeding bottles. An integrated analytical workflow was applied, combining pyrolysis–gas chromatography–mass spectrometry for polymer mass quantification, asymmetrical flow field-flow fractionation with multi-angle light scattering, nanoparticle tracking analysis, and electron microscopy to characterise particle size and morphology. Results demonstrate that FCMs can release substantial quantities of MNPs into food and beverages during normal use. Across products, particle release ranged from millions to billions per use, with the highest release typically observed during initial use. New electric kettles released up to 12 million nanoparticles per millilitre during first use, equivalent to approximately 3 billion particles in a single serving, with release persisting after more than 150 uses. Particle release increased significantly when hot food or liquids were applied, indicating a strong influence of temperature and food composition. Biopolymer-lined cups released more particles than polyethylene-lined equivalents, and recycled plastics exhibited higher initial particle release than virgin materials. These findings identify FCMs as a significant and underappreciated source of MNP exposure in food systems. The results highlight the need for standardised testing approaches, improved material design, and regulatory frameworks that incorporate MNP migration assessments. Addressing FCM-derived contamination is critical for reducing human exposure and advancing safer and more sustainable food systems.

2.09.T02 A Framework for Microplastic Flux and Polymer Transformation in Biscayne Bay

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Microplastic (MP;<5 mm) pollution has emerged as a pervasive environmental threat, with urban stormwater systems increasingly recognized as major pathways for MP transport into coastal ecosystems. Yet flux-based assessments linking watershed sources, transport, and polymer transformation remain limited. Biscayne Bay, one of Florida's most ecologically and economically important estuaries, is highly influenced by urban canal discharges, making it vulnerable to MP contamination and accumulation. This study evaluates the spatiotemporal distribution, transport, and early environmental transformation of MPs entering Biscayne Bay from major tributaries, assessing how weathering and biofilm accumulation alter

environmental behavior and analytical identification. MP concentrations (particles/L) were converted to mass concentrations (mg/L) using FTIR/Raman-derived polymer densities and microscopy-based particle volume estimates, with thickness approximated via z-axis focal depth. Polymer identity, concentration, and size-class data were integrated with SFWMD-DBHYDRO discharge records, precipitation datasets, and in situ hydrologic measurements to calculate daily, seasonal, and annual MP fluxes to Biscayne Bay. GIS-derived watershed delineations link MP abundance to anthropogenic indicators and storm-driven transport dynamics, supporting refinement of the Biscayne Bay Plastic Transport and Fate Model (BBLAST) to improve its predictive capacity for contaminant transport. Ten plastic types were deployed in Biscayne Bay to monitor early biofilm colonization and ATR-FTIR spectral changes over three months. After one month, all plastics showed visible surface dulling and biofilm accumulation. By three months, complex biofilm communities were observed on PVC, PC, PA, PP, HDPE, LDPE, and ABS. The most consistent spectral change was broadening of 1000-1250 cm^{-1} band in HDPE, LDPE, and PP, alongside broad 3000-3600 cm^{-1} features and possible carbonyl signals at the 1550-1750 cm^{-1}, suggesting surface oxidation and oxygen-rich organic fouling. PET, rPET, PC, PVC, and PA showed comparatively limited spectral alteration. By integrating analytical chemistry, environmental monitoring, hydrologic modeling, and plastic transformation studies, this work provides insights into land-to-sea MP fluxes and polymer weathering dynamics in urban coastal systems, offering a replicable framework for MP source tracking, polymer identification, and ecological risk assessment.</p>

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2.09.T03 Effects of long-term UV exposure on biodegradable plastics fragmentation in freshwater environments.

Biodegradable plastics have gained increasing attention as alternatives to conventional petroleum-based plastics, with their global usage continuing to rise. However, while these materials degrade effectively under industrial composting conditions, complete degradation rarely occurs in natural environments due to insufficient temperature, humidity, and microbial activity, where fragmentation into microplastics is instead the predominant process. In natural environments, plastics undergo fragmentation through various weathering factors, among which ultraviolet (UV) irradiation serves as a representative abiotic driver that induces polymer chain scission and oxidative reactions. This photochemical weathering constitutes a critical step that governs the rate and pattern of subsequent fragmentation. Nevertheless, systematic comparative studies on fragmentation characteristics among different polymers under identical photochemical conditions remain scarce.

In this study, UV irradiation was isolated as the primary weathering factor to comparatively analyze the fragmentation characteristics of four types of biodegradable plastic chips (1 × 1 × 0.2 cm) over a long-term exposure period of 120 days. Four biodegradable polymers were investigated: polylactic acid (PLA), polybutylene adipate terephthalate (PBAT), polybutylene succinate (PBS), and polyhydroxybutyrate (PHB). For comparison, two petroleum-based plastics, polyethylene terephthalate (PET) and polystyrene (PS), were also tested. Samples were collected at 40, 80, and 120 days. Surface alterations of the plastic chips were characterized using field emission scanning electron microscopy (FE-SEM), Fourier transform infrared spectroscopy (FT-IR), X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM). The mass of generated microplastics was quantified by calculating the difference between the initial and final weight of the plastic chips and confirmed the formation through FE-SEM analysis.

Degradation products were additionally characterized by LC/MS/MS. This study provides critical insights into the photodegradation mechanisms of biodegradable plastics under freshwater conditions.

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2.09.T04 Validation of a Method for Quantification of Bisphenols and Phthalate Metabolites in Post-mortem Human Brain Tissue

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Introduction: The apparent cost effectiveness and versatility of plastics have made them ubiquitous in our daily lives. These properties in part stem from the numerous plastic-associated chemicals used in their manufacturing, with phthalates (ortho-phthalic acid esters – PAEs) and bisphenols (BPs) amongst the most used. As a result, exposure to these chemicals is widespread as measured through human biomonitoring studies. PAEs and BPs are associated with known deleterious health impacts including hormonal effects and neurobehavioural outcomes. However, the bioavailability of these compounds to organs, such as the brain, is much less well understood. It is important to understand their presence in the brain to better assess their blood-brain barrier permeation and support animal model research. Herein we detail a method developed for the quantification of 14 phthalate metabolites and 7 bisphenols in human brain tissues and its application to the analysis of 10 postmortem human brains (occipital lobe; ethics approval: HC210189).

Methodology: For each sample, half a gram of brain tissue was cut and placed into a furnaced glass test-tube. Hydrolysation enzymes and internal standards (i.e. isotopically labelled phthalate metabolites and bisphenols) were added to the samples, which were then incubated for deconjugation. Acetonitrile and QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) powder were added to each sample to perform the sample extraction through sonication. Hexane was then added to remove lipids. The cleaned extracts were analysed using a SCIEX Triple QuadTM 7500 LC-MS/MS coupled to an ExionLCTM HPLC system. Quantification of target analytes was achieved using an isotope dilution method, against a six-point calibration curve.

Results: The method detection limit (MDL) for each analyte ranged from 0.02 to 2 ng/g of brain tissue. Analytical accuracy, defined as the recoveries of the target analytes in native-fortified samples, ranged between 80% and 120% for most cases. Analytical precision, reflected as the relative standard deviation of replicated measurements (n = 9; native-fortified samples), was mostly below 15%. Mono-n- and mono-i-butyl phthalate were the most frequently detected analytes (nine out of the 10 postmortem human brains), with concentrations ranging from 0.11 to 0.64 ng/g. Other analytes had less detections, including bisphenol A which was not detected above its MDL (0.14 ng/g) in any of the samples.

2.10.A.T - Environmental Chemistry and Exposure Assessment: Generic Session

2.10.A.T01 Quantification Before Identification: Exposure Estimation as a Prioritization Tool in Non-Target High-Resolution Mass Spectrometry Screening

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The large amount of chemicals in daily use puts a strain on already scarce water resources. Non-target liquid chromatography electrospray ionization high resolution mass spectrometry (LC/ESI/HRMS) screening is increasingly used to monitor chemicals in environmental water samples and often yields detection of thousands of features (combination of retention time, exact mass and intensity). Identifying all features is unfeasible, and the efforts should be directed towards toxicity drivers, that is chemicals that are most hazardous or present at high concentrations. Therefore, a quantification-based prioritization of the LC/HRMS features is suggested. Unfortunately, the signals obtained in ESI/MS vary widely from one chemical to another, leading to the need for calibration graph-based quantification. However, this is impossible for prioritization in non-target screening, where the chemicals of interest are unknown prior to analysis.

MS2Quant is a recently developed machine learning tool which can predict the ionization efficiency, and subsequently the concentration of features directly from the MS2 spectra. For this, it leverages probabilistic molecular fingerprints predicted from MS2 spectra via SIRIUS+CSI:FingerID. Here we present major updates for MS2Quant. Firstly, we improve the prediction accuracy. This includes incorporating the model for chemicals ionizing in negative mode ESI as well as substantially expanding the range of chemicals used for training MS2Quant to increase the range of chemicals for which reliable predictions can be made. Secondly, we aim to make the tool available as a package in both R and Python to accommodate as many users as possible and enable integration into a variety of non-target workflows. Moreover, a user-friendly web application will be provided for users with little to no coding experience. Finally, we ensure compatibility with dependency software updates since MS2Quant currently does not work with SIRIUS 6.

We anticipate that the updated MS2Quant 2.0 will be used both as a stand-alone prioritization tool and in combination with machine learning tools that predict toxic endpoints from MS2 spectra, to capture the complete risk profile of unidentified features.

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2.10.A.T02 Investigating the chemical modifications of pollen proteins on exposure to air pollutants using non-targeted mass spectrometry analysis

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While airborne pollen is a primary driver of respiratory allergies, urban pollutants can further exacerbate its impact by altering the structural and functional integrity of allergenic proteins. Air pollutants can act as adjuvants and modify the chemical characteristics of airborne allergens either during atmospheric transport or by influencing the protein transcription within pollen grains. Despite evidence of pollution induced changes, the specific effects of mixed pollen exposure and the resulting modifications in intact and ruptured grains remain inadequately characterised. Several studies have used allergens directly to

understand the modifications but extent of expulsion of these allergens from pollen, the concentrations of air pollutant and the modification for specific species is not well known. Hence, this study utilised a controlled environment to evaluate protein expression and chemical modifications in a pollen mixture comprising grasses (Lolium perenne and Phleum pratense) and birch (Betula pendula). The mixture was exposed to nitrogen dioxide NO2, ozone (O3), and ammonium nitrate (NH4NO3). High resolution proteomic profiling was conducted by non-targeted analysis (NTA) using nanoflow liquid chromatography electrospray ionisation tandem mass spectrometry (NanoLC-ESI-MS/MS). A total of 600 high confidence proteins were identified, with the majority originating from the Lolium species based on the library availability. Differential expression analysis revealed that NH4NO3 exposure significantly regulated allergens Lol p 4, Phl p 4, Bet v 1.02A, and Bet v 8. In ruptured pollen, NO2 exposure led to the upregulation of Lol p 4, Phl p 4, and Bet v 8. Among the post-translational modifications (PTMs), analysis identified 193 modified proteins, with methionine and proline oxidation being the most prevalent chemical modifications. Tyrosine nitration was detected within the Bet v 1 family under NO2 and O3 ruptured conditions, suggesting a link between nitration and altered birch protein expression. Additionally, cysteine carbamidomethylation and lysine carbamylation were observed in proteins treated with NO2 and NO2 and O3 conditions. These findings demonstrate that urban pollutants may induce species specific biochemical changes in pollen mixtures. The observed upregulation and chemical modifications particularly nitration and oxidation highlight the complex interaction between air quality and the allergenic potential of atmospheric bioaerosols.

2.10.A.T03 Detection and Quantification of Methomyl in Suspected Animal Poisoning Cases by Non-Target and Targeted Mass Spectrometry

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Pesticide poisoning in animals and wildlife is a significant concern in veterinary forensic toxicology due to the widespread use and misuse of agrochemicals. In Japan, limited information is available on pesticide-related deaths of animals, despite increasing incidents of sudden death among pets and wild animals. This study investigated pesticide exposure in dead-found animals in Japan, with particular emphasis on methomyl, a highly toxic carbamate insecticide.

Stomach content samples from 44 suspected poisoning cases, including cats, dogs, birds, and wild animals were analyzed using a two-tier analytical approach consisting of non-target screening by LC-Q-TOF/MS followed by targeted quantification using LC-MS/MS. The QuEChERS extraction technique was used to prepare samples.

Non-target screening detected a wide range of pesticide classes, including carbamates, herbicides, fungicides, insecticides, neonicotinoids, and rodenticides. Among the detected compounds, methomyl was the most frequently identified pesticide, occurring in 65.9% of the cases. Due to its high detection frequency and known acute toxicity, methomyl was selected for quantitative analysis.

Targeted LC-MS/MS analysis revealed high methomyl concentrations, reaching up to 157 mg/kg in cats, 75 mg/kg in a civet, and 30 mg/kg in a dog. These concentrations exceeded the reported oral median lethal dose (LD_{50}) values for most mammals, strongly suggesting acute lethal exposure. The findings provide strong forensic evidence implicating methomyl as the primary toxic agent in multiple animal deaths.

This study demonstrates the effectiveness of combining LC-Q-TOF/MS and LC-MS/MS for veterinary forensic investigations and highlights the need for improved monitoring and stricter control of highly toxic pesticides.

2.10.A.T04 Unveiling Emerging Contaminants in Urban Stormwater: An

Understudied Pollution Pathway

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Rapid urbanization in coastal cities has intensified stormwater discharge. Stormwater carries a complex mixture of emerging contaminants such as pharmaceuticals, pesticides, industrial chemicals and other persistent organic pollutants that may serve as a significant source of environmental pollution. Since, stormwater runoff is one of the crucial and understudied pathways for aquatic pollution, understanding the pollutant profile in stormwater is essential. Non-targeted analysis (NTA) using high resolution mass spectrometry provides a comprehensive approach to detect and characterize a wide range of known and unknown contaminants, offering deeper insight into stormwater chemistry. This study analyzed stormwater samples collected from a commercial site (Belapur: BEL) and a residential site (Koparkhairane: KOP) in Navi Mumbai, India at both the inlet and outlet of stormwater ponds. Initial method optimization was performed for various parameters such as concentration factor, run time and sample pH during extraction. Optimized parameter including concentration factor of 500, pH adjustment during sample extraction and 17 min run time were further used to assess the contaminant profile in the collected samples. A total of 748 and 722 compounds were detected at BEL, inlet and outlet respectively. Pharmaceuticals such as antibiotics, antidepressants steroids, alkaloids, along with pesticides and plasticizers were abundant in both inlet and outlet. Compared with the BEL-inlet, the BEL-outlet showed a significant increase in surfactants, transformation products, and organic acids. While, compounds such as beta blockers, industrial chemicals and anesthetics were more abundant in the inlet. On the other hand, a much larger contaminant load was observed at KOP where a total of 935 and 887 compounds were detected at the inlet and outlet, respectively. At KOP, the number of pharmaceuticals, pesticides, industrial chemicals, and transformation products were higher compared to BEL. Overall, both ponds showed only a small decrease in the number of compounds in the outlet compared to the inlet, indicating that these stormwater ponds are not capable of removing emerging contaminants and they may further accumulate in receiving water body. This study provides detailed contaminant profile of stormwater and highlights its role as a carrier of diverse pollutant, emphasizing the need for effective pre-treatment before discharging into aquatic systems.

2.10.B.T - Environmental Chemistry and Exposure Assessment: Generic Session

2.10.B.T01 Pesticide Watch: A new, community-driven pesticide monitoring strategy for Australian waterways

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Pesticides are among the greatest drivers of biodiversity loss in Australia, however no cohesive, national monitoring program exists, and monitoring data is often unavailable to the community. Barriers to establishing such a program include (1) the large geographical spread of Australian waterways, and (2) developing a streamlined analytical method for a large suite of pesticides at environmentally relevant concentrations. These challenges are being addressed by the development of an active community scientist network who obtain water grab samples, which are then analysed in a central laboratory using innovative, automated sample preparation methods. Samples from 135 monitoring sites have been analysed as part of Pesticide Watch, representing a range of land use areas. Samples are collected using a validated sampling protocol for 12 consecutive months from 2024-25. Analysis was performed using a fully automated trap-and-elute sample preparation coupled in-line with liquid chromatography tandem mass spectrometry (LC-MS/MS). The instrumental method was validated for quantitative analysis of 171 pesticide analytes, with method detection limits in the low ng L-1 range. A total of 470 pesticide analytes could be qualitatively screened for in a single analytical run. Triazine herbicides, neonicotinoid insecticides, and fiprole insecticides were frequently detected, particularly in urban areas. Exceedances of

Australian freshwater guideline values were observed for several priority residues, including fipronil, imidacloprid, dimethoate, and glyphosate, above which toxic effects are expected to occur. Pesticide Watch is a fit-for-purpose, scalable pesticide monitoring strategy which provides a framework for residue monitoring and community engagement concerning emerging contaminants, and the resulting data may be used to investigate land use trends, residue persistence, pesticide co-occurrences, and possible mixture toxicity. The data from this baseline study is being used to develop a publicly available resource with the aim of enhancing community engagement and supporting effective management of emerging contaminants to improve outcomes for waterways.

2.10.B.T02 Pharmaceutical and personal care product marker panels resolve semester rhythms and community health correspondence in campus wastewater

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Wastewater surveillance has expanded from pathogen tracking to chemical markers of population behavior, exposure, hygiene practice, and treatment use. However, marker selection remains insufficiently validated for small, well-defined, and behaviorally dynamic catchments, where daily activity, occupancy shifts, and local practices can reshape chemical loads. In these systems, useful markers must retain source relevance, wastewater stability, and temporal interpretability under local variability. Hence, this study evaluated 42 pharmaceuticals and personal care products in campus wastewater from 2 student dormitories and 1 recreational clubhouse to develop a context-resolved marker framework. Caffeine-based normalization estimated population normalized daily loads and back-calculated intake.

The framework resolved three marker types. Artificial sweeteners, salicylic acid, and stimulants formed a persistent campus baseline. Didecyldimethyl ammonium chloride, triclocarban, N,N-diethyl-m-toluamide, and benzophenone 1 captured context-responsive signals linked to hygiene practice, outdoor exposure, weekends, examinations, and seasonal conditions. Azithromycin, doxycycline, and dehydrated erythromycin captured episodic treatment-related signals. Hierarchical clustering showed coordinated marker modules that linked shared consumption and intake patterns with hygiene use, outdoor exposure, and episodic treatment. These modules supported panel coherence and recovered campus-level temporal structures, especially monthly shifts and examination week responses, while weekend and subpopulation differences were weaker.

Azithromycin, doxycycline, and dehydrated erythromycin aligned with acute upper respiratory infection records, while N,N-diethyl-m-toluamide, crotamiton, and benzophenone derivatives aligned with broader community dengue records. Harmonized comparison with 2021 and 2022 datasets showed significantly lower antibiotic, antiviral, and quaternary ammonium compound consumption in 2024, with reorganized co-occurrence structures. These results show that PPCP markers in campus wastewater can capture semester phase and campus-wide temporal changes while retaining correspondence with disease activity, hygiene practice, seasonal exposure, and treatment-related change. The three-tier framework supports chemical marker panels for small catchment wastewater surveillance and calls for periodic recalibration as population behavior and public health conditions change.

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2.10.B.T03 The Distribution of Pharmaceutical Pollutants in a Wastewater-Impacted Coastal Environment

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Pharmaceuticals are increasingly detected in the environment and are expected to become more pervasive with rising global demand. While the occurrence and distribution of pharmaceuticals in freshwater environments have been extensively studied, comparable research in marine ecosystems remains scarce. Coastal wastewater outfalls are widely recognized as a major source of pharmaceuticals in marine environments. In this study, we examined the distribution of pharmaceuticals along a wastewater gradient in Port Phillip Bay, Melbourne, Australia. Stable nitrogen isotope ratios (δ15N) were used as an indicator of wastewater influence to evaluate how pharmaceutical concentrations varied with wastewater input. Samples of marine invertebrates, macroalgae, and marine/terrestrial plants were collected from four locations at increasing distances from Melbourne's largest wastewater treatment facility. Samples were then analyzed for stable isotope ratios and the concentrations of 95 pharmaceuticals and personal care products. Across the locations, 15 pharmaceuticals were detected in total. The most frequently detected compounds were telmisartan (83%), flecainide (52%), memantine (37%), caffeine (28%) and tramadol (23%). Using a Bayesian mixed-effects model, we found a positive relationship between δ15N and pharmaceutical concentrations, supporting wastewater influence as a key driver of pharmaceutical burden. Notably, the highest concentrations were typically observed in plants and algae, including terrestrial plants. Additional sampling revealed that pharmaceutical concentrations were higher in sea foam compared to seawater, suggesting enrichment at the water-air interface. Coastal aerosols may therefore act as a potential vector for the transfer of pharmaceuticals from marine to terrestrial environments. In summary, our results highlight the role of wastewater in pharmaceutical pollution and identify plants and algae as promising bioindicators.

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2.10.B.T04 Long-term Variations in the Concentrations of Polycyclic Aromatic Hydrocarbons and Their Halogenated Derivatives in Shizuoka, Japan

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Polycyclic aromatic hydrocarbons (PAHs) and their halogenated derivatives (XPAHs) are trace atmospheric pollutants formed through incomplete combustion of organic compounds and secondary photochemical reactions of PAHs. Atmospheric concentrations of PAHs and XPAHs can serve as indicators of industrial activities and the effectiveness of environmental regulations. However, long-term trends in their atmospheric concentrations remain unclear. We show that the concentrations of particulate benzo[a]pyrene (BaP) and total PAHs decreased from 1992 to 2025 in Shizuoka Prefecture, Japan. The halving times of BaP and total PAH concentrations were 9.1 and 9.0 years, respectively. These results suggest that health risks associated with PAHs have gradually decreased in Japan due to environmental regulations and reduction technologies. In contrast, an analysis of the period including the COVID-19 pandemic (2018–2024) showed increasing trends in BaP and total PAH concentrations, suggesting that the resumption of social activities after the pandemic restrictions may have contributed to the deterioration of air quality. The median concentrations aggregated by month indicated that total PAH concentrations peaked in winter. This trend is consistent with previous studies and can be attributed to the meteological conditions, suppression of gas-phase partitioning and photodegradation of PAHs under low

temperature and low light-intensity conditions during winter. The monthly median concentrations of total PAHs ranged from 1.78 (July) to 3.96 (December) ng m^{-3}.

2.10.B.T05 Source apportionment of polycyclic aromatic hydrocarbons in harbor sediments adjacent to shipyard areas using dual compound-specific isotope analysis

Polycyclic aromatic hydrocarbons (PAHs) are major hazardous contaminants in sediments of shipbuilding and harbor industrial complexes; however, conventional diagnostic ratio-based source apportionment approaches have inherent limitations in environments affected by multiple contamination sources. This study applied compound-specific isotope analysis (CSIA) of carbon and hydrogen (δ13C and δ2H) to harbor sediments from the Okpo National Industrial Complex, Geoje, South Korea, to distinguish PAH sources and characterize their spatial distribution. Surface sediments were collected from 32 stations across the shipyard and adjacent coastal areas, and concentrations of 26 PAHs were determined. CSIA was performed for phenanthrene (Phe), fluoranthene (Fl), pyrene (Py), benzo[a]anthracene (BaA), and chrysene (Chr). The measured isotopic values were integrated with principal component analysis (PCA) and a dual-isotope mixing model to estimate source contributions. ΣPAHs concentrations reached approximately 2,000 ng g^{-1} dw, with a contamination hotspot identified in the central inner harbor of the shipyard. Diagnostic ratio analysis [Ant/(Ant+Phe), BaA/(BaA+Chr)) suggested a dominant petroleum combustion origin; however, CSIA revealed a wide isotopic range of –27 to –24.5‰ for δ13C and –160 to –50‰ for δ2H, with statistically significant differences among individual compounds. Notably, BaA exhibited markedly lower δ2H values (ca. –160‰) than the other target compounds, indicating a high-temperature coal tar origin. The dual-isotope mixing model and PCA resolved three distinct source groups: high-T coal tar, liquid fuel leakage, and background sources. Spatial distribution mapping further revealed that coal tar contamination was predominantly concentrated in the inner harbor, particularly around the drydock area, while liquid fuel leakage was the primary source in the eastern area. These results demonstrate that dual-isotope (δ13C and δ2H) CSIA improves source discrimination of PAHs in harbor sediments affected by multiple sources. The spatial separation of coal tar- and liquid fuel-derived PAHs highlights the applicability of CSIA for contamination assessment in industrial harbor environments.

2.10.C.T - Environmental Chemistry and Exposure Assessment: Generic Session

2.10.C.T01 Development of a Colorimetric Passive Air Sampler for Reactive Chlorine Species: A Field Study

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Chlorine-based disinfectants (e.g., NaOCl) are among the most widely used biocides, with applications ranging from household cleaning to industrial facilities. Despite their efficacy, they can generate toxic reactive chlorine species (RCS), such as chlorine gas and radicals, which can cause significant acute and chronic inhalation health risks. While quantifying personal exposure is essential, existing sampling methods often require expensive additional equipment, such as air pumps and analytical instruments, or fail to capture acute risks due to analytical delays. To address these limitations, we developed a colorimetric quantification method using o-dianisidine-containing polydimethylsiloxane (PDMS) passive samplers. This system enables users to immediately measure personal exposure either qualitatively, by visually comparing the color change to green with a reference color chart, or quantitatively, by accurately determining exposure levels with a portable color reader using the CIE L*a*b* color space (MDL: 35 ppbv·h) (Korean Patent No. 10-2695695-0000). To evaluate its field applicability, we monitored cafeteria workers across 15 school kitchens in Korea. Distinct green discoloration (Δa < 0) was observed at six

facilities, visually confirming RCS exposure during routine cleaning activities. The calculated time-weighted average (TWA) concentrations ranged from 17.9 to 35.9 ppbv, which were well below the Cal/OSHA permissible exposure limit of 500 ppbv, indicating safe working conditions. Ultimately, this study demonstrates that the developed sampler provides a reliable, low-cost system for immediate exposure monitoring that is practical for broader consumer use. Furthermore, its high sensitivity allows for the detection of low-concentration TWA exposures with exceptional precision.

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2.10.C.T02 Effect-Directed Analysis Combined with Machine Learning and QSAR Modeling Identifies Major Estrogen Receptor Agonists in Highly Industrialized Sediments

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Estrogen receptor (ER)-mediated activity in sediments remains poorly characterized despite its ecological relevance, largely due to the complexity of chemical mixtures and the limited explanatory power of conventional target analysis. This study applied an integrated framework combining effect-directed analysis (EDA), high-resolution mass spectrometry-based nontarget screening (NTS), and machine learning-assisted prioritization coupled with QSAR-based screening to identify major ER agonists in sediments from Lake Sihwa, a highly industrialized coastal system. ER-mediated activity, measured using the T47D-Kbluc bioassay, was detected at all sites and was predominantly associated with the polar fraction (F3) and its RP-HPLC subfraction (F3.3), particularly in inland creeks influenced by industrial inputs. Bioassay-derived activity frequently exceeded effect-based trigger values (EBTs; 4.0 × 10–3 ngE2 gdw–1 for freshwater and 2.0 × 10–3 ngE2 gdw–1 for marine sediments) derived from water quality guidelines in this study, indicating widespread estrogenic risk. However, four target ER agonists explained only 10–53% of the observed activity, suggesting substantial contributions from unidentified compounds. A stepwise prioritization workflow integrating bioassay-guided filtering, machine learning-assisted prioritization, and VEGA QSAR-based prediction reduced more than 15,000 detected features to a small number of biologically relevant candidates. Among these, diethylstilbestrol and heptyl paraben were newly identified and confirmed as ER agonists, with relative potency values of 1.5 and 1.6 × 10–5, respectively. Inclusion of diethylstilbestrol substantially improved the explanatory power of potency balance analysis, increasing the contribution to ER-mediated activity up to 41% and exceeding 100% at highly impacted sites. Diethylstilbestrol is a synthetic estrogen compound used in contraceptive and hormone-related therapies, suggesting that pharmaceutical-derived contaminants may contribute to estrogenic ecological disturbances in aquatic environments. Descriptor-based analysis indicated that ER activity was strongly associated with electronic distribution, aromaticity, and molecular connectivity. Overall, the results demonstrate that a limited number of high-potency compounds can dominate mixture-driven ER activity in sediments and highlight the utility of EDA-based approaches for sediment risk assessment.

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2.10.C.T03 Integrating Polychlorinated Alkane Biomonitoring into the Japan

Environment and Children's Study (JECS): A Harmonized Sweden–Japan Approach for Human Exposure Assessment

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Polychlorinated alkanes (PCAs), major components of chlorinated paraffins, are high-production-volume industrial chemicals widely used as flame retardants and plasticizers since the 1930s. Due to their persistence, bioaccumulation potential, and suspected toxicity, PCAs are increasingly recognized as contaminants of emerging concern. However, human biomonitoring data remain scarce because of analytical challenges and the lack of harmonized methodologies. Recent studies from Sweden showed that PCA concentrations in human serum and breast milk exceeded those of legacy persistent organic pollutants (POPs) such as polychlorinated biphenyls (PCBs) and polybrominated diphenyl ethers (PBDEs), highlighting the need for large-scale biomonitoring, particularly among vulnerable populations. This project aims to introduce PCA biomonitoring into the Japan Environment and Children's Study (JECS), one of the world's largest longitudinal birth cohort studies, including approximately 100,000 mother–child pairs. Previous work from our group has focused on PCA exposure in the Swedish population and the development of harmonized analytical workflows for PCA quantification, including CPxplorer. By implementing this workflow within JECS, the project will enable direct comparison of PCA exposure between Swedish and Japanese populations.
Preliminary results demonstrated successful adaptation of the original 2 mL serum extraction method to a streamlined 200 µL workflow suitable for large-scale biomonitoring. Both methods showed comparable analytical performance and sensitivity, although the reduced-volume method presented slightly lower recoveries, likely due to the SPE cartridge size relative to sample volume. Instrumental analysis was successfully transferred between Liquid Chromatography– quadrupole Time of Flight platforms, supporting implementation within the JECS framework. Ongoing optimization aims to improve recoveries and facilitate future automation using robotic high-throughput infrastructure.
This project represents the first harmonized PCA biomonitoring dataset between Japan and Sweden, enabling internationally comparable exposure assessments. Moreover, integrating PCA analysis into JECS will support future epidemiological studies, improve understanding of human exposure to these under-regulated chemicals, and strengthen the scientific basis for risk assessment and regulatory decision-making.

2.10.C.T04 Development and Application of a Multimedia Environmental Model for Assessing the Behavior of Chemical Warfare Agents

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Chemical warfare agents (CWAs) pose severe risks to human health due to their high toxicity and environmental persistence. Venomous Agent X (VX), in particular, persists as liquid-phase droplets owing to its low volatility and water solubility. To simulate the multimedia behavior of liquid-phase CWAs, a GIS-based Level IV fugacity model, DREAM-CWA (Dynamic fugacity-based Regional Environmental model for Air-surface exchange and Multimedia fate of Chemical Warfare Agents), was developed with an integrated droplet compartment. The model simulates phase partitioning and intermedia transport of droplets. To represent urban environmental characteristics, soil, asphalt, coated concrete (non-porous), and water were incorporated as distinct surface compartments. Model reliability was evaluated through comparison with the fugacity model CoZMo-POP 2. A hypothetical VX release scenario was simulated as an initial evaluation to optimize the multimedia framework, with a primary focus on liquid-phase persistence and dynamics. The simulation showed that VX was primarily retained within droplets and surface compartments, while subsequent volatilization increased air concentrations.

Soil and sediment served as the dominant short-term reservoir and long-term sink, respectively. To evaluate model applicability across CWAs, five representative agents were selected to encompass a wide range of volatility and persistence: a highly volatile gas (phosgene), a volatile liquid (sarin), semi-volatile liquids (soman and distilled mustard), and a highly persistent liquid (VX). Parameter sensitivity analyses were conducted to assess the influence of emission scenarios, environmental variables, and key physicochemical properties on environmental fate. The results indicated that secondary emissions from droplets and surfaces contributed to sustained atmospheric exposure following primary releases. Comparisons across agents showed differences in dominant environmental media, fugacity distributions, and potential exposure durations. By generating spatiotemporally resolved volatilization fluxes, DREAM-CWA outputs can be coupled with computational fluid dynamics simulations to evaluate near-surface dispersion and exposure. This framework serves as a robust tool for evaluating environmental risks of CWAs and supporting decision-making during chemical attack responses.

2.10.C.T05 Zone-specific co-occurrence of reactive chlorine species and VOCs in school cafeteria kitchens using passive sampling

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This study investigates the co-occurrence of reactive chlorine species (RCS) and volatile organic compounds (VOCs) in school cafeteria kitchens under real operating conditions using low-cost passive sampling techniques.

Passive samplers were deployed across functionally distinct zones (cooking, cleaning, and corridor areas) to capture spatial variability in indoor chemical environments. A colorimetric sampler was used to quantify integrated oxidative chlorine exposure, expressed as Cl_2-equivalent concentrations, while VOCs were measured using an ePTFE-based passive sampler coupled with GC–MS analysis.

Measured time-weighted average concentrations of reactive chlorine species ranged from 17.9 to 35.9 ppbv during working periods. Chlorine-related signals were primarily associated with cleaning activities, although elevated responses were also observed in cooking areas, suggesting additional oxidant formation during high-temperature processes. VOC concentrations showed relatively modest overall variation; however, benzene and limonene exhibited statistically significant increases during working periods. Benzene was elevated in cooking and adjacent zones, consistent with combustion-related emissions, while limonene increased across all zones, reflecting the use of fragranced cleaning products.

The simultaneous presence of reactive chlorine species and VOCs highlights the potential for secondary chemical interactions in cafeteria environments, even though specific byproducts were not directly measured. The results demonstrate that indoor kitchens represent spatially heterogeneous exposure environments influenced by multiple emission sources and reactive processes. This study provides field-based evidence supporting the importance of zone-specific measurements for understanding real-world exposure scenarios in complex indoor environments.

3.06.P - PFAS Treatment and Remediation: Linking Environmental Behavior to Sustainable Solutions

3.06.P–Mo093 (Ultra)short-chain Per- and polyfluoroalkyl Substances (PFAS) in Marine Environment: Method Development and Environmental Occurrence

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Kong

Ultrashort-chain per- and polyfluoroalkyl substances (PFAS) have attracted increasing attention because of their high mobility, environmental persistence, and the analytical challenges associated with their determination, particularly in high-salinity matrices. In this study, a robust analytical method was developed for the determination of ultrashort-chain PFAS in high-salinity matrices, which was based on the optimization of a previously established solid phase extraction (SPE)-based method for PFAS analysis, making it suitable for the efficient extraction and determination of ultrashort-chain compounds. The method integrated sample treatment and instrumental analysis, and the effects of key factors on extraction performance and recovery were systematically investigated. Through method optimization, an effective and reliable procedure was established for high-salinity samples. Under the optimized conditions, satisfactory recoveries (84.8%–100.1%) were achieved for six ultrashort-chain PFAS, while the method also enabled the simultaneous determination of other 43 short-chain and long-chain PFAS targets. The developed method was subsequently applied to seawater samples collected from the Pearl River Estuary in south China to investigate the occurrence of PFAS in this coastal region. This study provides a practical analytical approach for the monitoring of ultrashort-chain PFAS in complex saline environments and offers valuable data for understanding PFAS contamination in marine waters.

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3.06.P–Mo094 Addressing Analytical Challenges in PFAS Sorption Measurement Under Environmentally Relevant Conditions Using Online Soil Column Chromatography- Mass Spectrometry

Anh T. Ngoc Do[1] and Satoshi Endo[1] (1)Health and Environmental Risk Division, National Institute for Environmental Studies (NIES)

Sorption is a central process governing PFAS transport in soils; however, most available sorption data are generated using batch or conventional column methods that require long experimental times and extensive manual handling. Soil column chromatography (SCC), which employs a short packed column, offers a rapid and reproducible alternative with precise control of soil conditions. We developed an online SCC– mass spectrometry (MS) approach in which SCC – packed with peat as model soil organic matter and silica as a diluent – is coupled to MS through a post column dilution and flow splitting system, enabling PFAS sorption measurements under saline conditions (CaCl2 and NaCl). The post column configuration incorporates a static mixer for dilution and a tee union that splits the effluent flow into MS and a waste outlet. Using the SCC MS, we quantified the sorption coefficients of PFASs for peat across varying salt concentrations and pH conditions. Short and mid chain PFASs showed minimal competition in mixtures, while long chain PFASs exhibited competitive sorption compared with single compound systems. Relatively long-chain PFASs (PFNA, PFDA, PFOS, 8:2 FTCA and 5:3 FTCA) exhibited appreciable sorption to peat. Across the tested CaCl2 and NaCl concentrations and pH values (5–6.5), PFAS sorption showed only minor variation. A notable exception is 5:3 FTCA, whose sorption strongly varied with pH. For strongly acidic PFAS, sorption was significantly weaker in NH4HCOO solution, indicating a salt type effect. Notably, PFBSA (pKa 6.2) and MeFBSA (pKa 7.3), the weakest acids examined, showed no measurable response to salt type. Overall, the SCC–MS approach with flow dilution and splitting addresses key analytical limitations by delivering rapid, reproducible, and environmentally relevant PFAS sorption measurements.

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3.06.P–Mo095 Fluorescence “Turn-off” Indicator Displacement Method for Continuous Monitoring of PFAS in Soil Column Experiments

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Sorption to solid matrices plays a major role in the transport and bioavailability of per- and polyfluoroalkyl substances (PFAS) in soils. The strength of soil sorption is commonly expressed by the soil sorption coefficient (Kd), which is typically measured using batch suspension tests. As an alternative, soil column elution experiments offer several advantages. In particular, automated retention experiments using an HPLC system equipped with a miniaturized soil column (2-3 cm) are rapid and highly reproducible. However, most PFAS of concern require mass spectrometric (MS) detection due to their lack of UV and fluorescence activity. MS instrumentation is often not readily available for this specific application, and it is generally incompatible with nonvolatile, inorganic salts, such as calcium chloride, thereby limiting the determination of Kd in environmentally relevant solution conditions.
In this study, a fluorescence “turn-off” indicator displacement assay (OFF-FIDA) was applied for the continuous detection of PFAS in soil eluent. OFF-FIDA uses a fluorescence indicator (FI) that exhibits little or no fluorescence when freely dissolved in water but shows strong fluorescence enhancement upon binding to a macromolecular host, such as cyclodextrin (CD). While the FI-CD complex is fluorescent, the introduction of a target molecule (i.e., PFAS) leads to competitive binding to CD and displacement of the FI, resulting in a decrease in fluorescence intensity. This mechanism potentially enables continuous monitoring of PFAS in the soil eluent using a conventional fluorescence detector.
Here, four candidate FIs and seven β-cyclodextrin derivatives were evaluated with respect to their fluorescence spectra, on-off fluorescence behavior, and competitive host-guest binding properties with perfluorooctanoic acid (PFOA) using fluorescence spectroscopy. A post-column derivatization unit was hyphenated with an HPLC system with a fluorescence detector to test the feasibility of the method concept under flow-through conditions. As a proof of concept, 1-naphthol and β-cyclodextrin were selected as the OFF-FIDA system, and chromatograms of PFOA were obtained using a silica-filled column. Initial results indicate that improving method sensitivity to enable detection of low PFAS concentrations is a primary challenge.

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3.06.P–Mo097 Exploring the Reductive Transformation Pathways of Perfluoroalkyl Sulfonylimides to Short-chain Legacy Perfluoroalkyl Sulfonates and Perfluoroalkyl Sulfonamide Compounds

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<p>Bis(perfluoroalkyl sulfonyl)imides (NH(CnF2n+1O2S)2, FASIs), emerging alternatives to legacy PFAS, are widely used in industrial applications, particularly in semiconductor manufacturing and battery production. Their toxicity toward aquatic organisms, activated sludge bacteria, and Vibrio fischeri has been reported, and their occurrence has been documented in diverse environmental matrices. However, their behavior during water treatment processes remains largely unexplored. In this study, the degradation of FASIs during an advanced reduction process (ARP) was systematically investigated. FASIs exhibited negligible degradation under direct photolysis and advanced oxidation processes (<7%). In contrast, under UV/sulfite treatment, FBSI (n = 4) was removed by more than 99% within 45 min, achieving

46.4% defluorination after 24 h. LC-MS and LC-Q-Orbitrap HRMS analyses revealed that 5.0–10.3% and 12.9–48.5% of the fluorine mass from degraded FASIs was transformed into short-chain perfluoroalkyl sulfonamides (CnHF2n+1NO2S−, FASAs) and perfluoroalkyl sulfonic acids (CnF2n+1SO3−, PFSAs), respectively. Density functional theory (DFT) calculations indicated that the transformation of FASIs into FASAs and PFSAs, initiated by N–S and C–S bond cleavage, was both thermodynamically favorable and kinetically feasible. Based on the identified transformation products and DFT results, degradation pathways for FBSI, FESI (n = 2), and TFSI (n = 1) were proposed. Although the parent compounds degraded rapidly, the resulting FASAs and PFSAs exhibited substantially lower reactivity toward hydrated electrons, thereby limiting overall defluorination. These findings underscore the need to further develop treatment technologies capable of effectively degrading short- and ultra-short-chain PFAS. To the best of our knowledge, this study is the first to investigate the behavior of FASIs during ARP treatment and demonstrates that novel PFAS can act as precursors to persistent short- and ultra-short-chain FASAs and PFSAs.</p>

3.06.P–Mo098 Characterization of Known and Unknown PFAS in Groundwater and Surface Water at an AFFF-Contaminated Site Treated with a Colloidal Activated Carbon Barrier

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Per- and polyfluoroalkyl substances (PFAS) in contaminated soils and groundwater pose a significant risk to both human and environmental health. A major source of PFAS contamination worldwide is the historical use of aqueous film-forming foam (AFFF) at airports, military facilities, and firefighting training sites. Repeated AFFF application has resulted in extensive contamination of soil, groundwater, and nearby surface waters, often generating long-term contaminant plumes that threaten drinking water resources and aquatic ecosystems. Remediation of PFAS-contaminated sites remains challenging, as conventional treatment methods are often costly, energy intensive, and may generate secondary contaminated waste. In-situ stabilization approaches therefore represent a promising alternative for limiting PFAS migration at the source zone.
In this project, an in-situ remediation technique based on injection of colloidal activated carbon (CAC) was evaluated at an AFFF-contaminated site. Ground water and surface water from the site collected in May 2024 and 2025 were analyzed to assess the total PFAS levels. A comprehensive analytical approach was applied, including determination of extractable organofluorine (EOF) combined with fluorine mass balance, oxidation of both raw samples and extracts, and suspect screening.Results showed clear differences in PFAS profiles between groundwater and surface water samples collected at varying distances from the source zone. Groundwater samples closest to the barrier contained a higher proportion of ultra-short-chain PFAS. EOF analysis demonstrated lower concentrations of known EOF near the barrier, suggesting retention or transformation of target PFAS. In contrast, surface water samples further from the source area showed a larger fraction of unidentified EOF, indicating the presence of unknown fluorinated compounds. Oxidation experiments revealed substantial precursor formation, particularly in raw samples, demonstrating the presence of significant precursor fractions not captured by conventional target analysis. Differences in oxidation profiles between samples collected near and further from the barrier further indicated spatial variations in precursor composition and transformation potential.Overall, the results demonstrate the importance of combining target analysis with fluorine mass balance and oxidation-based approaches to better characterize PFAS contamination and evaluate remediation performance at AFFF-impacted sites.

3.06.P–Mo096 Spatial Distribution and Ecological Risks of Per- and Polyfluoroalkyl

Substances (PFAS) in the Yangtze River Basin, China

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Growing concern over per- and polyfluoroalkyl substances (PFAS) contamination is driven by their rising consumption and potential ecological risks; however, the environmental behavior of PFAS, especially the emerging ones, in the Yangtze River (a major sink) remains poorly understood. In this study, 46 target PFAS were comprehensively investigated within the Yangtze River Basin (20 sites), including surface water, suspended particulate matter (SPM), and sediment, as well as the Yangtze finless porpoises (YFP: Neophocaena asiaeorientalis asiaeorientalis; 12 individuals). Results showed that perfluorobutanoic acid (PFBA), perfluorooctanoic acid (PFOA), and perfluorobutanesulfonic acid (PFBS) were predominant in most of the abiotic samples, while perfluorooctanesulfonic acid (PFOS) and perfluoroundecanoic acid (PFUnDA) predominated in the YFP liver. Poyang Lake (the largest flood basin of Yangtze) exhibited a severe PFAS burden, as reflected by the average concentrations of total PFAS in the water phase (including dissolved and SPM phases: 205 ng/L) and stranded YFP (14200 ng/g dry weight) being significantly higher than those in the other regions (p < 0.05). YFP stranded in Poyang Lake showed a higher bioaccumulation potential of predominant PFAS [(i.e., PFOS and 6:2 chlorinated polyfluorinated ether sulfonate (6:2 Cl-PFESA)] than those from the region adjacent to Yichang (the confluence of the upper and middle Yangtze reaches). Ecological risk assessment based on toxicological prioritization index (ToxPi) identified PFOA as the highest-priority chemical, followed by PFBS and PFBA. The hazard quotients of 6:2 Cl-PFESA (100%), PFUnDA (92%), and PFOS (83%) were greater than 1, suggesting a high health risk posed to YFP. This study provides valuable insights into enhancing PFAS monitoring and regulatory management in aquatic ecosystems.

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3.06.P–Mo099 Pathway-Informed Prioritization of PFAS in Hong Kong Urban Stormwater Using Chemical Profiling and Bioactivity Assessment

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Urban stormwater is an important but under-characterized pathway for transporting emerging contaminants from urban surfaces to receiving waters. This concern is particularly relevant in Hong Kong, where intense seasonal rainfall, dense impervious surfaces, and extensive drainage networks allow untreated runoff to discharge into rivers and coastal waters. PFAS are of special concern because of their persistence, mobility, and potential biological activity, yet their occurrence and risk relevance in Hong Kong's stormwater remain poorly understood.

This study investigated PFAS in Hong Kong's urban stormwater across different land-use catchments and seasons. PFAS levels were compared with international studies and guideline values, and their spatial and seasonal patterns were linked to land use, rainfall, and drainage characteristics. Preliminary results showed widespread occurrence of PFAS in all stormwater samples, with short-chain PFCAs were dominant in the dissolved phase. Industrial and high-density urban catchments generally exhibited higher PFAS concentrations and greater compositional complexity than residential areas. Seasonal variations were also observed, with elevated PFAS levels during the wet season, suggesting enhanced mobilization and transport during rainfall events. Exposure–activity ratio analysis further identified several PFAS with

elevated bioactivity potential, highlighting the importance of toxicity-informed prioritization beyond concentration-based assessment alone. This study provides a pathway-informed framework linking urban runoff, PFAS transport, and predictive toxicological assessment. The findings improve current understanding of PFAS behavior in subtropical stormwater systems and support risk-based stormwater management and future monitoring strategies in Hong Kong.

3.06.P–Mo100 Versatile and Scalable Sorption Technology for Per- and Polyfluoroalkyl Substances (PFAS) Removal from Challenging Matrices

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Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants that pose significant challenges for water and waste management systems, particularly in complex matrices such as landfill leachate, wastewater effluent, and biosolids-derived streams. Conventional treatment technologies, including granular activated carbon and ion exchange resins, often suffer from limited selectivity, rapid fouling, and poor performance for short-chain PFAS in high organic load environments.

Here we present a versatile and scalable sorption technology designed for efficient PFAS removal across a wide range of challenging matrices. The platform is based on engineered polymeric sorbents with tunable surface chemistry and hierarchical structure, enabling enhanced affinity toward both long- and short-chain PFAS while maintaining resistance to natural organic matter interference. The sorbent can be deployed in multiple configurations, including fixed-bed columns, fluidised-bed processes and modular treatment units, supporting integration into existing treatment infrastructure.

Laboratory and pilot-scale evaluations demonstrate high removal efficiencies under realistic conditions, including elevated dissolved organic carbon and variable levels of co-contaminants. The system exhibits stable performance over extended operation, with favourable regeneration potential and reduced secondary waste generation compared to conventional sorbents. Importantly, the technology shows strong adaptability across different water streams, highlighting its potential as a unified solution for PFAS management.

This work advances sorption-based PFAS treatment toward practical implementation by addressing key limitations in selectivity, robustness, and scalability. The results support the deployment of next-generation sorbent systems for sustainable PFAS remediation in both municipal and industrial settings.

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3.06.P–Mo101 Legacy of Landfilling Connected With PFAS and Other Organic Pollutants: Comparison of Czech and Danish Landfill Leachates

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Landfill leachates represent an important source of emerging organic pollutants that may persist in the environment long after landfill closure. This study compared the occurrence of per- and polyfluoroalkyl substances (PFAS), pharmaceuticals and personal care products (PPCPs), endocrine-disrupting chemicals (EDCs), brominated flame retardants (BFRs), and polychlorinated biphenyls (PCBs) in landfill leachates

and sediments from the Czech Republic and Denmark, two countries with contrasting waste management strategies. While Denmark has minimized landfilling through long-term reliance on waste incineration and recycling, the Czech Republic still depends heavily on municipal waste landfills.
A total of 23 leachate samples were collected from 18 landfill sites, including operational and recently closed Czech municipal landfills and Danish landfills closed for more than 20 years. Target compounds included 32 PFAS, 59 PPCPs and EDCs, 55 BFRs, and congener-specific PCBs. Analyses were performed using liquid chromatography-tandem mass spectrometry and gas chromatography-mass spectrometry methods.
PFAS were detected in all leachate samples, with generally higher concentrations in Czech landfills (sum PFAS 691–9254 ng/L) than in Danish sites (415–2589 ng/L). Nearby Czech stream samples reached up to 11,011 ng/L, indicating migration of contaminants into surrounding waters. PPCPs and EDCs were also more diverse and abundant in Czech leachates, with pharmaceuticals such as diclofenac, ketoprofen, sulfamethazine, and carbamazepine detected at elevated concentrations. Danish samples showed lower diversity but persistent occurrence of compounds such as bisphenol A and carbamazepine even decades after landfill closure. PCBs and BFRs were primarily associated with sediments, confirming the importance of solid matrices for monitoring hydrophobic legacy contaminants.
The results demonstrate that landfill leachates remain a long-term source of environmental contamination regardless of landfill age. Active Czech municipal landfills exhibited broader pollutant spectra and higher concentrations, while Danish closed landfills still released persistent legacy contaminants more than two decades after closure. The study highlights the long-term environmental burden associated with landfilling and the importance of improved waste management and leachate treatment strategies.

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3.08.B.T - Integrated Approaches in Ecological and Human Health Risk Assessment (APAC Focus)

3.08.B.T01 Advancing Science-Based Environmental Risk Assessment in Asia through Scientific Engagement with Regulators and Industry–Regulator Collaboration

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The lack of a standard framework for environmental risk assessment (ERA) of crop protection products has increased pressure on less-regulated countries in Asia such as Taiwan, Malaysia, Vietnam, and Thailand. This has resulted in additional local data generation requirements and has limited farmers' access to robust crop protection tools. Identifying a locally best-fit ERA scheme from the many global models (e.g., US EPA, EU, China) is challenging for regulators, given current capability constraints. To address this, the CropLife Asia ERA team analyzed country needs and aligned with industry experts to design a framework for scientific engagement with regulators, with the aim of introducing science-based risk assessment that supports local environmental protection goals. Comprehensive ERA training workshops were organized in Malaysia (2022–23) and in Vietnam and Thailand (2024–25). Industry proposals—delivered through concise technical presentations and case studies using suitable ERA tools and models—were very well received by regulators. The hands-on trainings helped achieve two key objectives: (1) establish the CropLife-led industry expert group as a trusted partner in providing technical support to regulators on environmental safety topics; and (2) build regulators' internal capability in scientific risk assessment, enabling countries to transition from arbitrary, hazard-based systems to more

robust and predictable science-based safety evaluations. As a result, Malaysia, Vietnam, and Thailand are updating national guidance to adopt scientific ERA models, ultimately enabling more sustainable crop protection regulations through strengthened industry–regulator partnership and collaboration.

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3.08.B.T02 Advancing Environmental Risk Assessment of Fragrance Materials: Global Prioritization in Aquatic Systems Beyond Europe and North America

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

3.08.B.T03 Plastisphere Microbiome of the Red River Delta, Vietnam: Co-occurrence of Resistome, Metal Resistance, and Virulence Signatures as One Health Risk Indicators

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Microplastics (MPs) in river–estuary systems of the Red River Delta, Vietnam, are exposed to multiple pollution sources including urban wastewater, hospital effluents, and aquaculture discharge, creating distinct gradients from urban Hanoi to estuarine areas. Plastisphere biofilms on MP surfaces represent potential hotspots for co-accumulation of antibiotic resistance genes (ARGs), metal resistance genes (MRGs), and virulence-associated factors, yet their ecological and public health significance in tropical, highly impacted systems remains poorly understood.

Water, sediment, and MP samples (waterborne and sediment-associated) were collected across Hanoi, Ha Nam, and Ninh Binh. Six waterborne MP biofilm samples from contrasting land-use settings were subjected to shotgun metagenomic sequencing (Illumina 2×150 bp) to characterize plastisphere communities and functional resistance profiles. Remaining samples were screened by PCR for selected ARGs and MRGs; biofilm structure was visualized by scanning electron microscopy.

Plastisphere bacterial communities were dominated by Pseudomonadota and included genera with

pathogenic potential (Klebsiella, Vibrio, Aeromonas, Pseudomonas). Bray–Curtis beta-diversity analysis revealed site-specific community differentiation, with the first two PCoA axes explaining 65.8% of variation. Metagenomic profiling detected ARGs, MRGs, and mobile genetic element markers across all biofilm samples. VFDB analysis revealed prominent virulence-associated genes (acpXL, dnaK, fliG, lpxC) and strong co-occurrence of Arsenophonus with multiple VFDB signatures. PCR screening confirmed broad distribution of resistance markers (parE, copA, rsmA) across all sample types.
These findings demonstrate that MPs in tropical river–estuary systems act as colonizable surfaces that concentrate microbial communities carrying resistance and virulence signatures. The plastisphere represents a One Health-relevant microhabitat warranting integration into environmental monitoring frameworks in rapidly urbanizing Southeast Asian regions.

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3.08.B.T04 Operational Detection of Salinity Interference in Freshwater Toxicity Assessment Using a Bioassay-Informed Explainable Machine Learning Framework

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Salinity-induced interference represents a persistent challenge in freshwater ecotoxicity assessment, as elevated ionic strength can trigger organism-level stress responses indistinguishable from chemically mediated toxicity, potentially inflating toxicity units (TUs) and misrepresenting actual ecological risk. To address this, we developed a bioassay-informed machine learning framework for operationally identifying salinity-associated interference patterns in industrial wastewater. From 250 nationwide industrial wastewater samples, 27 high-salinity samples (>6 PSU) were selected for model development. TU responses from the freshwater crustacean Daphnia magna, freshwater macrophyte Lemna minor, and euryhaline macroalga Ulva australis were integrated to generate biologically grounded interference labels, with 11 samples classified as interference-positive. Ulva australis served as a salinity-tolerant reference species, enabling mechanistic separation of osmotic stress from intrinsic chemical toxicity.
Among logistic regression, random forest (RF), and gradient boosting classifiers evaluated under repeated stratified cross-validation (100 repeats), RF demonstrated the most balanced performance (AUROC = 0.715). A reduced five-variable RF model — using dissolved oxygen, copper, selenium, chromium, and zinc — achieved an AUROC of 0.781, retaining dominant predictive signals under dimensionality reduction. SHapley Additive exPlanations (SHAP) analysis identified dissolved oxygen and selected trace metals as primary contributors, consistent with redox-sensitive metal speciation pathways.
This framework translates multi-species TU fingerprints into an interpretable, ready-to-use screening tool that can be embedded into existing monitoring workflows without additional analytical burden. The proposed approach highlights the potential of coupling effect-based methods with explainable machine learning to improve ecotoxicity data interpretation under saline conditions — with direct implications for regulatory compliance assessment and industrial discharge management.

1.03.T - Adverse Outcome Pathways (AOPs): From Mechanistic Insight to Regulatory Impact

1.03.T01 Fenoxycarb Reduces Fecundity through Oocyte Apoptosis in Daphnia magna: A Mechanistic Framework for Adverse Outcome Pathways of Juvenile

Hormone Analogs

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Juvenile hormone analogs (JHAs) are commonly used insect growth regulators, but they can also disturb endocrine signaling and affect reproduction in non-target aquatic organisms. In Daphnia magna, reproduction occurs through parthenogenesis in healthy population, while environmental stresses or chemical cues can induce male production. Previous studies have shown that JHA exposure reduces fecundity and promotes male production in D. magna parthenogenesis. However, how JHAs cause the two different reproductive toxicities at the organism level is still not fully understood.
In this study, we examined the effect of the JHA fenoxycarb on D. magna fecundity using time-controlled exposure together with genetic and imaging approaches. First, we exposed D. magna to fenoxycarb with different start and end times (0–72 h post-oviposition) and across different exposure windows (24 h, 16 h, 8 h, and 4 h). The results showed that exposure during 16–32 h post-oviposition time window caused a significant decrease in D. magna fecundity, indicating that this period is particularly sensitive.
We also developed a germline-specific VASA:H2B-GFP CRISPR knock-in line to visualize ovarian development in vivo. When this line was exposed to fenoxycarb during the 16–32 h sensitive window, high resolution fluorescence and multiphoton imaging showed irregular nucleoli and nuclear collapse in developing oocytes, suggesting apoptosis-like processes. This indicates that oocyte degeneration is a key step leading to reduced fecundity.
We further found that the fenoxycarb sensitive periods for fecundity and sex determination are different in D. magna, since sex determination is sensitive at 62–68 h post-oviposition. This suggests that JHAs may disrupt multiple developmental checkpoints depending on exposure timing.
Overall, our results connect cellular-level effects to organism-level outcomes and support the Adverse Outcome Pathway (AOP) concept. This study also shows that genetically engineered Daphnia can be a useful model for understanding mechanisms of chemical toxicity and improving environmental risk assessment.

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1.03.T02 Development of Adverse Outcome Pathway (AOP) on Amyotrophic Lateral Sclerosis (ALS)

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Amyotrophic lateral sclerosis (ALS) is a fatal neurodegenerative disease characterized by the impairment of motor neurons in the brain and spinal cord, leading to skeletal muscle atrophy and eventual death due to respiratory muscle paralysis. Currently, fundamental curative treatments remain unestablished. The objective of this study is to develop an Adverse Outcome Pathway (AOP) for ALS to elucidate its underlying pathological mechanisms. By analyzing molecular networks using RNA-seq data and synthesizing existing literature, we have proposed a draft AOP. This pathway delineates the progression from an initial rise in reactive oxygen species (ROS) and oxidative stress to neurodegeneration and motor neuron death, mediated by key events such as TDP-43 aggregation, mitochondrial dysfunction, neuroinflammation, and axonal transport failure. In developing a quantitative AOP (qAOP), it is essential to assess the quantifiability of each Key Event (KE) and Key Event Relationship (KER) to accurately

model the network's functional relationships.

1.03.T03 Cross-Species Omics2AOP: Using Comparative Transcriptomics and Adverse Outcome Pathways to Support Chemical Safety Assessment

A major challenge in omics-based chemical safety assessment is translating complex molecular data into evidence that is biologically meaningful, adverse outcome-relevant and useful for decision-making across both human health and ecological contexts. New Approach Methodologies, including transcriptomics and in vitro cell models, can capture early mechanistic responses to chemical exposure, but these data often remain difficult to interpret chemical toxicity across species.

Cross-species Omics2AOP provides a practical framework to address this challenge by integrating comparative transcriptomics with the Adverse Outcome Pathway (AOP) framework. By linking gene expression changes to key events (KEs), this approach can help identify conserved toxicity pathways, distinguish species-specific responses, and organise complex omics data into a transparent mechanistic structure.

We illustrate this approach using methylmercury exposure in human, bird and fish neural cell lines as a case study. Concentration-dependent transcriptomic responses are compared across vertebrate neural models and interpreted through AOP network to identify molecular perturbations associated with impaired neural development and function. This case study demonstrates how comparative transcriptomics can move beyond descriptive profiling toward pathway-informed interpretation, supporting more predictive, transparent and animal-sparing chemical safety assessment.

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1.03.T04 Evaluating cross-chemical applicability of time-resolved quantitative Adverse Outcome Pathway (qAOP) models for mitochondrial uncouplers

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Quantitative Adverse Outcome Pathways (qAOPs) are increasingly proposed to support Next-Generation Risk Assessment (NGRA) of chemicals using New Approach Methodology (NAM) data. However, their applicability beyond calibration with a single chemical remains insufficiently evaluated. A key challenge is determining whether qAOPs can provide reliable predictions across chemicals that share a common mode of action but differ in physicochemical properties and toxicokinetics. This study evaluated the cross-chemical applicability of a time-resolved qAOP based on an OECD-endorsed AOP describing uncoupling of mitochondrial oxidative phosphorylation leading to growth inhibition. The zebrafish liver (ZFL) cell line was used as an in vitro model to generate temporal concentration-response data following exposure to a model uncoupler, carbonyl cyanide m-chlorophenyl hydrazone (CCCP), for qAOP development. Directional relationships among key events were quantified using piecewise structural equation modeling (PSEM), and model performance was assessed across temporal configurations and chemicals. The qAOP was subsequently challenged using five additional environmental uncouplers with distinct physicochemical properties to evaluate model robustness and predictive performance. Results showed that predictive performance increased systematically along the pathway. Early key events were

highly sensitive to chemical-specific properties and exhibited limited transferability, whereas downstream key events reflecting integrated bioenergetic stress demonstrated strong and consistent predictive performance across chemicals. Variability in early predictions was partly attributable to differences in uptake kinetics and the absence of internal concentration measurements for the additional compounds. These findings demonstrate that qAOPs can support mode-of-action-specific predictions across chemicals when anchored to integrative downstream key events. The study highlights the importance of time-resolved data, internal dosimetry, and clearly defined applicability domains. Overall, this work advances the development of qAOPs as tools for chemical screening and prioritization and supports their application in regulatory decision-making.

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1.04.T - Bridging Gaps in Microplastic Ecotoxicology: From Particle Characterization to Reliable Risk Assessment

1.04.T01 From Detection to Impact: Advancing the Assessment of Microplastic Exposure and Risk; a 10 year retrospect.

Leah Bendell[1] (1)Simon Fraser University

For the past 10 years (since 2016), my research group (Ecotoxicology Research Group (ERG) at Simon Fraser University), has worked towards advancing the understanding of microplastic sources, environmental distribution, and potential ecological and human-health impacts, while identifying critical methodological gaps in detection and risk assessment. A central challenge we have had to address is the difficulty of accurately quantifying microplastic occurrence, transport pathways, and biological effects across ecosystems and food webs, which limits confidence in risk-based management. To address this, our studies have integrated field observations, laboratory experiments, targeted literature reviews, and methodological evaluations to link environmental concentrations with biological exposure and effects. Approaches have included systematic sampling across water, sediment, and biota, controlled uptake experiments, and critical assessment of analytical protocols such as sampling design, size fractionation, and polymer identification. Overall our body of work has demonstrated the widespread presence of microplastics across habitats and trophic levels, along with evidence of uptake and possible sublethal effects under certain exposure scenarios. Importantly we have also identified substantial variability driven by particle size, polymer type, and environmental context. Overall, research from ERG has indicated both the ecological relevance of microplastics and the urgent need for improved methodological consistency.

1.04.T02 Comparative Study of Microplastic Egestion Patterns in Daphnia magna Based on Shape

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Microplastics are a major concern because of their potential effects on organisms through various pathways. Most studies have reported the direct or indirect effects of microplastics, but quantification has rarely been considered. Daphnia magna is a filter-feeder, that can uptake microplastics within its edible size range, and these particles move along the digestive tract. To bridge the gap in understanding the impact of microplastics, it is necessary to quantify the amount of ingested and residual particles. This

study aimed to quantify the ingestion and egestion of microplastics using a fluorescence intensity-based method without chemical or physical degradation. D. magna was exposed to green fluorescent microspheres and fragments for 24 hours, then transferred to clean media for egestion. Egestion rates of microplastics were observed based on ingestion rates, under both the presence and absence of food conditions. As a result, D. magna egested more microplastics in the presence of food than in its absence. Microplastic fragments persist longer than spheres in D. magna following a 24-hour egestion period. These results showed that microplastic egestion patterns can vary depending on shape, and this method allows for easier quantification of the amount of microplastics ingested and egested by D. magna compared to quantification using images or degradation methods.

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1.04.T03 Accurate Identification of Submicron-sized Plastic Particles using Submicron Infrared Technique

Michael K. F. Lo[1], Kevin Kjoller[1], Eoghan P. Dillon[1] and Mustafa Kansiz[1] (1)Photothermal Spectroscopy Corp

In recent years, interests in microplastics have captured significant attention due to their environmental impacts and potential effects toward health of living organisms. To accurately identify the chemical identities of such particles can be challenging, especially for the size groups smaller than 20 micrometers due in part to the detection limitations of conventional Fourier-transform Infrared and Raman spectroscopies. An effective approach would be using optical photothermal infrared spectroscopy (O-PTIR) to achieve sub 20-µm sensitivity reliably while retaining superior searchability in commercially available infrared databases. This novel type of analytical instrumentation makes use of co-illumination of an infrared and visible lasers simultaneously to provide a “pump-probe” excitation and detection through the same optical objective. With this arrangement, non-destructive analyses could be made without making physical contact with the specimen, thus preserving the integrity of the same. Notwithstanding, plastic particles smaller than 1 µm are even more challenging for identification but knowing their chemical identity can be highly rewarding. Other than mass spectrometry, there are no known analytical methods to reliably identify these matters in a non-destructive manner. In this presentation, we hereby demonstrate the feasibility of using O-PTIR for identifying particles in the sub-500 nm regime by using a counter-propagating approach where the pump and probe lasers beams co-illuminate through two separate objectives.

1.04.T04 Bayesian Species Sensitivity Distribution Modeling for Microplastic Particles: Toward Ecological Risk Assessment Informed by Particle Characteristics

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Scientifically defensible ecological risk assessment of microplastic particles remains challenging because their toxicity can depend on diverse particle characteristics, such as size and shape. Species sensitivity distributions (SSDs) are widely used to derive environmental quality benchmarks, but conventional SSD approaches have often failed to incorporate particle characteristics, species-level variation, and censored effect concentrations. To address these limitations, we developed hierarchical Bayesian SSD models for chronic no observed effect concentrations (NOECs) of microplastic particles. The models account for intra-species variation and examine how particle characteristics influence species sensitivity. They also allow highest observed no-effect concentrations to be incorporated as right-censored observations,

thereby making use of a substantial amount of information that is often excluded from conventional SSD analyses. Using an updated ecotoxicity dataset, we identify particle characteristics, such as particle length and shape, that are included in SSD models selected based on the widely applicable information criterion. Hazardous concentrations for 5% of species are then estimated while explicitly representing uncertainty. This modeling framework provides a flexible and data-informed approach for ecological risk assessment of microplastic particles as well as groups of chemically similar substances, such as per- and polyfluoroalkyl substances (PFAS).

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1.08.T - Integrating Experimental and Modeling Approaches To Unravel the Mechanisms of Multiple Stressor Effects on Aquatic Ecosystems Under Climate Change

1.08.T01 The Interactive Effects of Temperature and Zinc (Zn) on Four Species of Native Australian Shrimp (Family: Atyidae, Genera: Caridina, Paratya).

Gina Mondschein[1], Vincent Pettigrove[1] and Kathryn Hassell[1] (1)RMIT University

Climate change and pollution pose a significant global threat to biodiversity within freshwater ecosystems. Elevated water temperatures alone can be detrimental to aquatic organisms, but also increase the solubility of pollutants, exacerbating their toxicity. The interactive effects of these two stressors on aquatic ecosystems remain poorly understood. Freshwater shrimp (Family: Atyidae) are ecologically significant taxa widely used as bioindicators. There are 50 species in Australia. Only one, Paratya australiensis, is currently used as a bioindicator, however its distribution is limited to temperate and sub-temperate regions. In contrast, Caridina species richness is higher and its distribution spans most of Australia, including a range of climatic zones. Six Australian species are endemic to Africa and Asia, where they are used in ecotoxicology and biomonitoring. In Australia however, they remain significantly understudied.

This project explores how sensitivity to temperature and pollution varies between shrimp genera and species across different climatic regions of Australia, with the view of establishing native Caridina species as bioindicators. It integrates ecotoxicology, biogeography and climate science. Two temperate species (P. australiensis and C. mccullochi) and two tropical species (C. niloticaNT and C. gulf1) were exposed in separate experiments to multiple temperatures (20ºC, 26ºC and 32ºC) and concentrations of Zn, a common environmental pollutant, over a four day (96 hour) period. Mechanisms tested included thermal tolerance (survival) and zinc uptake in tissue. Survival in control treatments was high (>80%) for all species at 20ºC and 26ºC, and for one tropical species, C. niloticaNT at 32ºC. Survival decreased as temperature and zinc concentration increased, which was more pronounced in the tropical species. Caridina species were more tolerant to higher temperatures than P. australiensis but was more sensitive to pollution.

Response varied based on geography and genus, emphasising the importance of establishing local bioindicator species with broader Australian and international comparability and relevance. Using multiple temperatures, zinc concentrations and species over a climate gradient provides opportunities to

develop models to predict ecosystem response to climate change and associated stressors. The data generated can be used to predict ecosystem health and function in a changing climate.

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1.08.T02 Assessing the Interactive Effects of Climate Change-driven Temperature Variation and Chemical Pollution on Aquatic Communities: A Modelling Study.

Constanza Vega Olivares[1] and Andreu Rico[1] (1)University of Valencia

Aquatic ecosystems are currently experiencing severe biodiversity loss due to anthropogenic threats, such as climate change and chemical pollution. These human-induced stressors manifest concurrently rather than in isolation. However, the effects of stressors such as pesticides, rising temperatures, and heatwaves on aquatic organisms have primarily been investigated as isolated factors, thereby disregarding the potential interactive effects between the different stressors and at different ecological levels (e.g. communities). In this study, a temperature-explicit bioenergetic model for polluted food webs was employed. This model links individual-level physiological processes to emergent community-level responses. It was used to assess the interactive effects of global warming and chemical pollution on aquatic communities. Specifically, we considered different manners of thermal stress (prolongated warming and heatwaves), pollutants with different chemical properties and modes of action, and different sequences of stressors' application to the system. Subsequently, the effects of the various treatments on the stability of the communities were determined, and potential induced climate change sensitivity (TICS) and climate-induced toxicant sensitivity (CITS) were identified. In this study, we advance beyond the limitations of single-factor analyses by systematically quantifying the interactive effects of diverse forms of thermal stress with chemicals of varying properties and modes of action across entire food webs. Ecological models enable the assessment of community changes over temporal scales that are challenging to obtain empirically, such as stability, persistence, and recovery. Furthermore, the model outcomes can guide management by identifying pollutant types, warming patterns, and timing of exposure that most strongly compromise community stability. This, in turn, can support more targeted mitigation strategies and ecosystem-based climate adaptation in aquatic systems.

1.08.T03 Combined Effect of the Insecticide Methoxyfenozide and Elevated Temperatures on Freshwater Macroinvertebrate and Emergent Insect Communities and Populations

Paul van den Brink[1], Wout Hoppenreijs[1], Ivo Roessink[1] and Iim Imroatushshoolikhah[1] (1)Wageningen University and Research (WUR)

Agricultural intensification and climate change are increasingly threatening freshwater ecosystems, with aquatic invertebrates particularly vulnerable due to their sensitivity to agrochemical contamination and rising surface water temperatures. Moreover, pesticides can interact with warming, altering toxicity and producing unpredictable effects in aquatic ecosystems. To address this research gap, a 30-day outdoor mesocosm study was performed in the Netherlands to assess the single and combined effects of two methoxyfenozide treatments (30, 300 µg/L) and a control (0 µg/L) under two temperature scenarios (ambient, ambient +4°C) on macroinvertebrate and emergent insect communities and populations. Methoxyfenozide, a widely used ecdysone receptor agonist for controlling Lepidoptera pests, is persistent and highly prone to leaching. The results showed that both single- and combined-stressor treatments significantly altered macroinvertebrate community composition, with significantly lower abundances of larval Chaoborus sp. and Tanypodinae in chemical treatments relative to the chemical control. The

elevated temperature treatment significantly increased the abundance of Lumbriculus variegatus and Gyraulus albus, whereas it reduced the abundance of Gammarus pulex relative to the ambient control. The emergent insect community was dominated by Diptera and was significantly affected by temperature and the high-chemical treatment at multiple time points. Abundances of Chironomidae, Chaoboridae, and Culicidae were significantly lower at high chemical treatments relative to the chemical control, while Chironomidae and Culicidae abundances were also lower under the elevated temperature treatments relative to the ambient control at certain timepoints. Diptera biomass was consistently lower under elevated temperature, chemical, and combined stress. Although there were some indications of stressor interaction, they were not consistently significant, suggesting that the effects of multiple stressors were predominantly additive rather than antagonistic or synergistic.

1.08.T04 Multiple Stressor Effects of Heatwaves and Thiacloprid on Stream Ecosystems

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Multiple stressors posed by climate change and pesticides are major threats for aquatic ecosystems due to unpredictable interaction effects. Their impacts will increase in the future as weather extremes, such as heatwaves, are expected to become more frequent and severe, and the application of increasingly potent insecticides, like neonicotinoids, persists globally. To understand how climate extremes and pesticides affect lotic ecosystems, we conducted a 7-week outdoor mesocosm experiment employing the "POTAMOS" system consisting of 20 experimental flumes mimicking streams. All flumes were filled with a mixture of pebbles of different grain sizes and organic matter simulating realistic environmental conditions. Subsequently, all flumes were inoculated with macroinvertebrates from streams in the vicinity of the experimental site. Physical water parameters, including temperature, retention time, and flow velocity were steadily controlled. To investigate the effects of climate extremes, three heatwave events were simulated, each lasting 7 days and with +8°C above ambient temperatures following natural daily temperature fluctuations. The neonicotinoid thiacloprid was spiked at an environmentally relevant concentration (10 µg/L) simultaneously with each heatwave to investigate single and interactive effects (n=5 per treatment combination). We measured water quality parameters, invertebrate community structure, as well as ecosystem processes and functions during and after each stressor sequence. We observed strong stressor-induced changes in macroinvertebrate abundance and community composition. The most depleted and dissimilar communities (Bray-Curtis dissimilarity) occurred under the heatwave and the combined stressor treatments. Changes were driven by decreased abundances of sensitive taxa, including Gammarus sp., Chironomidae, Coleoptera, Hydracarina, Diptera, Baetidae, Hydropsychidae, and Sericostomatidae, and increased abundances of Physidae. In contrast, the thiacloprid treatment induced more moderate effects, albeit affecting the same sensitive taxa. Significant effects of both single and combined stressors on taxa richness and evenness confirm these findings. Whether significant co-occurences of certain species over time coincide with the observed changes in biodiversity and how direct and indirect relations between taxa, ecosystem processes and functions are altered by the stressors, is still under investigation.

1.10.A.T - Environmental and Human Toxicology and Ecology: Linking Contaminants, Wildlife Sentinels, and Ecological Risk Assessment

1.10.A.T01 Homing pigeons as biomonitors, what information can they provide?

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Atmospheric pollution is a global concern effecting animal and human health. Mechanical air monitoring can provide information regarding concentrations of hazardous chemicals in the air; however, biomonitoring provides tissue exposure and effects data not available from air monitoring alone. In many countries, homing pigeons are raised by hobbyist in urban and rural areas. Know age, location, and health history information facilitate the use of homing pigeons to evaluate air pollution exposure and effects data among various urban areas and regions. Our previous research demonstrated that homing pigeons collected from cities with known air pollution had similar gross lesions including gray/black discolorations of the lungs and several cases of enlarged and irregular testes (tumors) compared to pigeons collected from cities with no air pollution issues. Concentrations of polycyclic aromatic hydrocarbons (PAHs) and mercury in lung and liver tissue from pigeons collected from cities with air pollution issues were greater than concentrations in pigeons collected from cities with no air pollution. Our research suggests that avian species in some evaluated urban areas are adversely affected by air pollution and that homing pigeons provide specific in situ contaminant data useful in evaluating and managing environmental and potential human health issues. Biomonitoring data provided by monitored homing pigeons allows for direct evaluation of exposure and effects data not readily available using other forms of environmental monitoring.

1.10.A.T02 Exposure to Mercury and Polychlorinated Biphenyls affects the Thyroid Function of an Australian Seabird (Ardenna carneipes)

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Seabirds are top predators in the marine environment. They are therefore exposed to high levels of persistent pollutants that can bioaccumulate and biomagnify, making these predators excellent indicators of ecosystem health. Commonly found in the marine environment, mercury (Hg) and polychlorinated biphenyls (PCBs) are known to interfere with the thyroid system in wildlife. This study quantified PCBs and Hg concentrations and investigated the relationship with thyroxine (T4) and triiodothyronine (T3) levels in fledgling and adult sable shearwaters (Ardenna carneipes). Hg and PCBs were measured in feathers and red blood cells, respectively. The results indicate Hg and PCBs were more abundant in adult shearwaters than in fledglings. Negative associations were found between Hg/PCB body burdens and circulating thyroid hormone concentrations in both age categories. However, some of these correlations were not statistically significant. This study presents an empirical dataset of these contaminants and the thyroid function of adult and juvenile birds in the Australian coastal environment. This is a significant step towards better understanding the threat posed by Hg and PCBs to the health of seabirds.

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1.10.A.T03 Identification and Phylogenetic Analysis of CYP2 and CYP3 Family Genes in Morelet's Crocodile (Crocodylus moreletii)

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Cytochrome P450 (CYP) enzymes play central roles in the metabolism of xenobiotics, including

environmental chemicals. However, compared with those of humans and other mammals, reptilian CYP genes remain poorly characterized, particularly regarding their diversity and evolutionary relationships. This knowledge gap limits understanding of the molecular basis of contaminant responses in reptiles, including crocodilians that may be exposed to heavy metals and agricultural pesticides in the wild. Among CYP families, CYP2 and CYP3 are major contributors to xenobiotic metabolism in vertebrates. Therefore, this study aimed to characterize CYP2 and CYP3 family genes in Morelet's crocodile (Crocodylus moreletii) and evaluate their phylogenetic relationships among reptiles.

Candidate CYP sequences were identified from protein sequences predicted from de novo assembled scale-derived RNA-seq data and evaluated by phylogenetic analysis with representative reptilian CYP sequences. Multiple CYP2 candidate sequences were identified from Morelet's crocodile scale RNA-seq data, including CYP2A-, CYP2B-, CYP2D-, and CYP2J-like genes. These sequences phylogenetically clustered with corresponding reptilian CYP subfamilies, suggesting that CYP2 family genes with xenobiotic metabolism are shared among reptiles. In contrast, although several CYP3A-like hits were detected, no definitive CYP3A candidates were confirmed. This may reflect tissue-specific expression patterns because the analyzed RNA-seq data were derived from scale tissue, whereas CYP3 gene are typically highly expressed in liver and intestine.

These findings provide new insights into reptilian CYP diversity and suggest that reptilian scale tissue may possess xenobiotic metabolic capacity mediated by CYP2 family genes. This study also provides a foundation for understanding molecular responses to environmental contaminants in crocodilians and other reptiles.

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1.10.A.T04 Assessment of the Possibility of Metabolomics-Based Early Indication of Drug-Induced Liver Injury (DILI) Using In Vitro and In Vivo Approaches

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Hepatotoxicity remains one of the primary causes of post-market drug withdrawal, limiting the overall success of pharmaceutical development despite extensive safety evaluation processes. Drug-induced liver injury (DILI) is commonly assessed through both in vitro and in vivo screening during the preclinical stage, while chronic toxicity evaluation still relies predominantly on animal models. However, concerns regarding interspecies variability, experimental duration, and ethical issues have increased the demand for alternative testing strategies. Conventional in vitro assays also require relatively long experimental periods and involve destructive sampling of exposed cells, restricting the investigation of time- and physiology-dependent cellular and molecular responses. Therefore, this study applied extracellular metabolomics, a non-destructive approach, in combination with a conventional cytotoxicity assay. We hypothesize that changes in abundance of liver cell-derived biomolecules will be correlated with the magnitude of subsequent hepatotoxicity. We additionally expected that whether a drug is hepatotoxic or not could be predictable from the metabolomic profile patterns. HepaRG cell line was used for this experiment. Five DILI and non-DILI pharmaceutical substances were respectively selected, and exposure tests were conducted at high(>IC20) and low(

2.02.B.T - Advances in Environmental Chemistry for Quantitative Exposure Assessment and Risk-Informed Management of PFAS and Emerging Contaminants

2.02.B.T01 Unidentified Organofluorine in Human Serum: Insights from Fluorine Mass Balance and PFAS Biomonitoring

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Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants, yet conventional biomonitoring captures only a limited subset of these compounds. Increasing evidence suggests that a substantial fraction of total organofluorine in humans remains unidentified, posing challenges for accurate exposure assessment and risk evaluation .

This study aims to quantify the contribution of unidentified organofluorine (UOF) to human exposure and to evaluate the completeness of current PFAS biomonitoring approaches. We address this challenge by integrating targeted PFAS analysis with extractable organofluorine (EOF) measurements and fluorine mass balance in human serum.

Serum samples from the EuroMix cohort (Norway; n=215), including 72 paired samples collected 2–3 weeks apart, were analyzed for EOF and 64 PFAS, including trifluoroacetic acid (TFA). A complementary case study examined the influence of fluorinated pharmaceuticals using serum samples from individuals with and without fluoxetine use. Fluorine mass balance was applied to quantify the proportion of unidentified organofluorine and assess temporal variability in exposure.

Results show that UOF accounted for up to 81% of EOF (median 38%) in the cohort, indicating that a large fraction of human exposure is not captured by targeted analysis. TFA was the most abundant individual PFAS, with concentrations exceeding those of PFOS. Short-term variability was observed, with 36% of paired samples showing >25% change in EOF, suggesting exposure to compounds with relatively short biological half-lives. In the case study, fluoxetine use was associated with substantially elevated EOF and TFA levels, highlighting fluorinated pharmaceuticals as a potentially important and under-recognized source of exposure.

These findings demonstrate that current biomonitoring approaches capture only a fraction of total fluorinated chemical exposure and that unidentified organofluorine contributes significantly to human burden. Integrating EOF and fluorine mass balance with targeted analysis provides a more comprehensive framework for exposure assessment. This approach improves the robustness of risk evaluation and supports the development of more effective monitoring and regulatory strategies for PFAS and related substances.

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2.02.B.T02 Interlaboratory Evaluation of PFAS Total Approaches: Performance, Reproducibility, and Blank Effects across Target Analysis, TOP Assay, and EOF-CIC

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Poly- and perfluoroalkyl substances (PFAS) are persistent chemicals of global concern due to their environmental persistence and potential health impacts. Regulatory frameworks increasingly require comprehensive assessment, including the concept of “PFAS Total.” However, no single analytical method can directly quantify the full spectrum of PFAS. Therefore, proxy approaches such as target analysis, the total oxidizable precursor (TOP) assay, and extractable organofluorine (EOF) by combustion ion chromatography (CIC) are widely applied. Their comparability, reproducibility, and robustness across laboratories, however, remain insufficiently understood.

An interlaboratory trial (ILT) was conducted to evaluate these methods across river water, soil, and acrylonitrile–butadiene–styrene (ABS) resin. Ten laboratories in Japan participated using standardized samples and protocols. The evaluation focused on concentration, reproducibility (coefficient of variation, CV), recovery, and blank levels.

For most samples, target analysis and TOP assay yielded comparable concentrations for known PFAS. However, higher concentrations by TOP assay were observed in one river water sample, suggesting the presence of unidentified or precursor PFAS not captured by target analysis. Reproducibility was acceptable for water samples, with interlaboratory CV <40% at PFAS concentrations ≥0.2 ng/L, while variability increased at lower concentrations, likely due to blank contributions.

Recoveries were generally within 70–120% across methods and matrices. In the TOP assay, oxidation surrogate recoveries were mostly within 50–150%, indicating sufficient precursor conversion, although correction for ionization suppression was necessary. For ABS resin certified reference material, linear PFOS recovery by target analysis was approximately 72%.

Significant interlaboratory variability was observed in blanks, particularly for EOF and TOP assay, which were more susceptible to contamination than target analysis. Elevated blanks strongly affected low-concentration results and increased variability, highlighting the need for strict blank control.

This study demonstrates the strengths and limitations of current PFAS Total proxy methods and underscores the need for harmonized protocols, improved blank management, and standardized quality control to ensure reliable interlaboratory comparability and support regulatory implementation.

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2.02.B.T03 Characterizing Side-Chain Fluorinated Polymers via Non-Target Screening: Insights from Scotchgard Formulations

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Side-chain fluorinated polymers (SCFPs) remain a blind spot in PFAS research due to their structural complexity, lack of analytical standards, and absence from spectral libraries. Scotchgard products, widely used in consumer applications, are known sources of SCFPs; however, the composition and structures of their dominant fluorinated polymers remain poorly understood. This knowledge gap limits the assessment of PFAS contamination at impacted sites, including textile manufacturing facilities and biosolids, where SCFPs have been either tentatively detected or suspected, but not fully characterized. This study aims to characterize SCFPs in Scotchgard formulations and address key analytical challenges associated with SCFP. A non-target screening (NTS) framework was combined with complementary techniques to improve detection and structural interpretation. Scotchgard products manufactured between 1987 and 2022 were analyzed using LC-HRMS for targeted and non-targeted PFAS detection, pyrolysis-GC-MS for polymer decomposition products, and 19F NMR for fluorinated moiety characterization. Kendrick

mass defect (KMD) analysis and chemical reasoning were applied to identify homologous series, while historical patent data supported structural elucidation.
The results reveal multiple homologous SCFP series, including previously unreported polymeric PFAS. Rather than a few discrete compounds, older Scotchgard formulations consist of complex mixtures spanning a range of perfluoroalkyl chain lengths, with certain species dominating based on signal intensity. A temporal shift from C8 electrochemical fluorination (ECF)-based chemistries (1987–1997) to C4-ECF formulations after 2000 was observed, and no PFAS were detected in 2022 products. Pyrolysis confirmed characteristic fluorinated fragments, but MS2 fragmentation highlighted the difficulty of reconstructing full polymer structures. Given that most detected species had molecular weights below 2000 Da, LC-HRMS proved particularly effective for structural characterization. Overall, this work expands the known PFAS chemical space and provides a case study for identifying polymeric PFAS structures. The findings suggest that some SCFP structures likely remain unmonitored in contaminated industrial sites, especially those associated with the historical production of ECF-based products, as well as in biosolids. All point to the need for improved analytical strategies in risk assessment.

2.02.B.T04 Comparative Evaluation of Targeted and Total Fluorine Approaches for PFAS Monitoring in Harbour Sediments?

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Harbours are linchpins of global commerce, and the maintenance of harbours is essential. Key to keeping harbours operational is the regular removal of sediments – dredging. Dredged material has beneficial uses, but most of this material is dumped at sea. This can lead to sediment plumes, which pose an environmental hazard for the organisms in the area as harbour sediments are often contaminated with various legacy and emerging pollutants.
While different regions of the world have developed and use different risk assessment approach for dredged materials, they share one key challenge: per- and polyfluoroalkyl substances (PFAS) are not systematically monitored. PFAS represent a large group of organic pollutants, more than 4000 having been listed by the Organisation for Economic Co-operation and Development (OECD). These compounds have been linked to various adverse health effects, such as neurotoxicity , immunotoxicity, teratogenicity, and cancer. Although the use of some legacy PFAS has been limited since 2009, the levels of PFAS in the environment have persisted.
Our aim in this study was to compare different methodologies for comprehensive PFAS monitoring in harbour sediments. While conventional targeted methods (e.g. liquid chromatography tandem mass spectrometry (LC-MS/MS)) are highly sensitive and selective, they are unsuitable for monitoring thousands of compounds at once in practice. Consequently, alternative total fluorine methods have been developed. Total oxidizable precursor assay (TOP assay) converts perfluoroalkyl acid (PFAA) precursors into PFAAs, which are readily measurable by LC-MS/MS. Extractable organofluorine (EOF) analysis using combustion ion chromatography (CIC) converts all organofluorine compounds into inorganic fluoride.
We applied these methods to a selection of 20 sediment samples from harbours in south-east Sweden. The sum of target PFAS ranged from below the limit of quantification (LOQ) to 8.2 ng/g (dry weight). The presence of PFAA precursors was indicated by the TOP assay, which resulted in more than 300 % increase in PFAA levels in some samples. However, this was dwarfed by EOF analysis. For the 16 samples that had EOF levels above LOQ, the unidentified organofluorines (UOF) accounted for 71 % - 100 % of the EOF. These results indicate that the total fluorine methods are crucial for more comprehensive characterization of such sediment samples as the environmental impact of the UOF constituents is unknown.

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2.02.C.T - Advances in Environmental Chemistry for Quantitative Exposure Assessment and Risk-Informed Management of PFAS and Emerging Contaminants

2.02.C.T01 Global PFAS Pollution Needs to be Addressed on City and Local Levels – Some Experiences from Europe

PFAS pollution has exceeded planetary boundaries. Tens of thousands of PFAS-contaminated sites and presumptive contaminated sites have been mapped in the United States and Europe, respectively. These PFAS pollution legacies contaminate groundwater, surface water, and drinking water, threatening and impacting human health. PFAS pollution and human exposure need to be tackled and controlled on national level by a regulatory framework, but the practical assessment and remediation normally take place on the city and local level. A consortium of European cities published a position paper and highlighted that the costs for monitoring, remediation, and tackling the consequences of the pollution are rising rapidly and are compounded by growing concerns about the serious health impacts of long-term PFAS exposure. Local and regional authorities (LRAs) are on the front line: they must guarantee safe drinking water, manage soil and groundwater, operate waste and wastewater systems, and answer citizens' concerns —yet they have little control over PFAS sources and limited capacity to remove these persistent chemicals once released
(https://www.acrplus.org/global/gene/link.php?doc_id=434&fg=1).
The current study introduces a case study of a European city that assessed PFAS-contaminated sites, already starting in 2006 with a systematic inventory of PFAS-contaminated sites and controls and remediating PFAS-contaminated sites in the past 20 years. While good progress has been made on all major PFAS-contaminated sites in the city, the remediation will have to continue for the years and decades to come. Recently several European cities have developed a network of PFAS-contaminated cities to exchange such experiences on approaches and solutions and published a policy paper. Also, this activity will be shortly introduced. The policy paper suggests a stronger application of the polluter-pays principle, enabling local and regional authorities to hold polluters accountable and additionally propose an Extended Producer Responsibility (EPR) scheme for PFAS to fund the remediation of orphan pollution.

2.02.C.T02 Large-Scale Monitoring of PFAS Occurrence and Cross-Compartment Transport Across Groundwater to Coastal Systems Near Semiconductor and Municipal Sources in the Philippines

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Per- and polyfluoroalkyl substances (PFAS) are synthetic fluorinated compounds valued for their chemical and thermal stability. However, these same properties also confer high persistence in aquatic systems, leading to accumulation in environmental matrices and long-term risks to ecosystems and human health. The Philippines, undergoing rapid industrialization and lifestyle transitions, provides a compelling setting to investigate PFAS exposure across environmental and socioeconomic gradients. As an archipelagic nation, it is particularly vulnerable to cross-compartment transport of contaminants from groundwater to rivers and coastal waters. In this study, large-scale field monitoring was conducted across 66 sites nationwide, focusing on water systems proximal to semiconductor industrial zones. Targeted analysis of 32 PFAS compounds identified 11 that were consistently detected across all locations, representing the first comprehensive assessment spanning groundwater to coastal systems in the Philippine archipelago. Groundwater exhibited the highest total PFAS concentrations (up to 16 ng/L), exceeding those in river water (13 ng/L), indicating subsurface accumulation and delayed release. Short-chain PFAS were prevalent in both river and groundwater systems and were largely comprised by PFBA (13–65%), compared to long-chain PFAS, which were primarily dominated by PFOS (9.6–58%),

suggesting mixed legacy and emerging sources. Overall, these findings identify groundwater as a critical reservoir and transport pathway facilitating PFAS transfer to surface and coastal waters, with important implications for downstream water quality and human exposure risk.

2.02.C.T03 Emerging Per- and Polyfluoroalkyl Substances in Ho Chi Minh City: Spatiotemporal Profiling and Inhalation Exposure Evaluation

Cat Tuong Le Tong[1], Jheng-Jie Jiang[1] and Duy Dat Nguyen[2] (1)Chung Yuan Christian University, (2)HCMC University of Technology and Engineering

Southeast Asian megacities are rapidly urbanizing and sprawling, leading to complex atmospheric conditions; however, empirical data on the occurrence and transport of airborne per- and polyfluoroalkyl substances (PFASs) in these regions are alarmingly scarce. This study was conducted to supplement the pollution data in this region by providing a comprehensive study on atmospheric PFAS for Ho Chi Minh City (HCMC), Vietnam. We combined high-resolution source apportionment by advanced receptor modelling (Principal Component Analysis (PCA) and Positive Matrix Factorization (PMF)) with chromatographic analysis (LC-MS/MS) of indoor (n = 30) and outdoor (n = 40) airborne particulate matter for 75 distinct PFASs. Furthermore, backward trajectory analysis provided insight into the dynamics of long-range atmospheric transport. Our findings demonstrate the dominance of 6:2 fluorotelomer sulfonate (6:2 FTS) and perfluorobutanoic acid (PFBA) in the indoor microenvironment, shifting to short-chain alternatives. PMF identified indoor sources as infiltration from automobile manufacturing (38.9 %), thermal degradation of lubricants (31.0%) and fugitive emissions from laboratory equipment (30.1 %). Diffuse commercial packaging emissions dominated (42.8%) mixed with urban backgrounds. On the other hand, legacy signatures (e.g., NEtFOSA) in addition to 6:2 FTS preserved in outdoor profiles. In particular, high concentrations during the rainy season indicate that transboundary transport from the Indo-Pacific region dominates the usual wet scavenging effects. The presence of 6:2 FTS in HCMC points to a unique change in the chemical profile of the city, even though it has a lower atmospheric PFAS burden than established global industrial centers. Current risk assessments show negligible non-carcinogenic inhalation risks (Hazard Quotient < 1). However, the pervasive presence of commercial sources and transboundary pollution vectors necessitates ongoing longitudinal monitoring.

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2.02.C.T04 From Sink to Source: Sediment-Mediated Mobilisation of PFAS and Precursors in Tropical Catchments

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Understanding the mobilisation of per- and polyfluoroalkyl substances (PFAS) between sediment and aqueous phases is critical for assessing their environmental fate and persistence in aquatic systems. While liquid chromatography-mass spectrometry (LC-MS/MS) provides quantitative measurement of targeted PFAS in surface waters, it often underrepresents total PFAS burdens by overlooking sediment-associated fractions and precursor compounds that can transform and be remobilised over time. This obscures the role of sediments as both reservoirs and dynamic secondary sources of PFAS to the water column.
In this study, targeted LC-MS/MS and the total oxidisable precursor (TOP) assay were applied to paired surface water and sediment samples from tropical water catchments to investigate phase-resolved PFAS distribution and precursor dynamics. Targeted PFAS concentrations were consistently higher in sediments

than in overlying surface waters, with solid-phase partitioning reaching up to 2706-fold for ultra-long-chain compounds. TOP results indicated substantial precursor and intermediate contributions, with post-oxidation increases of 33%–73% in concentrations, particularly for short-chain terminal PFAS. Notably, despite the relatively low partitioning of short-chain compounds, their precursors and intermediates were relatively enriched in sediment. This suggests that preferential retention of precursors is a significant fraction of sediment-associated PFAS that can subsequently generate mobile short-chain PFAS upon release.
By comparing pre- and post-oxidation profiles across phases, this study evaluates the extent to which sediments act as long-term sinks versus dynamic sources of PFAS. Accumulated precursor pools in sediments can undergo transformation and contribute to mobile aqueous PFAS loads. Under seasonal rainfall and runoff, mobilisation of sediment-bound PFAS may drive episodic increases in water column concentrations, with suspended particulates interacting with bed sediments as coupled reservoirs and transport pathways. These findings highlight PFAS mobilisation cycles between phases and underscore the role of sediment-bound precursors in sustaining delayed release and downstream transport in aquatic systems.

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2.06.A.T - Emerging Contaminants in Agriculture and Food: Sources, Transport and Exposure Risks

2.06.A.T01 The Hidden Carbon Value of Southeast Asian Peatlands: Implications for Conservation and Climate Mitigation

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Peatlands in Southeast Asia (SEA) represent one of the most carbon-dense terrestrial ecosystems, yet their climate-regulating value remains persistently underestimated in land-use planning, commodity expansion and national development strategies. They store disproportionately large below-ground carbon stocks accumulated over millennia under waterlogged, anaerobic conditions. SEA contains approximately 23–30 million hectares of tropical peatlands, representing about 40–60% of the world's tropical peatland area. Indonesia contains the largest share estimated at 15 – 20 million hectares, while Malaysia contains about 2.7 million hectares. Indonesia's peatlands have been estimated to store up to about 57 Gt Carbon, while Malaysia's peatlands may store about 8.9 Gt Carbon. These values indicate that peat soils store far more carbon per hectare than most above-ground tropical forest biomass, making their protection crucial to climate mitigation. Peatlands in Indonesia and Malaysia have been rapidly degraded through drainage, logging, oil palm and pulpwood plantations, and recurrent fires. Drainage lowers the water table, exposes peat to oxygen, accelerates decomposition and converts long-term carbon sinks into persistent carbon sources. Regional assessments estimated peat swamp forest deforestation in SEA at 2.2% per year (2000-2010): 14 million hectares logged; 2.4 million hectares for oil palm; 1 million hectares for pulp and paper. Fires remain a critical threat, where drained peat ignites easily; produces massive greenhouse gas emissions resulting in a catastrophic 2015 transboundary haze over Indonesia, Singapore, and Malaysia. Priority conservation actions include: strict protection of intact peat swamp forests, moratoria on new drainage-based development; rewetting through canal blocking; revegetation with native peat swamp species; fire prevention; and community-based paludiculture. The ASEAN Peatland Management

Strategy 2023–2030 aim to support healthy and resilient peatlands through better governance, haze mitigation and sustainable management, while Indonesia's peat restoration programs have targeted millions of hectares of degraded peat landscapes. Ultimately, underestimating peatland value leads to climate, biodiversity, public health and economic losses that far exceed the short-term gains from conversion. Conserving SEA peatlands should be recognised as a high-impact, nature-based climate solution with regional and global significance.

2.06.A.T02 Distribution of PFAS in lettuce grown in hydroponic and soil systems with and without activated carbon amendment

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Per- and polyfluoroalkyl substances (PFAS) are a large class of synthetic chemicals characterized by exceptionally strong carbon–fluorine bonds, which confer high chemical stability, resistance to degradation, and long-term environmental persistence. These properties have led to their widespread use in industrial and consumer products. Among PFAS, perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) are two of the most extensively used compounds and are therefore frequently detected in the environment. Their occurrence in agro-ecosystems has raised concerns about potential human exposure through the consumption of contaminated crops. However, studies investigating the distribution of PFOA and PFOS in lettuce grown under different cultivation conditions remain limited, and effective strategies to mitigate crop uptake of these compounds are needed. In this study, lettuce was cultivated in both hydroponic and soil pot systems. Activated carbon was applied to soil as an amendment to evaluate its potential for reducing the bioavailability of PFOA and PFOS to lettuce. PFOA and PFOS in lettuce tissues were extracted using the QuEChERS method and analyzed by LC-QTOF/MS. Mass balance analysis showed that in the hydroponic system, PFOA mass in lettuce shoots increased from 10 to 72 hours, whereas PFOS primarily accumulated in roots over time. In the soil pot system, after 40 days of cultivation, both PFOA and PFOS were detected at higher levels in shoots than in roots. Moreover, the application of 2% activated carbon reduced the accumulation of PFOA and PFOS in lettuce shoots by more than 90%. Overall, the results indicate that both PFOA and PFOS can be translocated from roots to shoots with increasing exposure time. Activated carbon shows strong potential as a soil amendment to reduce PFAS accumulation in the edible parts of crops. These findings highlight the need for further research on the effectiveness of activated carbon in mitigating the uptake of other PFAS in agricultural systems.

2.06.A.T03 Screening of Benzotriazole UV Stabilizers and Legacy POPs in Philippine Aquatic-Derived Foods: Occurrence Patterns and Dietary Exposure Relevance

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Dried and processed fishery products are widely consumed in the Philippines, but they remain underexplored as food-related matrices for both emerging and legacy organic contaminants. This knowledge gap is particularly relevant for benzotriazole ultraviolet stabilizers (BUVs), a class of additives used in plastics and coatings that are characterized by persistence, hydrophobicity, and potential for dietary exposure. In this study, we investigated the occurrence, compositional profiles, and screening-level dietary exposure relevance of selected BUVs in dried fishery products purchased from six public markets in the Philippines. Sample extraction and clean up for BUVs were performed using a modified procedure adapted from previously reported methods for BUVs in biological matrices, followed by quantification by gas chromatography–tandem mass spectrometry (GC-MS/MS). Legacy persistent organic pollutants (POPs), including polychlorinated biphenyls (PCBs), polybrominated diphenyl ethers

(PBDEs), and selected pesticides were also analyzed to provide broader context on co-occurring organic contaminants in aquatic food matrices, with PCBs and PBDEs quantified by GC-MS and pesticides by GC-MS/MS. BUVs were detected in all samples, indicating their widespread presence in dried fishery products. Total BUV concentrations were highest in samples from Parañaque Market. The compositional profiles varied among locations, with the predominance of UV-326 in Parañaque and Butuan. Screening-level dietary intake estimates showed a similar spatial trend, with the highest estimated intake in Parañaque. Estimated exposure to UV-328, which was recently listed as POPs, was low relative to available hazard benchmarks, although this assessment remains preliminary. PCBs were detected in all analyzed products, with profiles mainly influenced by hexa-chlorinated PCBs. PBDEs occurrence was represented by BDE-47, which was measured at low concentrations. Overall, these results provide initial evidence of the presence of both BUVs and legacy POPs in dried fishery products in the Philippines. The findings highlight the need for expanded monitoring and further evaluation of contaminant sources, environmental transport pathways, and potential dietary exposure risks associated with aquatic-derived foods.

2.06.A.T04 Microplastic Burden in Commercial Seafood from Small Islands of Eastern Indonesia: Linking Coastal Contamination to Dietary Exposure

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Abstract Microplastic (MP) contamination in commercial seafood is an emerging concern for coastal and island communities that depend heavily on fisheries resources for food and livelihoods. This study assessed the abundance, characteristics, and potential dietary exposure implications of MPs in the gastrointestinal tracts (GIT) and edible tissues of commercially important seafood from small islands in North Maluku, eastern Indonesia. Triplicates of 7 fish and 7 molluscs representing locally consumed species were collected from local markets, followed by laboratory extraction, microscopic identification, and polymer confirmation of suspected MP particles. Fish GIT contained a mean of the MP burden of 89±99 items/100 g wet weight, followed by 3 species of fish flesh of 32±18 items/100 g wet weight, and edible tissue of molluscs of 198±154 items/100 g wet weight, respectively. Particles were predominantly fragments and filaments with less than 1 mm in size. Black colour is the most common in fish GIT (35%), while 60% is blue in fish flesh and white/transparent in mollusc (37%). Polyethylene (PE), polypropylene (PP), polystyrene (PS), and polyester were identified in several selected samples. Based on the estimation of the average MP consumption from seafood within a typical North Moluccan diet, the predicted MP accumulation per week was 36 items in the fish GIT (used in bakasang, a fermented fish sauce), 448 items in the fish flesh, and 468 items in the mollusc tissue. The dietary MPs' intake was 23,296 items/person/year for fish and 24,336 items/person/year for molluscs. This result highlights MP contamination in widely consumed seafood and emphasises a significant pathway of human exposure through daily consumption, with ramifications for human health and food security. Keywords: Commercial seafood, dietary exposure, microplastic contamination

2.08.A.T - Innovations in Understanding the Chemical Fate and Exposure of Plastics in the Environment

2.08.A.T01 Spatial distribution of tire-wear particles and microplastics in airborne suspended particles of Hanoi city, Vietnam

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Seoul 02841, Republic of Korea and cDivision of Environmental Science and Ecological Engineering, Korea University, Seongbuk-gu, Seoul 02841, Republic of Korea, (3)University of Science and Technology of Hanoi, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Nghia Do ward, Hanoi 113070, Vietnam, (4)OJEong Resilience Institute (OJERI), Korea University, Seoul 02841, Republic of Korea

Currently, Vietnam is a developing country with rapid urbanization and industrialization and express with high population density and crowded traffic. This trend has increased the frequency of tire-to-road interactions, resulting in a greater generation of tire wear particles (TWPs) and microplastics (MPs), which are significant sources of non-exhaust emissions that contribute to air pollution. In fact, tire wear particles (TWPs) have been identified across multiple environmental compartments worldwide, including air, soil, surface waters, and sediments; however, studies specifically examining total suspended particles (TSPs) remain relatively limited in Vietnam. This study provides the distribution of TWPs and MPs in airborne suspended particles in inner-city and suburban areas of Hanoi. TSPs samples were collected using a high volume air sampler and had concentrations ranging from 100.2 ± 31.3 to 242.4 ± 24.3 μg/m3 in inner-city area and from 170.6 ± 45.1 to 224.1 ± 40.2 μg/m3 in suburban area. The results show that TWPs concentrations in the urban area (218.8 ± 110.1 particles/m3) were higher than in the suburban area (84.1 ± 18.4 particles/m3). Similarly, MPs concentrations in the urban area (72.7 ± 35.1 particles/m³) were higher than in the suburban area (30.3 ± 1.2 particles/m³). By correlation analysis, the results showed that urban areas exhibited lower TSPs concentrations but higher levels of TWPs and MPs compared to suburban areas. The predominant size of TWPs was in the range of < 100 μm, while the majority size of MPs in fiber form was in the range of 1000-3000 μm.

2.08.A.T02 Spatiotemporal Distribution of Tire-wear Particles and Microplastics in Road Dust in Hanoi, Vietnam

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Tire wear particles (TWPs) are a major source of environmental microplastics (MPs). Generated by tire–road abrasion, they accumulate in road dust and can be transported into the environment via runoff. While TWP contamination may vary with season and traffic composition, its spatiotemporal patterns remain less studied than those of conventional MPs. Here, we investigated road dust in Hanoi, Vietnam—a city with distinct wet–dry seasons and mixed traffic (motorbikes, cars, and trucks). We developed a pyrolysis–GC/MS (Pyr-GC/MS) method to simultaneously quantify TWPs and MPs across urban and suburban sites, seasons, and peak/off-peak traffic periods. TWPs (mean 3.64 mg g^{-1}) exceeded MPs (mean 1.20 mg g^{-1}). Styrene–butadiene rubber dominated TWPs, while polyethylene (PE) dominated MPs. MP concentrations varied significantly across sites, whereas TWP levels did not. The styrene–butadiene rubber:natural rubber ratio was lower at suburban sites dominated by heavy vehicles than at urban roads dominated by motorbikes and passenger cars. Seasonally, TWP mass increased significantly from wet to dry season, while MPs showed no significant change. Peak-hour concentrations were ~39% (TWP) and ~22% (MP) higher than off-peak, but differences were not statistically significant. Overall, seasonal accumulation—rather than site-specific traffic intensity—appears to control TWP loading in Hanoi. These findings highlight the need for street-cleaning interventions before the monsoon to reduce the mobilization of tire-derived contaminants into urban stormwater.

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2.08.A.T03 Investigating Background Atmospheric Contamination During Analysis of Micro- and Nanoplastics Using Pyrolysis-Gas Chromatography-Mass Spectrometry

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Micro- and nanoplastics (MNPs) are prevalent in the air and may pose risks to humans through inhalation exposure. An increasing number of studies have used different analytical techniques on separate samples such as scanning electron microscopy (SEM; visualisation, no chemical characterisation), Raman spectroscopy (visualisation and chemical characterisation but only for particles > 0.5 μm), and pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS; all size ranges including nanoplastics, mass quantification and chemical characterisation). Although the use of multiple analytical techniques may improve certainty in the analysis, background contamination remains one of the biggest challenges due to the ubiquitousness of MNPs in the environment. Here we discuss challenges and lessons learnt in developing workflows for atmospheric MNP analysis, from sample collection to quantification.

To assess the impact of background contamination within the laboratory environment, deposition samples (glass containers: 14 cm × 20 cm) were deployed in laboratories with either low or high human access. Samples were filtered through 1 μm glass fibre filters to separate MPs (>1 μm) and nanoplastics (NPs; 1 μm in size-fractionated samples that should have only contained particles between 20 – 300 nm. This demonstrates that even with rigorous quality control procedures implemented, background contamination still needs to be assessed at every stage of the sample handling process and appropriate contamination control procedures implemented, for example restricting access to work areas.

2.08.A.T04 Playground pollutants: environmental release of elastomeric ecotoxins during outdoor wear and tear of recreational crumb rubber flooring

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The ubiquitous presence of cushioning crumb rubber flooring in outdoor playgrounds and sports facilities worldwide, whilst providing relief to the problem of tire recycling, is creating its own environmental pollution challenge. What happens when these elastomeric materials inevitably degrade and need running repairs then replacement after 10-15 years? The particulate microplastic mixtures used in such recreational surfaces typically comprise a combination of black ground tires and colored synthetic rubbers such as ethylene propylene diene monomer (EPDM), and they are chemically extremely complex. Here we report on the results of experiments and analytical procedures designed to improve our understanding of how crumb rubbers release pollutants from surfaces where children run and play.

We demonstrate how elastomeric organic pollutants such as organophosphate ester (OPE) plasticizers are present in all water leachates from these rubber materials, and how ground tire particles release metals such as Co, Cu and Zn, concentrations of which decrease through time as weathering proceeds. A particularly innovative study involved the collection and analysis of inhalable sized particulate matter (PM10) from crumb rubber surfaces using a portable vacuum sampler equipped with a PM10-selective separation chamber. These samples were used to develop an optimized pyr-GC-MS method which enabled the quantification of both natural and artificial (styrene-butadiene) rubbers using selective molecular markers and internal-standard calibration. Tire-derived natural and artificial rubber particles

known to contain plasticizers/softeners such as OPEs, phthalates and polycyclic aromatic hydrocarbons, were detected in PM10 samples, and ascorbic acid depletion assays show good correlations between metals typical of vulcanized rubber and EPDM coloring agents (e.g. Sn, V, Cu, Fe, Ti, Cd and Zn) and oxidative potential. Such findings demonstrate that these rubber surfaces, degrading with time under the effects of weathering and physical abrasion, act as a source of not only polluted leachate runoff but also potentially inhalable microplastic particles. They also emphasize the importance of applying good outdoor maintenance procedures to minimise the environmental release of loose, ecotoxic black used tire particles from ageing and damaged crumb rubber playground surfaces.

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2.08.B.T - Innovations in Understanding the Chemical Fate and Exposure of Plastics in the Environment

2.08.B.T01 Using multi-omics approaches to unfold pollutants' impacts on blue carbon dynamics

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Blue carbon ecosystems—including mangroves, salt marshes and seagrass—sequester disproportionately large amounts of contaminants, such as nutrients, plastic waste and PFAS from land and sea. These pollutants increasingly impair the carbon storage capacity of blue carbon ecosystems and undermine climate mitigation efforts. In this study, we used a multi-omics approach, combining 16S rRNA amplicon sequencing, Fourier Transform Ion Cyclotron Resonance Mass Spectrometry, and Ultra-Performance Liquid Chromatography–Mass Spectrometry, to examine how different pollutants (microplastics, nitrogen fertilisers and PFAS) alter blue carbon biogeochemistry. We found that hydrolysis of a polylactic acid biopolymer released carboxylic acids and related compounds into sediments, providing substrates for fermentative bacteria. In turn, these bacteria degraded plant polysaccharides and increased sediment CO_2 emissions. By contrast, polyethylene terephthalate had minimal effects on the microbial community, metabolomic profiles, and greenhouse gas emissions. Nitrogen fertilisation stimulated community-wide metabolic activity towards fermentation and further enhanced CO_2 release from sediments. Strikingly, PFAS-contaminated sediments emitted 350% more methane than uncontaminated sediments, driven by methanogens such as Methanolobus and Methanococcoides, while suppressing the broader microbial community. Collectively, our findings demonstrate the power of multi-omics approaches to resolve mechanistic pathways through which interacting pollutants disrupt blue carbon mineralisation. They also highlight that strategic pollutant management is critical for safeguarding global blue carbon under intensifying anthropogenic pressure.

2.08.B.T02 Influence of a Category 4 Hurricane on Microplastic Deposition in the Mountainous Southeastern United States

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Due to global warming, we can expect more intense hurricanes, leading to higher precipitation than previously observed. Historic storms, such as Hurricane Helene, that hit the southeastern United States in September 2024, deposited between 508 to 762 mm (20-30 in) of rainfall in rural, mountainous parts of

Western North Carolina, causing catastrophic damage from flooding. Less known is the extent of microplastic (MP) deposition in these less-developed areas, as MP levels are largely influenced by development, population, and traffic. While there is insight into MP deposition due to typhoon events in the eastern parts of the world, in our assessment, we conducted the first-ever study assessing MP deposition in a severely affected region at multiple locations (Iron Duff, Coweeta Hydrologic Laboratory, and Highlands Biological Station (HBS) in the southeastern US, months before (January to September), during (September), and weeks post-storm (October to November). Our findings show that Hurricane Helene contributed to elevated MP deposition at all sites, where total storm MP deposition was 1,280, 2,179, and 10,243 MP/m² at Iron Duff, Coweeta, and HBS, respectively. This historic storm accounted for 4.2%, 4.6%, and 18.8% of the annual MP deposition at Iron Duff, Coweeta, and HBS, respectively. Using backward trajectory analysis, we found that air masses reaching our sampling locations differed between the Helene and pre- and post-Helene periods. Our regression model estimated that the total anomalous deposition over the area affected by Hurricane Helene (3,798,756.55 km²) was 3.85×10^{15} MPs (385 quadrillion MPs). Polyamide, polystyrene, polyethylene terephthalate, polypropylene, and polyethylene were the main polymers detected before and during Helene. Our findings underscore how extreme storms can produce short-term spikes in MP deposition above ambient levels in a region and highlight how abundant MPs are in the atmosphere.

2.10.P - Environmental Chemistry and Exposure Assessment: Generic Session

2.10.P–We055 Environmental occurrence of octocrylene in marine and freshwater systems: A critical review

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The use of octocrylene has come under regulatory scrutiny, with concerns regarding its potential environmental risk. A main challenge in assessing environmental risk relates to uncertainties associated with exposure quantification, specifically with the use and release of octocrylene into marine and freshwater systems. A systematic and critical literature review is conducted in this study, consistent with the Criteria for Reporting and Evaluating Exposure Data (CREED), with the primary aim to collate measured environmental concentration (MECs) of octocrylene in surface water systems. The results of the study, consequently, include considerations regarding the reliability and usefulness of the available data, to quantify and/or represent reasonable approximations of environmentally relevant exposure to octocrylene. Significant procedural and methodological inconsistencies were involved among the available studies regarding surface water and sediment sample collection, processing, and analyses. Therefore, accompanying discussion in this study draws attention to the need for well-defined monitoring studies capable of acquiring concentration data that are representative of environmental systems and the need to either increase the number and frequency of samples collected or to consider the adoption of time-weighted passive sampling methods at sites to account for spatial, diurnal, and seasonal variabilities. Nonetheless, the existing data provides some understanding of central tendencies in MECs, which may be useful in ground truthing ongoing regulatory environmental risk assessments. The geometric mean concentrations for octocrylene in surface water reported at sites associated with recreational activities are similar in freshwater (30 ng/L) and marine (37 ng/L) systems. Similarly, the geometric mean concentrations of octocrylene in sediments influenced by potential sources of octocrylene are also relatively consistent for samples collected from both estuarine (6.9 ng/g dw) and freshwater riverine (4.3 ng/g dw) systems.

2.10.P–We057 Occurrence, bioaccumulation, and HRMS-based suspect screening of cyanotoxins in suspended particle matter and freshwater fish from Lake Asan, Korea

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Increasing harmful algal blooms (HABs) have raised concerns regarding cyanotoxin exposure and environmental risks in freshwater systems. This study investigated the occurrence, bioaccumulation, and potential analogs of cyanotoxins in Lake Asan, Korea. Suspended particulate matter (SPM) was collected by size fractionation (200 μm), and freshwater fish were sampled bimonthly from April to October 2024. Target analysis of 12 cyanotoxins, including seven microcystins (MCs), anatoxin-a (ANA), two anabaenopeptins (Apts), and cylindrospermopsin (CYN), was performed using LC-MS/MS. Suspect screening was conducted using high-resolution mass spectrometry (HRMS) to identify potential analogs of cyanotoxins. Cyanotoxins were consistently detected in all SPM samples, with total concentrations reaching 29 μg g-1 dry weight (dw) in October. The 20–200 μm SPM fraction exhibited the highest concentrations, corresponding with periods of cyanobacterial dominance (> 60% relative abundance) during August and October. MCs accounted for more than 90% of total cyanotoxin concentrations during bloom periods, with MC-LR and MC-RR as dominant variants. Fish tissues revealed significant tissue-specific accumulation patterns (p < 0.05). Liver and intestine tissues exhibited the highest accumulation, with MC-LR concentrations reaching 19 and 24 μg g-1 dw, respectively. Muscle tissue selectively accumulated MC-YR with a median of 91.2 ng g-1 dw. The SPM-biota accumulation factor of MC-YR varied significantly among particle size fractions, with the < 20 μm SPM showing approximately 100-fold greater bioaccumulation potential than the > 200 μm fraction. Trophic magnification factor analysis indicated no significant biomagnification of cyanotoxins within the food web. Suspect screening identified 44 potential cyanotoxin analogs in SPM, including 15 MCs, 4 Apts, 10 microginins, 9 cyanopeptolins, and 6 aeruginosins. In fish tissues, 10 compounds with structural modifications, including amino acid losses, were detected, suggesting metabolic transformation of cyanotoxins in fish. These findings demonstrate the occurrence of diverse cyanotoxin analogs beyond currently monitored compounds and highlight tissue-specific accumulation patterns in freshwater fish. The strong association between cyanobacterial dominance and cyanotoxin concentrations highlights the need for comprehensive monitoring and expanded risk assessment frameworks.

2.10.P–We058 Occurrence of β-N-methylamino-L-alanine (BMAA) in Phytoplankton and its Bioaccumulation in Shellfish from Korean Coastal Waters

Global climate change has intensified harmful algal blooms and marine biotoxin productions, highlighting the need to understand their impacts on marine ecosystems and human health. The neurotoxin β-N-methylamino-L-alanine (BMAA) and its isomer 2,4-diaminobutyric acid (DAB), produced by certain phytoplankton, exhibit neurotoxic properties, and BMAA has been implicated in neurodegenerative diseases. However, informations on their occurrence and bioaccumulation in Korean coastal waters remains limited. This study aimed to (1) investigate the distribution of BMAA and DAB in phytoplankton (20 – 200 μm, n = 38) and Mediterranean mussels (Mytilus galloprovincialis, n = 45) collected from 13 coastal stations in the Yellow Sea, South Sea, and East Sea of Korea between August 2020 and April 2021. (2) examine phytoplankton community composition to identify potential algal groups associated with BMAA occurrence. And (3) assess contamination levels in eight commercially available shellfish species (n = 70) collected from major seafood markets in Seoul and Busan in 2021. Neurotoxins were quantified using LC-MS/MS, and relationships between BMAA occurrence and phytoplankton composition were evaluated using correlation analysis. In phytoplankton, BMAA concentrations reached up to 9,782 ng g-1 dry weight (dw), whereas DAB was generally detected at lower concentrations. In coastal mussels, BMAA concentrations ranged from

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2.10.P–We059 Simultaneous Analysis of N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD) and Its Oxidation Product 6PPD Quinone in Tire Rubber Using a High-Performance Liquid Chromatography System

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Tires contain anti degradant additives such as N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD) that protect rubber from ozone and oxidative damage. Atmospheric oxidation of 6PPD produces 6PPD quinone, a transformation product reported to be highly toxic to aquatic organisms.
Here, we developed and validated a simple, robust method for simultaneous quantitation of 6PPD and 6PPD quinone in tire rubber to support environmental screening and alternative additive research. Samples were prepared following ISO 23075:2021. Extraction was performed by sonication of approximately 200 mg finely cut tire rubber in 10 mL of a 2:1 (v/v) mixture of isopropanol and dichloromethane solution for 3 hours at controlled temperature. Analyses used an integrated HPLC system (i Series LC 2070) with a Shim-pack GISS C18 column (150 × 4.6 mm, 5 µm). A gradient from 30% to 100% methanol (flow 1.0 mL/min, column temp. 40 °C) was employed. Detection used UV at 290 nm for 6PPD and 351 nm for 6PPD quinone. Calibration employed five-point standards for each compound.
Calibration curves demonstrated excellent linearity (r2 >0.999). Method detection limits in solution were 0.1 mg/L for 6PPD and 0.05 mg/L for 6PPD quinone, determined as the average concentration giving S/N = 3 across calibration standards. Spike recovery tests on tire samples (n=2, duplicate analyses) yielded mean recoveries of 96% for 6PPD and 92% for 6PPD quinone, indicating good accuracy and reproducibility. Chromatograms show clear separation and reliable peak identification for both analytes.
The developed integrated HPLC method permits simultaneous, sensitive, and reproducible quantification of 6PPD and 6PPD quinone in tire rubber with simple sample pretreatment. This approach is suitable for screening tire materials, assessing environmental release potential, and supporting research into alternative anti degradant compounds with reduced ecotoxicological risk.

2.10.P–We060 Identification of unknown per- and polyfluoroalkyl substances in anti-fog agents by comprehensive analysis

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Per- and polyfluoroalkyl substances (PFAS) have been widely used in industrial and consumer products because of their unique properties, including water/oil repellency and chemical/heat resistance. However, PFAS have received worldwide attention due to their environmental persistence and toxicity. The Conference of the Parties of the Stockholm Convention on Persistent Organic Pollutants listed PFOA and PFOA-related compounds in Annex A in May 2019. Anti-fog agents are one of the consumer products known to contain PFAS. A recent study has reported the presence of novel PFAS and unidentified fluorinated compounds in anti-fog agents manufactured in China and the United States; however, available information remains limited. Comprehensive investigations of PFAS in anti-fog agents are therefore needed. In this study, we determined the concentrations of individual PFAS in anti-fog agents sold in Japan and estimated the structures of unidentified fluorinated compounds in the anti-fog agents. Eight anti-fog agent products sold from 2007 to 2018 were purchased in Japan. The concentrations of 119 target PFAS in these products were determined by LC-MS/MS and GC-MS/MS. Concurrently, the concentrations of total fluorine (TF) were determined by combustion ion chromatography. The concentrations of individual PFAS accounted for up to only 1% of the TF concentrations, suggesting that

the major fluorinated components in the anti-fog agents were unidentified PFAS. Alkaline hydrolysis and oxidative decomposition using the total oxidizable precursor (TOP) assay were conducted to elucidate the partial structure of these unidentified PFAS in the anti-fog agents. The results of the alkaline hydrolysis and TOP assay suggest that the unidentified PFAS in the anti-fog agents have structures in which the perfluoroalkyl moiety is not adjacent to the ester moiety and contain perfluoroalkyl chains with a maximum chain length of C6F13. Screening analyses for unknown compounds were conducted by GC-MS and LC-Orbitrap-MS to identify the chemical structures of the unidentified PFAS detected in this study. Furthermore, the chemical structures of unidentified PFAS were estimated by using a in silico-type chemical-structure estimation tool (MetFrag). The structures of the candidate compounds were consistent with the results. These findings indicate that the comprehensive analysis enabled the identification of previously unknown PFAS in anti-fog agents.

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2.10.P–We061 Accurate Determination of Polycyclic Aromatic Hydrocarbons and Their Halogenated Derivatives Using a Silicone Passive Sampler

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Polycyclic aromatic hydrocarbons (PAHs) and halogenated PAHs are emitted by anthropogenic activities with incomplete combustion. Certain PAHs and halogenated PAHs have adverse effects on human health. The silicone passive sampling method has attracted attention as an individual exposure assessment tool. The silicone passive sampling method is less burdensome for participants because the sampler is compact and requires no electrical power. Passive samplers are generally affected by wind speed, and information on the effects of meteorological factors on silicone passive samplers remains limited. Here, we evaluated the effects of wind speed on the sampling rates (SRs) of PAHs and halogenated PAHs and corrected wind effects during the sampling.

Passive sampling using silicone sheets and active sampling using mini pumps were simultaneously performed to evaluate the relationships between the atmospheric concentrations and their collection amounts in the silicone sheet. To assess the wind speed effects, air sampling was conducted with wind speed control using an electric fan. Ultrahigh-purity silicone rubber was used as the passive sampler. The samples were analyzed by using a gas chromatograph-triple quadrupole mass spectrometer.

Previous studies reported that the sampling mechanism of gaseous compounds is based on molecular diffusion. For laminar flow along a flat-plate passive sampler, the SR is proportional to the square root of the wind speed. For two- and three-ring PAHs and halogenated PAHs, the relationship between the wind speed and SRs on the silicone passive sampler regressed with high accuracy using this model. For four-ring PAHs, the regression accuracy was lower than that for two- and three-ring PAHs and halogenated PAHs. The relationships between the SR and the wind speed inadequately accounts for gas–particle phase partitioning and particle movement because it is based on molecular diffusion. This limitation results in poor regression accuracy for four-ring PAHs within the model. Wind speed had a negligible effect on the SRs for five- and six-ring PAHs because of their fine particle sizes.

The amounts of two- to four-ring PAHs and halogenated PAHs collected using the silicone passive sampler were corrected by setting the same wind speed. The concentrations of atmospheric PAHs and halogenated PAHs were accurately estimated up to four or five orders of magnitude within errors of 1/3–3 times the theoretical consideration of the wind speed effects.

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2.10.P–We062 Simultaneous Determination of Multi-Pesticide Residues in Honeybees (Apis mellifera) using LC-MS/MS and GC-MS/MS

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(1)Animal and Plant Quarantine Agency (APQA)

Despite the crucial role of honeybees in the ecosystem, pesticide exposure is considered a major factor of their population decline. This study aimed to evaluate actual exposure levels and potential toxicological impacts on honeybees in South Korea using optimized liquid chromatography-tandem mass spectrometry (LC-MS/MS) and gas chromatography-tandem mass spectrometry (GC-MS/MS) analytical methods for 104 pesticide substances.

In 2025, a total of 62 dead honeybee samples, suspected of pesticide poisoning, were collected and submitted to APQA for diagnostic testing from apiaries nationwide. Sample preparation involved acetonitrile (ACN) extraction followed by dispersive solid-phase extraction (d-SPE) cleanup. The instrumental analysis was performed using both LC-MS/MS and GC-MS/MS in Multiple Reaction Monitoring (MRM) mode.

Among the target substances, 25 were detected. The herbicide MCPB showed the highest detection rate at 59.7% (37 samples), followed by clothianidin (35.5%), tebuconazole (21.0%), thiamethoxam and indoxacarb (8.1% each), and fenitrothion and pendimethalin (6.5% each). Notably, the analysis revealed exceptionally high maximum concentrations: clothianidin reached 34,025 μg/kg, and phorate (including its metabolites) was detected at 4,712.0 μg/kg. Furthermore, the maximum concentration of indoxacarb (1,895.2 μg/kg) significantly exceeded its contact acute median lethal dose (LD50, 0.08 μg/bee). Multiple pesticide residues co-occurred frequently, with up to six different substances identified in a single sample, suggesting potential synergistic effects. Several detected substances exhibited high lipophilicity (log P > 3.0), suggesting a high potential for accumulation in beeswax and long-term chronic exposure within the hive.

The widespread detection of highly toxic pesticides at extreme concentrations indicates substantial field exposure risks for honeybees. The synergistic toxicity from multiple pesticide exposure, combined with the risk of chronic exposure due to high bioaccumulation potential, poses a significant threat to pollinator health. Continuous monitoring using robust LC-MS/MS and GC-MS/MS methodologies is essential for developing effective conservation strategies.

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2.10.P–We063 High-Resolution Mass Spectrometry-Based Non-Target Analysis and Molecular Annotation of Exogenous Chemicals and Metabolites in Pet Urine

Pets share living environments with humans and can serve as indicators of exposure to lifestyle-related chemicals. Although biomonitoring studies using pets have recently increased, most have focused on a limited number of hazardous chemicals. In this study, urine samples from 45 dogs were pooled by breed and grouped into seven sets. Target, suspect, and non-target analyses were performed using high-resolution mass spectrometry. Target analysis was conducted based on an in-house database, while suspect screening was performed using Compound Discoverer. Non-target analysis was carried out using MZmine3 and SIRIUS. A total of 478 chemicals were detected and classified into confidence levels: Level 1 (18 compounds), Level 2 (18 compounds), Level 3 (13 compounds), and Level 4 (429 compounds). Of the Level 1–3 compounds, 28 were identified as parent compounds, 16 as metabolites, and 5 were confirmed in both forms. Personal care product-related chemicals accounted for the largest

proportion, followed by pharmaceuticals, dietary-derived compounds, plasticizers and flame retardants, and pesticides. To expand metabolite information, molecular structure candidates for unknown compounds were predicted using SIRIUS in combination with the in-silico metabolism tool Biotransformer3.0, generating approximately 8,000 candidate parent compounds and metabolites. The chemical profiles obtained from non-target analysis and breed-specific characteristics will be presented at the conference.

2.10.P–We064 Bioaccumulation and Temporal Trends of Per- and Polyfluoroalkyl Substances in Fish from the Seto Inland Sea Region, Japan

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Per- and polyfluoroalkyl substances (PFAS) are persistent chemicals of concern because some compounds bioaccumulate in aquatic food webs and may pose risks to wildlife and humans. Although monitoring data are available for regulated substances such as PFOS, PFOA and PFHxS, information remains limited for other PFAS, including long-chain perfluorocarboxylic acids (LC-PFCAs), which have attracted regulatory attention under the Stockholm Convention.
This study investigates bioaccumulation profiles and temporal trends of PFAS in fish from the Seto Inland Sea region, Japan. Red seabream and largehead hairtail collected in 2010 and 2025 were initially analyzed, and additional coastal and freshwater fish species are being analyzed. The 2010 samples were archived specimens from the Ehime University es-BANK, whereas 2025 samples were purchased from local markets. Target analytes comprised 33 PFAS, including LC-PFCAs (C9–C18). Fish tissues were extracted after alkaline digestion, cleaned up using lipid-removal and solid-phase extraction, and analyzed by liquid chromatography tandem mass spectrometry.
In muscle samples of red seabream (n = 16) and largehead hairtail (n = 16), six PFAS were detected, and total PFAS concentrations ranged from below the detection limit to 3.2 ng/g wet weight. PFTrDA showed the highest detection frequency, followed by PFUnDA and PFOS. No significant differences were observed between fishing areas within the same species. In addition, PFOS, PFUnDA, PFTrDA and total PFAS concentrations were higher in largehead hairtail than in red seabream, suggesting food web magnification in the higher-trophic species. PFOS, PFUnDA and total PFAS concentrations in largehead hairtail were lower or below detection limits in 2025 than in 2010, possibly reflecting regulatory controls and changes in environmental inputs.
Estimated weekly intakes were calculated for four PFAS relevant to health-based guidance values and compared with the tolerable weekly intake established by the European Food Safety Authority. The estimated intake for largehead hairtail in 2010 exceeded the guidance value, whereas values for both species in 2025 were below it. This study provides insight into temporal changes in contamination status by emerging and regulated PFAS, including LC-PFCAs, in aquatic biota.
This study was supported by the Environment Research and Technology Development Fund, Japan (JPMEERF20255M03). We thank Ehime University es-BANK for providing archived samples.

2.10.P–We065 Temporal Trends of Legacy and Alternative Brominated Flame Retardants in a Dated Sediment Core from Osaka Bay, Japan

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Contaminants of emerging concern (CECs), such as pharmaceuticals and brominated flame retardants (BFRs), have gained increasing attention due to their uncertain environmental behavior, persistence, and ecological effects. Their accumulation is also relevant to global discussions on chemical pollution within the planetary boundaries framework. Osaka Bay, a semi-enclosed and highly industrialized coastal system

in western Japan, has long been recognized as a major sink for anthropogenic pollutants. Previous sediment core studies have shown that legacy BFRs, including polybrominated diphenyl ethers (PBDEs) and hexabromocyclododecane (HBCDD), peaked between the 1990s and mid-2000s, but long-term trends of alternative BFRs (a-BFRs) remain unclear. In this study, a sediment core from Osaka Bay was analyzed to reconstruct temporal trends of BFRs from 1990 to 2019 using lead-210 dating. The target compounds included PBDE, decabromodiphenyl ethane (DBDPE), and BTBPE. Results showed that BDE-209 and DBDPE were dominant, while BTBPE was detected only at trace levels. Despite its regulation in 2017, BDE-209 was still present in recent sediments, suggesting continued release from legacy sources. In contrast, DBDPE showed increasing concentrations, reflecting its ongoing use as a replacement for PBDEs. BTBPE remained low due to its limited historical usage.Compared to other Asian coastal regions, BTBPE concentrations in Osaka Bay were relatively low. This is likely due to the bay's hydrodynamic characteristics, including water exchange through the Kii Channel, tidal mixing, and sediment resuspension, which enhance dilution and reduce long-term accumulation. These processes may lead to underestimation of actual contaminant inputs in sediment records.

Overall, BFR accumulation in Osaka Bay is influenced not only by usage patterns but also by environmental transport and hydrodynamics. Future research should include multiple sampling sites, additional transport pathways, and emerging compounds to better understand contamination dynamics and support environmental risk assessment.

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2.10.P–We066 Tracing Landfill Impacts Through Stream Benthic Invertebrates

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Landfill runoff can alter stream ecosystems by introducing nutrients, contaminants, and organic matter that modify ecological communities and ecosystem processes. These effects may vary with distance from the discharge point and habitat characteristics such as vegetation, substrate, channel structure, as well as seasonal variation in temperature and hydrology, but the combined influence of these factors remains poorly resolved. This study examined how landfill runoff, habitat context, and seasonality influence benthic invertebrate composition in a small stream, as these organisms are widely used indicators of ecological condition.

Invertebrates were sampled at three sites: a forested upstream reference site 800 m above the landfill outlet, the outlet reach receiving runoff, and a forested downstream reach 100 m below the outlet. The upstream site had muddy and sandy substrate, a narrow channel, and forested riparian cover. The outlet reach had muddy substrate, reed vegetation, and an open grass-dominated riparian zone, whereas the downstream site was forested and muddy. Samples were collected in spring at all three sites and in autumn at the outlet and downstream sites. Specimens were identified morphologically to the finest possible level, with eDNA used to improve resolution for difficult taxa.

We tested whether communities differed between the upstream reference site and landfill-influenced sites, whether outlet and downstream assemblages differed because of contrasting habitats, and whether these patterns changed seasonally. We expected landfill-influenced sites to show reduced diversity and altered composition, outlet and downstream communities to differ due to habitat conditions, and season to affect community structure.

The upstream site supported a more diverse and sensitive benthic community, whereas the outlet and downstream sites showed reduced diversity and altered composition. Outlet and downstream communities were similar despite riparian differences, suggesting that landfill runoff influenced the stream beyond the

discharge point. Nutrient enrichment likely contributed to these patterns, while seasonal differences in water temperature and hydrology modified community structure. These findings show that landfill runoff can shape benthic invertebrate assemblages downstream and demonstrate the importance of habitat context and seasonal variation when assessing ecological impacts in small streams.

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2.10.P–We067 Environmental Dust as a Reservoir for Anthropogenic and Geogenic Contamination in the Erongo Region, Namibia.

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Environmental dust in Namibia is influenced by both natural and human activities and can act as a reservoir for trace contaminants in the environment. Major dust-generating sources such as the Namib Desert and Etosha Pan contribute to regional dust transport, which may be further affected by mining, urbanisation, industrial activity, traffic emissions, and deteriorating infrastructure. Indoor household dust has been identified in previous studies as an important medium for trace metal exposure, yet information remains limited in the Erongo Region, particularly in relation to how indoor and roadside dust differ within arid urban environments.

This study investigates dust contaminant concentrations and chemical characteristics within indoor household and roadside dust samples (<100 µm) collected from residential areas in three major towns of the Erongo region. Samples will be analysed using Inductively Coupled Plasma – Mass Spectrometry (ICP-MS) to determine elemental concentrations. In addition, samples will be examined using Scanning Electron Microscopy – Energy Dispersive Spectroscopy (SEM-EDS) for particle morphology and elemental composition. Pollution indices and multivariate statistics will be used to interpret contamination patterns and variability within the dataset.

It is expected that indoor household dust will show higher accumulation of trace elements than roadside dust due to greater particle retention in enclosed environments. Roadside samples will reflect ambient outdoor dust composition for comparison, with differences in elemental composition and particle characteristics anticipated between the sample types.

The study will provide important baseline data on dust-associated contamination in an arid urban-industrial environment and will highlight how indoor dust can act as an important environmental reservoir for trace elements. These findings will improve our understanding of contaminant behaviour in dust systems and support future environmental monitoring and exposure assessment in Namibia.

2.10.P–We068 Source-Specific Risks and Spatial Correlation of Polycyclic Aromatic Hydrocarbons and Their Derivatives for Respiratory Health in Ulsan, South Korea

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Polycyclic aromatic hydrocarbons (PAHs) and their derivatives, including nitrated PAHs (NPAHs), oxygenated PAHs (OPAHs), chlorinated PAHs (ClPAHs), and brominated PAHs (BrPAHs), are mainly emitted from incomplete combustion processes, with industrial activities representing important sources. Some PAH derivatives may induce greater oxidative stress and toxicity than parent PAHs. However,

information on these derivatives and their associations with respiratory diseases remains limited. In this study, atmospheric concentrations of 21 PAHs, 17 NPAHs, 9 OPAHs, 13 ClPAHs, and 12 BrPAHs were investigated in Ulsan, one of the largest industrial cities in South Korea. The objectives were to characterize ambient concentrations, assess inhalation health risks by age and sex, and evaluate associations with respiratory diseases, including asthma and chronic obstructive pulmonary disease (COPD). Polyurethane foam-based passive air samplers (PUF-PASs) were deployed at urban and industrial sites in the summer and winter of 2023. The samples were Soxhlet-extracted, cleaned up using silica gel and alumina columns, and analyzed using gas chromatography-mass spectrometry. Assoications between PAH and PAH derivative concentrations and respiratory disease prevalence were evaluated using a local indicator of spatial association (LISA) and a distance-decay model. Concentrations of most compounds were higher in winter than in summer. In contrast, several NPAHs showed higher concentrations in summer, possibly reflecting enhanced secondary atmospheric formation under photochemical conditions. Health risk assessment showed that PAHs contributed more to inhalation risk than their derivatives. The estimated risks were higher for children than for adolescents and adults, and higher for males than for females. Elevated risks were observed mainly near the petrochemical industrial complex, where PAH, ClPAH, and BrPAH levels were high. LISA and distance-decay analyses suggested that respiratory disease prevalence tended to be higher in areas closer to major industrial sources, indicating an influence of source-related emissions on health outcomes. Although the estimated risks were below the acceptable risk level of the US EPA (10-6), continuous monitoring is needed to manage unregulated PAHs and their derivatives in industrial areas.

2.10.P–We069 Multispectral Image-Based Quantification of Organic and Elemental Carbon in $PM_{2.5}$ Quartz Filters via Machine Learning

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Organic carbon (OC) and elemental carbon (EC) are dominant constituents of $PM_{2.5}$ with distinct optical properties and important implications for air quality, climate forcing, and human health, yet their quantification remains dependent on costly and labor-intensive techniques (e.g., thermo-optical analysis). Image-based techniques have emerged as a promising low-cost and rapid alternative for assessing carbonaceous aerosols; however, their reliability is sensitive to imaging conditions and calibration, and current applications are largely limited to strongly light-absorbing fractions such as Black Carbon (BC) and EC. To address these limitations, this study explores a controlled multi-illumination imaging approach combined with machine learning (ML) to capture robust optical signatures of carbonaceous aerosols. $PM_{2.5}$ samples were collected at urban sites in Astana and Almaty, Kazakhstan, using low-volume aerosol samplers and 24 h quartz filter sampling. OC and EC concentrations were quantified using a thermo-optical analyzer (NIOSH 870 protocol). Optical imaging was performed using a mobile phone camera under controlled multi-wavelength illumination (i.e., warm, red, green, cold, blue) with fixed camera settings (e.g., RAW (DNG) image format, ISO 64, shutter speed of 1/1000 s) to ensure consistency between samples. An eXtreme Gradient Boosting (XGBoost) regression model was developed using engineered features extracted from multi-illumination filter images and trained within a cross-validated framework. The model achieved relatively strong predictive performance, with R^2 values of 0.768 for OC and 0.841 for EC, respectively. Feature importance analysis identified red-channel intensity under warm illumination as the dominant predictor, highlighting the role of illumination conditions in enhancing signal sensitivity and reflecting the optical response of deposited carbonaceous material. By linking image-derived features to OC/EC concentrations, this study demonstrates the

potential of optical indicators for carbonaceous aerosol quantification, supporting the development of a computationally efficient and cost-effective approach for air quality monitoring, particularly in resource-limited settings.

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2.10.P–We070 Source Identification of Ammonium of PM2.5 in Bangladesh Using Nitrogen Stable Isotope Ratios

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Particulate matter (PM2.5) is a type of aerosol that floats in the atmosphere and has become a major concern due to its adverse effects on the respiratory and circulatory systems. In Bangladesh, PM2.5 concentrations reach 66.1 μg/m3 (2025), which is more than 10 times the World Health Organization (WHO) environmental standard. In that country, traditional brick production has been compounded in recent years by increases in the number of vehicles, the use of agricultural fertilizers, and waste generation, resulting in the highest levels in Asia for eight consecutive years through 2025.
Ammonia gas (NH3), which forms secondary PM2.5 particles, has a wide range of sources, ranging from agricultural sources such as soil and livestock waste to non-agricultural sources such as vehicle exhaust. In Bangladesh, approximately half of the NH3 emissions from March to November are considered non-agricultural in origin, but the long-term trends in these sources remain unclear. Therefore, this study measured water-soluble ion concentrations in PM2.5 and the nitrogen stable isotope ratio of ammonium (δ15N-NH4+) for five years. The objective was to estimate the sources of PM2.5 and NH3 considering Bangladesh's recent economic growth.
At Dhaka University in Bangladesh, PM2.5 was collected using a high-volume air sampler from March 2019 to April 2024. Water-soluble ions were measured using an ion chromatograph. δ15N-NH4+ was converted to N2O through oxidation using bromic acid and reduction using denitrifying bacteria and then measured using GasBench II and a stable isotope ratio mass spectrometer. Finally, the source contribution ratios were calculated using the isotope mixing model (SIAR).
The annual average of NH4+ concentrations, excluding the dry season, increased more than threefold from 2019 (0.53 μg/m3) to 2023 (2.03 μg/m3). It was suggested that NH4+ played a more significant role in aerosol formation than previously. The δ15N-NH4+ values fluctuated significantly between 0.4‰ and 34.4‰ over the five years. Additionally, the average (15.7 ± 5.4‰) is approximately 5‰ lower than in previous research at the same site, suggesting an increasing contribution of agriculture-derived NH3. As a result of SIAR, it was estimated that agricultural contributions such as waste and agricultural fertilizers account for 60% to 70% of NH3 gas generation, and this trend did not fluctuate significantly by year or season.

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2.10.P–We071 Effects of Food Composition on the Decomposition and Chemical Characteristics of By-products in Biological Processors

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As food waste management shifts from mere disposal to biological reduction and composting at the source, the use of biological food waste processors is increasing. The biological decomposition process

emits various volatile organic compounds (VOCs), raising concerns about odor generation and indoor air quality degradation; therefore, evaluating the environmental safety of such devices has become crucial. It is essential to understand the physicochemical characteristics of by-products generated after processing by biological food waste processors. Since the chemical composition of decomposition products and the emission patterns of secondary pollutants, such as VOCs, vary depending on the composition of the input food waste, precise component analysis of waste and by-products must be conducted. In this study, we investigated the decomposition characteristics of four food groups (rice, meat, vegetables, and fruit) input into three types of biological food waste processing devices (A, B, and C). We identified that the constituent components of food waste are the primary factors determining the chemical characteristics of the generated by-products as well as the types and concentrations of volatile organic compounds (VOCs). Furthermore, we suggest that ensuring environmental safety during the composting process of by-products is essential for effective waste management. Therefore, in addition to improving the sealing performance of the treatment device, ventilation and management guidelines must be established to minimize secondary environmental pollution that may occur during the on-site treatment process.
Key words: Food waste processor, Microbial fermentation, Byproduct analysis, VOCs

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2.10.P–We072 A Comprehensive Analysis of Sr-90 in Calcified Tissues of the Benthic Organisms Collected off Coast of Fukushima Prefecture

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A large amount of radioactive nuclides was released into the coastal region after the Fukushima Daiichi Nuclear Power Plant (FDNPP) accident in 2011. Among the major radionuclides, radioactive strontium (90Sr), which has a long half-life (28.8 years), accumulates in calcified tissues such as bones, due to its chemical similarity to calcium, and thus its biological half-life might also be long. However, because the amount of released 90Sr was smaller than that of radioactive cesium, there have been relatively few studies on 90Sr. In this study, we analyzed 90Sr in calcified tissues of benthic fish and invertebrates collected off the coast of Fukushima Prefecture.
Calcified tissues examined in this study were vertebrae in fish, and exoskeletons in invertebrates. Sampling was conducted at nine stations off the coast: northern (off Soma), central (in front of FDNPP), and southern (off Iwaki) areas, at depths of 10 m, 20 m, and 30 m, respectively. Calcified tissues were dissolved in nitric acid. Radioactive nuclides were purified using DGA Resin and measured with 2π gas flow counter
A comprehensive analysis of 90Sr in various fish species collected in January and July 2014 revealed that elasmobranchs, particularly Okamejei kenojei showed higher 90Sr concentrations. Focusing on O. kenojei, we examined temporal changes in 90Sr concentrations from 2013 to 2015. Although 90Sr concentrations showed a gradual decreasing trend, measurable levels were still detected in 2015. The average body weight of individuals where 90Sr was detected showed an increasing trend and individuals with high body weight (i.e., aged individuals) were not observed as the years passed, indicating that gradual decrease of 90Sr is likely due to the growth dilution and natural mortality related to their lifespan.
A comprehensive analysis of 90Sr in various invertebrates collected in 2013 and 2014 showed that high concentrations of 90Sr (4.42–1362 Bq/kg) were detected in the starfish Asterias amurensis, while concentrations in other species were below 10 Bq/kg. By comparing the size of detected individuals of A. amurensis with previously reported growth rates of this species, they are likely to be exposed to the radioactive contaminated water released from FDNPP in their early life stages. Because growth rate might be faster during early life stages, which would lead to the rapid incorporation of inorganic components,

higher concentrations of 90Sr was also suggested to occur in A. amurensis.

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2.10.P–We073 Illegal gold mining alters soil organic matter, increases mercury availability, and filters bacterial communities across Brazilian tropical biomes

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Artisanal and illegal gold mining is a major driver of mercury (Hg) contamination in humid tropical soils, yet its interaction with seasonal variability and soil organic matter (SOM) dynamics remains poorly understood. In this study we investigated how mining-induced changes in SOM quality and seasonal climatic conditions influence Hg mobility, environmental exposure potential, and soil bacterial communities across four Brazilian biomes: Amazon, Cerrado (Savannah), Pantanal (Wetland), and Atlantic Forest. Soils from mining sites and adjacent pastures were sampled during wet and dry seasons and analyzed using an integrated approach combining SOM characterization (diffuse reflectance infrared Fourier transform spectroscopy), Hg fractionation, and 16S rRNA gene sequencing. Mining reduced soil organic carbon (SOC) and nitrogen (N) contents (~40–60% across biomes) and altered SOM composition, decreasing aromatic and carboxylated fractions while enriching more labile compounds (p 30 mg/L). Hg mobility had strong seasonal control, with bioavailable Hg reaching ~0.4–0.5 mg/kg, and active Hg up to ~5 mg/kg, both enhanced during the dry season, likely driven by increased oxidation and reduced stabilization by SOM. Across biomes, Hg bioavailability was positively associated with WEOC contents, highlighting the role of organic ligands in facilitating Hg transport and environmental exposure pathways. Bacterial diversity was consistently lower in mining soils, reflecting strong environmental filtering driven by Hg availability and reduced nutrient inputs. Microbial communities showed negative correlations with aromatic SOM (r= –0.44) and mobile Hg fractions (r = –0.32), and positive associations with SOC, nitrogen, and pH (r > 0.6). Functional predictions indicated reductions in pathways related to organic matter decomposition and N cycling in mining-impacted soils. Seasonal effects further modulated these patterns, with increased microbial turnover linked to labile carbon inputs during the wet season. Overall, illegal gold mining promotes persistent alterations in soil biogeochemistry that enhance Hg mobility and increase environmental exposure and dispersion across humid tropical ecosystems, with implications for ecosystem resilience and human health.

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2.10.P–We074 Soil Components Control Biochar-Mediated Arsenate Immobilization and Phosphate Retention

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Arsenate and phosphate are structurally similar oxyanions, but their environmental implications differ sharply: arsenate is a toxic metalloid that can move through soil–water and food-chain exposure pathways, whereas phosphate is an essential nutrient whose excessive mobility can accelerate

eutrophication. Biochar is increasingly considered for simultaneous contaminant immobilization and nutrient retention, yet its performance in real soils remains difficult to predict because mineral ions, dissolved silica, and organic matter can alter access to reactive surfaces and pores. This study evaluated how common soil components regulate biochar-mediated arsenate immobilization and phosphate retention.
Miscanthus-derived biochars produced at 400 °C and 700 °C were reacted with binary arsenate–phosphate solutions under acidic, neutral, and alkaline conditions. Aluminum, calcium, iron, silicate, humic acid, and a mixed-component treatment were used to represent major cationic, anionic, and organic soil constituents. Bulk retention was quantified by inductively coupled plasma optical emission spectroscopy, while surface and pore-scale mechanisms were examined using depth-profiling X-ray photoelectron spectroscopy and X-ray diffraction.
Soil components substantially changed both total oxyanion retention and arsenate–phosphate selectivity. Aluminum and calcium promoted phosphate retention through cation bridging, mineral-associated binding, and pore-scale enrichment. Iron produced a more arsenate-favorable response than the other cations, consistent with iron-associated oxyhydroxide domains that provide strong binding environments for arsenate. In contrast, silicate and humic acid suppressed retention by masking reactive sites, competing for sorption domains, and limiting access to internal pores. In the mixed-component system, cation-enhanced retention was partly offset by silica and organic matter, showing that biochar performance depends on the combined geochemical setting rather than on isolated soil constituents.
These results demonstrate that soil chemistry can shift biochar function between arsenic immobilization, phosphorus conservation, and reduced overall sorption. The findings provide mechanistic guidance for selecting or engineering biochar amendments for agricultural soils where contaminant exposure reduction and nutrient management must be balanced.

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2.10.P–We075 Release Behaviour and Kinetics of Phosphate from Nano-Hydroxyapatite in Simulated Irrigation Water

The reduced phosphorus use efficiency of conventional fertilisers remains a major agronomic and environmental challenge, due to the accumulation of immobilised legacy P and mobilised losses. Under various simulated irrigation water conditions, the phosphorus release behaviour and kinetics of nano-hydroxyapatite (nHAP) were studied and systematically compared with conventional granular single superphosphate (SSP). Phosphate released from nHAP and SSP was investigated over 15 days in aqueous system with varying pH (6, 7, 8) and salinity (0.75-3.00 dS/m), simulating irrigation water, and was interpreted as relative phosphorus release (%). Granular SSP demonstrated an immediate burst release, highest at pH 6, peaking 48.0565 ± 5.002% on day 2, governed by Fickian diffusion through its porous matrix and largely independent of salinity variations. In contrast, nHAP demonstrated sustained release (16.257 ± 0.861% at pH 6 on day 5), with release kinetics regulated by water chemistry, exhibited by a zero-order model under a slightly acidic and moderately saline system, indicative of surface-controlled hydrolysis. Whereas significantly lower release was observed under pH 7 (11.782 ± 2.45% on day 4), and pH 8 (2.61 ± 1.67% on day 1), demonstrating a diffusion-dominated Higuchi kinetics. These results showed that P release from nHAP is majorly influenced by proton availability, whereas granular SSP exhibited burst release behavior leading to inefficient nutrient utilization and losses. The mechanistic insights into nHA release indicated its potential as a sustained-release nanofertilizer, with reduced environmental loss risk.

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2.10.P–We076 Toxic elements in heated tobacco products marketed in Japan and exploration of tobacco-specific markers

Heated tobacco products (HTPs) have rapidly expanded in the Japanese tobacco market; however, information regarding exposure to toxic elements from HTP aerosols remains limited. Here we quantified elemental concentrations in tobacco sticks and mainstream aerosols from commercially available HTPs marketed by three manufacturers in Japan and conducted a preliminary assessment of associated non-carcinogenic and carcinogenic risks. Mainstream aerosols were collected using the Health Canada Intense protocol and analyzed by inductively coupled plasma mass spectrometry. Chromium (Cr) and copper (Cu), which were not detected in conventional cigarette mainstream smoke, were detected in aerosols from all investigated HTPs, suggesting contributions from metallic heating components. Median Cr and Cu concentrations in HTP aerosols ranged from 1.3–2.0 and 0.50–0.90 ng stick^{-1}, respectively. In contrast, concentrations of Zn, Cd, As, Ni and Pb in HTP aerosols were significantly lower than those in cigarette smoke, indicating reduced emission amounts of toxic elements under non-combustion conditions. Elemental concentrations in HTP tobacco sticks were comparable to those in conventional cigarettes, suggesting that differences in aerosol composition were primarily due to the aerosol generation mechanisms rather than tobacco leave components. Screening-level risk assessment indicated that Cr represented the dominant contributor to both carcinogenic risk (CR) and hazard quotient (HQ) values associated with HTP use. The 90th percentile CR values for Cr ranged from 3.8×10^{-4} to 4.6×10^{-4}, whereas the HQ value reached 1.5. Although CR values for Ni and As were lower than those for combustible cigarettes, they exceeded the benchmark value of 1×10^{-6} under conservative exposure assumptions. These findings suggest that, despite generally lower elemental emissions from HTPs than from cigarettes, emissions of specific metals associated with heating devices may represent a distinct toxicological concern. Further studies incorporating elemental speciation and real-world exposure characterization will be warranted to refine health risk estimates for HTP aerosols.

2.10.P–We077 Experimental Validation of the Groundwater Ubiquity Score Leaching Index Using Site-Specific Physicochemical Parameters Across 16 Pesticides in Two South Korean Agricultural Soils

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The Groundwater Ubiquity Score (GUS) is a widely utilized first-tier screening tool for predicting pesticide leaching potential. However, its accuracy in regulatory risk assessments often depends on literature-derived values for the organic carbon-water partition coefficient (Koc) and soil half-life (DT50), which may not accurately represent regional soil conditions. This study evaluated the predictive reliability of the GUS index by comparing site-specific experimental parameters with literature data and validating them against observed leaching in two distinct agricultural soils from South Korea.

We determined Koc values for 16 pesticides across five chemical classes using reverse-phase high-performance liquid chromatography (HPLC) following OECD Test Guideline 121. Simultaneously, DT50 values were established via 30-day dark soil incubation at 25°C in a loam (Jinju; organic matter 1.54%) and a silty clay loam (Wanju; organic matter 10.42%). Leaching experiments were conducted using duplicate Wagner pots under four simulated rainfall intensities (56.3–241.7 mm h^{-1}), representing return periods of 2 to 50 years.

Significant discrepancies were found between measured log Koc and literature values, with differences reaching 1.3 log units. For instance, the measured log Koc for dinotefuran was -0.065, whereas the literature value was 0.74. These variances necessitated the reclassification of GUS categories for several

compounds. Notably, chlorantraniliprole (GUS 3.17, 'Leacher') showed negligible leaching, likely due to its low water solubility (0.88 mg L^{-1}) and high measured log Koc (2.465), suggesting that the GUS index inadequately accounts for solubility constraints. Conversely, boscalid (GUS 1.76, 'Non-Leacher') exhibited detectable leaching in the loam soil during extreme rainfall. The correlation between GUS and cumulative leaching was stronger in the loam soil (r = 0.82) than in the silty clay loam (r = 0.61), indicating that soil texture and organic matter significantly influence the reliability of the index. These results underscore the necessity of site-specific measurements for accurate leaching assessments and suggest that incorporating water solubility could improve the precision of screening indices in South Korean agricultural contexts.

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2.10.P–We078 Neonicotinoid Insecticide Leaching Under Variable Rainfall Return-Period Scenarios: Exceedance of Groundwater Quality Thresholds in South Korean Upland Soils

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Despite the global prevalence of neonicotinoid insecticides in groundwater, their specific leaching dynamics under the high-intensity rainfall regimes characteristic of the East Asian monsoon remain insufficiently characterized. This study quantified the vertical mobility of four neonicotinoids—thiamethoxam, imidacloprid, dinotefuran, and clothianidin—within two representative South Korean upland soils (Jinju loam and Wanju silty clay loam) under simulated rainfall return periods ranging from 2 to 50 years. Our primary objective was to evaluate the frequency and magnitude by which leachate concentrations surpass the European Union (EU) groundwater quality threshold of 0.1 μg L^{-1}.

To simulate realistic field conditions, we utilized indoor rainfall simulators and Wagner pots, monitoring leaching over nine consecutive events per intensity pattern (56.3 to 241.7 mm h^{-1}). In the loam soil, all neonicotinoids exhibited persistent leaching across all scenarios, with mean concentrations (117.1–288.7 μg L^{-1}) exceeding the EU threshold by approximately three orders of magnitude. Although the higher organic matter and clay content in the silty clay loam attenuated these concentrations by 30–50%, levels remained consistently above the 0.1 μg L^{-1} limit from the initial event. Notably, an unexpected attenuation in clothianidin leaching occurred in the loam soil under the most extreme rainfall scenario (50-year return period) relative to less intense patterns. This phenomenon suggests that extreme, short-duration intensities may trigger preferential flow that bypasses the soil matrix, rather than promoting sustained matrix-flow leaching. Dinotefuran, characterized by the lowest measured organic carbon-water partition coefficient (log Koc -0.065) and highest water solubility, mirrored the behavior of a bromide tracer, indicating near-zero soil retardation. These findings signal a substantial risk to subsurface water quality in regions experiencing climate-driven increases in extreme weather frequency, highlighting an urgent need for targeted groundwater monitoring and refined application guidelines.

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2.10.P–We079 Local History Improves Water-Quality Forecasts

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Routine surface-water monitoring produces large environmental datasets, but chemical measurements are often sparse and irregular at the level of individual station-compound time series. Predicting future concentrations, therefore, requires models that can exploit local monitoring history while remaining applicable across heterogeneous monitoring networks. In this study, we used FOTO-NL Data on Long-term chemical pollution monitoring data of surface waters in the Netherlands, which collates monitoring data from 21 Dutch regional waterboards and the national Rijkswaterstaat authority.

We compared local and pooled forecasting strategies under a strict final-year holdout setup, training on observations from 2015-2018 and predicting measurements from 2019. Prophet models were tested in multiple scopes: separate station-compound models, pooled compound-level models trained across stations, and pooled compound-level models calibrated by station-compound historical medians.

Results showed that the best performance was obtained by local station-compound Prophet models, with a log-scale RMSE of 0.51 and MAE of 0.34 on 996 well-monitored station-compound series in the 2019 holdout year.

These results suggest that forecast accuracy in routine water-quality monitoring is strongly controlled by the availability of repeated historical measurements at the same station for the same compound. Local time-series models are highly effective where sufficient monitoring history exists, while dataset-wide machine-learning models remain important for sparse compounds, newly monitored stations, and broader spatial generalization. The findings motivate further analysis of how much station-compound history is required before local forecasting becomes reliable, and whether auxiliary environmental data can reduce this requirement in data-limited settings.

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2.10.P–We080 Comprehensive evaluation for assessing multigenerational pirimicarb tolerance in Daphnia magna and the significance of fitness costs

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Aquatic organisms are continuously exposed to non-target anthropogenic chemicals (e.g., pesticides) in the environment. To evaluate chemical effects under environmentally relevant conditions, it is essential to understand their long-term and multigenerational consequences.
Our laboratory performed multigenerational studies in Daphnia magna continuously exposed to the carbamate insecticide pirimicarb for 15 generations. Here, we synthesize our work to propose a framework linking tolerance mechanisms, their associated fitness-costs, and environmental modifiers. We observed pirimicarb-sensitive neonates (relative to controls) by generation 5, followed by the acquisition of pirimicarb tolerance over continued exposure through generation 15. To ascertain mechanisms underlying tolerance, we quantified mRNA expression in D. magna. RNA-seq and RT-qPCR approach showed that increased acetylcholinesterase (AChE) genes, and antioxidant-defense genes (e.g., CYP4c3 and peroxidase) were significantly associated with pirimicarb tolerance. Consistent with our follow-up inhibitor assay, phenylhydrazine (a peroxidase-related inhibitor) reduced carbamate tolerance in tolerant lineages, strengthening the possibility that peroxidase activity contributes to the tolerant phenotype. In addition, DNA methylation increased in tolerant lineages, which may suggest that an epigenetic

component contributes to plasticity of the tolerant phenotype. Importantly, tolerance was not uniformly beneficial because tolerant lineages also showed altered physiological characteristics, including increased extinction probability in Daphnia population. Environmental factors strongly modulated long-term pirimicarb effects; in particular, thermal stress constrained the multigenerational build-up of carbamate tolerance by offsetting enhanced antioxidant defenses. Together, these findings suggest that carbamate tolerance can arise through complex, multi-pathway molecular responses and can be strengthened or constrained by external stressors. Thus, we need to evaluate environmental modifiers rather than attributing long-term outcomes to chemical exposure alone. Moreover, because tolerance is accompanied by fitness costs that can alter multigenerational effects, which may not be captured by guideline endpoints. Future assessments may require endpoints that better quantify trade-offs and population-relevant performance.

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2.10.P–We081 Post-fire ash runoff effects on physiological and behavioural stress responses in the South-west glass shrimp (Palaemon australis)

Bushfires can have significant but often overlooked impacts on aquatic ecosystems, particularly when rainfall after fire transports ash, sediment, and dissolved materials into waterways. These post-fire runoff events can alter water quality and expose aquatic organisms to stress, yet the early behavioural and physiological responses of small estuarine invertebrates remain poorly understood. This project will investigate how whole bushfire ash affects the South-west glass shrimp (Palaemon australis), a small crustacean that is ecologically important and potentially sensitive to changes in water quality.

The study will use a controlled laboratory experiment to expose shrimp to a range of ash concentrations and monitor their behaviour and oxygen use during exposure. Behavioural responses such as surface respiration, movement, and activity will be recorded, alongside physiological stress measured through oxygen use. After exposure, shrimp will be transferred to clean water to assess recovery and determine whether responses are temporary or persistent. By comparing responses across treatments and through time, the project aims to identify the concentration at which ash exposure begins to cause measurable stress and whether shrimp are able to recover once conditions improve.

This research is significant because it will improve understanding of how post-fire ash runoff affects a neglected but ecologically important aquatic species. The findings may help identify early warning signs of stress in waterways affected by bushfires and contribute to more effective monitoring and management of post-fire aquatic environments.

2.10.P–We082 No Bile? No Worries. Vitreous Humour to Assess Exposure of Fish to PAHs

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Biliary metabolites are commonly utilised in fish as biomarkers for recent exposure to polycyclic aromatic hydrocarbons (PAHs). A frequent challenge encountered with field-collected fish is the absence of biliary secretions in the gall bladder. The lack of biliary secretions following feeding diminishes sample size and consequently reduces the statistical power to detect inter-site differences in biliary PAH metabolite concentrations.

In commercial environments, fluorescent compounds present in fish vitreous humour have served as indicators for evaluating reductions in freshness during storage. Furthermore, eye fluids have been used to determine PAH contamination in porcine and bovine livestock.
The current study examined whether vitreous humour can be used in fish to evaluate recent exposure to PAH contamination. Specimens of robalo (Centropomus undecimalis) and pufferfish (Sphoeroides testudineus) were sampled from the port of Santos, Brazil, and from a reference location at Barra do Una on the central coast of São Paulo State, Brazil. Both vitreous humour and biliary secretions were collected for analysis.
Metabolites of naphthalene, pyrene, and benzo(a)pyrene were quantified using fixed wavelength fluorescence, while protein concentrations were assessed by spectrophotometry. All PAH metabolites measured in vitreous humour displayed similar patterns to those observed in biliary secretions; specifically, significantly elevated metabolite levels were detected at the contaminated port of Santos compared to the reference site.
These findings suggest that measuring PAH metabolites in the vitreous humour of fish eyes constitutes a reliable alternative to the assessment of PAH metabolites in biliary secretions.

2.10.P–We083 What did Contribute Induction of Serious Effects on Fish Embryos Exposed to 1,2-benzanthraquinone?

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OxyPAHs have been widely detected in the aquatic environments, raising concerns about their effects on the aquatic organisms. However, the toxic mechanism of OxyPAHs remains unclear. In general, toxicities of PAH derivatives are possibly caused by themselves or their metabolites. In this study, we aimed to elucidate the mechanism in fish embryos using metabolism inhibitor. Sometimes OxyPAHs induce specific effects, for example, 1,2-benzanthoraquinone (BAQ) induces the discoloration of oil droplets in fish embryos that leads to mortality in a few days, during embryonic developmental growth. OxyPAHs could activate the aryl hydrocarbon receptor (AhR) and induce Cytochrome P450 (CYP) enzymes like parent PAHs. AhR-CYP mediated pathway possibly contribute to the inductions of their certain toxicities. However, owing to the specification for toxicities, the metabolism and the toxic mechanism in fish embryo exposed to OxyPAHs might differ from those of PAHs. In the present study, we focused on BAQ, which is ubiquitous in the environment and has known the effects on Japanese medaka (Oryzias lapites) embryo, and investigated the mechanism underlying the toxic effects using Piperonyl butoxide (PBO), CYP inhibitor. At first, the embryos were exposed to DMSO and BAQ alone or BAQ+PBO. As the results, the discoloration in oil droplets in a few embryos exposed to BAQ for 200 µg/L was observed on 5 days after starting the exposure. The induction rate was 6% on 6 days. Meanwhile, the discolorations in BAQ for 200 µg/L+PBO were 70% and 90% in 200 µg/L+PBO at 4 and 5 days, respectively. Ultimately, all individuals were dead by 8 days. Furthermore, the discoloration was not observed in BAQ alone for 12 µg/L, but 11.5% of embryos exposed to BAQ for 12 µg/L+PBO was induced that at 7 days. We also analyzed the gene expression and ethoxyresorfin-O-deethylase (EROD) to evaluate CYP1A1 activity. As the results, cyp1a1expression was significantly higher in all groups treated with BAQ+PBO than BAQ alone group. On the other hand, there were no differences in EROD activity between BAQ for 12 µg/L+ PBO and BAQ alone group. They suggested that PBO inhibited the metabolism of BAQ by CYP enzymes and resulted to promote the binding of BAQ to AhR and excessively inducing cyp1a1. In conclusion, BAQ metabolites might contribute only minimally to discoloration of oil droplets induced by BAQ exposure.

2.10.P–We084 Effect of oral exposure to silica nanoparticles on fetal development in

mice

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Nanoparticles are integrated into diverse fields, including food additives and cosmetics. However, their minute size raises concerns regarding unexpected biological effects. Given our daily exposure to these materials, it is particularly important to examine the effects on pregnant women, who are highly vulnerable to chemicals. In this regard, we have been evaluating a safety assessment of nanoparticles, with a specific focus on reproductive and developmental toxicity. Among the various types, silica nanoparticles are some of the most used nanoparticles. We previously showed that intravenous injection of 10 nm silica nanoparticle (nSP10) can impair fetal development in mice. However, data on oral administration—which more closely simulates actual human exposure—remain scarce. In this study, we aimed to assess the reproductive and developmental toxicity of silica nanoparticles following oral administration, specifically focusing on the influence of particle size. Pregnant ICR mice were orally administered with nSP10, 100 nm silica nanoparticle (nSP100), or 1000 nm silica particle (mSP1000) (125 mg/kg) for three consecutive days from gestation day 15 to 17. On gestation day 18, anesthetized with isoflurane inhalation, mice were euthanized, and blood was collected through cardiocentesis. After that, fetuses and placentae were collected and weighed. Maternal body weight did not differ significantly among the groups, and biochemical analysis of maternal serum showed no abnormalities in liver or kidney functions, indicating no overt maternal toxicity. Although there was no significant difference in fetal weight, the nSP10-treated group exhibited a significant decrease in placental weight. Consequently, the fetus-to-placenta weight ratio was significantly elevated in this group. While the mSP1000-treated group showed a marginal reduction in placental weight, this did not result in a significant change in the fetus-to-placenta weight ratio. In contrast, no weight-related changes were observed in the nSP100-treated group. These findings suggest that nSP10 may impair placental function, potentially leading to fetal developmental abnormalities and long-term health risks. We are currently investigating the effect of nSP10 on placental structure via histopathology and on placental function by measuring maternal serum sFlt-1 levels.

2.10.P–We085 Heterogeneous Persulfate Activation by Water Treatment Sludge–Bamboo Carbon Composite for Sulfamethoxazole Degradation in Water

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Antibiotic contamination of aquatic environment is increasingly recognized as major pressure on aquatic ecosystems. Sulfamethoxazole, a widely used sulfonamide antibiotic, is frequently detected in surface, ground, and wastewater because discharges from agricultural runoff, municipal sewage, and hospitals are not fully removed by conventional treatment. This study evaluates a water treatment sludge–bamboo carbon composite (WTSBCC) as a heterogeneous catalyst for persulfate driven SMX degradation. WTSBCCx (x denotes pyrolysis temperature) was obtained by co pyrolysis at 600–900 °C with varying sludge:bamboo ratios. Among them WTSBCC700 with sludge:bamboo mass ration of 2:1 delivered the highest degradation. The Brunauer–Emmett–Teller (BET) analysis was used to determine surface area and porosity, X ray diffraction (XRD) and Raman spectroscopy to probe mineral phases and structural ordering, and X ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM) to analyze surface chemistry and morphology of the catalyst. Batch experiments were conducted at an initial SMX concentration of 3 mg $L^{-}1$, WTSBCC700 loading of 200 mg $L^{-}1$ and sodium persulfate concentration of 1 mmol $L^{-}1$. Under these conditions, more than 99% of SMX was removed within 120 min, and the time profile followed apparent pseudo first order kinetics (k = 0.041 $min^{-}1$). Adsorption isotherms showed favorable SMX uptake, well described by both Langmuir (R2 = 0.945) and Freundlich

(R2 = 0.993) models, indicating strong interaction between SMX and the heterogeneous carbon surface. Radical quenching-scavenger test and electron spin resonance (ESR) experiments indicated that non radical pathways dominate, with singlet oxygen (1O2) and interfacial electron transfer processes at the carbon–persulfate interface acting co–operatively in SMX degradation. Electrochemical analysis (LSV and EIS) showed a conductive carbon framework with abundant redox active sites that favors electron transfer to persulfate. The catalyst maintained high activity over multiple reuse cycles. This research demonstrates that a bamboo–water treatment sludge composite carbon is a robust and efficient persulfate activator for SMX removal. The work links pharmaceutical pollution control with beneficial reuse of treatment residuals and supports the development of circular, low waste advanced oxidation technologies for environmental management in the Asia Pacific region.

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2.10.P–We086 MXene-Optimized Ternary Z-Scheme Photocatalyst for Desorption-Coupled Visible-Light Degradation of Simazine.

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The persistence of herbicide residues in aquatic systems poses significant environmental and health risks due to their recalcitrance and resistance to conventional treatment processes. Simazine (SIM), a widely used triazine herbicide, exhibits strong affinity for solid media due to hydrophobicity, leading to secondary contamination and limiting the efficiency of sequential adsorption–regeneration processes. In this study, a visible-light (VL) responsive ternary photocatalyst (TCU-x, where x denotes MXene loading wt%) composed of a zirconium-based metal–organic framework (NH2-UiO-66), graphitic carbon nitride (g-C3N4), and titanium carbide MXene (Ti3C2) was rationally synthesized via a one-step in-situ approach. The MXene content was systematically varied (3, 5, and 10 wt%), with TCU-5 exhibiting optimal performance due to a favorable balance between electrical conductivity and interfacial active site availability. Structural and optical properties were confirmed by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FE-SEM), X-ray photoelectron spectroscopy (XPS), Brunauer-Emmett-Teller (BET) analysis, photoluminescence (PL), and time-resolved photoluminescence (TR-PL), indicating efficient suppression of e□-h+ recombination. Under VL irradiation, the optimized system ([SIM] = 1 mg L□1, TCU-5 dosage = 100 mg L□1, pH = 5.49) achieved more than 94% degradation of SIM within 120 min. The system was further evaluated for its ability to couple adsorption and photocatalytic degradation by treating SIM preloaded onto Amberlite XAD-4, enabling in situ desorption and subsequent oxidative transformation. Mechanistic analysis indicates a Z-scheme e□ transfer pathway mediated by conductive Ti3C2, wherein photogenerated e□ in the conduction band of the NH2-UiO-66 recombine with h+ in the valence band of g-C3N4. Radical quenching-scavenger test and electron spin resonance (ESR) experiments showed that the retained charge carriers promote the generation of O2•− and •OH, which drive efficient oxidative degradation of SIM while suppressing charge recombination losses. The system exhibited excellent stability and reusability, and maintained performance in real water matrices, indicating robustness against coexisting ions and natural organic matter. This work demonstrates a mechanistically informed, integrated desorption–photocatalysis strategy for scalable removal of persistent organic pollutants.

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2.10.P–We087 Visible-Light-Responsive Cu-BDC MOF Films for Surface Microbial Exposure Control

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Frequently touched indoor surfaces can act as reservoirs for microbial contamination, leading to potential exposure in healthcare and shared indoor environments. Cu-based antimicrobial films are promising for surface disinfection, but their performance is often limited by insufficient surface exposure of active copper species and gradual deactivation caused by the oxidation of Cu^{+} to Cu^{2+}.

Here, we developed a Cu-BDC metal–organic framework (MOF) based antimicrobial film to maintain active copper species under indoor visible-light conditions. The Cu-BDC MOF consists of aromatic ligands and copper centers, enabling visible-light-induced ligand-to-metal charge transfer (LMCT), which may promote Cu^{2+} reduction to Cu^{+} and support Cu^{+}/Cu^{2+} redox cycling. The MOF was incorporated into a polyurethane support, and sodium carboxymethyl cellulose was used as a binder to improve film stability, particle dispersion, and surface exposure of the MOF.

The film showed up to a 3-log microbial reduction under visible-light irradiation and maintained more than a 1-log reduction under dark ambient conditions. These results suggest that the Cu-BDC MOF film combines intrinsic copper toxicity with light-assisted redox activity, enhancing microbial inactivation under indoor-relevant conditions.

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2.10.P–We088 Mechanism of Levofloxacin Sorption by the Metal-Organic Framework MIL-88b (Fe)

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In recent years, the antibiotic levofloxacin has been detected in surface water, groundwater, wastewater treatment plant effluents, and even drinking water in many countries [8], which may lead to the emergence of antibiotic-resistant bacteria and genes. Various target sorbents (metal nanoparticles with an N-doped carbon surface, activated carbon) are used for the sorption of amphiphilic levofloxacin molecules [14, 15]. However, they operate in a narrow pH range or have low sorption capacity.

In this work, the mechanism of levofloxacin sorption by metal-organic coordination polymers (MOF), in particular, MIL-88b, was investigated. MIL-88b is a mesoporous MOF consisting of iron trimers linked by terephthalic acid ligands. The sorption capacity of MOF samples for levofloxacin at different pH was 51, 59, and 50 mg per g for pH 5.0, 7.0, and 9.0, respectively. The sorption isotherms show a specific local maximum, a desorption section, which is indicated by the release of iron ions into the solution, a local minimum, and then an increase in the sorption parameter. The deviation of the isotherm shape from linear in this section characterizes the competitive process of micelle formation and sorption absorption on the sorbent surface, characterized by the values of adsorption and association energies. The micelle formation of levofloxacin is confirmed by the presence of an inflection on the curve of the dependence of UV absorption on the concentration of the pharmaceutical, obtained at the absorption maximum at a wavelength of $\lambda = 287$ nm. Thus, for the drug after 30 minutes of shaking, a concentration of 285 mg / L corresponds to the critical micelle concentration (CMC). An increase in the shaking time leads to a decrease in the CMC to 75 mg / L. In this case, the highest value of the CMC corresponds to pH 7, at which levofloxacin exists in a zwitterionic form. Dynamic light scattering data indicate the formation of dispersed particles with an average hydrodynamic diameter of 130 nm at a levofloxacin concentration of

75 mg/L after 24 hours on a shaker. Thus, the presence of impurity ions is a key factor influencing the behavior of levofloxacin in solution, leading to the formation of micelles and drug desorption.

2.10.P–We089 Metal-Polymer Nanocomposites for Heavy Metals and Radionuclides Remediation: Formation, Properties, and Sorption Mechanisms

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This study investigates the development and characterization of metal-polymer nanocomposites as advanced sorbents for the removal of heavy metal ions (Pb2+, Cd2+, Zn2+, Cu2+, Cr3+) and radionuclides (UO22+) from contaminated environments. The primary objective is to enhance environmental quality and human health by mitigating the presence of these contaminants in water sources, food products, and other affected sites. The research focuses on a comprehensive study of nanocomposite formation, particularly those based on matrix-stabilized polymers, including natural polymers, and magnetoactive nanoparticles. Special attention is given to the in-situ self-organization and stabilization processes of nanoparticles through their interaction with the polymer matrix. The study also examines how the nature of stabilizing media and transformation conditions influence the physicochemical properties of the resulting nanocomposites. A key aspect involves predicting and identifying critical parameters that govern these properties.
The study establishes correlations between the fundamental characteristics of the nanocomposites, such as microstructure, nanoparticle dispersion, size distribution, spatial distribution within the matrix, and morphology, with their sorption properties, including capacity, selectivity, and stability. Furthermore, the research delves into the molecular mechanisms of adsorption processes within the polymer nanocomposite–metal ion system. Detailed analysis of sorption isotherms, mathematical description of static equilibria, and determination of quantitative sorption parameters provide insights into the sorbent surface characteristics, sorbent-sorbate interactions, and the overall detoxification efficacy of the proposed nanocomposite sorbents.

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2.10.P–We090 Zero-Valent Iron Nanoparticles from Poly(vinylpyrrolidone)-Iron Complexes: Green Synthesis and Environmental Potential

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Nanoscale zero-valent iron (nZVI) is a highly reactive material for environmental remediation, but its preparation in a truly metallic state is difficult because water and oxygen rapidly convert iron into oxide or oxyhydroxide phases. Here, we present a photochemical route in anhydrous isopropanol that uses a poly(vinylpyrrolidone) (PVP)-iron(III) complex as both a molecular precursor and a stabilizing polymer matrix. This approach avoids borohydride and aqueous reducing media and therefore provides a greener route to highly reactive iron nanophases.
The precursor was structurally characterized using ultraviolet-visible, infrared, Raman and Mössbauer spectroscopy, supported by density functional theory calculations. Model studies with N-methylpyrrolidone showed the formation of an ionic pair, [Fe(NMP)2Cl2]+[FeCl4]-, while the polymer system forms a related PVP-stabilized structure, [Fe(PVP)2Cl2]+[FeCl4]-. Carbonyl groups coordinate the iron(III) center through oxygen atoms, and the polymer matrix retains chloride-containing iron fragments. Complexes with PVP of different molecular weights, 10, 30, 40, 90 and 360 kDa, were also

obtained and tested as agents for correcting iron-deficiency chlorosis in cucumber plants; [FePVP30kDa] showed the best performance.
Under ultraviolet irradiation in deaerated isopropanol, the [FePVP] precursor enabled the first solution-phase formation of truly zero-valent iron nanoparticles. The Fe(0) state was verified by a methyl viologen assay, demonstrating high reducing ability rather than only the presence of iron-rich particles. The formation process proceeds through Fe(III)→Fe(II)→Fe(0) stages and follows a topochemical Erofeev-Kolmogorov-type kinetic profile with induction, autocatalytic growth and deceleration. Water and oxygen switch the pathway from nZVI formation to mixed iron oxide/oxyhydroxide particles, with a critical water threshold near 15%. Thus, the same polymer-iron platform links plant-available iron delivery with controllable production of environmentally relevant nZVI and oxide nanoparticles.

2.10.P–We091 Development of High-Performance PFAS Adsorbent Using PET Bottles

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This study presents a novel approach for upcycling waste PET bottles into powdered activated carbon (PAC) for removing per- and polyfluoroalkyl substances (PFAS) from water. PET was pyrolyzed at 800°C, activated using KOH and K2CO3, and then heated under a hydrogen atmosphere to remove oxygen-containing functional groups. The resulting materials were characterized using SEM-EDS, BET, FT-IR, XPS, and elemental analysis.
KOH activation produced a predominantly microporous PAC with a high specific surface area of 1,743 m2/g, whereas K2CO3 activation generated a mesopore-dominant PAC with a surface area of 1,018 m2/g. Hydrogen treatment effectively reduced surface oxygen content while maintaining similar pore structures and specific surface areas.
Adsorption experiments using a 20 mg/L dose showed that hydrogen-treated PACs removed over 99% of eight PFAS compounds at an initial concentration of 50 ppb, representing a significant improvement relative to untreated PACs. Kinetic tests further demonstrated rapid PFAS removal, achieving 95% removal within 27 minutes for the KOH-activated PAC and 97 minutes for the K2CO3-activated PAC, outperforming a commercial PAC.
Additional adsorption experiments using drinking water treatment plant influent (TOC: 2 mg/L) and sewage treatment plant secondary effluent (TOC: 5 mg/L) showed that dissolved organic matter reduced PFAS removal efficiency. However, PET-derived PACs consistently exhibited superior adsorption performance for all PFAS species compared to the commercial PAC. These results demonstrate the strong potential of PET-derived PACs as high-performance adsorbents for PFAS removal. The valorization of waste PET bottles into PFAS adsorbents offers a sustainable solution for both water treatment and plastic waste management.

2.10.P–We092 Development of Novel Biofilm Monitoring Platform using Non-ohmic Fringe Field Electrodes

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Biological treatment processes utilizing biofilms in wastewater treatment are inherently susceptible to biofouling. For effective management, it is critical to detect, predict, and quantify the degree of fouling in its early stages. Conventional methods for biofouling detection have primarily relied on invasive strategies, such as physical scraping followed by biomass quantification, or indirect indicators, including flux decline and microbial activity assessments. However, these traditional approaches are largely destructive, ex-situ, and have a limitation to provide real-time data. Such limitations make it difficult to

achieve fully quantitative analysis or to predict fouling trend, particularly during the initial stages of formation. Consequently, there is an urgent need for non-disruptive, real-time monitoring technology that can replace post-methods. A promising solution is the use of non-ohmic electrical fringe fields. Lee et al. have proposed a novel electrode design using interdigitated electrodes to generate fringe fields. Unlike line-of-sight electric fields, the fringe field design allows for high field strength at the surface using low voltages (e.g., 10 V) while permitting unimpeded water flow. Notably, the fringe field selectively concentrates within the biofilm due to the difference in relative permittivity between the biofilm matrix and the surrounding water, enhancing its interaction with the attached microbial growth. In this study, we present an electrochemical monitoring platform based on the fringe field electrode for the non-invasive and on-site detection of biofouling. To establish this platform, an instrumentation setup was designed to measure impedance signals, reflecting the attachment and growth of Escherichia coli K12 on the electrode surface. To validate the reliability of this impedance-based sensor, the harvested biomass was independently quantified using ATP bioluminescence assays and spectrophotometry (OD600). Through analysis of impedance signal variations, we established a correlation between impedance response and the concentration of E. coli K12, without destroying the sample. Therefore, we demonstrated the potential of this platform as a robust, quantitative tool for real-time biofouling monitoring in wastewater treatment systems.

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2.10.P–We093 Environmental Challenges and Bioprocessing Opportunities for e-Waste Printed Circuit Boards (PCBs): Findings and the Road Ahead

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Waste Electrical and Electronic Equipment (e-waste) is the fastest-growing waste stream worldwide, intensifying pressure on waste management systems due to complex structures and heterogeneous compositions, comprising metals, plastics, and persistent contaminants that pose challenges for recycling and disposal processes. Conventional treatments and informal recycling pathways are often energy-intensive, environmentally harmful, and focused on the recovery of metals, frequently neglecting other hazardous constituents. These limitations highlight a need for integrated strategies that promote both resource valorisation and environmental protection.

Bioprocessing approaches have attracted increasing attention as sustainable alternatives, but most studies remain focused on metal recovery, overlooking the fate of polymeric fractions. PCBs, which pose additional waste management challenges due to miniaturisation and increasing ubiquity, are often used in such studies due to high concentrations of strategic metals such as copper, zinc, and gold. However, different materials have been used across such studies, compromising comparability. In our studies, materials derived from the same printed circuit boards were used to ensure consistency, having been previously characterised (using Attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR), Scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDS), and X-ray diffraction (XRD), among others).

Bioprocessing experiments using the filamentous fungus Penicillium brevicompactum (conducted over 28 days each) revealed its capacity to promote polymer degradation, evidenced by increased particle fragmentation, mass reduction (up to 75%), the potential occurrence of chain scission and oxidation events (assessed through ATR-FTIR), and metal solubilisation (up to 26 mg Cu/L). Fungal biomass exhibited stable growth in the presence of PCB particles, with increases in ATR-FTIR spectra regions attributable to carbohydrate-associated functional groups, suggesting their potential as a carbon source for the fungus.

These findings highlight the potential of filamentous fungi (specifically P. brevicompactum) for the bioprocessing of multiple e-waste constituents (i.e., polymers and metals) within a single process. The development of such integrative and multifaceted processes is key for resource recovery and environmentally-sustainable management of e-waste under a circular economy framework.

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2.10.P–We094 Suspect Screening Workflow to Detect Emerging Contaminants Using Silicone Rubber Passive Samplers Deployed across Global Waters─Insights from AQUA-GAPS/MONET

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Aquatic environments worldwide are increasingly impacted by emerging contaminants (ECs), including pesticides, industrial chemicals, and personal care products. Despite growing evidence of their occurrence in the environment, many ECs remain outside the scope of existing regulatory frameworks. The global aquatic passive sampling network AQUA-GAPS/MONET has demonstrated the ability to provide highly comparable data across freshwater and marine environments, thereby supporting the Stockholm Convention on Persistent Organic Pollutants and delivering data on ECs including novel brominated and organophosphate flame retardants, polycyclic aromatic hydrocarbons, and synthetic musks. Building on this foundation, the network offers a powerful platform for broadening chemical surveillance through suspect and non-target screening approaches. The aim of this study is to develop an analytical workflow for the suspect screening of ECs in silicone rubber passive samplers deployed worldwide, including sites in Australia and China, and to demonstrate the feasibility of identifying new hydrophobic ECs. Fifty exposed silicone rubber passive samplers from AQUA-GAPS/MONET and the corresponding quality assurance and quality control (QA/QC) samples were analysed by gas chromatography coupled to high-resolution mass spectrometry with electron ionization (GC-EI-HRMS) in full-scan mode. An in-house data processing workflow was developed, with spiked internal standards and previously detected target analytes serving as benchmarks. The compound identification was based on the retention index and mass spectral matching against GC-Orbitrap-HRMS libraries. The successful identification of spiked standards and previously detected target analytes confirms the reliability of the workflow as a foundation for a broader suspect screening. It is hypothesised that application of this workflow on the entire AQUA-GAPS/MONET sample archive will enable the tentative identification of a wide range of hydrophobic ECs across diverse geographic regions. This work contributes to ongoing efforts towards more comprehensive chemical surveillance of aquatic environments on a global scale.

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2.10.P–We095 Associations Between Polycyclic Aromatic Hydrocarbons (PAHs) and Pro-inflammatory Cytokines in the Kidney of Grass Carp (Ctenopharyngodon idella)

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The accumulation of polycyclic aromatic hydrocarbons (PAHs) in aquatic environments represents an important toxicological concern for freshwater teleosts. The kidney, a key excretory organ with important immunoregulatory functions in fish, is susceptible to the toxic effects of these compounds. Therefore, this organ is a suitable target for studying immune responses induced by environmental toxicants. The aim of the study was to analyse the relationships between tissue PAHs exposure and the renal immune response in grass carp (C. idella) during two sampling periods (June and July). Tissue samples from grass carp (4-year-old individuals) were collected during June and July (location: Kolíňany University Experimental Pond, Slovakia). The tissues were sonicated (lysis buffer with a protease inhibitor) o ice and used for the analysis of pro-inflammatory cytokines: interleukin-1 beta (IL-1β), interleukin-6 (IL-6), tumor necrosis factor alpha (TNF-α). Twelve priority PAHs (BcFL, BaA, CPP, Cry, 5MCH, BbF, BjF, BkF, BaP, Ind, Dda, Bgp) were quantified using GC–MS. Statistical analysis included the nonparametric Mann–Whitney U test, Spearman's correlations, principal component analysis (PCA), calculation of total toxic equivalents (Total BaPeq), and hierarchical clustering. The analysis revealed significantly higher concentrations of all 12 PAHs in the kidneys in June compared with July (all p < 0.05). In contrast, cytokine levels did not show statistically significant differences between the months. The PCA biplot showed a clear separation of the profiles for both months, with June associated with PAHs pollution vectors. To integrate the toxicity of the PAHs mixture, individual concentrations were converted to benzo[a]pyrene toxic equivalents using toxic equivalency factors. This metric summarized the potential toxicity of the PAHs mixture accumulated in the kidney. In June, overall toxicity (BaPeq) was positively correlated with cytokine levels, whereas in July these associations were weak or absent. Hierarchical clustering revealed a sub-cluster linking TNF-α with indeno[1,2,3-cd]pyrene, indicating a potential association that warrants further investigation. The results suggest that the renal immune response in June is positively associated with acute exposure to PAHs. However, the loss of correlation in July, despite relatively stable cytokine levels, may reflect the influence of PAH metabolites or persistent immune activation following the initial exposure.

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2.10.P–We096 Effects of Polycyclic Aromatic Hydrocarbons and Chlorophenols on Heart Rate Patterns in Medaka Embryos

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Cardiac dysfunction in fish embryos, including arrhythmia and impaired contractility, disrupts circulation and can lead to developmental abnormalities and mortality. Therefore, heart rate and cardiac function are considered useful indicators for assessing the toxic effects of chemicals. However, the specific cardiac effects induced by different chemical substances remain insufficiently characterized.
Polycyclic aromatic hydrocarbons (PAHs) and dichlorophenols (DCPs) are among the environmental contaminants frequently detected in aquatic ecosystems. Notably, pyrene (Pyr), a four-ring PAH, has been detected in heavily contaminated aquatic environments, raising concerns regarding its potential impact on aquatic organisms.
One challenge in fish embryo studies is the difficulty of accurately measuring heart rate. In this study, heart rate was therefore defined based on periodic changes in brightness associated with blood inflow and outflow during cardiac contraction. Using this approach, we evaluated cardiac functions and its temporal

dynamics in Japanese medaka (Oryzias latipes) embryos exposed to some PAHs and DCPs.
DCPs induced robust concentration-dependent tachycardia, and exposure to 2,4-DCP and 3,5-DCP resulted in tubular heart formation with exposures of at higher concentrations. In contrast, PAHs elicited distinct patterns of cardiac dysfunction. Naphthalene caused time-dependent alterations in heart rate, whereas phenanthrene and dibenzothiophene induced a 2:1 atrioventricular (AV) block indicative of impaired electrical conduction, accompanied by yolk sac retention and defective fin development. Fluorene caused bradycardia without conduction block, while pyrene induced pronounced bradycardia and pericardial edema.
The predicted no-effect concentration (PNEC), estimated from the EC50 value for pyrene-induced bradycardia, was approximately 3 µg/L. In contrast, the measured environmental concentration (MEC) of pyrene reported in the Gulf of Suez, a highly contaminated aquatic environment, reached 443 µg/L, resulting in MEC/PNEC ratios far exceeding 1. These findings indicate substantial ecological risk under heavily polluted conditions and suggest that pyrene contamination may contribute to cardiac dysfunction and developmental abnormalities in fish embryos.
Taken together, these findings suggest that exposure to environmentally relevant concentrations of PAHs and DCPs can induce diverse forms of cardiac dysfunction in fish embryos.

3.03.T - Genomic Instability And Biomarkers of Environmental Stressors with Implications for Long-Term Ecological and Human Health

3.03.T01 DNA Repair Deficiency and Telomere Dysfunction as Determinants of Sensitivity to Environmental Carcinogens

Genetic susceptibility plays an important role in determining how individuals respond to environmental carcinogens, particularly when cellular mechanisms that safeguard genomic integrity are compromised. This study investigates how deficiencies in DNA repair pathways and telomere maintenance influence cellular responses to environmental toxicants, with implications for biomarker discovery and cancer risk assessment.

Using mammalian cell models deficient in key DNA repair pathways, including non-homologous end joining (NHEJ) and nucleotide excision repair (NER), we evaluated genotoxic responses to environmentally relevant stressors, including sodium arsenite, silver nanoparticles (Ag-np), bisphenol A, ionising radiation, and oxidative stress. Cells with impaired DNA repair capacity or telomere dysfunction exhibited significantly increased DNA damage, reactive oxygen species (ROS) generation, cell cycle arrest, and reduced viability following exposure.

Notably, Ag-np exposure induced γ-H2AX foci formation, telomere attrition, mitochondrial dysfunction, and elevated oxidative stress. These responses were more pronounced in DNA-PKcs–deficient cells, highlighting the critical role of the NHEJ pathway in maintaining genome stability and regulating cellular responses to oxidative stress.

Gene expression profiling revealed activation of stress-response pathways alongside downregulation of DNA repair effectors, providing insight into early molecular events triggered by toxicant exposure. These findings reinforce the concept that DNA repair capacity and telomere integrity are key determinants of cellular sensitivity to environmental mutagens and carcinogens.
Overall, our results demonstrate how genomic instability–based biomarkers can help identify susceptible populations and improve understanding of mechanisms underlying environmental carcinogenesis. Integrating such mechanistic insights into environmental toxicology may support improved exposure assessment, biomarker development, and risk evaluation for environmentally and occupationally exposed

populations.

3.03.T02 Genome Stability under Environmental Stress: Real-time Visualization of Holliday Junction Processing

Environmental stressors can induce DNA lesions and replication-associated intermediates that must be accurately repaired to prevent persistent genomic instability. Although biomarkers such as DNA damage, chromosomal instability, oxidative stress and cellular senescence provide early indicators of exposure and effect, the repair processes that determine whether damaged genomes are restored or destabilized remain less directly observable. Holliday junctions are central intermediates in homologous recombination, a key pathway for repairing DNA double-strand breaks and replication-associated DNA damage. Failure to process these structures accurately can lead to chromosome aberrations, genome rearrangements and loss of genome stability. We recently used high-speed atomic force microscopy to directly visualize how the bacterial Holliday junction resolvase RuvC interacts with junction-like DNA structures at the single-molecule level under near-physiological ionic conditions. This label-free approach revealed that RuvC exists as both monomeric and dimeric species, whereas stable junction binding is associated with the dimeric form. Magnesium ions markedly prolonged the lifetime of RuvC–junction complexes, suggesting that metal ions contribute not only to catalysis but also to structural preorganization of the repair complex. Complementary structural predictions supported a model in which magnesium promotes a more symmetric and coordinated protein–DNA interface. These findings provide a real-time view of an early molecular step that safeguards genome stability: the transition from transient DNA encounter to stable repair-complex formation before catalytic resolution. In the context of environmental risk assessment, visualization of DNA repair dynamics can complement conventional genotoxicity biomarkers by offering mechanistic insight into genome maintenance, biological resilience and the interpretation of delayed or cumulative effects of environmental stressors.

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3.03.T03 Environmental Microplastics Induced Oxidative Stress Mediates Genotoxicity in Field and Laboratory Models: An Insight into Long-term Ecological and Human Health Implications

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Microplastics (MPs) are emerging contaminants of concern, widely present in ecosystems, and have the potential to act as chronic biological stressors. Whether environmental MPs disrupt cellular redox balance and induce genotoxicity under real-world conditions remains unclear, raising concerns about long-term ecological and human health impacts. This study integrates field and experimental model systems to assess the genotoxic potential of environmental MPs and the role of oxidative stress in genomic instability. MPs were characterized in water and fish samples from the Karamana River, followed by genotoxicity assessment in fish. These field observations were extended to laboratory studies in Drosophila melanogaster reared in culture media prepared with MP-contaminated river water. The role of MPs in oxidative stress–induced genotoxicity was validated using polystyrene MPs. Multigenerational analyses were subsequently performed to examine whether chronic exposure promotes oxidative stress-mediated genotoxicity through assessment of oxidative stress biomarkers, comet assay-based DNA damage, and DNA repair gene expression. MPs were found in river water and fish, confirming freshwater contamination and biological uptake. Fish collected from the river exhibit significant DNA damage,

indicating measurable genotoxic stress under natural exposure. In D. melanogaster, river water and polystyrene MPs produced comparable toxic responses, including impaired development, reduced reproductive fitness, elevated oxidative stress, and increased genotoxicity. Multigenerational findings revealed persistent oxidative imbalance, sustained DNA damage, and altered DNA repair gene-expression, supporting oxidative stress as a key driver of MP-induced genotoxicity. Overall, this study provides direct evidence that environmental MPs induce oxidative stress–associated genotoxicity across field and experimental systems. By integrating ecological observations with model validation, the findings highlight MPs as persistent genotoxic agents with long-term ecological and human health risks, underscoring the urgent need for mitigation strategies and regulatory frameworks.

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3.03.T04 Development of a Human iPSC-Derived Liver Organoid Model for In Vitro Genotoxicity Assessment

Genotoxicity testing is an essential component of chemical and pharmaceutical safety assessment. However, commonly used in vitro systems, such as bacterial assays and conventional cell cultures, do not always reproduce human liver-specific metabolic activation. This limitation creates a need for test models with greater human relevance. Although organoids have emerged as promising in vitro systems, their application to genotoxicity studies remains limited because animal-derived matrices can reduce reproducibility and complicate chemical exposure, while the low proliferative activity of three-dimensional tissues restricts the use of endpoints that depend on cell division.

In this study, we developed a human iPSC-derived liver organoid using a scaffold-free culture approach and evaluated its potential for in vitro genotoxicity assessment under simplified exposure conditions. To assess DNA damage in a three-dimensional tissue with low proliferative activity, H2AX phosphorylation (γ-H2AX) was used as the endpoint. The organoids retained a stable three-dimensional morphology and exhibited hepatic characteristics, including albumin secretion and CYP3A4 activity. Immunostaining also confirmed the presence of hepatocyte and cholangiocyte marker expression. Treatment with aflatoxin B1 caused concentration-dependent reductions in cell viability and increases in γ-H2AX levels in the liver organoids, whereas undifferentiated iPS cells did not show the same response. These results suggest that this human iPSC-derived liver organoid model may serve as a useful in vitro tool for detecting metabolism-related DNA damage.

3.06.C.T - PFAS Treatment and Remediation: Linking Environmental Behavior to Sustainable Solutions

3.06.C.T01 Experience from Germany in the treatment of PFAS-contaminated water and solid surfaces affected by PFAS

The first major PFAS contamination case in Germany became public in 2005. The author was commissioned by the German Environment Agency to develop a treatment solution for PFAS-contaminated groundwater in order to prevent contamination of nearby surface waters used as a drinking water source for several million people. As no experience with PFAS treatment existed in Germany at that time, a multi-stage treatment system was developed consisting of extensive pre-treatment for organic and inorganic co-contaminants, followed by activated carbon adsorption and ion-exchange resin treatment. This represented one of the first large-scale PFAS treatment systems in Germany and was

followed by several additional projects between 2005 and 2008. The operational experience gained demonstrated that conventional adsorption technologies alone are often not sufficiently optimised for PFAS removal and that more targeted and complementary treatment mechanisms are required. In 2008, a research alliance between Cornelsen and the Fraunhofer Institute was established to develop PFAS-specific technologies. Initially, a PFAS-selective adsorbent with higher loading capacities than conventional activated carbon and ion-exchange resins was developed. However, the wide variability of PFAS contamination and water matrices showed that adsorption technologies should be selected on a project-specific basis and combined with complementary treatment approaches. As a result, a precipitation-based technology for dissolved PFAS compounds was developed and introduced to the German market in 2010 under the brand name PerfluorAd. This presentation provides an overview of more than 20 years of experience in PFAS-contaminated water treatment and discusses the applications and limitations of activated carbon, ion-exchange resins and precipitation technologies. In addition, combination models integrating different treatment principles for improved PFAS removal efficiency will be presented. Finally, the presentation will address the decontamination of PFAS-contaminated solid surfaces, particularly fire-fighting systems exposed to PFAS-containing foams. The principles of replacing PFAS-containing fire-fighting foams and preventing recontamination of tanks, pipes and pumps during conversion to PFAS-free foams will be briefly outlined.

3.06.C.T02 Applied Smouldering to Treat PFAS: From Fundamentals to Recent Developments

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Per- and polyfluoroalkyl substances (PFAS) have been used to manufacture many modern materials for over 80 years – from non-stick cookware to fire fighting foams. PFAS are now recognised as a challenging class of emerging contaminants that pose environmental risks at low concentrations. Thousands of types of PFAS have been produced and their environmental release has led to widespread contamination. Therefore, there is a need for environmental remediation solutions to treat these compounds sustainably, economically, and robustly. Applied smouldering treatment is a thermal technology that can drive PFAS remediation. Smouldering is a flameless and low-temperature form of combustion, commonly seen as the glowing red surface in a traditional charcoal barbecue. Smouldering is a highly resilient form of combustion that can be harnessed in engineering systems for sustainable and cost-effective remediation that can remove >99% of organic contamination in soils. Ongoing research has shown that smouldering can also treat challenging wastes, e.g., contaminated-sludges and digestates, to destroy organic contaminants while also recovering energy and resources to support a circular economy. That is, organic contaminants (e.g., hydrocarbons) within soil or the organic matrix in waste (e.g., sewage sludge) can be used to drive smouldering treatment with small energy footprints. Upon modest energy inputs for ignition, subsequent treatment can be self-sustained with low airflows – provided the rate of energy released from smouldering exceeds energy loss rates, e.g., from heat losses. For PFAS remediation, the contamination is often at low concentrations that cannot sustain smouldering. Therefore, PFAS-contaminated matrices must foster smouldering with another fuel source, e.g., another waste stream. For example, in soil remediation applications – nearby wastes can be used, such as spent granular activated carbon from groundwater treatment. In contaminated sewage sludge treatment, the sludge matrix itself can provide sufficient energy to drive PFAS treatment. This presentation will overview smouldering treatment fundamentals for PFAS remediation, ongoing research and application advances, and key knowledge gaps. Altogether, smouldering treatment demonstrates strong potential to provide a sustainable, economical, and robust PFAS remediation solution.

3.06.C.T03 Isolation of a Paenibacillus Strain Encoding a Fluoroacetate

Dehalogenase–Like Protein from a a Per- and Polyfluoroalkyl substances (PFAS) Contaminated Site

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Per- and polyfluoroalkyl substances (PFAS) are highly persistent synthetic chemicals whose recalcitrance stems from the exceptional stability of the carbon–fluorine bond, rendering them resistant to thermal, chemical, and biological degradation. In contrast, naturally occurring organofluorides are rare and predominantly monofluorinated. To date, only one enzyme class, fluoroacetate dehalogenase (FAcD), has been shown to catalyse biological C–F bond cleavage in naturally occurring organofluorides. Despite this, FAcDs have not been demonstrated to catalyse defluorination of PFAS. The aim of this study was to advance the understanding of microbial PFAS degradation by investigating defluorination processes in enrichment cultures derived from PFAS-contaminated environments.

Anaerobic enrichment cultures were optained from soil collected at two aqueous film forming foam (AFFF) contaminated sites in Sweden. Cultures were spiked with high concentrations of perfluorooctanesulfonic acid (PFOS, ≥98.0%) and perfluorooctanoic acid (PFOA, ≥96%). Fluoride release, monitored with an ion-selective electrode, was observed in a single enrichment dominated by Paenibacillus (36.6%). However, targeted chemical analysis revealed no concomitant decrease in PFOS or PFOA concentrations in the incubation. The absence of fluoride release when using higher-purity PFOA (≥98.0%) indicates that defluorination originated from an impurity present in the lower-purity standard rather than the target PFAS themselves.

Nevertheless, Paenibacillus sp. was successfully isolated and genome sequencing revealed the presence of a gene encoding a protein with high similarity to known fluoroacetate dehalogenases. To our knowledge, this represents the first report of a bacterium encoding FAcD isolated from a PFAS-contaminated site, suggesting possible microbial adaptation and a potential role in the transformation of PFAS at the site. Ongoing work is evaluating the substrate scope of this isolate to resolve its role in the potential PFAS degradation at the contaminated site.

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3.06.C.T04 Sustainable Innovative Drinking Water Treatment Solutions for PFAS Removal

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Safe and sustainable drinking water supply is increasingly challenged by the widespread occurrence of per- and polyfluoroalkyl substances (PFAS), dissolved organic matter (DOM), and other emerging contaminants in surface and groundwater resources. New regulatory limits for PFAS in drinking water, such as 4 ng/L for four PFAS in Sweden, highlight the urgency of developing more effective treatment solutions, particularly as current technologies are often insufficient to meet these standards at full scale. This study addresses this challenge by developing and evaluating innovative, scalable, and sustainable treatment trains for drinking water production and reuse. The overarching aim is to remove PFAS and thereby breaking the continuous “treat and release” cycle that leads to environmental recirculation of PFAS and other pollutants. This is achieved through four full-scale case studies representing different water sources and contamination scenarios, in collaboration with drinking water utilities. These systems

provide a realistic basis for testing treatment performance under operational conditions. This study evaluates a combination of advanced and innovative treatment processes, including foam fractionation, granular activated carbon (GAC), anion exchange (AIX), membrane technologies, electrochemical oxidation destruction (EO), and integrated multi-stage treatment trains. These approaches are assessed for their ability to remove PFAS from raw water, infiltration systems, and process streams. Results indicate that membrane filtration and foam fractionation can achieve high PFAS concentrations in the treated fractions; however, foam fractionation shows reduced removal efficiency for shorter-chain PFAS. GAC and AIX both demonstrated strong overall performance for PFAS removal, although a gradual breakthrough of shorter-chain PFAS was observed over time. The destructive treatment approach using EO effectively degraded PFAS. However, careful assessment is required due to the formation of shorter-chain PFAS and other transformation products, which appear to be dependent on the water matrix. Overall, this study will provide practical tools and knowledge to water utilities and regulators, supporting the implementation of sustainable water treatment solutions at scale and contributing to improved protection of both human health and aquatic environments.

3.07.T - Soil Contaminant Bioavailability and Remediation

3.07.T01 Developing bioavailability-based assays for refining exposure to PFAS-impacted matrices

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Per- and polyfluoroalkyl substances (PFAS) comprise a large class of >15,000 man-made fluorinated compounds, with >1,400 used in consumer and industrial applications due to their oil, water and stain repellence, chemical stability and surfactant properties. Many PFAS are environmentally persistent and bioaccumulative, leading to widespread human exposure, with oral ingestion recognised as the predominant pathway. Exposure magnitude is modulated by matrix-specific parameters that influence desorption and absorption kinetics under physiological conditions (i.e. bioavailability) although approaches for its assessment are lacking. As such, this study used Sprague-Dawley rats to develop an in vivo assay to quantify PFAS relative bioavailability in impacted matrices based on PFAS toxicokinetics. Cannulated female rats, housed in individual metabolic cages, were administered a single dose of PFOA, PFOS or PFHxS by either oral gavage (~0.2-2,000 µg kg-1 body weight) or by intravenous injection (5 µg). Time course blood samples (200 µl) were collected prior to dosing and throughout the 120-hour exposure period. At 120 hours, rats were humane killed with livers and kidneys collected for PFAS analysis. Pooled urine and faecal samples were also collected to quantify PFAS concentration in excreta. When PFAS relative bioavailability was determined, exposure matrices (soil, food) were administered as slurries via gavage with endpoints collected as per toxicokinetic studies. PFAS concentration in samples was determined using targeted LC-MS/MS analysis using USEPA-based extraction and analysis methodologies. Toxicokinetic differences were observed in PFAS blood, organ and excreta concentrations. However, linear dose responses were observed for area under the blood plasma time curve (PFOA, PFHxS), liver accumulation (PFOS) and urinary excretion (PFOA, PFHxS) indicating the potential of these endpoints for relative bioavailability quantification. When oral and intravenous doses were compared, PFOA, PFOS and PFHxS absolute bioavailability values ranged from 88.3-102.9% highlighting high gastrointestinal permeability of these compounds. Assessment of PFAS relative bioavailability in soil (n = 20) and food (n = 6) resulted in a wide range of bioavailability outcomes (5-105%) depending on matrix physicochemical properties which influenced matrix-driven sorption-desorption equilibria influencing the freely available fraction for gastrointestinal uptake.

3.07.T02 Metabolomics and Lipidomics Reveal Granulated Activated Carbon (GAC) Impacts Molecular Level Health of Earthworm (Eisenia fetida) During Per- and Polyfluoroalkyl Substances (PFAS) Immobilization

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Remediation of PFAS impacted soil is a critical environmental challenge due to the ubiquitous nature of PFAS contamination, mobility, persistence and toxicity. One of the most widely used amendments to immobilise soil PFAS is GAC. Although its efficacy in reducing PFAS bioavailability is established, the health impacts of GAC on sentinel soil organisms such as earthworms are unclear, particularly at sub-lethal, low environmental concentrations. This study used targeted metabolomics and untargeted lipidomics to elucidate molecular level impacts on Eisenia fetida exposed to soil containing PFAS (10-1000 µg/kg), GAC (0.5-2.5%) and PFAS (1000 µg/kg) + GAC (0.5-2.5%) for 28 days (n=3, 10 worms per replicate).

Results showed that although earthworm mortality was not significantly different among treatments, dry biomass was significantly reduced by 2.5% GAC application (31.7% and 35.9% reduction in 2.5% GAC and 1000 µg/kg PFAS + 2.5% GAC treatments respectively, p<0.01). One-way ANOVA and post hoc Tukey's HSD (p<0.05) testing identified 120 significantly different metabolites. Further analysis using a combination of t-test (α=0.05) and fold change (FC=2) between control and treatment revealed that 10, 100 and 1000 µg/kg PFAS resulted in significantly higher levels of 5, 14 and 21 metabolites, respectively. These changes suggest disruptions to lipid metabolism, cell signalling and oxidative stress. However, 0.5%, 1.0% and 2.5% GAC significantly affected 16, 19 and 75 metabolites respectively, indicating disruptions to lipid, carbohydrate, amino acid and energy metabolism, cell signalling and oxidative stress. Interestingly, comparison between 2.5% GAC and 1000 µg/kg PFAS + 2.5% GAC treatments showed that fewer metabolites (n=57) were significantly altered in the latter. However, metabolite profiles associated with disruptions to carbohydrate, amino acid and energy metabolism remained mostly similar between the 2.5% GAC and 1000 µg/kg PFAS + 2.5% GAC exposure, which were not observed in the 1000 µg/kg PFAS treatment alone, suggesting that they were primarily associated with the presence of GAC in soil. Glutathione was the only common polar metabolite among these three groups, suggesting that both 1000 mg/kg PFAS and 2.5% GAC may cause earthworm oxidative stress.

Overall, the results suggest that minimizing weight loss and adverse molecular level effects on earthworms should be a key consideration when choosing the application rate of GAC during soil remediation.

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3.07.T03 Pre-soaked Biochar to Mitigate Methylmercury Formation in Coastal Sediments

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Mercury is a pervasive environmental contaminant, and among different chemical species methylmercury (MeHg) is the most toxic and bioavailable. MeHg bioaccumulates and biomagnifies through food webs, posing serious risks to ecosystems and human health. Biochar is an effective, low-cost remediation amendment with tunable surface chemistry and soil co-benefits. However, surface-associated dissolved organic matter (DOM) and other redox-active leachates from biochar can transiently trigger MeHg

formation after biochar application in paddy soils and coastal sediments. Here, we focus on microwave-derived biochar for aqueous Hg(II) sorption and evaluate whether simple pre-soaking in deionized water that can effectively remove labile DOM can mitigate MeHg formation in anoxic coastal sediment incubations. Aqueous sorption tests confirmed high Hg(II) uptake by microwave biochar in both seawater and freshwater (within the observed range of 15.77-17.31 mg/g). In the incubation experiment, raw microwave biochar showed a dose-dependent transient response. At 0.5 % addition, sediment MeHg was approximately 49 % higher than the blank in Week 1, whereas at 1 % addition the Week 1 increase was only approximately 6 % and shifted to a net suppression by Weeks 2-3. Pre-soaked microwave biochar consistently reduced sediment MeHg relative to the blank, with stronger suppression at 1 % addition. In the 1 % incubation, UV254 showed the strongest association with sediment MeHg (Pearson r = 0.83 overall; r = 0.94 in Week 1), suggesting that UV-absorbing DOM was closely linked to MeHg dynamics. Raw biochar also increased aqueous pH to 7.6, indicating release of slightly alkaline ash components. SUVA254 measurement identified that raw biochar released high amounts of DOM with relatively low aromaticity, consistent with water-extractable and potentially labile DOM. Overall, the results strongly suggest that pre-soaking can mitigate early MeHg stimulation by removing reactive leachable fractions of DOM and perhaps Hg while preserving the solid-phase Hg stabilization effect of biochar. Within the tested range, an appropriate increase in biochar application rate may help counteract the MeHg impact associated with DOM leaching by strengthening solid-phase Hg sorption and stabilization.

3.07.T04 Ecosystem Functioning Overrides Metal Load Legacy in Regulating Soil Carbon Storage in Smelter Affected Boreal Forests

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Historical metal emissions from the Industrial Brassworks have affected boreal and nemoboreal conifer forests for centuries. The present study area, Gusum's Bruk, the smelter, has been active for >300 years, was relocated by ~1 km, and emissions were markedly reduced from 1982 onward, yet legacy contamination persists in near-source stands. We evaluated how ecosystem functioning mediates soil carbon (C) storage under this metal-load legacy by revisiting long-studied forest sites spanning ~0.44–7.91 km from the current smelter and including reference conditions further away.

We quantified soil C stocks and indicators of C–N cycling from 0–20 cm depth (0–5, 5–10, 10–20 cm), combining depth-resolved soil and vegetation $\delta^{13}C/\delta^{15}N$, vegetation surveys (with emphasis on moss recovery), microbial activity proxies, soil physicochemical variables, and metal concentrations and isotope ratios (Zn, Cu, and Pb). Legacy Cu exposure in another study system spanning a ~100-year gradient (50–2300 mg kg^{-1}) in soils supports the evaluation of persistent metal-load effects on ecosystem processes.

At Gusum, across the gradient, moss cover ranged from ~12% near the new smelter to ~100% at reference sites, paralleling shifts in biogeochemical organization and nutrient cycling. Surface-soil pH varied from ~4.6 to ~5.1 among site groups. Partial least squares regression showed that ecosystem-function indicators explained most variation in soil C: the final model explained 71.7% of soil C-stock variance ($Q^2 \approx 0.68$), with $\delta^{15}N$ slope and moss cover as the strongest predictors; a reduced model with these variables retained high predictive ability ($Q^2 \approx 0.61$). Metal isotope ratios primarily traced contamination sources and mixing, but contributed only marginally to explaining soil C variability once biological functioning was included.

These results indicate that legacy metal loads leave persistent imprints, but recovery of ecosystem functioning—especially moss re-establishment and depth-structured N cycling—best predicts long-term

soil C storage in smelter-affected boreal forests.
Keywords: Soil carbon storage, biological recovery, smelter impacted forests, nitrogen cycling, stable isotopes

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5.01.A.T - Application of Novel Approach Methodologies (NAMs) to Improve Risk Assessment and Management of Contaminants of Emerging Concern (CEC)

5.01.A.T01 In Vitro Assays for Evaluating Adverse Health Effects of Environmental Pollutants

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Environmental pollutants released throughout the life cycle of industrial and consumer chemicals are widespread in aquatic environments and pose global health risks. Understanding their toxicological effects is essential for effective public health policies. This review summarizes current methodologies for toxicological evaluation of environmental pollutants, with emphasis on new approach methods (NAMs), particularly in vitro cell-based assays. A key challenge is to select biologically relevant and fit-for-purpose in vitro models and endpoints that are explicitly matched to pollutant-specific exposure scenarios, modes of action, and associated adverse health outcomes. In vitro assays targeting cytotoxicity and genotoxicity endpoints have enabled comparative toxicity profiling across pollutant classes. Moving beyond, we underscore the potential of in vitro mechanistic toxicology (including immunotoxicity and endocrine-disrupting effects) and the adoption of emerging stem cell-based models to assess the developmental toxicity of pollutants in early embryogenesis. By applying the iceberg model to mixture toxicity, we highlight the significant yet often-underestimated risks of complex pollutant mixtures. Collectively, we outline critical gaps in experimental design and data interpretation, and propose a decision-making framework to better evaluate the risks of environmental pollutants.

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5.01.A.T02 Establishment of an In Vitro Platform for Developmental Toxicity Screening Using Human iPS Cells and Their Differentiated Definitive Endoderm Cells

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In vitro new approach methodologies (NAMs) have long emphasized human relevance through complex multicellular and multicompartmental models. However, while informative, these prove challenging to scale and standardize, leaving a gap in fit-for-purpose models for the developmental toxicity screening and prioritization of the large number of untested chemicals.

To address this methodological gap, we established and technically validated a scalable, reproducible, and cost-effective in vitro platform comprising two models based on human iPS cells and their induced

definitive endoderm (DE) cells. The first model (h-iPSCs-S9) combined human iPS cells with human liver S9 fractions as an external metabolizing system; it measured cell viability, oxidative stress, and targeted gene expression changes using qPCR. The second model (iDE) treated DE cells differentiating from iPS cells with novel, chemically defined media; it measured cell viability, differentiation efficiency, and transcriptomic responses using RNAseq. We then benchmarked the platform against short-, medium-, and long-chain chlorinated paraffins (CPs) (SCCPs 63% Cl, MCCPs 57% Cl, and LCCPs 47% Cl) at human exposure levels (1–1000 µg/L).

Results revealed that CPs altered the viability of iPS cells during differentiation (IC_{10} of 262 and 187 µg/L for SCCPs and MCCPs, respectively), while undifferentiated cells were less sensitive (IC_{10} > 500 µg/L), suggesting a higher risk during development. At sub-cytotoxic concentrations (≤ 100 µg/L), the h-iPSCs-S9 model revealed that, consistent with in vivo observations and depending on cellular metabolic potency, SCCPs and MCCPs either downregulated DNA damage repair genes or upregulated the damage tolerance gene REV3L. Also, CPs induced oxidative stress with signs of antagonism toward PPARα-Nrf2 signaling, again consistent with in vivo observations. Further, the iDE model revealed that SCCPs downregulated CXCR4 and inhibited pathways related to cell migration and cytoskeletal homeostasis, while MCCPs downregulated FOXA2 and enriched pathways favouring mesodermal over endodermal commitment, suggesting possible developmental hazards.

By concomitantly screening for the developmental hazards of CPs across 3 experimental conditions, our platform not only replicated their in vivo effects but also prioritized SCCPs and MCCPs over LCCPs for further investigations, strengthening its stance as a scalable, reproducible, and fit-for-purpose NAM for faster decision-making.

5.01.A.T03 Exposure Assessment in In Vitro NAMs for Improved Hazard Ranking of Bisphenol A Alternatives

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Bisphenol A (BPA) has been a key industrial chemical to produce plastics and color developers for several decades, but its use is now restricted in many legislations worldwide due to its endocrine disrupting properties. Numerous BPA alternatives have entered the market, but the toxicological profiles remain insufficiently characterized for the majority of the alternatives. To fill these data gaps, we evaluated BPA and 26 alternatives in six cell-based in vitro bioassays covering cytotoxicity, endocrine disruption, xenobiotic metabolism, adaptive stress responses, mitochondrial toxicity and neurotoxicity. To enable direct comparison of BPA with its alternatives we used a newly developed cumulative specificity ratio score that integrates the degree of specific activation and overall toxicological activity across the test battery. Several structurally related alternatives activated estrogen receptor α as strongly as, or more strongly than, BPA. Some non-estrogenic alternatives, including BPS-MPE, showed shifted activity towards peroxisome proliferator-activated receptor γ, while others caused mitochondrial dysfunction or neurotoxicity. To refine the hazard ranking, chemical stability and freely dissolved concentrations (Cfree) were determined for BPA and 24 alternatives in bioassay medium. BPA and 22 alternatives were stable for up to 48 h, whereas BADGE degraded completely in medium and BPPH decreased by 40%. Cfree values predicted with a mass-balance model were validated experimentally for BPA and 15 alternatives and agreed within a factor of 10. Relative effect potencies (REPs) based on nominal concentrations and Cfree were similar for hydrophilic and moderately hydrophobic alternatives but differed for hydrophobic or highly protein-bound chemicals. For TCBPA and BPAF the Cfree-based REP was up to 147-fold higher than the nominal REP. Based on nominal concentrations BP-MIBK was ranked highest for estrogenicity. Considering Cfree, the highest ranked compound was BPAF. TCBPA appeared less

estrogenic than BPA based on nominal REP but more potent after Cfree-correction. Overall, many BPA alternatives constitute regrettable substitutes based on their in vitro effects. Only TMCD was identified as a more benign replacement.Furthermore, Cfree-based exposure correction further improves hazard rankings and supports prioritization of safer alternatives.

5.01.A.T04 Building Confidence in In Vitro Permeability Data as a New Approach Method for Chemical Absorption Assessment

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New Approach Methodologies (NAMs) have gained increased popularity in chemical risk assessment to provide mechanistic insight, reduce reliance on animal testing, and improve predictions of internal exposure. For orally ingested chemicals, intestinal permeability is a key determinant of absorption. However, in vitro permeability data have not been widely adopted in NAM-based risk assessment for two main reasons. First, many exposure and toxicokinetic models do not recognize and explicitly incorporate the independent mechanistic role of permeability and instead rely on hydrophobicity as a convenient, expedient surrogate. Second, the reliability of published in vitro intestinal permeability measurements has not been systematically evaluated, and it remains uncertain to what extent they can reasonably characterize intestinal absorption. In this presentation, we assess the role and reliability of in vitro intestinal permeability data for more than 1,800 diverse chemicals, including pharmaceuticals, pesticides, and industrial compounds. We first show that permeability and hydrophobicity jointly influence fractional gut absorption, but they are not interchangeable: permeability reflects additional transport processes (such as paracellular and active transport) that hydrophobicity cannot capture. We then use a mechanistic model to identify three key sources of uncertainty in reported permeability measurements: loss of chemical mass to membranes or headspace, limited experimental windows between steady-state and equilibrium transport, and interference from aqueous boundary layers or paracellular resistance that can obscure true membrane permeability. These results indicate that permeability should be considered a fundamental NAM-relevant property, comparable in importance to partitioning and reactivity, but only when supported by transparent reporting and appropriate evaluation of data quality. We suggest that intestinal permeability data can strengthen next-generation chemical assessments by improving predictions of absorption and internal dose, while also underscoring the need for structured data management, clear applicability domains, and rigorous quality-screening criteria before such data are used in regulatory or decision-support contexts.

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5.03.T - From Plastic Leakage and Emission Assessment to Treaty Implementation: Developing and Harmonizing Monitoring Approaches

5.03.T01 Utilizing harmonized leakage and emission data towards establishment of risk assessment methods for microplastics, in case of aquatic organisms

The Ministry of the Environment (MOEJ) is currently conducting expert reviews with the aim of establishing a method for risk assessment of the effects of microplastics present in aquatic environments,

including the ocean, on aquatic organisms, based on the assumption of exposure via the environment. The objective of this project is to collect scientific evidence regarding microplastic exposure, environmental fate, and toxicity to aquatic organisms, and to establish a risk assessment methodology to quantitatively assess the impact on organisms and ecosystems, with the aim of estimating risks that will serve as a basis for future administrative decision, which is also important for negotiating treaty implementation. We have established several committees and been advancing discussions in collaboration with domestic experts.
With regard to exposure data, most current measurements of MicP microplastic particles in aquatic environments target particles with a diameter of 300 μm or larger, and use particle concentration (particles/m³) as the unit of concentration. In contrast, toxicity testing often uses MicP microplastic particles ranging from a few to several tens of μm in size and evaluates them in terms of weight concentration (μg/L). It is necessary to convert particle number concentration to weight concentration, taking into account particle size, shape, and material (bulk density). To address these issues, experts has been convened to examine the estimation of fine MicP microplastic particle number concentrations and the conversion between particle number concentration and weight concentration, by utilizing MOEJ's research data gained in line with the harmonized monitoring methods.
With regard to toxicity, while many studies provide quantitative assessments such as the LOEC, it is currently not possible to comprehensively evaluate these results with lack of test guidelines. For this project, through a review of relevant literature by expert group, we have formulated and scrutinized “Key Considerations for Literature Reviews (a kind of criteria)” regarding necessary experimental conditions and other factors, serving as the fundamental approach for selecting endpoints to be adopted in toxicity assessments and for evaluating the reliability of toxicity data. Based on these points to ensure a certain level of quality, categorization of hazard data for each species have been explored.

Disclaimer/Disclosure: The presentation is based on the outcome of the project in FY2025. This may be updated in the future.

5.03.T02 Occurrence and Management Implications of Additive-Derived Chemicals in Marine-Leaked Micro- and Macroplastics

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Plastic pollution is increasingly recognized not only as litter accumulation and fragmentation, but also as a pathway for chemicals contained in or associated with plastics. However, limited information is available on how additive-derived chemicals differ between environmental microplastics (MicP) and macroplastics (MacP), or how such data can support risk-based management.
This study investigated additive-derived chemicals in marine-leaked MicP and MacP from surface waters, coastal and seafloor environments, and riverine inputs around Japan. Polymer types were identified by attenuated total reflectance Fourier-transform infrared spectroscopy, and target chemicals were extracted and analyzed by gas chromatography–mass spectrometry. In total, 48 MicP composite samples and 308 MacP samples were analyzed. We focused on three substances with different environmental and management implications: Irgafos 168-related compounds, di(2-ethylhexyl) phthalate (DEHP), and hexabromocyclododecane (HBCD).
Irgafos 168-related compounds and DEHP were frequently detected in polyethylene and polypropylene MicP and MacP. Irgafos 168-related compounds showed polymer- and size-dependent patterns, suggesting different degrees of oxidation, leaching, and migration from the plastic matrix. In contrast, DEHP tended to be higher in MicP than in seafloor MacP, indicating that external sorptive uptake from surrounding water, particles, or organic matter may contribute to its concentrations. HBCD was detected at elevated concentrations in polystyrene-containing MicP fractions, suggesting that fragmented expanded

polystyrene can transport regulated flame retardants after weathering and marine drift.
These findings indicate that fragmentation from MacP to MicP does not necessarily reduce chemical concerns. Increased mobility and dispersion may allow additive-derived chemicals to act as secondary exposure sources in coastal ecosystems. The results highlight a gap between product-based chemical regulation and environmental management of plastic debris. Integrating additive content, persistence, and size-dependent transport into monitoring and risk assessment can support science-based plastic pollution mitigation.

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5.03.T03 Tyre wear particles and tyre associated chemicals in the Moreton Bay region, Australia – Spatial trends and hydrodynamic influences

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Plastic pollution is one of the biggest environmental challenges the world is facing, with microplastics (particles <5mm) of particular concern. Tyre wear particles (formed through abrasion of tyre tread during use) are now considered one of the largest sources of microplastics to urban environments, yet information on their occurrence, transport and fate within the environment is still limited. Additionally, TWPs contain a wide range of tyre associated chemicals (TACs) which are added during the manufacturing process or occur as transformation products within the final material. They have been shown to readily leach into environmental compartments with 6PPD-Quinone of particular concern due to demonstrated toxicity towards certain salmon species.

There is a distinct lack of environmental monitoring data in the Australian environment, particularly in sensitive habitats such as the Great Barrier Reef catchments. Therefore, this study aimed to investigate occurrence and distribution of TWPs and 15 common TACs in surface water and sediment across 15 river and bay water systems within the Moreton Bay catchment of Brisbane, Australia. Over the whole study, TACs were detected widespread in surface water and sediment (9.3 to 2043 ng/L and

5.03.T04 Collecting microfibres and behavioural insights through a citizen science study on microfibre emissions from household clothes washing

Antonia Praetorius[1], Allison Moll[1], Anna Bosshard[1], Riko Kimura[1], Suhas Puranik[1], Cameron Brick[1] and Lies Jacobs[1] (1)University of Amsterdam (UVA)

The release of microfibers during washing of synthetic textiles (e.g. polyester) is a major contributor to the emissions of microplastics to the environment. However, mechanisms driving microfibre emissions are poorly understood and little is known about the willingness of individuals to adopt pollution-reducing measures. Existing studies on the impact of textile properties or of washing conditions on microfibre release are limited by non-realistic laboratory set-ups or case-by-case assessments and do not include behavioral dimensions.
Here we present a unique citizen science project on synthetic microfibre release, designed in collaboration with environmental scientists and psychologists. Washing practices and related microfibre release were studied in 2 different home-washing campaigns in the Netherlands (involving 60-80 citizens each), allowing for a fine-grained data collection in real-life settings. Citizens were equiped with either washing

bags or external washing machine filters (both commercially available) to collect microfibres released from their everyday clothes during typical home washing conditions over several months. In addition to collecting the microfibres, participants reported data on textile characteristics and washing conditions. The collected fibres were analyzed in the laboratory to yield information on total mass and/or number of microfibres released per mass of clothing, as well as identification of fibre material through pyrolysis–gas chromatography–mass spectrometry. Alongside this data collection, psychological surveys, before and after participation, were completed by the citizen scientists to assess (changes in) perception, behaviours and pro-environmental attitudes.
This study yields insights into total amounts, typical ranges and characteristics of microfibres released under different washing conditions and for different clothing items; and also reveals that participation in such a data collection impacted problem awareness and perceived responsibllity, but did not significantly change personal norms, social norms about sustainability or perceived behavioural control. We demonstrate that citizen science can serve the dual purpose of contributing to scientific data collection as well as to assess citizen's perceptions and behaviours with respect to a topic of interest. This provides invaluable insights to inform effective interventions and holistic policies to reduces synthetic microfibre emissions to the environment.

6.01.B.T - Trajectories in Environmental Science & Technology: From Biodiversity and Public Health to Sustainable Solutions

6.01.B.T01 Using Adverse Outcome Pathway Paradigms in evaluating risks of chemical and climate change induced environmental impacts in estuarine fish species

Sea Level rise has led to the intrusion of saltwater into estuarine coastal areas. In areas were anthropogenic contaminants co-occur, the increase in salinity may significantly alter biological responses to the contaminants. Effects are species-specific with organisms having euryhaline life histories such as salmonids showing dramatic alterations. Hormonal changes as a result of osmoregulatory responses from hypersalinization impact a host of physiological targets and include numerous neuro-endocrine signalling pathways that may alter reproduction. Using adverse outcome pathway paradigms may allow a pathway to estimate toxicity from combined chemical and non-chemical stressors which may be used in weight of evidence components of ecological risk assessments.

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6.01.B.T02 Epidemiological Studies as a Cornerstone for Evaluating Novel Chemical Exposures and Protecting Human Health

Rapid advances in chemical synthesis technologies have led to the production of vast numbers of novel chemicals that did not previously exist in nature. Many of these substances have substantially improved safety, comfort, and convenience in modern societies. At the same time, their intentional and unintentional release into the environment has resulted in widespread and persistent exposure of humans and ecosystems. From a planetary boundaries perspective, growing evidence suggests that the scale and pace of novel chemical production may be approaching or exceeding the Earth's capacity for safe assimilation.
While experimental toxicology relies on in vitro assays and animal models, understanding real-world health effects fundamentally requires epidemiological evidence. Since the 1990s, birth cohort studies have played an essential role in elucidating long-term and intergenerational effects of chemical exposures during sensitive developmental periods such as fetal life. We initiated the "Hokkaido Study on Environment and Children's Health" in 2001 as a long-term birth cohort to investigate health effects of

chemical exposures in pregnant women and their children. Prenatal exposure has been assessed by measuring persistent organic pollutants in maternal blood, and more recently emerging contaminants such as plastic additives in children's urine. Evaluated health outcomes include physical growth, allergic diseases, and metabolic and endocrine biomarkers to explore underlying mechanisms. By tracking exposures from the fetal period across the life course, we aim to improve individual health risk prediction and preventive strategies.
The exposome concept—capturing the totality of environmental exposures across the lifespan—has become central to systems-oriented environmental health research. Advances in analytical technologies now enable comprehensive characterization of external exposures and internal biomarker profiles. As data complexity increases, simple single exposure–single outcome models are no longer sufficient. We emphasize the role of birth cohort studies as a transdisciplinary foundation for integrating exposure science, toxicology, epidemiology, and omics technologies. Such integrative approaches are essential for sustainable chemical assessment and management, strengthening the science–policy interface, and advancing environmental science and technology to protect public health, biodiversity, and ecosystem services within planetary boundaries.

6.01.B.T03 Identifying Sources of VOCs and Hazardous Air Pollutants in Japan Using Regional Air Quality Simulations Constrained by Background Measurements

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Volatile organic compounds (VOCs) contribute to air pollution through the formation of secondary pollutants, including ozone and fine particulate matter with an aerodynamic diameter of less than 2.5 μm (PM2.5), as well as through direct adverse impacts on human health as hazardous air pollutants (HAPs). Regional air quality simulations are used to identify sources of VOCs and HAPs and to develop mitigation strategies; however, reproducing their ambient concentrations remains challenging due to limited availability of reliable input datasets. In this study, model performance for simulating ambient concentrations of VOCs and HAPs over Japan was improved by combining observations with regional air quality modeling. Emission inventories commonly used for ozone and PM2.5 simulations were replaced with inventories derived from the Pollutant Release and Transfer Register (PRTR) system. In addition, ambient concentrations of VOCs and HAPs were measured at three spatial scales—nationwide background sites, background sites for the Tokyo metropolitan (Kanto) region, and urban sites within Kanto—to independently constrain boundary concentrations and emissions. Initial simulations substantially underestimated observed VOC and HAP concentrations. Model performance improved markedly after incorporating PRTR-based emissions and applying observational constraints. The improved simulations were used to identify sources of VOCs and HAPs in the Kanto region. Local emissions dominated reactive VOCs, whereas background contributions were substantial for less reactive VOCs and most HAPs, underscoring the importance of long-range transport and international cooperation in reducing their ambient concentrations.

6.01.B.T04 Unrecognized Anesthetic Gas Exposure in Operating Rooms and Strategies for Healthcare Worker Protection

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<p dir="ltr">Hospital air quality management has traditionally centered on infection control, while chemical hazards in hospital workplaces have remained largely unrecognized. Healthcare workers in operating rooms are routinely exposed to hazardous chemical agents such as anesthetic gases, yet their air

quality has rarely been treated as an occupational health priority. An operating room was designated as a living lab for a multi-year investigation of anesthetic gas contamination. Sevoflurane, desflurane, and N2O concentrations were continuously monitored at multiple locations over three years. Substantial anesthetic gas leakage persisted even after surgical procedures, with contamination patterns varying by surgery type and anesthesia method. The accumulation of equipment has produced dead spaces that impede designed airflow, resulting in localized air stagnation and elevated pollution concentrations. Computational simulations confirmed that residual anesthetic gases continuously expose healthcare workers throughout and beyond the surgical procedure. A large language model based predictive tool was developed to estimate contamination levels under varying surgical conditions, offering a practical means to anticipate and manage exposure risk in real time. These findings highlight an urgent need to expand hospital air quality management beyond infectious agents to include chemical exposure risks, and point to a broader need for occupational health strategies and policies tailored to the operating room environment.

5. Environmental Policy, Regulation, Risk Management, and Science Communication

2.10.D.T - Environmental Chemistry and Exposure Assessment: Generic Session

2.10.D.T01 Degradation of Acetaminophen via Persulfate Activation using O-Doped Polyimide-Derived Carbon Catalyst

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The ubiquitous detection of pharmaceuticals, such as acetaminophen, in aquatic environments poses a significant threat to ecosystem health due to their potential to foster antibiotic resistance and disrupt endocrine systems. Traditional wastewater treatment processes often struggle to achieve complete removal of these persistent organic pollutants, necessitating the development of efficient advanced oxidation processes. This study aims to develop a metal-free, high-efficiency carbon catalyst derived from polyimide to activate persulfate for the sustainable remediation of contaminated water.

To achieve this, an oxygen-doped polyimide-derived carbon catalyst was synthesized via a controlled pyrolysis process. The structural and chemical transformations of the catalyst were characterized using X-ray photoelectron spectroscopy and Raman spectroscopy to correlate surface functionalities with catalytic performance. The catalytic activity was evaluated through the degradation of acetaminophen, and the study further investigated the inhibitory effects of common inorganic ions, such as phosphate and bicarbonate, using real water samples collected from the Geumho River and Shinchon wastewater treatment plant to ensure environmental relevance.

Results indicated that the pyrolysis temperature significantly influences the nitrogen configuration within the carbon lattice, with the sample treated at 800°C showing the highest catalytic activity. The incorporation of oxygen into the polyimide precursor was found to optimize the formation of active sites, specifically graphitic nitrogen and oxygen-containing functional groups. Mechanistic investigations involving chemical scavenging experiments and electron spin resonance analysis revealed that the degradation was predominantly governed by a non-radical pathway, where singlet oxygen and superoxide radicals served as the primary reactive species.

The research demonstrates that oxygen-doped polyimide-derived carbon is a robust and reusable catalyst, maintaining high stability over multiple cycles. While high concentrations of phosphate and bicarbonate in real-world water matrices can suppress oxidation rates, the system remained highly effective for pharmaceutical removal. These findings may provide a sustainable, metal-free alternative for persulfate

activation, offering a practical strategy for protecting aquatic ecosystems from emerging chemical threats

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2.10.D.T02 Microbubble-mediated deep oxidation of gaseous VOCs via interfacial non-radical pathway

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Gas–solid catalytic oxidation has been widely explored for volatile organic compound VOC abatement, yet incomplete oxidation, catalyst deactivation, and the formation of toxic oxygenated byproducts remain critical challenges. In this study, we develop a microbubble-mediated wet air purification system that exploits the gas–liquid interface as a reactive microdomain for deep VOC oxidation. An amphiphilic Co single-atom catalyst CoSA@N–C was engineered to localize at the microbubble–water interface, enabling spatially confined activation of peroxymonosulfate PMS directly at the VOC transfer boundary. Mechanistic investigations suggest that VOC oxidation proceeds predominantly through a non-radical pathway, associated with Co(IV)-oxo species and singlet oxygen (1O2). This interfacial non-radical oxidation pathway allows hydrophobic VOCs to be efficiently converted into water-soluble intermediates, thereby suppressing gaseous byproduct emission and promoting further aqueous-phase mineralization. As representative target pollutants, toluene, chlorobenzene, and acetaldehyde were removed with efficiencies exceeding 99%, accompanied by near-complete mineralization. The results indicate that microbubble–liquid interfacial catalysis can overcome key limitations of conventional gas-phase catalytic oxidation by integrating VOC mass transfer, localized oxidant activation, and wet-phase mineralization. This work provides a new strategy for wet air purification and suggests broader applicability for the simultaneous removal of gaseous pollutants and particulate matter in practical air treatment systems.

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2.10.D.T03 Rapid bacterial sensing strategy for live bacteria quantification via electric-field induced change in membrane potential

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Bacteria pose constant public health risks, as evidenced by the recent global infection incidents linked to contaminated health supplements and infant formula. The persistence of these outbreaks is rendered difficult to prevent by the inherent limitations of current gold-standard methods. Traditional culture-based assay is too slow for real-time clinical emergencies. The enzyme-substrate and molecular methods which are alternatives of culture-based to detect bacteria rapidly, however they have a critical drawback in that cannot distinguish live and dead cells. To overcome these challenges, we propose a rapid biosensing strategy for the selective quantification of live bacteria using electric-field enabled fluorescence measurement. An electric field (100 V/cm) was applied to Escherichia coli K12 via a bespoke sensor platform to induce specific changes in bacterial membrane potential. Membrane potential indicates the differential distribution and activity of cations such as Na+, H+, and K+ and hence an indicator of cellular metabolism and viability. Strong stimuli such as an electric field, change the membrane potential, which is a specific response that occurs only in living cells. Changes in membrane potential are usually monitored using membrane potential dyes using microscopes. By switching the electric field off and on,

this allowed the membrane potential dyes to enter and then be expelled from the live bacteria. This platform monitored dyes interaction in real- time via fluorescence measurement and demonstrated quantification of live bacteria over a range of concentrations (OD600nm = 0.0 to 1.0) within only 180 seconds (y = 15.06x – 1.39, R2 = 0.85). Furthermore, while commercial adenosine triphosphate (ATP) kits resulted in false positives, our proposed method clearly differentiated and quantified live versus dead bacteria. Consequently, this approach serves as a useful tool for rapid detection of live intact bacterial cells, especially in scenarios eliminating both false negative and positive results. Finally, we designed an easy-to-use bespoke sensor platform that brings out the application of membrane potential dyes, in this way, the role of dyes would be re-purposed and expanded beyond niche microscopy visualization to the broader studies of fluorescence-base bacterial sensors and quantification.

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2.10.D.T04 When Emergency Actions End but Contamination and Exposure Continues: Multimedia Fate and Exposure Modeling in East Palestine, Ohio

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Chemical accident-related environmental disasters have become increasingly frequent and consequential in industrialized societies. The sudden, large-scale, and uncertain releases of contaminants during such accidents pose substantial challenges for assessing environmental and health risks and remediation decision-making. Using the train derailment happening in East Palestine, Ohio, United States, in 2023 as a case study, we developed a generalizable workflow integrating post-disaster monitoring data with reverse modeling approaches to reconstruct pre-event environmental baselines, estimate disaster-phase emissions, simulate post-event chemical variability, and conduct public health risk assessments.

We selected phenanthrene (Phe), pyrene (Pyr), and benzo[a]pyrene (BaP) as representative compounds because of relatively abundant monitoring data, contrasting physicochemical properties, and differing toxicological relevance. With chemical concentrations measured in water, sediment, and soil across different locations in 2023 and 2024, we used reverse modeling to estimate emissions to air, nearby water bodies, and the derailment site during and after the accident, expressed as central tendency values and 95% confidence intervals (reflecting uncertainty accumulation from the reverse model approach to fitting measurements). Statistical estimates indicated that BaP emissions exceeded the U.S. Superfund Reportable Threshold more than two orders of magnitude. Simulation results further revealed environmental behavior governed by physicochemical properties, with lipophilic contaminants showing strong accumulation in the contaminated site during the derailment and subsequent redistribution into aquatic compartments. However, the emission estimates should be interpreted with caution for their wide confidence intervals; for example, for Pyr emission, the upper 97.5th percentile is 136 times the central tendency estimate.

Our reconstructed contamination history indicates that the train derailment caused a short-term spike in water BaP concentration (83 times the pre-emergency baseline level in the impacted region), and environmental concentrations declined shortly afterwards to pre-event levels after one year. However, this transient spike may have driven high contaminant accumulation in local aquatic food during the immediate post-derailment period, potentially leading to doubling life-long cancer risk.

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2.10.D.T05 Swedish Landfill Leachate: Mapping and Seasonal Profiling of Contamination of Emerging Concern (CECs)

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Landfilling is a primary waste management method but remains a critical source of contaminants of emerging concern (CECs) to the environment. These contaminants, including pharmaceuticals and personal care products (PPCPs), per- and polyfluoroalkyl substances (PFASs), and industrial chemicals (ICs), can leach from landfills even decades after closure. Many of these CECs are particularly hazardous due to their persistence, mobility, and potential for endocrine disruption or carcinogenicity. Despite the potential risks, the spatio-temporal profiles of CECs in Nordic, cold-climate regions are largely understudied. This study addresses this gap by utilizing high-resolution mass spectrometry (HRMS) and non-target screening (NTS) to provide a comprehensive snapshot of CEC occurrence and variability across five Swedish sites.

This study identified 79 CECs, with 68 of them confirmed with level 1 confidence. This profile comprised 31 ICs, 23 PPCPs, 13 PFASs, 9 pesticides, 3 stimulants, and 1 sweetener. Notably, triisopropyl phosphate, 1,3-diphenylguanidine, and 1,3-di-o-tolylguanidine were reported in landfill leachate for the first time.

Spatial anaylsis revealed that around 55% of detected CECs were found in all locations, suggesting these chemicals stem from widespread usage rather than localized activities. A core set of 34 CECs was detected in the treated leachate of all landfills, indicating that the current treatment technologies are largely insufficient at removing those CECs. PPCPs demonstrated higher site-specific variation, likely linked to the acceptance of sewage sludge at certain landfills.

Temporal monitoring presented moderate seasonal fluctuation. Around 66% of the detected CECs, particularly PFASs and ICs, were present in high frequency across all seasons, underscoring their environmental persistence and the continuous risk they pose to recipient ecosystems. Winter exhibited the highest and summer showed the lowest number of detected CECs. Precipitation, temperature, sunlight duration, and operational factors can possibly explain the temporal variation.

This study underscores that landfill leachates are significant sources of diverse CECs. The consistent presence of a wide array of contaminants across all sites, regardless of treatment, highlights a critical need for advanced monitoring and the development of removal technologies. The spatio-temporal snapshots provided serve as a vital reference for environmental risk assessment in Nordic regions.

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3.08.P - Integrated Approaches in Ecological and Human Health Risk Assessment (APAC Focus)

3.08.P–We098 Guidance on Risk Assessment of Combined Exposure to Multiple Chemicals in the Environment

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Under the conventional risk assessment (RA) practices for regulatory objectives, such as identifying high-priority chemicals, developing guidance values or selecting candidates for refined assessment, chemical-by-chemical RAs have been conducted without explicit consideration on combined exposure to multiple chemicals. It may have been underestimating risks caused by substances in the environment.

Ministry of the Environment, Japan has compiled the first version of “Guidance on Risk Assessment of

Combined Exposure to Multiple Chemicals in the Environment" in Spring 2026. Referring to OECD document "Considerations for Assessing the Risks of Combined Exposure to Multiple Chemicals", dose additivity within target group of chemicals with structural/toxicological similarities has been adopted as a default assumption. Considering the different phases of the regulatory RA, a tiered approach (Levels 0-3) to be flexibly applied to the existing RA practices has been developed by modifying the tiered framework for RA of combined exposure to multiple chemicals by WHO/IPCS. A complementary guidance on Level 2 ecotoxicological hazard assessment as well as several case studies on RA of combined exposure to certain groups of chemicals are under development.
Outlines of the Guidance, its potential implications for existing regulatory RA practices and prospects of relevant supporting materials will be discussed at the conference.

3.08.P–We099 Multi-stressor Influences under a Changing Climate in Tropical Ephemeral Systems

Shelley Templeman[1] and Chris Williams[1] (1)TropWATER, James Cook University

Anthropogenic climate change is increasing hydrological irregularity in tropical ephemeral systems in the dry tropics. These systems, although naturally adapted to seasonal extremes, are now experiencing greater instability with more severe floods interspersed with prolonged dry phases and greater unpredictable flow timing. Such changes are disrupting the unique ecological stability of these systems by exceeding historical disturbance thresholds, reducing recovery time, and degrading key refugia such as persistent pools and hyporheic zones. These effects can be seen in both the aquatic systems, adjacent riparian communities and often more widely into the adjacent terrestrial systems.

Superimposing chemical and physical stressors on these systems under a changing climate has the potential to further disrupt ecological resilience and potentially drive ecological change to simpler less diverse ecologies with more rapid encroachment of pests and weeds into these ecosystems. This presentation will review outcomes from a range of ecological assessments across the dry tropics in Northern Australia over the last 15 years. It will outline some of the challenges associated with establishing and understanding the baseline conditions in these ephemeral systems. It will also identify where potential increased pressures from a mix of natural and anthropogenic stressors on these environments have greater potential to drive shifts in community structures. The findings will provide some insight into the current resilience and vulnerabilities identified across these systems. Forward risk from increased climate instability will also be discussed.

3.08.P–We100 Risk characterisation and source identification of mercury in migratory shorebirds in a subtropical wetland

Along with habitat destruction and land use changes, chemical pollution has been widely considered as a contributing factor to the global decline in population of migratory shorebirds. A recent study in East Asia showed that feathers of migratory shorebirds can contain elevated levels of mercury (Hg), particularly those caught at southern China coastal zone in Mai Po Nature Reserve (MPNR) in Hong Kong. In this study, breast feather and blood samples from migratory shorebirds, along with other environmental samples (e.g. biota, and sediment) were collected from various habitats within MPNR and the nearby habitats. Analysis of Hg on 318 bird feather samples revealed that slightly less than half of the sampled birds (~46 %) exceeded the toxicity threshold, with 8.4 % of birds deemed to have moderate risk, 0.8 % to have high risk and 0.4 % to have severe risk. Stable carbon and nitrogen analyses on a subset of feather samples identified that these birds feed in vastly different habitats (freshwater vs. marine) and occupied different trophic levels. Selenium, a potential antagonist against Hg toxicity, did not show elevated levels in bird feathers (n = 86). The findings showed that Hg pollution pose a potential risk to the shorebirds in

the region, albeit to a lesser extent due to the co-occurrence and antagonistic nature of Se

3.08.P–We101 A Framework for Environmentally Realistic Risk Assessment of Sunscreen UV Filters in Japanese Subtropical Waters

Rie Tai[1], Hiroyuki Mano[1] and Wataru Naito[1] (1)National Institute of Advanced Industrial Science and Technology (AIST)

Ultraviolet (UV) filters are indispensable components of sunscreens and other personal care products, as they protect human skin from solar radiation. After use, these compounds enter coastal waters either indirectly via domestic wastewater or directly during recreational activities. The global growth in UV filter production and consumption has intensified concerns about their ecological effects, particularly on coral reefs. Japanese subtropical waters, linked to the Coral Triangle through the Kuroshio Current, may, therefore, face regulatory scrutiny comparable to that emerging elsewhere; however, ecotoxicity testing and risk assessment tailored to Japanese reef ecosystems remain limited.
This study aims to evaluate the risks that representative UV scattering and absorbing agents pose to coral growth and reef sustainability under environmentally realistic conditions. First, chronic toxicity protocols will be established for native coral species such as Acropora digitifera and used to examine the effects of priority UV filters. Concurrent field sampling will determine ambient concentrations of target compounds in reef waters. In the second phase, exposure models will integrate effect thresholds with predicted discharge scenarios to assess the efficacy of proposed risk-mitigation measures.
The presentation will outline the overall study design, describe the newly developed test protocol for A. digitifera, and summarize preliminary toxicity findings for selected UV filter ingredients.

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3.08.P–We102 Comparative Analysis of Environmental Registration Requirements for Pesticides and Consumer Products Across Japan, Singapore, the United States, and the European Union

Aileen Maldonado[1] (1)UPL Limited

Environmental registration requirements for pesticides and consumer products vary substantially across jurisdictions, reflecting differences in regulatory philosophy, scientific tradition, and risk tolerance. A formulation cleared for market in one country may require additional ecotoxicity testing, exposure modeling, or reformulation to meet the data expectations of another. These divergences carry real consequences for product availability, environmental protection, and the global movement of chemical goods, yet they are often described in isolation rather than in direct comparison.
This work presents a comparative analysis of the environmental registration frameworks governing pesticides and selected consumer products across four jurisdictions: Japan, Singapore, the United States, and the European Union. The consumer product scope is intentionally focused on categories that frequently cross the regulatory boundary between “pesticide” and “consumer good” — household insecticides, cosmetics, and cleaning products including antimicrobial formulations — where classification itself drives substantially different submission pathways.
The analysis examines the governing legislation and competent authorities in each jurisdiction; the environmental data packages required for submission, including ecotoxicity endpoints, environmental fate and persistence studies, and exposure assessment approaches; the review process, including timelines, the use of risk-based versus hazard-based decision frameworks, and provisions for data waivers or read-across; and post-approval obligations such as labeling, re-registration intervals, and post-market

surveillance.
Pesticides and consumer products occupy distinct regulatory spaces shaped by the conditions under which each is used, the populations and environmental compartments they reach, and the historical development of the laws that govern them. Pesticides are generally subject to more intensive pre-market environmental scrutiny owing to their intended biological activity and direct release into the environment, while consumer products are more often assessed through frameworks emphasizing human exposure, with environmental considerations addressed through downstream or ingredient-level controls. Examining these two classes side by side across jurisdictions offers a useful lens for understanding how scientific evidence, regulatory structure, and environmental protection objectives come together in practice.

3.08.P–We103 Antioxidant and Behavioral Responses to Antimony Exposure in the Brackish Water Flea Diaphanosoma celebensis

Chaerin Park[1], Sang-Hyun Cho[1] and Je-Won Yoo[1] (1)Sangmyung University

Antimony (Sb) is a metalloid widely used in various industrial applications, including flame retardants, alloys, glass refining, plastic catalysts, and semiconductors. These anthropogenic activities have led to a rapid increase in Sb concentrations in the environment. Once released, Sb can be transported into marine ecosystems via rainfall and surface runoff, with aquatic environments ultimately acting as sinks for these contaminants. Nevertheless, the toxic effects of Sb on marine organisms remain poorly understood. Therefore, this study aimed to evaluate the toxicity of two Sb compounds, antimony trichloride ($SbCl_3$) and antimony pentachloride ($SbCl_5$), in the brackish water flea Diaphanosoma celebensis. We assessed the physiological effects of Sb exposure on survival and reproduction in D. celebensis. In addition, antioxidant responses and neurotoxicity were evaluated at both molecular and organismal levels using behavioral assays, gene expression analysis, and enzyme activity assays. In acute toxicity tests, both Sb compounds induced concentration-dependent mortality, with $SbCl_5$ exhibiting greater toxicity than $SbCl_3$. The 48 h LC_{50} values of $SbCl_3$ and $SbCl_5$ were 1.594 (1.339–1.896) mg/L and 0.311 (0.273–0.399) mg/L, respectively. Chronic exposure did not cause significant changes in reproduction. However, behavioral assays revealed an expansion of the swimming range with increasing exposure concentrations, particularly in the $SbCl_5$-exposed groups. At the molecular level, significant downregulation of dopamine- and GABA-related genes was observed, accompanied by significant alterations in acetylcholinesterase (AChE) activity. The antioxidant system was also significantly modulated, especially through increased GST expression and GST activity. Overall, our findings demonstrate that Sb can induce toxic effects on the antioxidant and nervous systems of marine zooplankton. This study provides important insights into the toxic mechanisms of Sb in marine organisms.

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5.01.P - Application of Novel Approach Methodologies (NAMs) to Improve Risk Assessment and Management of Contaminants of Emerging Concern (CEC)

5.01.P–Tu094 An Interdisciplinary Framework for Comparative Antimicrobial Efficacy and Environmental Risk Assessment of Antibiotics Integrating Human and Environmental Health: A Case Study From Patient to River

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Pharmaceutical residues in freshwater environments are a global concern. In response, the European Union funded project TransPharm (https://transforming-pharma.eu/) follows the 'Benign by Design' concept to develop novel fluoroquinolone (FQ) antibiotics to mitigate the environmental persistence of traditional FQs. This study introduces an interdisciplinary framework for comparative environmental risk assessment (ERA), applied to a new FQ derivative, ciprofloxacin-hemi (CIP-hemi), in comparison to its conventional counterpart, ciprofloxacin (CIP). This framework integrates multiple dimensions: antibiotic efficacy, human pharmacokinetics, environmental degradability, and ecotoxicity to non-target organisms. By combining experimental data from microbial assays, in vitro safety tests, and ecological toxicity studies, with in silico p hysiologically based pharmacokinetic (PBPK) modelling, the framework aims to assess trade-offs between human health need (i.e. therapeutic efficacy) and environmental protection (i.e. risk to freshwater ecosystems).
Using this framework, we show that the expected environmental risk to aquatic ecosystems (RQeco) caused by CIP-hemi exceeds that of CIP in most scenarios when the two antibiotics reach equivalent efficacy levels. Although CIP-hemi degrades faster than CIP through hydrolysis in human urine, as well as lower ecotoxicity to sensitive non-target organism Microcystis aeruginosa, the minimum inhibitory concentrations (MICs) of CIP-hemi is 17-71 times higher than those of CIP for clinically relevant pathogens. As a result, higher doses of CIP-hemi are required to achieve equivalent therapeutic outcomes, making the RQeco of CIP-hemi surpassing that of CIP. Only under highly specific conditions: intravenous administration at clinically unrealistic high doses, CIP-hemi shows the potential for lower risk than CIP regarding the spread of antimicrobial resistance (RQMIC).
Our study indicates that prioritizing degradability alone is not sufficient in designing environmentally safe and sustainable pharmaceuticals. Instead, the interdisciplinary approach developed in this study is essential, which can offer a more robust basis for identifying antibiotic derivatives that are both clinically effective and environmentally responsible.

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5.01.P–Tu095 Target sequencing of environmental RNA enables in situ assessment of stress responses: a case study of Japanese medaka

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Freshwater ecosystems are under increasing pressure from human activities, creating an urgent need for monitoring tools that can assess not only biodiversity but also the physiological status of aquatic organisms. Environmental RNA (eRNA) has attracted attention as a complementary approach to environmental DNA because it may provide more recent and physiologically informative signals of organismal condition. However, comprehensive transcriptomic analysis of extra-organismal RNA in field settings remains technically challenging, because eRNA is typically present at low concentrations, degraded, and mixed with abundant RNA derived from non-target organisms.

In this study, we developed a targeted sequencing approach for non-invasive transcriptomic profiling of Japanese medaka (Oryzias latipes) eRNA in water using a custom AmpliSeq panel targeting 1,687 genes associated with major biological pathways and toxicologically relevant processes. We applied the AmpliSeq panel to medaka-derived eRNA collected from laboratory water and from a field waterway at six different time points at the National Institute for Environmental Studies, Japan.
AmpliSeq successfully detected medaka transcripts in both lab and field eRNA and achieved near-saturation of gene detection, indicating sufficient depth for reliable expression quantification. In field eRNA samples, 1,044 of 1,687 target genes were detected. Gene detection was highest in winter (December and February), when more than 850 genes were detected, and lower in spring and summer. Temporal variation in expression profiles were also observed across seasons. Of the 1,044 genes, 255 were consistently detected across all sampling periods. We found that heat responsive genes, such as hsp90b1 and id1, showed seasonal trends consistent with established temperature-response patterns reported in the literature.
These results demonstrate that targeted AmpliSeq can provide robust transcriptomic profiling of extra-organismal RNA in water and can extend eRNA analysis beyond simple detection toward physiological assessment. This approach offers a practical framework for non-invasive monitoring of freshwater organisms in both experimental and natural environments.

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5.01.P–Tu096 MINTOX: A Computational Framework for Early-Stage Assessment of Joint Toxicity in Binary Nanoparticle-Ion Mixtures

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Innovative advanced materials often act as multicomponent systems, so their environmental hazard cannot be inferred reliably from single-substance tests alone. A key challenge is predicting joint toxicity when the effective contribution of each component within a binary mixture is unknown. Here we present mintox, a computational framework for early-stage assessment of binary nanoparticle-ion mixtures that combines dose-response reconstruction with multiple mixture-toxicity indices. The approach uses available mixture composition and effect data to derive component-specific dose-response curves, estimate the concentrations of individual components contributing to mixture EC50, and then calculate a set of toxicity indexes (Sum of Toxic Unit, Additivity Index, Mixture Toxicity Index, Model Deviation Ratio) to classify additivity, synergism, or antagonism. We demonstrated the framework on literature data for 18 mixtures composed of TiO2, ZnO, and Fe3O4 nanoparticles combined with Cu2+, Ag+, or Zn2+, using Daphnia magna acute toxicity data. Across the analyzed set, antagonism was the dominant interaction pattern, whereas synergy was observed for selected systems, particularly TiO2-Ag+ and ZnO-Ag+. Agreement among indices showed that classical concentration-addition based metrics frequently converged, while MDR provided complementary sensitivity to deviations from additivity. These results indicate that mintox can support safe-and-sustainable-by-design decisions by identifying mixture combinations that may mitigate toxicity and flagging formulations that warrant redesign because of synergistic effects. The framework provides a practical in silico screening tool for prioritizing safer innovative materials before synthesis or market introduction.

5.01.P–Tu097 Scientifically Grounded and Mechanistically Anchored in silico NAMs in Practice: From Evidence Generation to Dissemination

Tomasz Puzyn[1] (1)University of Gdansk

New Approach Methodologies (NAMs) are rapidly expanding, offering alternatives to traditional toxicity testing. However, despite their growth, the identification, validation, and regulatory uptake of scientifically credible NAMs remain limited. This work addresses the need to develop mechanistically anchored in silico NAMs that support regulatory decision-making, while also enabling their effective dissemination through an accessible and interoperable digital platform. A modeling framework is developed that integrates physicochemical properties of nanomaterials with transcriptomic responses anchored in Adverse Outcome Pathways (AOPs). This approach shifts from traditional phenotype-based Nano-QSAR models toward models describing early key events (KEs) in toxicity pathways, thereby improving biological relevance and mechanistic interpretability. Transcriptomic perturbations linked to KEs from established AOPs (e.g., lung fibrosis and cardiovascular toxicity pathways such as AOP33 and AOP237) are used as modeling endpoints. This AOP-anchored strategy strengthens the causal linkage between molecular-level changes and adverse outcomes at higher levels of biological organization. The results demonstrate that integrating transcriptomics with AOP-informed modeling enhances mechanistic interpretability and supports the development of scientifically robust in silico NAMs. Such models provide biologically meaningful predictors and increase confidence in their application for human hazard assessment. In addition, to facilitate transparency, comparability, and uptake, the developed methods are implemented within available platforms, enabling access to state-of-the-art knowledge on diverse NAMs, thereby facilitating their integration into regulatory workflows. Advancing NAM-based risk assessment requires prioritizing the development of mechanistically grounded methods, complemented by digital infrastructures that enable their dissemination and practical implementation. This combined approach supports the transition of NAMs from scientific innovation to regulatory application, improving the transparency and reliability of chemical and material safety assessment.

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5.01.P–Tu098 Direct Toxicity Estimation of Unknowns Based on GC-MS Nontarget Analytical Signals

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In recent years, nontarget analysis based on GC- or LC-MS has been increasingly applied in environmental studies, enabling the detection of thousands of chemical-derived peaks from a single sample. With these advances, risk assessment of complex chemical mixtures is expected to become feasible. However, most detected peaks remain structurally unknown, awaiting future elucidation. Although various chemicals potentially affecting humans and ecosystems can be detected, substantial knowledge is required to understand the characterization and understand the magnitude of the risks they pose. The accumulation of such knowledge takes considerable time and effort even for a limited number of chemicals. Nevertheless, the continual emergence of new substances, together with improved detection capabilities, further increases the number of compounds requiring evaluation, thereby hindering conventional risk assessment. In this study, we propose a distinct approach that leverages data from nontarget analysis to estimate environmental fate-related parameters and toxicity-relevant properties without structural identification. Analytical signals (i.e., retention time and mass spectrum) obtained for each peak by GC-MS nontarget analysis are considered to reflect intrinsic chemical structure. Based on structure-activity relationships, we investigated whether such information can be used to estimate

toxicity-relevant properties. Approx. 68,000 compound data were collected and their GC-MS retention times and mass spectra were used as inputs, while toxicity data, including LC50 for fish and EC50 for algae, were collected as target values. Although the ECOTOX database contains over 60,000 toxicity records for Danio rerio, only about 100 compounds were available for the GC-MS data, which is insufficient for machine learning models. Therefore, despite being based on in vitro assay, the ToxCast was used due to its broader compound coverage. For assays associated with marine organism toxicity, approx. 1,000 compound data were available for endpoints such as estrogen receptor activity and androgen receptor antagonism, and high predictive performance was demonstrated with XGBoost. In contrast, predictive performance remained limited for several assays, suggesting insufficient training data. These results indicate that expanding the dataset and exploring a wider range of toxicity markers are key for the broader application of this approach.</p>

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5.01.P–Tu099 Transcriptomic Assay Assesses Hazard of 6PPD-Quinone to Fish Species-At-Risk

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Transcriptomic novel approach methodologies can support the assessment of emerging contaminants by quickly producing hazard data. Hazard data for 6PPD-Quinone, a degradation product of a key constituent of tires and contaminant of emerging concern. Here, we combine early-life stage fish assays and transcriptomic benchmarking to rapidly test the toxicity of 6PPD-Quinone in fish species of interest. Our study included model species, as well as species at risk that are native to Canada. Eleutheroembryos (<24 hours post-hatch) for each species were exposed for 24-hours across 12 concentrations of 6PPD-Quinone. We designed the dose-range to capture mortality and concentrations at which no transcriptomic response was expected. Mortality was noted and surviving eleutheroembryos were pooled (n = 3 per concentration) prior to RNA extraction and sequencing. Sequenced RNA fragments were aligned to a curated fish protein database using Seq2Fun to obtain count tables. Dose-responsive genes were then modelled to obtain a benchmark dose for each of them. Benchmark doses were used to derive the concentration at which significant molecular changes occur, hereafter known as the transcriptomic point-of-departure (tPOD). The first peak of the distribution of logged-transformed benchmark doses was used as the tPOD. Acute 24-hour LC50s were obtained for two species, rainbow trout (Oncorhynchus mykiss; 5.6 µg/L, all concentrations hereafter in nominal) and chinook salmon (Oncorhynchus tshawytscha; 9048 µg/L). tPODs were obtained for four species, rainbow trout (0.00528 µg/L), chinook salmon (34.9 µg/L), zebrafish (Danio rerio; 0.607 µg/L) and copper redhorse (Moxostoma hubbsi; 0.135 µg/L). No tPODs were obtained for Atlantic salmon (Salmo salar), and river redhorse (Moxostoma carinatum). Notably, the tPODs of rainbow trout, zebrafish and copper redhorse are below the concentrations detected in some environments, raising concerns as more tire-wear particles are washed into their habitat. Our study demonstrates that transcriptomic approaches can be combined with early-life stage fish assays to quickly generate hazard data for a variety of fish species, including species-at-risk. With further validation, these data, such as the tPOD for copper redhorse, could become part of the weight-of-evidence for rapid prioritization, and even maybe for the risk assessment, of these emerging contaminants.

5.02.P - Environmental Risk Assessment of Metals in the Asia-Pacific Region

5.02.P–Tu100 Deriving and Implementing an Ecologically Relevant Environmental Quality Standard for Aluminium: The Challenges Remaining.

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The importance of accounting for the bioavailability of aluminium is now well established, with bioavailability-based standards for freshwaters now set for aluminium in both the USA and Canada. The need for an approach for setting scientifically robust site-specific standards for aluminium in UK freshwaters is acknowledged, although differences in the approaches used mean that the existing US and Canadian standards are not suitable. The water quality standards for aluminium in the USA and Canada do not account for differences between algae (or plants) and invertebrates or fish in terms of their sensitivity to aluminium under different water chemistry conditions, due to limitations of the bioavailability models that are currently available. Taking account of the sensitivity of algae and aquatic plants to aluminium within a bioavailability-based water quality standard requires extrapolation of the bioavailability model for algae for the approach to be applicable to most UK surface waters. However, the most sensitive waters do not require extrapolation of the algal bioavailability model. It extrapolation of the bioavailability model for algae is applied then the bioavailability normalisation approach used for the proposed standard for aluminium can be applied to 87% of sites in the UK.
The most sensitive region of the UK to aluminium is the South West due to low pH, low organic matter concentrations, and low water hardness. The reference standard for aluminium in UK freshwaters is 54.1 µg L-1 bioavailable aluminium, expressed as an annual average. It is set for highly sensitive waters and is protective of 99% of UK waters. Bioavailable aluminium is calculated from measured total aluminium concentrations. The maximum achievable ecological quality, expressed as the number of benthic invertebrate taxa, will not be significantly affected when the proposed site-specific standard is met. Based on the analysis of field evidence the proposed standard for aluminium is protective of local benthic invertebrate communities even in the presence of other additional stressors, including other toxic metals. Further development and validation of bioavailability normalisation models and measurements of "bioavailable aluminium" could reduce the uncertainty associated with the approach. Accounting for aluminium bioavailability ensures that sensitive areas can be protected without requiring excessively stringent standards in less sensitive areas.

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5.02.P–Tu101 Comparative Metal Stress Profiling in Freshwater Cladocerans using Relative Oxygen Species and Immobilization Endpoints

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Cadmium and lead are persistent metal contaminants in freshwater ecosystems, where they can cause acute toxicity and cellular stress in aquatic organisms. Conventional ecotoxicological assessments

commonly rely on immobilization-based endpoints, but these responses may not fully capture early sublethal stress before observable toxicity occurs. This study applied a comparative endpoint framework to evaluate metal-specific stress responses in two freshwater cladocerans (i.e., Moina macrocopa and Daphnia magna) exposed to Cd and Pb. Acute immobilization was used to estimate species- and metal-specific EC50 values, while ROS-based assessment was applied as a complementary stress endpoint to compare cellular-level responses across treatments. Preliminary results showed measurable ROS species-specific responses in both species, with Pb generally inducing stronger stress patterns than Cd. In one cladoceran species, Pb exposure produced a marked ROS increase at low treatment levels, while Cd induced a weaker response across the tested range. A similar trend was observed in D. magna, where Pb-related ROS elevation appeared at lower concentrations than Cd. Acute immobilization results also indicated higher toxicity of Pb than Cd, with estimated EC50 values of 0.040 ppm for Pb and 0.639 ppm for Cd in the non-standard cladoceran species. Although additional replication and statistical validation are ongoing, the current findings suggest that Pb may exert stronger acute and cellular stress effects than Cd under the tested conditions. The comparison between cladoceran species further indicates that reliance on a single standard test organism may limit the ecological interpretation of metal toxicity. By integrating ROS-based stress assessment with conventional immobilization endpoints, this study provides a more informative framework for evaluating metal-specific toxicity and species-dependent sensitivity in freshwater ecotoxicological testing.

5.02.P–Tu102 Study on Bioavailability-Based Short-Term Chronic Ecotoxicity of Five Metals and Their Mixtures on Reproduction of Ceriodaphnia dubia

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To assess the ecological risks of metal mixtures at environmentally relevant concentrations, it is essential to predict their effects on aquatic organisms under realistic exposure profiles. For this purpose, ecotoxicity data for individual metals, particularly under long-term and low-concentration conditions (i.e., chronic toxicity), are critically important. In addition, metal toxicity should be evaluated based on bioavailability while accounting for the influence of water quality. Previously, we conducted short-term chronic toxicity tests using Ceriodaphnia dubia for five individual metals as well as for metal mixtures reflecting the composition and concentration ratios observed in Japanese rivers. In those tests, diffusive gradients in thin films (DGT) devices were deployed in 100 mL test solutions for 48 h to measure bioavailable metal concentrations, which were then used to estimate individual metal toxicity and their contributions to the toxicity of the metal mixtures. However, because the test solution volume was insufficient relative to the DGT deployment time, bioavailable metal concentrations may not have been adequately measured under those conditions. Therefore, in the present study, DGT devices were deployed for 48 h in 1 L test solutions under the same environmental conditions as the toxicity tests, across the exposure concentration ranges used for the five metals. Relationships between dissolved metal concentrations at the start of the tests and bioavailable metal concentrations were derived. The results indicated that, at the same initial dissolved metal concentrations, bioavailable metal concentrations measured in 1 L test solutions were higher than those obtained from 100 mL test solutions. This finding suggests that the toxicity of individual metals to C. dubia reproduction may have been overestimated in the previous assessment. In this poster presentation, we will report revised toxicity values for individual metals based on bioavailable concentrations recalculated using the derived relationships, and present a re-evaluated estimation of the contributions of individual metals to the overall toxicity of metal mixtures.

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5.02.P–Tu103 Two Guidance Documents for Point-of-use Management and Ecological Impact Assessment: Toward Sustainable Mine Drainage Management in Japan

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Long-term management of mine drainage remains a critical challenge in Japan, particularly for abandoned and closed mines where treatment may be required for decades or longer. A previous study suggested that treatment requirements may persist at many mines even after more than a century (Iwasaki et al. 2021, STOTEN). Conventional effluent management at mine outlets can impose substantial economic and operational burdens, highlighting the need for more flexible and sustainable management approaches. To address this issue, two national guidance documents were developed and published in Japan in 2022. The Guidance for Point-of-Use Management of Mine Drainage introduces a framework that focuses on ensuring environmental safety at downstream points of water use, rather than relying solely on strict compliance at discharge outlets. The Guidance for Ecological Impact Assessment in Rivers Receiving Mine Drainage provides a stepwise approach for evaluating potential ecological risks associated with mine drainage, combining water quality surveys, biological assessments, and bioassays. In this presentation, we introduce the background, conceptual frameworks, and assessment approaches described in these two guidance documents.

Disclaimer/Disclosure: The guidance documents (in Japanese) introduced are available from the Ministry of Economy, Trade and Industry, Japan:
Guidance for Mine Drainage Management for Point-of-Use Risk Reduction:
https://www.meti.go.jp/policy/safety_security/industrial_safety/sangyo/mine/portal/report/risuiten_guidance1.pdf
Guidance for Ecological Impact Assessments in Rivers Receiving Mine Discharges:
https://www.meti.go.jp/policy/safety_security/industrial_safety/sangyo/mine/portal/report/seitai_guidance1.pdf

5.02.T - Environmental Risk Assessment of Metals in the Asia-Pacific Region

5.02.T01 A New Framework for the Implementation of Bioavailability-based Metal Guideline Values in Australia and New Zealand

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The bioavailability and toxicity of metals in freshwaters is influenced by the water chemistry of the specific water body, including such Toxicity Modifying Factors (TMFs) as pH, hardness ions (calcium and magnesium), and dissolved organic matter. Following recommendations from several workshops of scientists and regulators in Australia and New Zealand, we have developed a new framework for deriving and implementing bioavailability-based default guideline values (DGVs) for copper, nickel and zinc under the Australian and New Zealand Guidelines for Fresh and Marine Water Quality (ANZG 2018). The tiered assessment framework, which builds on similar approaches in Europe, introduces a screening level at Tier 1, where measured dissolved concentrations of copper, nickel and zinc are compared to a high-bioavailability DGV. The high-bioavailability DGV was developed from a probability distribution identifying highly sensitive waters in Australia and New Zealand. If the DGV is exceeded at Tier 1, a metal bioavailability tool is used at Tier 2 to either normalize the metal concentration to represent the

bioavailable fraction or adjust the guideline value for the sample water chemistry, yielding a bioavailability-adjusted guideline value (BAGV). The metal bioavailability tool is an on-line, publicly-available and user-friendly tool that automatically undertakes these computations and also calculates a Hazard Quotient for use in risk assessment. If the sample still fails at Tier 2 (i.e., the bioavailable metal fraction exceeds the DGV or the dissolved metal fraction exceeds the BAGV), then, at Tier 3, multiple lines of evidence can be used to determine the likely risks of an exceedance.
The outputs from the project include: new DGVs and updated technical briefs for copper, nickel and zinc in freshwaters; technical reports describing the process of deriving the high bioavailability DGVs; a guidance document on how to use the tiered approach and tool, including case studies; and training materials and other relevant updates to the ANZG (2018) website.

5.02.T02 Not All Plants Are Equal: The Role of Species Choice in DOM-Mediated Metal Toxicity Mitigation

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Urban streams are among the most valued and most degraded waterways globally, where copper (Cu) and zinc (Zn) concentrations frequently exceed ecological guideline values and can harm aquatic species. Dissolved organic matter (DOM) can reduce metal bioavailability through complexation, but the amount of DOM leached form plant material and its quality vary widely among plant species.

In an MBIE-funded programme led by Earth Sciences NZ, we are testing whether native plant "DOM super producers" can mitigate metal toxicity in urban waters. We have quantified DOM yields, screened leaf leachates for toxicity mitigation, characterised DOM chemistry and metal binding, and measured acute and chronic responses of key taxa across DOM concentration gradients.

Results to date show DOM generally reduces Cu, Zn and Cu–Zn mixture toxicity, but effects vary (and can reverse) with DOM source/composition and test species. Pōhutukawa and Mānuka sourced DOM provided the greatest protection to the native cladoceran, Daphnia thomsoni despite low DOM yields, supporting their potential as culturally relevant components of nature-based metal remediation systems. Conversely, some DOM sources/concentrations increased sensitivity in selected taxa (e.g., microalgae and glochidia), highlighting species-specific risk. DOM–metal binding was rapid (~30 s), with fast uptake at high-affinity sites followed by slower stabilisation as lower-affinity groups are occupied. Across sources, optical indices and acid–base titration metrics indicate aromaticity, molecular weight, and carboxylic/intermediate phenolic group abundance underpin binding and toxicity modification, supporting their use as rapid screening tools.

These datasets are being integrated into a DOM–metal mixture bioavailability model to predict Cu–Zn mixture toxicity across DOM sources and concentrations. Outputs will support targeted mitigation design (e.g., riparian/roadside planting, raingardens, tree pits, infiltration systems, green roofs and constructed wetlands) and improve interpretation of monitoring data. We will summarise model performance and key data gaps, and outline translation into practitioner guidance for selecting and deploying native plants to maximise beneficial DOM production and enable risk assessment and management.

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5.02.T03 The Development and Implementation of a Bioavailability-based Environmental Quality Standard for Uranium under the European Water Framework Directive

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In parts of Europe, including Sweden, natural background concentrations of uranium can exceed the existing Environmental Quality Standard (EQS). It is widely recognised that many biological and chemical factors can influence the behaviour and ecotoxicity of metals, including uranium, in surface freshwaters. Existing uranium EQS do not account for these factors and so lack ecological relevance and can be both under and over protective of aquatic ecosystems.
In line with bioavailability model developments in recent years for regulatory application for other metals, such as copper, nickel, zinc, cobalt, we have developed the first chronic bioavailability model for uranium in freshwaters. The model development is based on the results of long-term toxicity tests with algae, aquatic invertebrates and fish, which have investigated the influence of several toxicity modifying factors including pH, dissolved organic carbon (DOC) and hardness. The model has also been validated from tests on species not used in the development tests, but in the same respective taxa, in natural field-collected waters covering a wide range of water chemistry conditions. All these tests were specifically undertaken for this project as the existing chronic uranium ecotoxicity dataset is relatively limited and did not allow account to be taken of bioavailability.
In Europe, under the Water Framework Directive, national and Europe-wide EQS can be derived. For substances where account can be taken of bioavailability, both ecotoxicological effects data and water chemistry data for the area for which the EQS is being derived (i.e. a country or the whole of Europe). We have derived an EQSbioavailable for uranium for Sweden and for the whole of Europe, using the developed generalised bioavailability model, and water chemistry data from the last fives years for >98,000 samples, from > 38,000 sites, for 32 countries.
In order to ensure the routine regulatory implementation of this approach, a simplified tool has been developed for uranium, that requires inputs of measured uranium, pH, hardness/calcium and dissolved organic carbon for the site under consideration. This approach provides an ecologically relevant metric to assess potential freshwater risks from uranium that can readily and routinely implemented into existing sampling and monitoring schemes, as well as use for site-specific and targeted assessments.

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5.02.T04 Redistribution and Soil–Water–Biota Dynamics of Battery-Derived Metals in a Central California Estuary Following the World's Largest Energy Storage System Fire

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Catastrophic fires at large energy storage systems and industrial facilities are an emerging source of metal contamination at the urban–wildland interface, yet their environmental fate in adjacent coastal environments remains poorly constrained. In January 2025, a large-scale fire at the world's largest battery energy storage (BES) facility in Moss Landing (California) released Ni–Co–Mn-bearing cathode particulates to the adjacent Elkhorn Slough estuary (~25 metric tons). The EMBER (Estuary Monitoring

of Battery Emissions and Residues) collaboration integrates high-resolution soil mapping, tidal water-column time series, and multi-taxa biological monitoring to evaluate the transport, transformation, and uptake of these metals across soil–water–biota compartments.

Marsh soils within several kilometers of the BES exhibited shallow, spatially heterogeneous enrichment of Ni, Co, and Mn (Ni:Co ≈ 2), consistent with a cathode signature, that attenuated within weeks following precipitation and tidal inundation. In contrast, suspended particulate matter (SPM) shows persistent Ni–Co coupling with Ni:Co ratios (~6), distinct from both source material and pre-fire baseline conditions, indicating fractionation during estuarine transport and processing. Biological samples showed varied concentrations across species, with highest concentrations in deposit-feeding and suspension-feeding taxa during early post-fire sampling, followed by declines over subsequent months. Early tissue Ni–Co relationships are consistent with a shared source, while absolute concentrations of Ni fall within the upper range of historical observations.

These results indicate substantial redistribution of fire-derived metals mediated by hydrologic exchange and sediment transport. We propose that metal release from soils is modulated by redox gradients across marsh interiors, ecotones, and tidally flushed channels, producing episodic remobilization and higher availability for biota. While early biological incorporation is likely, longer-term retention and bioaccumulation remain unresolved. This study highlights the importance of multidisciplinary monitoring at high temporal and spatial resolutions following large-scale lithium-ion battery fires in coastal wetlands.

5.02.T05 Practicalities of Sampling and Sample Delivery to Account for Metal Bioavailability in Remote Locations

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The move towards accounting for metal bioavailability is important for managing environmental risks in a consistent manner between different locations, and arguably particularly so for the Asia Pacific with the wide range of geographic and geological settings that exist across the region. However, that can require undertaking trace analyses and sample manipulations that are difficult to undertake in the field, and are unfamiliar to laboratories in the region. Many sampling locations are very remote from any laboratories, and likely more so from laboratories who are able to undertake the required procedures to the limits of reporting and quality assurance required for reliable bioavailability assessments. While we acknowledge that this is a developing field and uptake of the approaches will become more widespread, we will discuss currently appropriate practical considerations and implementation gaps regarding sample hold times, limits of reporting to request from the laboratories, considerations on the logistics and practicalities of in-field sample manipulations, and for some cases, the need for ecotoxicological validation.

5.03.P - From Plastic Leakage and Emission Assessment to Treaty Implementation: Developing and Harmonizing Monitoring Approaches

5.03.P–We106 Development and Harmonization of Analytical Methods for Measuring Small Microplastics in Surface Water and Sediments

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Increasing concern has recently focused on microplastics (MPs) smaller than 100 μm and their impact on organisms and ecosystems. However, variations in sampling and analytical methods among studies hinder regions and media comparisons, leaving many aspects of the current state and accumulation mechanisms

of small MPs unclear.
This study aims to develop a standard operating procedure (SOP) for analytical methods targeting small MPs (20–300 μm) in surface water and sediments, and to verify its accuracy through inter-laboratory comparison tests. The draft SOP outlines methods for sample pre-treatment, polymer identification by instrumental analysis, and quality control. Multiple approaches are presented as “mandatory” and “recommended”, allowing selection based on research facilities and sample conditions. Pre-treatment procedures—including extraction, oxidation, density separation and collection of small MPs candidate particles on filters —are described separately for surface water and sediments. Polymer identification covers imaging and point-based measurements of particles collected on filters, primarily assuming μFTIR but allowing application to other instruments. Methods for particle size and shape measurement are also included. Quality control procedures address blank and recovery tests, working environment requirements and equipment cleaning. In addition, the SOP recommends water and sediment parameters to support method selection and data interpretation.

The inter-laboratory comparison test will be conducted in three phases. Phase 1 will assess analytical agreement and misidentification rates using spike test and blanks from participating institutions. Spiking particles will be prepared by freeze-crushing polypropylene, polyethylene, and polyethylene terephthalate, with a median particle size of 50–100 μm. Phase 2 will use ultrapure water and artificial sediment spiked with these particles to evaluate detection limits and recovery rates across particle sizes and materials while reducing laboratory blanks. Phase 3 will use surface water and sediments collected from semi-enclosed waters to verify intra-laboratory repeatability and inter-laboratory reproducibility. The SOP will then be revised based on the findings of these comparison tests and published together with quality control templates and data reporting forms. The results of the inter-laboratory comparison tests will also be made publicly available.

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5.03.P–We107 Investigation of Reducing Measurement and Analysis Time in μFTIR Analysis of Microplastics in Low Suspended Solids Water, Compliant with ISO 16094-2.

Kazumi Kawahara[1], Kazuki Sobue[1] and Riki Kitano[2] (1)Shimadzu Corporation, (2)Shimadzu Coporation

ISO 16094-2 provides fundamental guidance for the analysis of microplastics (MPs) in waters with low suspended solids, including drinking water, using microscopy combined with vibrational spectroscopy. The standard defines measurement methodologies for particle size determination, particle counting, and polymer identification. In recent years, as regulatory and monitoring frameworks for microplastics in drinking water have expanded internationally, there has been a strong demand for analytical methods that are not only reliable but also suitable for practical implementation.

According to ISO 16094-2, if the number of particles is less than 1000, measurement of the whole filter surface is recommended.; however, such exhaustive measurements substantially increase analysis time. This is a major challenge for samples containing large numbers of particles and for analytical workflows that involve manual operations, to achieve a balance between analytical throughput and completeness.

In this study, an ISO 16094-2–compliant micro–Fourier transform infrared (micro-FTIR) analytical workflow was established, and methods to reduce measurement and data-processing time while maintaining analytical quality were systematically investigated. Microplastics collected on filters were analyzed in accordance with ISO 16094-2 procedures. To suppress increases in analysis time associated

with wide-area measurements, spectral acquisition was omitted in regions where no microplastic candidate particles were detected, thereby reducing unnecessary measurements and improving overall measurement efficiency.
This workflow enables the simultaneous determination of polymer composition, particle size distribution, and particle number. Furthermore, particle mass—an important parameter in toxicological assessment—was also estimated concurrently within a single analytical workflow.

The method proposed here maintains consistency with ISO 16094-2 while substantially improving the measurement and data-analysis efficiency of micro-FTIR–based microplastic analysis. This approach is expected to support reliable monitoring of microplastics in low suspended solids water, including drinking water, and to contribute to the establishment of standardized reporting frameworks for exposure assessment and environmental risk evaluation .

5.03.P–We108 Total organic carbon-based proxy for QuEChERS estimation of microplastic mass in soils

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Total organic carbon (TOC) analysis has emerged as a simple and rapid proxy for quantifying total microplastic (MP) contamination, though its application to soils remains limited. This study proposes a QuEChERS (Quick, Easy, Cheap, Effective, Rugged, Safe) approach to estimate MP mass from carbon content in soils, involving organic matter removal using 6% NaClO, density separation with K2CO3 (1.54 g/mL), and TOC quantification. The method achieved 96.8 ± 3.5% removal of soil organic matter (peat moss) and 90.0 ± 2.0% recovery of common polymers, with minimal carbon loss. The optimized protocol was applied to field soils across different land uses and validated against pyrolysis–gas chromatography/mass spectrometry (Py-GC/MS). MPs accounted for only 0.09–3.54% of total soil organic carbon, with estimated concentrations ranging from 21.8 to 2023.4 ppm (TOC) and 21.3 to 133.9 ppm (PyGC/MS). Both methods showed consistent spatial trends and a strong correlation (R = 0.82). However, TOC may overestimate MP mass in soils enriched with emerging tire-wear particles and/or non-plastic anthropogenic particles (e.g., black carbon). Nonetheless, recent perspectives emphasize assessing pollutant persistence over polymer specificity. In this context, TOC offers a more inclusive measure of persistent anthropogenic particles, supporting broader environmental risk assessments beyond plastics.

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5.03.P–We109 Development of a Continuous Flow Method for the Preparation of Nanoplastic Particles

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In recent years, increasing attention has been directed toward environmental contamination by nanoplastics (NPs, <1 μm). Concerns regarding their toxic effects have grown due to their high propensity for uptake into biological systems. However, a major challenge in NP risk research is the lack of suitable reference materials required for toxicity testing and quantitative analysis. To address this issue,

we previously developed a method for producing impurity-free spherical particles with diameters below 1 μm for five major polymers. In this method, particles are formed by mixing a polymer solution with an organic nonsolvent under appropriate conditions, inducing polymer precipitation. However, because the mixing process was carried out in a single vessel (batch method), the production volume was limited by the container size, and precise control of particle size was difficult. In this study, we introduced a continuous-flow approach to overcome these limitations. Our aim was to enable scalable and stable particle production and to achieve precise control of particle size by adjusting the mixing conditions. We found that particle size can be controlled by adjusting the residence time of the particle dispersion at a given temperature after mixing, by varying the tube length. In the conventional batch method, the average particle sizes were 226 nm for PS and 430 nm for LDPE, and smaller particles could not be obtained. In contrast, the continuous-flow method enabled particle size control over a wide range (49–503 nm for polystyrene and 96–460 nm for low-density polyethylene), including the production of particles smaller than 100 nm. Furthermore, particle size variability was reduced in the continuous-flow method. The developed method enables the production of polyolefin particles smaller than 100 nm. By enabling stable and scalable production of nanoplastic particles, this method is expected to contribute to the establishment of standardized materials and to advance environmental risk research on nanoplastics.

5.03.P–We110 Overview of NITE-CHRIP contribution to chemical management

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The accessibility and transparency of chemical hazard information are essential for effective chemical management in industry, regulatory decision-making, and research activities. NITE Chemical Hazard Risk Information Platform (NITE-CHRIP) is an integrated and reliable database that contains variety of regulatory and hazard-related data and serves an indispensable resource for Japanese industries and regulators involved in chemical management.

This poster presents a comprehensive overview of the functions and information-provision framework of the NITE -CHRIP, a system developed by the National Institute of Technology and Evaluation of Japan. The objective of NITE-CHRIP is to provide a centralized platform that compiles diverse chemical information into a structured and user-friendly system to support decision-making by regulators, industry, and researchers.

The poster presents a comparison of regulatory status using NITE-CHRIP in various countries regarding substances that are currently in the spotlight. NITE-CHRIP places significant emphasis on data traceability, transparency of sources, and regular updates, while providing flexible search, filtering, and comparison functions. Furthermore, NITE-CHRIP integrates data from a wide range of authoritative domestic and international sources, offering a comprehensive array of information on chemical identifiers, hazard and risk assessment information, and regulatory information free of charge. The integrating information from the Asian region, including data from the ASEAN-Japan Chemical Safety Database (AJCSD), has been demonstrated to enhance access to regulatory information in Asian countries by NITE-CHRIP. Additionally, NITE-CHRIP and AJCSD provide hazard classifications and related information in accordance with the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). These features enable users to efficiently obtain and compare hazard information across substances, regardless of their level of expertise. The poster provides an example.

Moreover, NITE is considering the integration of additional information to facilitate chemical management across the life cycle in industry, including active utilization of recycled materials. We welcome your feedback on this matter.

In conclusion, this poster introduces how to utilize comprehensive chemical regulatory information available through NITE-CHRIP.

5.03.P–We111 Are Bioavailability-Based Water Quality Standards Sufficiently Protective of Aquatic Ecosystems?

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The use of single species laboratory tests conducted under highly controlled conditions to derive Environmental Quality Standards (EQS) for the protection of freshwater ecosystems requires a degree of extrapolation to ensure that natural ecosystems are sufficiently protected. Bioavailability models can be used to adjust the level of an EQS to the conditions at a specific site, to ensure that the ecosystem is adequately protected but without requiring excessive overprotection at insensitive sites. This helps to ensure that limited resources can be targeted towards the most sensitive areas. However, uncertainty remains about the protectiveness of a bioavailability-based EQS when applied to real ecosystems containing a multitude of both chemical and physical stressors. Ecological monitoring data can be used to ensure that aquatic communities remain unaffected by the implementation of bioavailability based EQS, and to evaluate the protectiveness of the standards. Datasets of benthic macroinvertebrate communities, and benthic diatom communities, have been combined with chemical monitoring data to facilitate such assessments. These assessments have identified especially sensitive indigenous taxa to some metals, and whether mixtures of metals cause greater levels of effects than an additive assessment of their individual risks indicates. Quantile regression based approaches enable assessments to be performed on datasets where it is impossible to fully account for impacts due to other stressors such as sanitary pollution, eutrophication, agrochemicals, sedimentation, flow conditions, and habitat loss. The approaches used to analyse and interpret the data need to be able to account for the highly variable nature of ecological communities, and the fact that specific species, or even families, may be completely absent from some locations for reasons other than stressors, such as inappropriate habitat conditions. In some cases it is possible to use predictive models of the communities that would be expected to occur under unimpacted, or reference, conditions, although these tools may not be applicable to all situations. This presentation will summarise how these approaches can help inform policy in relation to environmental standards and provide examples of how they have been applied.

5.03.P–We112 Hazard Quotient Screening of Chilean Pesticides in accordance with the New Bee Protection Law

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Chile is introducing a new requirement under the Bee Law to protect pollinators, which calls for advance notice when applying pesticides that are toxic or moderately toxic to bees. This rule aims to improve communication between pesticide applicators and beekeepers, although its effectiveness in lowering risk depends on whether the communication addresses the actual toxicity of the active ingredients in use.

This study developed a theoretical hazard screening for pesticide ingredients listed in Chilean regulations relevant to bee health. The ingredients were divided into two groups: those considered highly dangerous based on criteria from the Food and Agriculture Organization, World Health Organization, and Pesticide Action Network, and those not classified as highly hazardous. For each ingredient, the maximum recommended application rate was combined with the most sensitive measure of honeybee toxicity, using lethal dose values from scientific and regulatory sources. The hazard levels were then categorized using international thresholds to prioritize pollinator risk.

The assessment identified a subset of authorized insecticides of particular concern, especially those classified as highly hazardous, with low lethal doses to bees and high field application rates. These remained in the highest risk category even after conservative adjustments to application rates. Conversely, many fungicides and herbicides showed lower levels of concern, though there are gaps in data on long-

term effects, sublethal impacts, formulations, and native pollinators.

The findings suggest that while Chile's Bee Law improves risk communication around pesticides, it doesn't fully eliminate the danger posed by the most hazardous chemicals. Advance notice helps reduce direct exposure if beekeepers receive prompt, reliable information, but it doesn't change the inherent toxicity of ingredients with extreme acute effects on bees. To better protect pollinators, the law could be strengthened with risk-based prioritization, stricter use conditions, seasonal restrictions, buffer zones, clearer label instructions, incentives for safer alternatives, and ongoing monitoring.

Overall, this work offers a clear tool to support science-based efforts to protect pollinators in Chile. It also provides a practical framework for regulators to identify which active ingredients need urgent review, mitigation, or replacement.

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5.03.P–We104 Discharge characteristics of tire and road wear particles derived from highways with stormwater drainage facilities

Kanako Yamamoto[1], Kosuke Tanaka[1] and Go Suzuki[1] (1)National Institute for Environmental Studies (NIES)

Tire and road wear particles (TRWP) are partially discharged into rivers and oceans with stormwater runoff. Additionally, 6PPD-quinone (6PPD-Q), an oxidation product of the tire antioxidant 6PPD (N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylenediamine), has been reported to exhibit toxicity to certain fish species. Consequently, there is growing need to evaluate TRWP emissions from highways, and understanding TRWP behavior in stormwater drainage facilities is essential for refining emission inventories and risk management strategies. In this study, the influence of catchment basins on these substance behaviors during transport from highways to the outfall was investigated through the pollutant transport simulation, using Storm Water Management Model (SWMM).

The model domain comprised a 700-m elevated bridge section of the Matsuyama Expressway. TRWP derived from the road surface was washed into 61 catchment basins installed beneath bridge piers and was subsequently transported to the model terminus (hereafter referred to as "outfall") through a single open drainage channel. To conduct scenario analysis based on the presence or absence of catchment basins. Simulation was conducted with a total duration of 226 hours, including two rainfall events and preceding and succeeding dry periods. For pollutant simulation, the dry-weather accumulation rate constant for TRWP was set to 0.029 kg/ha/day. Leaching and degradation equations for 6PPD derived from TRWP were adopted from the previous study.

Under the catchment basin installation scenario, TRWP mass balance on the model area indicated that 38% remained on the road surface, 0.0047% was retained within catchment basins, and 62% reached the outfall. When catchment basins were present, peak 6PPD concentrations at the outfall were 1.3-fold and 1.9-fold higher for the two rainfall events, respectively, compared to the no-basin scenario. Mass balance analysis for 6PPD showed that with catchment basins installed, the pollutant load discharged from the outfall was approximately 1.5-fold greater.

These findings suggest that the installation of catchment basins may affect the transport behavior of TRWP and additive-related substances through the leaching of 6PPD during TRWP retention. Therefore, in the development of emission inventories and risk management frameworks for TRWP-derived substances, it is necessary to account for the fate and behavior of these substances within stormwater drainage facilities.

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5.03.P–We105 Estimating Microplastic Dynamics in Urban Tidal Rivers of Osaka City, Japan, Based on Field Investigations

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Urban rivers are an important pathway for transporting microplastics (MPs) from urban areas to coastal seas; however, the presence of tidal forcing makes it relatively difficult to quantify MPs dynamics in tidal rivers. This study estimated MPs dynamics in rivers in Osaka City, Japan, based on field surveys conducted in FY2023–FY2025 (Japanese fiscal years). Seasonal and interannual variability was assessed at a midstream site on the Dainineya River, where sampling was conducted four times per year. Additional surveys were carried out at upstream sites with no or weaker tidal influence (the Hirano River and an upstream site on the Dainineya River) and at downstream sites (the Ajigawa and Shirinashi rivers). Surface-water MPs were collected primarily using a Natural Water Flow Method; Towing Method was applied when flow velocity was low. The target MPs size class was 1–5 mm. At the midstream Dainineya site, MPs number density ranged from 4.05 to 59.9 items/m³ (mean: 16.0 ± 17.2 items/m³). High values were observed in summer FY2023 and spring FY2024, whereas FY2025 remained relatively stable (8.76–14.2 items/m³), indicating no consistent seasonal pattern. Across Osaka City, mean MPs number density increased downstream, from 5.12 items/m³ at upstream sites to 15.9 items/m³ at the midstream site, and to 281 items/m³ at downstream sites (range: 69.8–492 items/m³). At the Ajigawa site, a particularly high density (492 items/m³) observed on a clear summer day suggests upstream intrusion of MPs-rich coastal water from Osaka Bay.

At the Dainineya River, polymer composition was dominated by polyethylene (PE) and polypropylene (PP), with PP being slightly more abundant. Fragments were the most common morphology. In the mass-based assessment for FY2025, mass was estimated by converting projected area to mass using a conversion equation previously published for Japanese rivers; the results indicated that fragment-shaped PE accounted for approximately 28% of the total MPs mass. In addition, PP “fiber-resin” particles (fiber-like, resin-pellet–like particles) also contributed about 28% of the total mass, suggesting that they should be prioritized for mitigation.

Overall, MPs dynamics in Osaka City were considered to be strongly influenced not only by inputs from urban areas but also by tidal processes, including upstream intrusion from Osaka Bay and temporary retention/accumulation within the river system.

3. Ecological and Human Health Risk Assessment

3.01.P - Advances in Effect-Directed Analysis for Chemical Mixture Risk Assessment

3.01.P–Tu088 A Spectral Imaging-Based Machine Learning Approach for the Rapid Detection of Heavy Metals and Inorganic Disinfection By-Products in Drinking Water

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Drinking water safety is essential to human health and daily life. As water contamination becomes increasingly complex, certain contaminants can pose potential health risks even at low concentrations.

This underscores the need for sensitive, selective, and faster detection methods for environmental monitoring. However, classical analytical methods often follow a pretreatment-before-analysis workflow and rely on large-scale instruments, which can be costly. This limits the detection speed and analytical throughput for on-site applications. In this study, we developed a rapid multi-indicator detection method for heavy metals and disinfection by-products in drinking water by integrating long-optical-path spectral imaging with machine learning. The method targets low-concentration, multi-component contaminants and uses an extended optical path to enhance the optical response generated by colorimetric reactions between combined chemical probes and contaminants in complex sample matrices. A spectral imaging system was used to capture changes in optical features and fingerprint information of the target contaminants, enabling high-throughput acquisition of spectral image data from water samples. Deep convolutional neural network (CNN) models (ResNet-50, Inception V1, and SqueezeNet V1.1) were then developed to establish and analyze relationships between image features and contaminant concentrations. This enabled rapid detection and concentration prediction of heavy metals (Hg^{2+}, As, Cr(VI), Pb^{2+}, Cu^{2+}, and Al^{3+}), as well as inorganic disinfection by-products (ClO_2^-, ClO_3^-, ClO_4^-, and BrO_3^-) in drinking water. The tested concentration range was 1–250 µg/L, with the lowest detectable concentrations below drinking water guideline values. The results showed that the developed CNN models effectively learned feature information from the spectral images and accurately predicted the concentrations of multiple drinking water contaminants, with R^2 values reaching 0.8–0.9. The proposed method does not require complex sample pretreatment and has low detection costs. It was able to acquire data, learn and analyze the image feature information in a short time, demonstrating promising potential for rapid detection. This study provides a new technical perspective for the rapid detection of multiple trace inorganic contaminants in complex water matrices and offers insights into drinking water quality monitoring and digital water quality management.

3.01.T - Advances in Effect-Directed Analysis for Chemical Mixture Risk Assessment

3.01.T01 High Throughput Effect-Directed Analysis for Toxicant Identification in the Environment-Food-Human Continuum

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In modern daily life, everyone is exposed to a multitude of chemicals embedded in our living environment, food, air, the products we use, etc. To investigate the presence and distribution of chemicals in the natural and urban environment, and also in wildlife and humans, there is a need to develop methods to assess the identity of chemicals.

The development and application of a huge variety of approaches using high resolution mass spectrometry for chemical identification has significantly improved the knowledge on the environmental and human exposome. Although major steps towards improved identification success rate are being taken, the evaluation of the wealth of HRMS data leading to a concrete toxicant identification is still a bottleneck.

At the Vrije Universiteit, Amsterdam, we use High Throughput Effect-Directed Analysis (HT-EDA) in which suspect and nontarget screening is combined with in vitro effect-based testing, for which samples are fractionated with high resolution into multi-well plates. In the last decade, we have worked towards high resolution fractionation using an in-house developed instrument, the FractioMate, in combination with advanced workflows to achieve an easier, straightforward evaluation of the HRMS data ultimately resulting in a higher identification success rate. Effect-based testing serves as a prioritization tool to focus the identification efforts in the HRMS chromatograms on those time intervals (of several seconds wide)

where a response is being observed in the in vitro bioassay used.
To expand the scope of our work, we have developed several in vitro tools of varying complexity, ranging from simple protein binding assays to cell-based, to facilitate the identification of several classes of pharmaceuticals and their transformation products, focusing on water quality.
In recent years, we have used HT-EDA for a variety of other matrices. With the increasingly widespread acceptance of the use of in vitro bioassays, for example in the European Water Framework Directive, we have broadened the scope of our work to cover the environment-food-human continuum. Within the EU Horizon2020 Panoramix project, we have developed EDA strategies for (breast)milk and (umbilical cord) blood, based on the idea that - besides unravelling the identity of chemical mixtures - rapid effect-based tests could add a new dimension to traditional human biomonitoring.

3.01.T02 Mechanism-supported Deep Learning Frameworks to Identify Key Toxicants in Environmental Mixtures Responsible for Transcriptomic Perturbations in Cetaceans In Vitro

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Marine mammals such as the Indo-Pacific humpback dolphin (Sousa chinensis), inhabiting increasingly urbanized coastal environments are continuously exposed to complex mixtures of environmental pollutants. Unlike single-compound exposures, such mixtures can induce multiple interconnected biological responses, making it inherently difficult to identify key toxicants and elucidate their underlying mechanisms. Conventional toxicological approaches, which rely on targeted chemical analyses and predefined biological endpoints, are often insufficient to detect unknown contaminants or capture subtle perturbations at the molecular pathway level. To address this challenge, an integrative analytical framework is proposed to link non-target chemical exposures with pathway-level biological responses in cetacean cells through a data-driven integration strategy. To capture the complex composition of environmental mixtures that may drive biological perturbations, high-resolution mass spectrometry (HRMS) is used to generate non-target chemical feature profiles from seawater. In parallel, transcriptomic data are summarized at the pathway level to represent biological responses, providing a unified basis for subsequent association analysis. Building upon these data, random forest models are applied to establish associations between chemical features and pathway perturbations, and model interpretability is achieved using SHapley Additive exPlanations (SHAP) to identify candidate chemicals contributing to biological responses. These chemicals are further integrated with knowledge-based and structure-based toxicological evidence to strengthen mechanistic interpretation. Preliminary analyses suggest that a limited subset of chemical features may contribute disproportionately to pathway-level perturbations, indicating non-uniform contribution patterns in complex environmental mixtures. By integrating non-target exposomics, machine learning, and mechanistic evidence, this study advances mixture toxicity assessment and provides insights for environmental risk evaluation and marine ecosystem protection.

3.01.T03 Effect-Directed Identification of Primary Toxicants Causing Chronic Effects on Algae and Daphnids in Environmental Waters

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The increasing presence of new chemical substances that are neither evaluated nor regulated under current chemical management systems may pose adverse effects on ecosystems. To elucidate the actual impacts of chemical substances on aquatic organisms and to identify the primary causative chemicals, effect-based monitoring (EBM) using bioassays and effect-directed analysis (EDA), which integrates bioassays with chemical analysis, are required. Although numerous studies have demonstrated that EDA

using in vitro assays targeting specific mode of actions (MOAs) is an effective approach, the application of EDA using in vivo assays remains challenging.
In this study, we conducted a case study of EDA employing short-term chronic toxicity test with alga and daphnid, combined with multiple-component chemical analysis using Automated Identification and Quantification System (AIQS) with GC/MS and LC-QTof/MS, to develop an EDA methodology tailored to environmental waters in Japan. Through EBM using Raphidocelis subcapitata algal growth inhibition test and Ceriodaphnis dubia reproduction test, sampling sites were selected where solid-phase extracts exhibited toxic effects on alga and daphnid, respectively. Sequential elution of solid phase extraction cartridges using organic solvent of different polarities, followed by toxicity testing, revealed that 100% methanol fraction (F3) exerted the most significant effects on each organism among the five fractions. Multiple-component chemical analysis using AIQS identified the pesticide metabolite carbofuran as the primary toxicant for daphnid, and exposure to a carbofuran-spiked sample induced effects comparable to those observed in the corresponding environmental sample. The herbicide thiobencarb was also identified by AIQS analysis as a candidate toxicant for alga; however, its predicted contribution to the observed toxicity in the sample was low. Furthermore, suspect analysis of each fraction detected 11 F3-specific chemical substances, and one of these—a bisphenol S (BPS) substitute—was identified as a potential toxicant based on the toxicity prediction tool and actual toxicity tests.
This study demonstrated the practical applicability of EDA for assessing chronic effects with unknown MOA by incorporating suspect analysis and toxicity databases, including toxicity prediction tools.

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3.01.T04 The application of 3D printing for Single-cell ICP-MS analysis

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3D printing technology, characterized by high design freedom and the ability to achieve integrated forming of complex structures, has been widely applied in scientific research. Over the past decade, our team has focused on the application of 3D printing technology in the development of customized environmental analysis devices, particularly for single-cell inductively coupled plasma-mass spectrometry (ICP-MS) analysis.
We established a novel development paradigm for analytical devices based on “simulation-assisted design—precise 3D printing—rapid experimental validation.” A customized ICP-MS sampling interface was developed and 3D-printed for the time-resolved analysis (TRA) of heterogeneous samples, such as single particles and single cells. Through the integration of a microfluidic droplet separation module and an optimized nebulizer and spray chamber design, sample transport efficiency was improved from 60%, significantly enhancing the accuracy of heterogeneous sample analysis.[1] Additionally, we further developed a 3D-printed droplet microfluidic platform ahead of the ICP-MS sample introduction system to investigate the uptake behavior of single algal cells exposed to Cd and Eu-containing polystyrene (PS) NPs. The 3D-printed droplet platform offers high-throughput single-cell encapsulation, minimizes cross-contamination and enhances sensitivity for multielement single-cell analysis. Our results revealed that coexposure increased both the proportion of Eu/Cd-containing cells and the uptaken Eu/Cd content, which resulted in synergistic effects, including enhanced growth inhibition, photosynthetic impairment, membrane damage, and increased secretion of extracellular polymers.[2]
These results advance the application of 3D printing in environmental analysis, promoting the innovation of customized and miniaturized devices for MS analysis.

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3.01.T05 Knowledge-based Suspect Screening Workflow for the Identification of Main Contributing Pollutants to the Biological Endpoints

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The threat posed by mixtures of environmental pollutants to ecosystems and human health remains an enduring issue. Challenges exist in current research that the chemical space of analyte covered by the analytical methods in individual studies is limited and the known chemical pollutants typically account for only a small fraction of the toxicity observed in real environmental samples. For instance, the activation of peroxisome proliferator-activated receptor γ (PPARγ) represents a primary biological mechanism underlying the adverse effects of environmental adipogens. However, a holistic understanding on the composition profiles of PPARγ agonists in complex environmental matrices remains elusive. We show that an integrated workflow of knowledge-based suspect screening combined with in vitro bioassays enabled the comprehensive identification and prioritization of main contributing components in indoor dust samples. A total of 123 putative agonists covering 35 structural categories were found, among which 30 chemicals were verified as specific PPARγ agonists through reference standards and in vitro assays. These agonists could explain up to 84% of the effect in the mixed dust extracts. Phthalates, fatty acids, quaternary ammonium compounds and hydrocarbon surfactants were further found as the major contributors. Concentration addition model was also validated to effectively characterize the combined effects of these PPARγ agonists via artificial mixture experiments. These results suggest the workflow holds promise for the overall perception of bioactive components related to multiple toxicological endpoints in environmental samples.

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3.02.T - Evaluating Non-conventional Plant Protection Products (Biopesticides, Nanopesticides etc)

3.02.T01 Biopesticides vs Conventional Synthetic Pesticides: Combining Insights from a Systematic Review and Field Trial

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Current agriculture relies on conventional synthetic pesticides (CP) for effective crop protection, whose long-term use raises concerns of environmental sustainability. Derived from natural materials, biopesticides (BP) have been proposed as eco-friendly alternatives. However, critical comparisons of CP and BP across multiple metrics remain scarce.
As a first step, we systematically assessed existing literature comparing CP, BP and untreated controls in

terms of agriculture productivity (efficacy, yield and revenue) and impacts on environmental health (non-target organisms, soil fertility and greenhouse gas emissions). On average, CP agronomic performances were superior (48% for BP vs 56% for CP of efficacy; 17% for BP vs 19% for CP of yield improvement), but the gap is relatively small: more than 30% of existing studies reported better agricultural productivity for BP compared to CP. Although available evidence remains limited, BP were associated with environmental benefits, including reduced non-target animal mortality (24% for BP vs 56% for CP). Nevertheless, BP are not necessarily "benign", as exemplified by some studies with greater negative effects on non-target organisms for BP compared to CP.
To provide more insights beyond ecological impacts, field trials were conducted to compare the effects of the BP carvacrol and the CP dimethomorph with an untreated control in a potato production system. By integrating untargeted metabolomics and metabarcoding, we characterized tissue-specific metabolic responses, rhizosphere microbial communities, and potato quality traits. Compared with the untreated control, both pesticide treatments enhanced tuber lipid metabolism and downregulated secondary metabolism in leaves. For rhizosphere communities, while both treatments reduced beneficial bacterial taxa, carvacrol exerted less suppressive effects on plant-growth beneficial bacteria and resulted in superior suppression of fungal pathogens than dimethomorph. Compared with untreated control, both treatments increased starch content but decrease the contents of flavonoid and phenolic. Moreover, higher starch, flavonoid, and vitamin C contents were observed in carvacrol treatments compared to dimethomorph.
Collectively, our results demonstrate that three-way comparisons among BP, CP, and untreated controls are essential for systematically identifying the trade-off of pesticide use, thereby contributing to the integration of BP into sustainable crop production systems.

3.02.T02 Next Generation Risk Assessment applied to Nanopesticides

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The application of nanotechnology to develop and improve pesticides has been the topic of intense research and development activities over the last decade. Current challenges associated with the regulatory risk assessment of nanopesticides are one reason for their slow market uptake, which may be a missed opportunity to improve current agricultural practices. Guiding principles to adapt ecological and human health risk assessments were previously developed through a series of multisectoral workshops involving scientists, regulators, and industry, and supported by the IUPAC.
Our latest workshop evaluated the potential application of Next Generation Risk Assessment (NGRA) to nanopesticides. The main drivers for NGRA are the incorporation of molecular, computational and system biology developments in risk assessment, with a focus on animal-free New Approach Methodologies (NAMs). NGRA entails a more mechanistically based risk assessment paradigm and the use of hypotheses, based on this mechanistic understanding and a comprehensive evaluation of exposure potential. NGRA is an emerging approach that is particularly relevant for assessments at the nano-scale. In this presentation, we will illustrate how NGRA can be applied to nanopesticides. Several case studies have been selected to illustrate how hypotheses driving the NGRA can be established on the basis of three main information sources: (1) the expected exposure pathway for each human group or ecological taxa, (2) the previous knowledge on toxicity of the active substance and relevant co-formulants, and (3) the characteristics and benefits expected by the nano design of the plant protection product. We hope that the proposed framework can serve as a foundation to advance the risk assessment of nanopesticides as well as other advanced materials that do not easily fit in with existing approaches.

3.02.T03 Fate of CuS Nanoformulations in Soil

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Over the last decade, copper-based nanoparticles containing Cu(OH)2 or CuO have been extensively studied as promising novel agrochemicals for controlling plant diseases and supplying micronutrients. Most recently, copper sulfide nanoparticles (CuS NPs) have also received attention for their potential agronomic benefits. However, there is a very limited understanding of the fate of CuS NPs after field application, including the potential impact of the CuS formulation, which is an important gap in assessing potential risks and benefits. Our study focused on three key processes controlling fate in soils: (i) transport in saturated porous media, (ii) dissolution, and (iii) Cu speciation in soil. We compared the fate of non-formulated CuS NPs with that of CuS NPs formulated with nanocarrier systems made of lignin and poly-lactic co-glycolic acid. CuSO4,was also used as an ionic benchmark.

Column transport experiments with saturated quartz sand showed that formulated CuS NPs exhibited fast solute-like transport compared to non-formulated CuS NPs, which displayed a typical colloidal behaviour. This result is inconsistent with the dissolution experiments, which showed that formulated CuS NPs release Cu ions very slowly. Sequential extraction of soil after 90 days of incubation suggested that formulated CuS NPs formed more residual Cu than non-formulated CuS NPs. Regardless of formulation, CuS formed much lower proportions of Cu in the exchangeable and acid-soluble fractions than CuSO4, which has consequences on the long-term availability of Cu. Overall, our results show the strong influence of both the form and formulation on the environmental fate of Cu. The findings are important to guide the design of more performant and safer nano-enabled agrochemicals.

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3.02.T04 From grapevine to soil: Understanding the fate and ecological effects of nanosulfur in wine growing

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Nanosulfur has emerged as a promising treatment for controlling powdery mildew in grape growing. Several field studies have demonstrated improved efficacy or efficiency relative to commercial bulk sulfur while maintaining adequate crop protection against powdery mildew. However, key knowledge gaps remain regarding the environmental fate and ecological impacts of nanosulfur.
This study investigated the behaviour of foliarly-applied nanosulfur on grapevines and its effects on soil organisms. To understand the effect of nanoparticle size and surface coating on plant surface retention, rainfastness tests were performed on detached grapevine leaves and grape bunches. On grapevine leaves, uncoated and stearic acid-coated nanosulfur exhibited improved rainfastness compared to commercial bulk sulfur. On grape bunches, only stearic acid-coated nanosulfur showed relative improvement in rainfastness compared to commercial bulk sulfur. Enhanced rainfastness and absorption have the potential to reduce off-site transport and environmental contamination. The majority of the applied coated nanosulfur (PVP and stearic acid-coated) was absorbed into the leaf and berry tissue, which is expected to affect the characteristics of the wine produced.
The ecological effect of nanosulfur in soil was evaluated using soil microcosms with earthworms (Eisenia fetida). Soil exposure did not result in acute or chronic mortality, oxidative stress, or tissue damage in earthworms after 5-day and 21-day exposure. The absence of adverse effects in earthworms suggested a low short-term risk to soil macrofauna, although further studies across a broader range of soil organisms and exposure conditions are needed. Stearic-coated nanosulfur exhibited lower microbial oxidation from

elemental sulfur to water-soluble sulfur compared to both bulk sulfur and uncoated nanosulfur. The reduced oxidation of coated nanosulfur to water-soluble sulfur has the potential to influence sulfur cycling, soil bioavailability, and leaching in soil environments.
These findings provided new insights into the environmental behaviour and ecological risks of nanosulfur applied in grape growing. Nanosulfur has potential benefits in winegrowing, including lowering pesticide inputs while maintaining adequate crop protection against powdery mildew and reducing potential impacts on non-target organisms.

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3.02.T05 An Interpretable Machine Learning Approach for Predicting (Nano)pesticide Wash Off from Leaf Surfaces

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Pesticide wash off from crop leaves reduces pesticide efficiency and results in environmental contamination. Wash off is known to be influenced by many factors including rainfall conditions, leaf and pesticide properties and it is challenging to predict under realistic multi-factor scenarios. Here, we take advantage of artificial intelligence and introduce a model in which pesticide formulation properties and environmental factors are considered simultaneously to investigate the key drivers governing pesticide wash off on leaf surfaces. The wash off of nanoformulations (zein nanoparticles loaded with methoxyfenozide, MFZ) was systematically measured across a range of conditions (leaf type, concentration, rain water chemistry) and compared to a commercial MFZ formulation as well as unformulated MFZ. The Random Forest model showed good predictive performance (R^2 >0.9), effectively capturing non-linear relationships. Model interpretation showed that leaf type, particle size and formulation type were the main factors influencing wash off, whereas rainwater conditions played a secondary role. Lower wash off was generally associated with tomato leaves, smaller particle size, moderately negative to positive zeta potential, lower contact angle, and mildly acidic formulation pH. The developed model was further applied to a wash off dataset of copper-based (nano)formulations, achieving an R^2 of 0.93 for test set and validating the generalization capability across different formulation systems. Our study demonstrates that machine learning models can help identify and prioritize key factors driving pesticide wash off under complex multi-factor scenarios, supporting wash off potential evaluation under experimental conditions and early-stage screening and optimization in nanopesticide development.

3.03.P - Genomic Instability And Biomarkers of Environmental Stressors with Implications for Long-Term Ecological and Human Health

3.03.P–Mo089 Occupational exposure modifies host factor associations with buccal cytome biomarkers in artisanal gold miners

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<p>In human biomonitoring, the Buccal Micronucleus Cytome (BMCyt) assay typically treats host factors such as age, smoking, and alcohol as static statistical covariates. This assumes uniform influence across exposure contexts. However, chronic occupational exposures may modify these relationships. We hypothesized that occupational exposure acts as an effect modifier, altering host factor–biomarker associations. We tested this using cross-sectional data from 125 adult Filipino males (63 healthy reference individuals and 62 artisanal gold miners). Eight BMCyt endpoints were analyzed via Jonckheere–Terpstra

trend tests, Spearman correlations, stratified multivariable Negative Binomial regression, pooled interaction models, and Principal Component Analysis (PCA). In multivariable models adjusted for intra-group confounding, smoking was significantly associated with micronuclei and nuclear buds in both groups. However, smoking showed significant associations with cell death markers, condensed chromatin (CC; IRR = 1.05, p < 0.001) and karyolysis (KL; IRR = 1.01, p = 0.016), exclusively in the exposed group. Age was negatively associated with basal cells (IRR = 0.99, p = 0.020) and positively associated with KL (IRR = 1.01, p = 0.015) only among exposed workers. Pooled interaction analyses demonstrated significant effect modification by occupational exposure: smoking with CC (IRR = 1.04, p_adj = 0.044), KL (IRR = 1.01, p_adj = 0.044), and binucleated cells (BN; IRR = 1.04, p_adj = 0.044), as well as age with KL (IRR = 1.01, p_adj = 0.021). Exploratory PCA illustrated distinct multivariate correlation structures, with the first two dimensions explaining 53.2% of variance in the exposed group versus 32.0% in the reference group. These results indicate that standard additive models may misclassify exposure-dependent associations as uniform background noise, potentially underestimating risk in co-exposed populations. Future exfoliative cytome research should prioritize stratified and interaction-based approaches for accurate real-world risk assessment.

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Full manuscript currently under review at a toxicology journal.

3.03.P–Mo088 AOP-directed Placental Multi-omics Study: Molecular Trajectories of Prenatal PFAS Exposure Inducing Large-for-Gestational-Age Infants

Prenatal exposure to per- and polyfluoroalkyl substances (PFAS) is closely associated with adverse birth outcomes, but the complex molecular mechanisms by which it induces fetal overgrowth-large for gestational age (LGA)-remain unclear. In this study, 30 PFASs were quantified in the serum of 797 pregnant women, among which 16 had a detection rate exceeding 50%. Restricted cubic spline (RCS) and generalized linear models revealed that exposures to PFHxA, PFHxS, PFOA, PFOS, PFHpA, PFNA, and PFTrDA were significantly and positively associated with the risk of LGA. Bayesian kernel machine regression (BKMR) models further identified PFHxA, PFHxS, and PFHpA as the key components driving the joint effect of the mixture exposure, with the overall joint effect demonstrating a positive direction. Placental transcriptome sequencing, weighted gene co-expression network analysis (WGCNA), and hierarchical dimensionality reduction via network topology identified a gene network comprising 66 genes. These genes were significantly enriched in biological processes including transmembrane amino acid transport, gas transport, and development, pinpointing RICTOR and PSEN1 as the highest-weighted hub genes among the core genes and suggesting their central role in mediating abnormal placental amino acid transport. Furthermore, cord blood metabolomics analysis confirmed that glutamic acid and pyroglutamic acid exhibited the highest contributions in the LGA group. Mediation analysis demonstrated that cord blood glutamic acid and pyroglutamic acid mediated 28.15% and 23.66% of the association between PFHxS exposure and LGA risk, respectively. By utilizing a multi-omics integration strategy within the Adverse Outcome Pathway (AOP) framework, this study identified placental hub genes and cord blood core mediating metabolites that drive fetal overgrowth, successfully mapping the molecular trajectory from prenatal PFAS exposure to large-for-gestational-age (LGA) infants. Our findings not only reshape the scientific understanding of the bidirectional developmental effects of environmental

endocrine disruptors but also provide novel molecular targets rooted in biological causality for the precision prevention of environment-related LGA and the optimization of prenatal risk monitoring. KEYWORDS: Prenatal PFAS exposure; Large for gestational age; Placental transcriptomics; Hub genes; Cord blood metabolomics; Adverse Outcome Pathway.</p>

3.05.P - One Health Perspective on NAMs: Bridging the Gap Between Human Toxicology and Ecotoxicology

3.05.P–Mo090 Approach for Assessing Developmental Neurotoxicity Using Zebrafish Swimming Behavior

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Neurodevelopmental disorders such as autism spectrum disorder and attention deficit hyperactivity disorder have been increasing recently. Exposure to chemicals during fetal and developmental stages has been suggested as one of the risks for developmental neurotoxicity (DNT). OPPTS 876.6300 and OECD TG426 are test guidelines for DNT. These tests are long-term, complex, and costly. Therefore, the development of low-cost and simple methods for DNT assessment is desired. Besides, alternative methods to animal testing for the safety assessment of chemicals have been developed from the perspectives of animal welfare and cost. Alternative methods include in silico approaches, such as QSAR models and read-across, as well as in vitro assays using tissues and cells. Zebrafish test is one of the alternative methods and has been available to assess developmental toxicity and DNT potential of chemicals. Zebrafish are small, prolific, easy to rear, develop quickly, and the development of various organs is well conserved between zebrafish and mammals. For these reasons, zebrafish are attracting attention as a model capable of comprehensive analysis of the developmental and neurodevelopmental processes of chemical substances.
We are studying a DNT assessment method based on changes in swimming behavior using zebrafish. Fertilized eggs of zebrafish were exposed to chemical substances until the larval stage and reared in a flow-through system for over two months. The behavioral analysis of these zebrafish was performed using a simple image analysis method. This presentation will report on the results of exposure to sodium valproate and ethanol. We will also assess and report morphological characteristics of neurons at the time of exposure, in conjunction with DNT assessments based on behavioral analysis.

3.05.P–Mo091 Comparative transcriptomics and tPOD estimation reveal cross-species sensitivity to chemical stress

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Transcriptomics is increasingly applied as a New Approach Methodology (NAM) in (eco)toxicology to support mechanistic interpretation of chemical effects and Next-Generation Risk Assessment (NGRA) within a One Health context. However, the cross-species comparability of transcriptomic responses and derived transcriptomic points of departure (tPODs) remains insufficiently understood, limiting their broader application in chemical hazard assessment and prioritization. This study compared transcriptomic responses and tPODs across three standard OECD aquatic test species: zebrafish (Danio rerio) embryos, Daphnia magna, and Lemna minor, representing three trophic levels within an ecosystem. A major challenge is integrating species-specific molecular responses into a harmonized framework that enables cross-species sensitivity assessment and mechanistic comparison. Organisms were exposed to the model oxidative phosphorylation uncoupler carbonyl cyanide m-chlorophenyl hydrazone (CCCP) under standardized laboratory conditions for species-specific exposure durations of 4, 6, and 7 days,

respectively. RNA sequencing was conducted to generate extensive temporal and concentration-response datasets. To enable direct comparison across taxa, a harmonized bioinformatic workflow was applied to all datasets, including differential gene expression analysis and functional enrichment using GO, KEGG, and Reactome databases. Gene- and functional-level tPODs were subsequently derived using benchmark dose (BMD) modeling. Preliminary analyses revealed both conserved and species-specific transcriptional responses, particularly in pathways associated with mitochondrial function, energy metabolism, and cellular stress responses. Comparative tPOD analyses further indicated differences in species sensitivity depending on the biological level of organization considered, while also identifying conserved pathway-level responses across taxa. Overall, this work demonstrates the utility of comparative transcriptomics and tPOD estimation as NAM-based approaches for evaluating chemical effects across species. The findings contribute to improving cross-species interpretation of omics responses and support the integration of transcriptomics into One Health risk assessment, chemical screening, and prioritization frameworks.

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3.05.P–Mo092 A zebrafish hepatic 3D spheroid-based high-throughput screening platform for assessing chronic effects of chemicals promoting MASLD

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New Approach Methodologies (NAMs) are transforming chemical risk assessment by enabling mechanistic, non-animal testing strategies. However, integration across biological domains remains limited, restricting alignment between human toxicology and ecotoxicology within a One Health framework. This study addresses this challenge by developing a high-throughput screening (HTS) NAM based on a zebrafish hepatic three-dimensional (3D) spheroid model to assess chronic metabolic effects relevant to both environmental and human health. Zebrafish liver (ZFL) cells were assembled into 3D spheroids in a 384-well format, enabling integrated long-term exposure and endpoint analysis within the same well. This configuration supports reproducible chronic exposure testing while maintaining high throughput and experimental consistency. Spheroids were exposed for 10 days to six environmentally relevant chemicals: perfluorooctanoic acid, perfluorononanoic acid, permethrin, triphenyl phosphate, dichlorodiphenyldichloroethylene, and bisphenol S, either alone or in combination with oleic acid to simulate a metabolically stressed, steatotic condition associated with metabolic dysfunction-associated steatotic liver disease (MASLD). Lipid accumulation and adenosine triphosphate (ATP) content were measured as indicators of metabolic disruption and viability. The model detected clear concentration-dependent increases in lipid accumulation, particularly for perfluorinated compounds. Co-exposure with oleic acid further enhanced steatotic responses, demonstrating increased sensitivity under metabolically relevant conditions. ATP levels remained largely stable, indicating that the observed effects were associated with metabolic perturbation rather than overt cytotoxicity. This work demonstrates how a 3D spheroid-based HTS NAM can generate mechanistically relevant data on chronic metabolic disruption while supporting higher-throughput chemical screening. By using a non-mammalian vertebrate system with conserved hepatic functions, the platform contributes to bridging ecotoxicological and human health perspectives within a One Health context. The approach further supports comparative evaluation of chemical-induced steatosis and provides a framework for integration into adverse outcome pathway-informed and weight-of-evidence-based risk assessment strategies.

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3.05.T - One Health Perspective on NAMs: Bridging the Gap Between Human Toxicology and Ecotoxicology

3.05.T01 Bridging Environment to Exposome: In Vitro Evidence for Chemical Mixture Propagation to Humans

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Synthetic organic chemicals are pervasive in the environment, forming complex mixtures with diverse toxic potentials. Their number, diversity, and co-occurrence pose major challenges for assessing risks to ecosystems and human health, particularly at low concentrations. In vitro bioassays are well-suited for evaluating both known and unknown mixtures. In the Panoramix project [1], we examined how environmental chemicals propagate through food webs to humans. Samples from 5–10 European countries were pooled, covering wastewater influent and effluent (human waste and emissions), surface water and fish (aquatic and dietary exposure), and conventional and organic cow milk (terrestrial mammal exposure). Human dietary exposure was represented by drinking water, bottled water, milk, and fish, while breast milk, adult serum, and cord serum captured direct human exposure. All samples were extracted using harmonized protocols and analyzed with targeted and nontarget chemical screening [2]. Extracts and reconstituted mixtures of 24 commonly detected chemicals were tested in 22 in vitro bioassays covering neurotoxicity, thyroid disruption, reproductive toxicity, and genotoxicity. Most bioassays responded, with strongest effects in samples from higher trophic levels like fish and humans. Reconstituted mixtures conformed to concentration addition predictions, but accounted for only a fraction of the observed bioactivity—pointing to the presence of uncharacterized toxicants and underscoring the limitations of current analytical coverage. Preliminary effect-based trigger (EBT) values defined for water and food by extrapolation from safe levels of individual chemicals suggests minimal immediate health risks.These findings illustrate how synthetic chemicals cross ecological and physiological boundaries, impacting ecosystems and human health alike, highlighting the value of in vitro tools and a One Health approach to integrated risk assessment. [1] Escher et al. (2022) Int J Environ Res Public Health, 19, 12990. [2] Motteau, et al. (2025). Environ Sci Technol. 10.1021/acs.est.4c12608. PANORAMIX project https://panoramix-h2020.eu/.

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3.05.T02 Precision Toxicology: Towards cross-species extrapolation of chemical risk using multi-omics bioactivity profiling

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Most environmental chemicals are poorly characterized, with only a few known mechanisms of action in limited model species. This limits our ability to assess chemical pollution risks and protect health. Efforts to reduce animal testing have spurred the development of New Approach Methodologies (NAMs), which detect early biological changes and provide mechanistic insights that complement or precede traditional endpoints. Bioactivity profiling via omics techniques like transcriptomics and metabolomics is a key NAM, identifying molecular signatures linked to chemical exposure that indicate adversity and may be conserved across species. These insights aid risk assessment and allow chemical grouping based on biological responses, not just structure.

The EU-funded PrecisionTox project uses omics-based assays to study biomolecular responses in five species—Danio rerio, Xenopus laevis, Caenorhabditis elegans, Drosophila melanogaster, and Daphnia magna—exposed to chemicals. Its goal is to create a mechanistic framework that predicts toxic effects by identifying conserved responses across species, improving prediction while reducing animal testing. This helps bridge environmental and human toxicology.

We present a case study using transcriptomic and metabolomic profiles from five species exposed to four chemicals with different modes of action: cadmium chloride, sodium arsenite, ethoprophos, and Wyeth-14643. Samples were collected at 3-5 time points within 48 hours. Pooled biomass was used to extract RNA, metabolites, and lipids. Co-expression networks were built for each species–chemical-omic pair, with module eigengenes used in multiblock correlation analysis to identify temporal patterns across omics. Biomolecular signatures for species-chemical pairs were used for comparison.

Notably, transcriptomic results used for cross-species comparison revealed significant overlap of orthologous genes beyond random expectation, indicating conserved response signatures with potential utility for cross-species extrapolation. Conserved responses were primarily associated with detoxification, oxidative stress, and proteostasis pathways. Comparison with human HepG2 datasets identified 15, 79, and 43 shared ortholog groups for $CdCl_2$, $NaAsO_2$, and pirinixic acid, respectively. The identified pattern of shared functional orthologues with species-specific temporal dynamics demonstrated the potential of ecological models to inform human toxicity and to support a One Health approach.

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3.05.T03 Behaviour-Transcriptomics Screening in Daphnia and Drosophila to Support One Health Toxicology

Lautaro Gandara[1] and John Colbourne[2] (1)European Molecular Biology Laboratory, (2)University of Birmingham

A key challenge for One Health toxicology is to decipher the molecular mechanisms underlying cross-species toxicity. Behavioural phenotyping can detect early functional changes in movement and activity, but behavioural endpoints alone do not explain the molecular pathways that drive these effects. Integrating behavioural screening with transcriptomics provides a route to connect functional disruption with mechanism-based interpretation across model systems.

Here, we present a cross-species behaviour-transcriptomics framework using Daphnia magna and

Drosophila melanogaster as complementary invertebrate models. A library of 200 environmentally relevant chemicals prioritised within the PrecisionTox programme was screened using automated video tracking under sublethal exposure conditions. Behavioural trajectories were analysed to identify chemicals that altered locomotor activity and movement profiles. Cross-species comparison was then used to distinguish shared behavioural perturbations from species-specific responses, providing insight into conserved functional disruption and model-specific sensitivity.

Transcriptomic profiling of selected behavioural responses will be used to explore the molecular mechanisms associated with these functional effects. These molecular signals can then be interpreted alongside chemical mode of action, Adverse Outcome Pathway knowledge and existing human bioactivity data. By combining functional screening, cross-species comparison and molecular profiling, this study provides a mechanism-oriented framework for prioritising chemicals and interpreting ecological toxicity evidence in a broader One Health toxicology context.

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3.05.T04 Marine Ecotoxicology as the Missing Pillar of One Health: Evidence from Industrial Coastal Zones in Northern Chile

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The One Health framework integrates human, animal, and environmental health, yet ecotoxicology remains largely absent from its implementation, particularly in marine ecosystems. In developing countries with extensive industrial coastlines, this gap has direct consequences for ecosystem integrity and human health.
Northern Chile concentrates several industrial sacrifice zones where metal contamination poses simultaneous risks to marine biota and coastal communities dependent on shellfish consumption. Despite this, ecotoxicological evidence from these areas is rarely framed within a One Health context. This study synthesises ecotoxicological data from native marine organisms across multiple trophic levels — the bivalves Perumytilus purpuratus and Leukoma thaca, and the benthic fish Labrisomus philippii — sampled at contaminated sites in San Jorge Bay (Antofagasta) and Tocopilla, a recognised sacrifice zone. Parameters evaluated included metal concentrations in tissues, histopathological lesions, parasite and pathogen loads, and immunological indices. Copper and lead concentrations in bivalve tissues consistently exceeded Chilean regulatory limits for human consumption across sites. Rickettsia-like organisms and haemocytic infiltration were associated with elevated cadmium and copper, while trematode infections showed site-specific gradients linked to temperature and organic matter — indicating that multiple environmental stressors simultaneously modulate host health across locations and species.
This represents one of the first case studies from the Global South to explicitly integrate marine ecotoxicology into a One Health perspective, illustrating how native marine organisms function as integrative sentinels linking environmental contamination, organismal health, and human exposure risk through seafood consumption. We argue that marine ecotoxicology must be formally incorporated into One Health frameworks, especially in nations where sacrifice zones concentrate environmental and social vulnerability

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3.06.A.T - PFAS Treatment and Remediation: Linking Environmental Behavior to Sustainable Solutions

3.06.A.T01 Validation of new materials for PFAS analysis in ambient air

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Per- and polyfluoroalkyl substances (PFAS) are subjects of environmental monitoring on a global scale. Although river water, ground water and soil were well subjected to their pollution even in nationwide surveys in many countries, atmospheric measurement is still limited because of lack of well validated standard methods. We developed several research tools including cryogenic air sampler, NS20, FM4, GAIAC, Triporous rice husk activated carbon and so. for the last ten years. In this report, currently available materials for sample collection of ambient air including normal activated charcoal filter, GAIAC, Triporous, two types of ion exchange filter were validated for their potency of trace measurement of PFAS in ambient air sample. To verification of PFAS adsorption efficiency of each material, several trials of recovery test were evaluated because there was uncertainty of spiking chemicals on filter surface. There was black box to understand real mechanisms of adsorption of volatile PFAS to adsorbent materials, procedural result of spiking test and adsorption were not same phenomenon, theoretically. Therefore, “non-touch spiking experiment” was used to compare adsorption and recovery of both volatile and non-volatile PFAS for each adsorbent. Experimental design was similar to Asakawa (2025) and Lin (2022). Briefly described as follows. Air samples were collected by using particle and gas sampler (NS20; Sibata Scientific Technology Co., Ltd., Japan). The air sampler was assembled with a four-stage cascade impactor equipped with quartz fiber filters to collect particulate matter with different aerodynamic diameters, reaching the submicron range in the last stage, followed by an adsorbent cartridge containing one polyurethane foam (PUF) and several new material adsorbents to collect the gaseous phase. After the pretreatment methods for PFAS in different sampling media described by Asakawa (2025), emerging PFAS, FOSAAs, FTSAs, FTUCAs, 8:2diPAP, and FOSA were measured by LCMSMS. The remaining pre-PFAAs were measured using Orbitrap Exploris GC Mass Spectrometer were used to detect additional pre-PFAAs and six HOCs in a portion of the collected samples. GC-Orbitrap MS was operated using selected ion monitoring in electron ion mode.
Finally, a developed method was applied to real sampling of ambient air from Osaka in March 2025 and validation result of new adsorbent materials were discussed in this report.

3.06.A.T02 Risks of Per- and Polyfluoroalkyl Substances Exposure to Fish and Human Health Through Fish Consumption

Minhao Wang[1], Ge Yang[1] and Wenhui Qiu[1] (1)Southern University of Science and Technology (SUSTech)

Global food trade expansion has enriched diets worldwide but has also heightened concerns about the spread of contaminants. Among these, per- and polyfluoroalkyl substances (PFAS) are recognised worldwide as “forever chemicals”. Yet the risk posed by PFAS from consuming marine fish is not well understood. Here, we integrate ecotoxicological evidence, machine-learning-based toxicity prediction, global field survey data, marine food-web modelling, seafood trade analysis, and human dietary exposure assessment to evaluate PFAS-related risks to fish and human health. From an ecotoxicological perspective, our studies show that PFAS can induce multiple adverse outcomes in fish. PFAS exposure disrupted neurotransmitter-related metabolism and locomotor behaviour, impaired antibacterial defence by altering immune cell responses, lysozyme activity, and inflammatory signalling, and interfered with

endocrine regulation along the hypothalamic-pituitary-gonadal axis, leading to reproductive impairment and intergenerational effects. For example, long-chain PFAS, such as PFDA, and PFAS precursors, such as PFOSA, showed pronounced immunotoxicity through TLR/MyD88 and NF-κB signalling pathways. Together, these findings suggest that PFAS exposure may impair fish health and ecological resilience before entering the human food chain. To broaden risk screening beyond experimentally tested compounds, we further developed a machine-learning framework to predict fish NOECs for diverse PFAS, revealing substantial toxicity variation shaped by molecular structure and species traits. Regarding human exposure, we predicted a global median C8-PFAS concentration of 0.34 ng/g wet weight across 212 marine fish species, with a median estimated daily intake of 0.023 ng/kg/day through marine fish consumption and PFOS as the dominant contributor. Higher exposure was observed in North America, Oceania, and Europe, while seafood trade further redistributed PFAS exposure pathways globally. These findings highlight the need to integrate fish ecotoxicology, predictive toxicology, seafood monitoring, dietary exposure assessment, and trade-informed regulation to protect aquatic ecosystems and human health.

3.06.A.T03 Sorption Behavior and Treatment of Fluorinated Electrolyte Anions from Lithium-Ion Batteries

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The expansion of lithium-ion battery (LIB) manufacturing has led to the large-scale use of fluorinated electrolyte anions, including trifluoromethanesulfonate (triflate), sulfonimide-based anions such as bis(fluorosulfonyl)imide (FSI^-), bis(trifluoromethanesulfonyl)imide ($TFSI^-$), and fluoroalkyl-substituted analogs (e.g., $FTFSI^-$ and $BETI^-$), and inorganic anions including tetrafluoroborate ($BF4^-$) and hexafluorophosphate ($PF6^-$). These species are critical to battery performance, but their increasing production raises concerns about environmental release. Lessons from PFAS research show that highly stable fluorinated chemistries can become persistent contaminants, yet the environmental behavior and treatment of LIB-derived fluorinated anions remain largely unexplored. This study investigates the removal of common LIB fluorinated anions using a range of sorbent materials and examines how their behavior differs from legacy PFAS. Batch isotherm and competitive sorption experiments were conducted across five aqueous matrices, including two landfill leachates, using four classes of sorbents: strong-base anion-exchange resins, modified organoclays, granular activated carbon (GAC), and a composite aluminum-carbon sorbent. Strong-base anion exchange resins achieved near-complete removal of sulfonimide anions (FSI^-, $TFSI^-$, $FTFSI^-$, $BETI^-$) across all matrices, including highly saline leachate, without evidence of saturation. ATR-FTIR analysis indicates that this performance arises from specific interactions between charge-delocalized sulfonimide anions and quaternary ammonium functional groups, rather than conventional electrostatic exchange. Modified organoclays showed moderate, matrix-dependent removal, while GAC performance declined substantially in DOC-rich leachate. Triflate showed good removal in deionized water but minimal retention in complex matrices due to competition from background anions. $BF4^-$ exhibited negligible sorption on GAC and limited uptake on organoclays, while $PF6^-$ showed instability in water and was excluded from the results. These results demonstrate that LIB-derived fluorinated anions exhibit distinct sorption behavior compared to PFAS and cannot be managed under existing assumptions. This work provides a comparative evaluation of treatment options for this emerging class of contaminants and establishes a mechanistic basis for selecting appropriate removal strategies in complex environmental systems.

3.06.A.T04 Does AI help us solve PFAS problems?

Nobuyoshi Yamashita[1] (1)AIST

Artificial Intelligent supportive non-target analysis of PFAS (AI-PFAS) was firstly reported in 2025 (Jiao

and Yu) by international cooperation between National Institute for Advanced Industrial Science and Technology (AIST), Japan and Nanjing University, China. Jiao (2025 Nature communications), the first to use AI for mass spectrometry and analysis of PFAS (PFAS-AI), used the expression "prediction analysis" instead of "suspect screening" for the first time, and Yu's report (2025 nature machine intelligence), the second report of PFAS-AI, developed a generative AI (Molecular Structure Generator: MSgo).By machine learning not only the mass spectral data of the measured samples, but also the vast amount of public data, such as the open database of chemical substances that have already been released and the analytical data available as supporting information for research papers, we can achieve "PFAS structures including CF2 and/or CF3", which are the OECD definitions of PFAS. To put it succinctly, the technology has been completed, "if there is a certain concentration or more of a molecule in a sample that meets the OECD definition of PFAS, it can be identified, not limited to unknown or known."
Furthermore, PFAS-AI basically eliminates the need for essential reference materials for target measurements. Instead of commercially available reference materials, the "precise mass number yardstick" for identifying PFAS in samples is itself a "yardstick" of giant mass spectral data of 1 GB or more per analysis, which averages the ionic intensity bias using SWATH technology. PFAS-AI described above is open source, and the following technology is rapidly spreading around the world.
PFAS-AI in 2025 is just beginning. Not only a standalone technology but also "cloud base platform" for big data analysis cooperating with industry and stakeholders is necessary. More than twenty big industries and manufactures of PFAS in the Consortium for analysis and remediation of per- and poly-fluoroalkyl substances (CAR-PFAS Japan) have started to develop "national platform; PFAS-AI Japan" to solve PFAS problem in Japan. In this report, current status and timeline of this project will be described.
PFAS-AI is only an example. AI and machine learning are significantly accelerating efforts to solve the PFAS problem by improving detection, speeding up the discovery of alternatives, and optimizing cleanup technologies.

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3.06.A.T05 Linking Sediment Records, Food Web Dynamics, and Toxicokinetics to Guide PFAS Remediation Priorities

Yuefei Ruan[1], Qi Wang[2], Kenneth Leung[1] and Paul Lam[3] (1)City University of Hong Kong, (2)The Education University of Hong Kong, (3)Hong Kong Metropolitan University

Effective remediation of PFAS requires understanding their long-term environmental behavior, trophic transfer potential, and species-specific toxicokinetics. This talk integrates our systematic investigations from the Pearl River Estuary and northern South China Sea across three interconnected compartments.
First, sediment core records spanning about 80 years reveal a critical shift. Perfluorooctanesulfonate (PFOS) levels have declined over the past decade due to regulatory actions, but its chlorinated substitutes, chlorinated polyfluoroalkyl ether sulfonic acids (Cl-PFESAs), have maintained persistent medium to high ecological risks for 40 years. We report the first in-situ evidence of 6:2 Cl-PFESA transforming into its hydrogen-substituted analog in sediments. Using equilibrium partitioning to derive interim sediment quality criteria, our risk assessment shows that emerging alternatives now dominate the ecological threat, while perfluorooctanoate poses low risk. Establishing sediment quality criteria for these persistent alternatives is urgent to avoid trading a regulated burden for an unregulated one.
Second, food web analysis of 15 fish, 21 crustaceans, and two cetaceans identified 22 PFAS with significant trophic magnification in the northern South China Sea. We report the first trophic magnification factors for cis- and trans-perfluoroethylcyclohexane sulfonic acid (PFECHS) isomers at 1.92 and 2.25, respectively. Perfluorohexanoic acid also undergoes trophic magnification, likely via

precursor degradation. Thus, emerging PFAS propagate through food webs, increasing exposure at higher trophic levels.
Third, toxicokinetic studies in marine medaka (Oryzias melastigma) revealed tissue-specific uptake and clearance of PFECHS and 6:2/8:2 Cl-PFESAs. All three compounds showed significant bioaccumulation, with the longest residence times in the eyes. Trans-PFECHS accumulated more than cis-PFECHS. PFECHS exposure also altered multiple eye-related proteins, indicating organ-specific toxicity. Such kinetic data are essential for predicting internal exposure and informing remediation endpoints.
Together, these findings link environmental fate, food web transfer, and biological responses into a coherent framework. We advocate that sustainable PFAS remediation strategies should prioritize emerging alternatives with proven persistence, trophic magnification, and slow organ clearance, alongside establishing water/sediment quality criteria for emerging compounds.

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3.06.B.T - PFAS Treatment and Remediation: Linking Environmental Behavior to Sustainable Solutions

3.06.B.T01 Enhanced Sorption of Per- and Polyfluoroalkyl Substances Across Chain Lengths Using Next-Generation Sorbents with Mechanistic Insight

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Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants with high mobility, particularly short-chain compounds such as perfluorobutanoic acid (PFBA) and ultrashort-chain compounds such as trifluoroacetic acid (TFA), posing ongoing challenges for water and soil remediation. Conventional sorbents often show limited performance for these mobile species due to weak interactions with anionic PFAS, highlighting the need for sorbents with cationic functionalities to enhance PFAS–sorbent interactions.

This study developed and evaluated next-generation mineral-based sorbents with cationic surface functionalities designed to enhance PFAS–sorbent interactions across a range of chain lengths. Sorption performance was assessed using batch experiments with mixed PFAS systems containing short- and long-chain compounds, with additional evaluation of ultrashort-chain PFAS. Sorption kinetics and isotherm studies characterised uptake behaviour and capacity, while soil incubation experiments assessed sorbent effectiveness in reducing PFAS leachability in field-collected soils.

The sorbents demonstrated high removal efficiencies across a wide PFAS range. In mixed systems, where short- and long-chain compounds compete for sorption sites, removal efficiencies of up to 93% for ∑PFAS were achieved, indicating effective sorption under competitive conditions. Kinetic results showed rapid sorption at early contact times, while isotherm analysis indicated strong affinity and high sorption capacity (≈100–900 µg/g), comparable to or exceeding values reported for commercial sorbents. High removal efficiencies were also observed for ultrashort-chain PFAS, reaching up to 90%. Soil application reduced PFAS leaching by up to 99% for ∑PFAS, supporting effective immobilisation.

Computational approaches, including density functional theory and molecular dynamics simulations, have been applied to elucidate PFAS–sorbent interactions at the molecular scale, including electrostatic and hydrophobic interactions and their dependence on PFAS chain length. These approaches provide mechanistic insight and support interpretation of experimental results.
These findings demonstrate that the developed sorbents achieve strong and consistent removal across a wide range of PFAS and conditions, with soil application further highlighting their potential for PFAS immobilisation. The study supports development of effective sorbents and improved understanding of PFAS remediation.

Disclaimer/Disclosure: This research was conducted as part of an industry PhD collaboration.

3.06.B.T02 Enhancing the Pollution Retention of Short-Chain Per- and Polyfluoroalkyl Substances (PFAS) using a Biological-Based Superabsorbent Polymer (SAP) Approach

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Per- and polyfluoroalkyl substances (PFAS), or “forever chemicals”, are contaminants of escalating global concern. Superabsorbent polymers (SAPs), known for their high-water retention capacity, offer a potential new approach for enhancing PFAS removal within green stormwater infrastructure, particularly in the face of climate change-driven weather events in urban environments. To test this, the study aimed at evaluating the retention potential for a group of highly mobile, short-chain PFAS, using a biological (lignin)-based, superabsorbent polymer (SAP). The polymer’s ability to trap short-chain PFAS was examined by evaluating the retention capacity of the SAP, using batch retention experiments and the following PFAS of interest: (short-chain: perfluorobutanoic acid (PFBA), hexafluoropropylene oxide dimer acid (HFPO-DA) and 4,8-dioxa-3H-perfluorononanoic acid (DONA). Adsorption was assessed at a single concentration of 10 µg/L for each compound. Spiked PFAS test solutions were added to polymer granules, and the adsorption (retention) was derived from the difference between the concentration of each PFAS initially present in the solution and the concentration remaining after 72 hours. Adsorption by the SAP varied for different PFAS, with decreasing order of percent retention as follows: DONA > HFPO-DA > PFBA. Additionally, retention of DONA (70.84 %, SD = 7.06) was approximately 50 % higher than that of the other compounds. Despite the postulation of smaller-sized PFAS molecules (e.g. PFBA: 4 carbons) having relatively faster kinetics, these compounds typically have lower hydrophobicity when compared to their ‘larger’ short-chain PFAS counterparts (e.g. DONA: 7 carbons), thus alluding to an overall low adsorption of PFBA to the natural lignin composition of the bio-based polymer. These findings represent the first crucial phase of a stepwise assessment of this polymer’s adsorption capability. Consequently, it provides the foundation for later experiments that will assess the SAP’s efficacy for removing short-chain PFAS when incorporated into lab-scaled microcosms (simplified framework of green infrastructure) and flow-through, planted mesocosms that represent near real-world conditions (vegetated prototype of green infrastructure).

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3.06.B.T03 PFAS Immobilisation in Soils: Insights from Laboratory to Long-Term

Durability Studies

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Per- and polyfluoroalkyl substances (PFAS) are among the most persistent and challenging contaminants in soil. Once released, PFAS interact variably with soil particles, migrate through the subsurface, and can leach or run off into groundwater and surface water, posing long-term risks to ecosystems and human health. As both a temporary sink and a potential secondary source, soil plays a critical role in the environmental cycling of PFAS. Immobilisation using sorbents has emerged as a practical strategy to limit PFAS mobility. However, a key concern among regulators and stakeholders is the longevity of PFAS immobilisation, specifically, how they may become remobilised.
Over the past five years, we have systematically evaluated PFAS immobilisation in soils through both standardised and novel leaching assessments. Laboratory- and field-scale experiments were conducted on various AFFF-contaminated soils treated with 1–5% (w/w) of over 20 different sorbents. Standard leaching protocols, including the Australian Standard Leaching Procedure (ASLP) and Leaching Environmental Assessment Framework (LEAF), were used to quantify PFAS retention in soils amended with granular and powder activated carbon (PAC/GAC), RemBind, and biochar. In parallel, non-standard approaches such as rainfall simulation were applied to examine leaching, runoff, and long-term stability (up to one year) under realistic field conditions. PFAS uptake in plants grown in immobilised soils was also evaluated to assess potential bioavailability and secondary transport. Additionally, sorbents were subjected to accelerated physical, chemical, and biological aging to determine the persistence of PFAS immobilisation efficiency over time.
Results demonstrated that certain sorbents are highly effective at immobilising ∑PFAS in soil, maintaining over 99% immobilisation even under extreme conditions, including vigorous shaking, acidic or alkaline pH, and high ionic competition. Long-term assessments revealed that sorbent efficiency can decline over time due to changes in surface chemistry and structure, emphasising the importance of incorporating aging studies under diverse environmental conditions. These experiments showed that sorbents with high specific surface area and strong initial sorption capacity, particularly activated carbon (AC)-based materials and RemBind, exhibited superior durability, retaining more than 95% PFAS immobilisation following physical, chemical, and biological aging.

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3.06.B.T04 Mechanistic Insights into Air Sparging Enhanced PFAS Desorption, Mobilisation, and Removal in Contaminated Soil

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Air sparging is a promising in situ remediation technique for mobilizing per- and polyfluoroalkyl substances (PFAS) in saturated soils through air–water interfacial processes and advective mixing. This study evaluated the short-term effects of air sparging on PFAS desorption and redistribution using field-contaminated soil from the Sundsvall Timra Airport site, Sweden, in controlled column experiments. Two

trials were conducted at a constant influent flow of 50 mL/min: i) a pilot test with a half-filled column operated sequentially under water-only and water–air conditions, and ii) a paired full-column comparison between water-only and water–air configurations. Air sparging substantially enhanced PFAS mobilization relative to hydraulic leaching alone. In the pilot trial, perfluorooctane sulfonate (PFOS) increased 30-fold in the aqueous phase, while 6:2 fluorotelomer betaine (6:2 FTAB) showed high enrichment in the foam. In the parallel-column trial, water-only flow caused mainly redistribution, whereas air sparging produced pronounced transport, foam formation, and phase partitioning upward. Long-chain perfluoroalkane sulfonates (PFSAs) such as C6 (PFHxS), C7 (PFHpS), and C8 (PFOS) showed the strongest sparging response, with foam capturing a substantial fraction of exported mass. In contrast, short-chain perfluoroalkyl carboxylic acids (PFCAs) were mainly redistributed within the water phase and showed limited foam enrichment. Overall, the results show that air sparging can enhance PFAS transfer from soil to mobile phases and promote foam-mediated removal, particularly for surface-active PFSAs and fluorotelomer precursors. These findings support the potential of air sparging for targeted in situ management of PFAS source zones.

Keywords: Per- and polyfluoroalkyl substances (PFAS); air sparging; soil remediation; PFAS desorption; foam fractionation; column experiment

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3.06.B.T05 PFAS Remediation Trade Offs: Granular Activated Carbon Lowers Bioavailability Yet Disrupts Earthworm Biology

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Per- and polyfluoroalkyl substances (PFAS) and aqueous film-forming foams (AFFF) are persistent soil contaminants of global concern due to their mobility, bioaccumulation potential, and ecotoxicological effects. We assessed the effects of a defined PFAS mixture [PFOS (perfluorooctane sulfonate), PFOA (perfluorooctanoic acid), PFHxS (perfluorohexane sulfonate)] and a diluted AFFF, with and without a 5% (w/w) granular activated carbon (GAC) amendment, on the earthworm Eisenia fetida. 28-day exposure integrated (1) organism level endpoints (survival, biomass change, cocoon production), (2) PFAS concentrations in soil and tissue, and (3) untargeted metabolomics to link exposure reduction with biological outcomes.

Survival did not differ among treatments; however, both PFAS and AFFF markedly reduced cocoon production and increased weight loss, confirming reproduction and condition as more sensitive indicators than lethality. Notably, GAC alone also decreased cocoon output and contributed to weight loss, suggesting indirect effects of the sorbent on soil properties and/or nutrient availability. Earthworms accumulated multiple PFAS, with PFOS and PFHxS dominating tissue burdens. Adding 5% GAC substantially lowered PFAS concentrations in soils and earthworm tissues, demonstrating effective sorption and reduced bioavailability, but without corresponding improvement in organism performance. Metabolomics revealed 72 annotated metabolites significantly altered across treatments. PFAS exposure changed 27 metabolites, whereas AFFF affected 58, with 19 shared responses, indicating broader biochemical disturbance from AFFF beyond the PFAS fraction alone. Pathway enrichment identified 20 impacted pathways spanning amino acid, carbohydrate, lipid, vitamin/cofactor, and nucleotide metabolism, with amino acid metabolism most responsive overall. PFAS uniquely perturbed glutathione, pyrimidine, and porphyrin metabolism, while AFFF preferentially disrupted central energy and lipid related pathways, consistent with distinct modes of action and mixture complexity.

Collectively, our results show that although GAC can reduce PFAS bioavailability and uptake, it may

introduce ecological trade-offs by altering soil conditions and eliciting reproductive and metabolic costs. Optimising GAC dose and pairing sorbents with ecologically supportive amendments may be necessary to achieve risk reduction without unintended harm to soil biota.

3.07.P - Soil Contaminant Bioavailability and Remediation

3.07.P–Tu089 Soil Lead (Pb) Immobilization Efficacy using Jarosite Treatment via Bioaccessibility, Relative Bioavailability and Speciation Approaches

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Lead (Pb) is a ubiquitous toxic metal that has been linked to developmental neurotoxicity at low exposure levels in children. Traditional remediation methods, e.g., soil washing/capping or replacement with clean soil may be unsustainable due to the scale of global Pb contamination. Similarly, in situ immobilization using soil amendments, e.g., phosphate, organic matter, lime and metal oxides are criticized for their low efficacy and/or the possibility of increasing toxic metalloid mobility in soil.
This study utilized a novel “Jarosite Treatment” technique to transform soil Pb into plumbojarosite [PbFe6(SO4)4(OH)12] minerals to reduce childhood Pb exposure. Twelve Pb contaminated soils (764-8,392 mg/kg) from mining, smelting, shooting and industrial activities were treated with ferric sulphate (0.4-1.0 M) + sulphuric acid (0.05 M) at a soil: solution ratio of 1:1 at 105℃. Lead bioaccessibility (dissolution in simulated gastric solution using US EPA method 1340) was assessed in pre- and post-treated <250 µm soil particle fraction (ingestible SPF) to determine the optimum reagent concentrations for immobilization. After treating with the optimised strategy, soils were neutralized with lime, and ingestible pre- and post-treated SPF were assessed for Pb bioaccessibility and relative bioavailability (RBA, dose normalised bioaccumulation in femur, kidney, liver compared to Pb-acetate following 9-day dietary exposure using 1% soil in mouse chow). Lead speciation was also investigated in these SPF using X-ray Absorption Near Edge Structure (XANES; Australian Synchrotron).
Lead bioaccessibility and RBA in the untreated samples were 5.58-78.2% and 0.60-42.9% respectively. Although a 40.3-90.3% reduction in Pb bioaccessibility was seen in all treated samples, a 36.2-75.6% reduction in Pb RBA occurred in ten samples, while an increase in Pb RBA was observed in the remaining two. Speciation analysis using XANES confirmed the presence of plumbojarosite minerals in the treated soils where bioaccessibility/bioavailability was reduced. However, predominant Pb species in the remaining two samples were identified as anglesite and Pb adsorbed to clay, which may be attributed to the inefficacy of the treatment. Overall, the outcomes of this study highlight that jarosite treatment may be highly effective in mitigating childhood lead exposure, however, more research is needed to elucidate factors that affect plumbojarosite formation.

3.07.P–Tu090 Enhanced Fenton-Type Degradation of Ciprofloxacin at Wide pH Range Using In Statu Nascendi Modified Magnetite Nanoparticles

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The search for effective methods for removing persistent pharmaceutical pollutants from aquatic environments is a pressing issue in modern environmental chemistry. Ciprofloxacin (CIP), a second-generation fluoroquinolone antibiotic, can accumulate in ecosystems and promote the development of resistance in microorganisms. The presence of a strong C–F bond in the CIP molecule, which has one of the highest energies among single bonds in organic chemistry (~105.4 kcal mol-1), determines its high resistance to degradation. Heterogeneous Fenton catalysts being developed based on magnetic iron oxides face agglomeration, iron leaching, and a narrow optimal pH. This work aims to synthesize magnetic

nanocomposites with high active site density and stability across pH 5–9 for CIP removal via Fenton-type reactions.
The approach uses in statu nascendi reduction of iron ions to magnetite nanoparticles on a mesoporous silica matrix pre-modified with humic acids (HA), yielding TAM (magnetite on silica) and TAHA-M (with HA). This approach provides additional steric stabilization of M during NPs formation. The presence of the Fe3+/Fe2+ pair on the surface of the NCs allows them to be used as catalysts in redox processes such as the Fenton reaction.The physicochemical properties of the obtained compounds were studied using X-ray diffraction, Fourier transform infrared spectroscopy, low-temperature N2 adsorption, surface fractal analysis, and vibromagnetometry. Sorption/catalytic experiments with CIP were conducted in H2O2-free and H2O2-free environments at pH 5, 7, and 9. Iron leaching was also quantified.
TAM achieved a specific surface area of 256 m2/g and a hierarchical inkwell pore architecture (blocking factor L=1.75). CIP degradation reached 84% at pH 5 and 68% at pH 9, up to 8-fold over sorption. Kinetics showed biexponential decay: fast radical oxidation, then slower intermediate breakdown. HA increased sorption but limited catalytic activity; however, HA reduced iron leaching to <3 wt.%. Micropores contributed ~62% of total pore volume. In statu nascendi synthesis preserved the matrix's fractal geometry, tripling surface area and creating optimal mass transport. TAM's performance stems from accessible Fe2+/Fe3+ sites and low blocking factor. HA provides chelate stabilization, ensuring reusability.
This study confirms the high efficiency of these synthesized heterogeneous magnetic HA-silica catalysts in degrading persistent pharmaceuticals through demineralization.

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3.07.P–Tu091 Tracking the fate and effects of nanoplastics in soil-dwelling arthropods using Pd doping

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Nanoplastics (NPs) are of growing concern due to their uptake by organisms, ability to cross biological barriers, and potentially greater toxicity compared to microplastics. However, their behavior and effects in terrestrial ecosystems remain poorly understood, particularly in soil-dwelling organisms where exposure pathways are complex and quantification at low concentrations remains challenging. Building on a previously developed palladium (Pd)-doped NP exposure system for agricultural food webs, this study expands the approach to additional arthropod species. We established NP exposure assays for two representative terrestrial arthropods: a predatory rove beetle (Dalotia coriaria) and a decomposing springtail (Folsomia candida). Adult rove beetles and springtails were exposed to Pd-doped NPs via spiked dry yeast feed (1%) for short-term (up to 1 week) and/or long-term (up to 6 weeks) durations, while rove beetle larvae were exposed throughout their developmental period. NPs in all species were quantified using inductively coupled plasma–mass spectrometry (ICP–MS), with Pd serving as a tracer. Across both species, no evidence of NP accumulation was observed, even under long-term exposure conditions. No significant effects on survival, growth, or reproduction were detected. In rove beetles, NP body burdens decreased after pupation, suggesting partial elimination prior to pupation. In addition, fewer adults emerged in the exposed group. These findings indicate limited bioaccumulation and toxicity of NPs in terrestrial arthropods under the tested conditions. The validated Pd-doped NP exposure system provides a robust framework for assessing NP fate in soil ecosystems and contributes to improved ecological risk assessment in agricultural environments.

3.08.A.T - Integrated Approaches in Ecological and Human Health Risk Assessment (APAC Focus)

3.08.A.T01 Gestational Exposure to Per- and Polyfluoroalkyl Substances and Non-Ideal Early-Life Growth: The Mediating Role of Cord Blood Fatty Acids

Yue Luo[1] and Yichao Huang[1] (1)Anhui Medical University

Abstract:
Prenatal exposure to per- and polyfluoroalkyl substances (PFAS) has been linked to adverse birth outcomes, but its long-term effects on early childhood growth patterns remain unclear. To address this knowledge gap, we investigated the longitudinal impact of prenatal PFAS exposure on infant growth and the potential mediating role of metabolic markers. This study included mother-infant pairs from a birth cohort in Hefei, China. We measured maternal serum PFAS concentrations and cord blood fatty acids. Longitudinal changes in weight-for-age, length-for-age, and weight-for-length z-scores from birth to two years were classified into stable, faltering, and accelerated growth trajectories. Multinomial logistic regression and mediation models were applied to assess these relationships.

Among the targeted PFAS, several substances were frequently detected in maternal serum samples and exhibited distinct associations with infant growth. Notably, prenatal perfluorohexanesulfonic acid (PFHxS) exposure demonstrated robust and divergent effects after multiple testing corrections. Compared to the stable group, PFHxS was significantly associated with altered risks of both faltering and accelerated weight-for-age trajectories. Sex-stratified analyses revealed these divergent associations were observed exclusively in female infants. Furthermore, cord blood very-long-chain saturated fatty acids (VLCFAs, including C20:0, C22:0, C24:0) were positively associated with the risk of faltering growth and served as significant mediators in the pathway between prenatal PFAS exposure and faltering development.

Prenatal PFAS exposure may shift early-life growth toward non-ideal growth patterns by altering cord blood fatty acid profiles. These findings advance our understanding of environmental developmental toxicity and highlight the clinical need for early metabolic monitoring in exposed populations, with particular attention to the heightened susceptibility of female infants.

Keywords: Per- and polyfluoroalkyl substance; Fatty acid; Growth pattern; Birth cohort; Sex-specific effect.

3.08.A.T02 Non-negligible Source of PFAS: Biochemical Fate and Metabolic Activation of Precursors

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The widespread detection of PFAS precursors in environment and human matrices raises new wave of health concerns. However, their ADME fates and toxicity profiles in mammalians remain largely unexplored. Here, we investigated the toxicokinetic, metabolic transformation, and toxicity of three overlooked precursors, N-MeFOSA, N-EtFOSA, and N-EtFOSAA, by integrating toxicokinetic modeling in mice, rat liver microsomes metabolism, and hepatocellular toxicity assays. N-MeFOSA and N-EtFOSA were rapidly eliminated in vivo and exhibited high efficiencies of conversion to legacy PFAS in liver microsomes, surpassing the typically low transformation rates in mammals reported for other precursors. Notably, N-MeFOSA showed the greatest metabolic transformation potential (25% legacy PFAS and 22% PFOS in 3 hours). Moreover, in hepatocellular toxicity assays both precursors exhibited weaker direct metabolic perturbations than their metabolites (PFOS and FOSA), indicating that their toxicity is

primarily enhanced via metabolic activation. In contrast, N-EtFOSAA displayed persistence and stability in vivo and in vitro, and induced lipid accumulation comparable to PFOS, together with stronger inhibition of cellular energy metabolism. Collectively, our study provides crucial ADME data identifying N-alkyl-FOSA-type precursors as non-negligible internal PFOS sources, underscoring a dual-risk paradigm where toxicity is driven either by metabolic activation or intrinsic parent compound toxicity.

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3.08.A.T03 Demonstrating Mitigation of Phenotypic Alterations by Targeted Removal of Key Risk Drivers in Embryo-larval Zebrafish: Based on Children-Relevant Exposure Profiles in Four Asian Countries

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Children are widely exposed to mixtures of plasticizers, with exposure profiles varying substantially across regions. Biomonitoring studies indicate that children are simultaneously exposed to multiple plasticizers, yet identifying the key contributors to mixture toxicity remains challenging due to complex interactions among components and limited ability to predict mixture effects.
In this study, we evaluated morphological and behavioral alterations in zebrafish larvae (Danio rerio) following a 5-day exposure to plasticizer mixtures designed to simulate the exposure profiles of children in four Asian countries (Korea, Thailand, Indonesia, and Bangladesh). Mixtures consisted of seven plasticizers at concentrations representing the 75th percentile of exposure for each country. To identify major contributors to mixture toxicity, reduced mixtures were generated by removing two plasticizers prioritized as risk drivers based on ToxPi analysis. Following a 120-hour exposure to either full or reduced mixtures, 57 quantitative endpoints across 11 categories (eye, head/jaw, otolith, yolk, heart/pericardium, intestine, fin, tail/notochord, somite, body contour, and behavior) were assessed. Partial least squares discriminant analysis (PLS-DA) revealed clear dose-dependent separation among treatment groups across all countries. Removal of the two predicted risk drivers led to substantial reductions in effect sizes across multiple endpoints, with 55–88% of endpoints losing statistical significance relative to the full mixture. Eye area, yolk sac area, pericardial area, fin fold length, and placode area were the most consistently affected endpoints across countries. In addition, pronounced upward shifts in lowest observed effect concentrations (LOECs) were observed following removal of the risk drivers, particularly in mixtures representing Korea and Indonesia. By reconstructing region-specific exposure mixtures, this study demonstrates a practical framework for identifying dominant toxicity drivers within complex environmental mixtures. Ultimately, these observations provide a proof of concept that a small subset of plasticizers can disproportionately drive the toxicity of complex mixtures, reinforcing the value of targeted prioritization strategies for mixture risk management.

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3.08.A.T04 Short-Term Variability of Urinary Oxidative Stress Biomarkers (OSBs) Associated with Exposure-Relevant Dietary and Lifestyle Factors

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Urinary oxidative stress biomarkers (OSBs) derived from cellular molecule damage, are relatively stable and non-invasive indicators of oxidative stress, and are increasingly used to evaluate disease progression and biological responses to environmental chemical exposure. However, the interpretation of their levels can be complicated by short-term variability driven by potential dietary and lifestyle factors, as well as diurnal variation.

In this study, 162 spot urine samples were collected from 10 healthy participants (five males and five females), over three consecutive days. A questionnaire was completed at each sample collection to track recent dietary behaviours, personal care product use, and activities that serve as potential sources of chemical exposure or factors potentially influence OSB levels. Eight urinary OSBs reflecting nucleic acid, protein, lipid, and glycoxidation damage, including 8-hydroxyguanosine, 8-hydroxy-2′-deoxyguanosine, 3-chlorotyrosine (Cl-Tyr), 3-bromotyrosine, 4-hydroxynonenal mercapturic acid (HNE-MA), 8-isoprostaglandin F2α, Nε-(carboxymethyl)-lysine (CML), Nε-(carboxyethyl)-lysine, were measured to evaluate their inter- and intra-individual variability and associations with questionnaire factors.

Across all urine samples, coefficients of variation ranged from 62% to 160% for the eight OSBs, and intraclass correlation coefficients ranged from 0.17 to 0.62, suggesting substantial short-term variability largely attributable to intra-individual variance. Specific gravity adjustment and first-morning void sampling reduced the overall variability. Intake of food mostly in contact with plastic within the previous 12 h was associated with 44% higher Cl-Tyr concentrations, (95% CI: 3.9% to 99%; $p = 0.043$). Grain-based food (e.g., pasta and rice) intake in the past 12 h showed significant positive associations with several urinary OSBs, including Cl-Tyr, Br-Tyr, HNE-MA, and CML.

These findings can support future exposure–OSB association studies by informing sampling strategies and questionnaire design to better account for potential confounding factors, such as diurnal variation and recent dietary behaviours. As part of this ongoing study, plastic exposure biomarkers, including bisphenols and phthalate metabolites, will be measured to further evaluate whether plastic-related dietary exposures associated with elevated OSB levels.

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6. Transdisciplinary, Emerging Topics, and Digital Innovation

5.01.B.T - Application of Novel Approach Methodologies (NAMs) to Improve Risk Assessment and Management of Contaminants of Emerging Concern (CEC)

5.01.B.T01 Beyond the Black Box: Mechanistic Interpretation as a Prerequisite for Trustworthy QSAR-like In Silico NAMs

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Considering the rapid development of artificial intelligence, we are observing growing interest in the use of predictive models for chemical risk assessment. Among these models, often referred to as in silico

NAMs (New Approach Methodologies), Quantitative Structure–Activity Relationship (QSAR) methods occupy a prominent position.

Validation standards for QSAR methods, described for example in the QSAR Assessment Framework (QAF), recommend not only reporting the validation statistics of the model itself and defining the compounds for which the model is applicable (the so-called applicability domain), but also providing a mechanistic interpretation of the model. However, the document states “if possible.” In the reality of the rapidly evolving fields of machine learning and AI, many newly developed models function as “black boxes,” where the causal relationship between descriptors and the modeled toxicity endpoint is not explicitly considered. Such models are particularly vulnerable to the phenomenon of “correlation by chance,” as described in the seminal work of John G. Topliss and Robert P. Edwards.

We postulate that, in order to increase the credibility and regulatory acceptance of QSAR models, providing a mechanistic interpretation is essential. In this presentation, we will demonstrate through selected examples how such interpretation can and should be performed, even for models based on highly advanced machine learning approaches and for the prediction of such toxicological endpoints as the transcriptomic response.

Ultimately, we aim to show that mechanistic interpretability should not be viewed as an optional addition to modern predictive toxicology, but rather as a fundamental prerequisite for building scientifically robust, transparent, and regulatorily trustworthy in silico methodologies. As predictive models become increasingly complex, ensuring their biological plausibility and mechanistic consistency will be critical for their future integration into regulatory decision-making frameworks.

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5.01.B.T02 Integrating Biological Activity with the Fish Plasma Model to Prioritize Antidepressants of Concern in Wastewater: A Case Study in Dalian, China

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Antidepressants have been widely detected in aquatic environments, raising concerns about their potential adverse effects on aquatic species. To date, the environmental risks of antidepressants to fish have been primarily assessed using the risk quotient approach and the classical fish plasma model. However, these methods do not consider the mode-of-action of antidepressants or interspecies variability in toxicokinetic parameters. In this study, wastewater effluent concentrations of antidepressants in China were predicted based on consumption, and then were used to estimate internal exposure in zebrafish using an adjusted fish plasma model. The pH-dependent octanol-water partition coefficient (Dow) and fathead minnow (Pimephales promelas) parameters were adopted in the fish plasma model to improve the accuracy of predicted fish steady-state plasma concentrations (FssPCs) of antidepressants. Antidepressants more strongly inhibited the zebrafish serotonin transporter (zSERT) than that against human transporter (hSERT). Fish therapeutic plasma concentrations (FTPCs) were proposed as an alternative to human therapeutic plasma concentrations, derived from the fold-change in IC50 values between zSERT and hSERT. The ratio of FssPCs to FTPCs were calculated to assess environmental risks of antidepressants in China, England, and Japan. Overall, the fish plasma model using Dow, fathead minnow parameters, and FTPCs provides an improved framework to predict environmental risks of pharmaceuticals.

5.01.B.T03 Predicting Synergistic Effects on Reproduction from Consumer Product

Mixtures Using Deep Learning Models

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Chemical risk assessment has shifted its focus from evaluating individual substances to adopting more comprehensive methods from assessing joint toxicity in mixtures. Testing all possible mixture combinations is logically challenging due to their vast number. To address this, machine learning-driven computational toxicology techniques have been rapidly advancing to predict chemical toxicology techniques have been rapidly advancing to predict chemical toxicity. Over 1000 potential endocrine-disrupting chemicals (EDCs) have been identified and are present in various consumer products, subsequently released into the environment. While numerous studies have focused on individual EDCs, predicting their synergistic effects remains a significant gap that requires further investigation. To examine this, we conducted an extensive study to screen substances in consumer products with potential reproductive toxicity. High-throughput screening (HTS) assays were constructed based on OECD Test Guidelines 455 and 458. Using the HTS method, potential estrogenic agonists and anti-androgenic antagonists were identified, followed by testing binary mixtures. Leveraging the HTS data, deep neural network models were developed to predict potential synergistic estrogenic (area under the curve (AUC): 0.837–0.881) and anti-androgenic (AUC: 0.826-0.907) activities of binary mixtures. This study provide novel tools for supporting the risk assessment of mixtures used in consumer products.

Keyword: Endocrine disruption, estrogen receptor, androgen receptor, mixture toxicity, deep learning model

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5.01.B.T04 Development of Exo-metabolomics and Deep Learning-Based Toxicity Quantification Tools as New Approach Methods for Ecotoxicity Assessment

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Traditional ecological risk assessment is often limited by high costs and time, and the ethical issue is another emerging concern for some species. To address these challenges, this study develops and validates New Approach Methods (NAMs)—specifically exo-metabolomics and deep learning-based behavioral analytics—using domestically adapted Daphnia magna across diverse river sites. To improve accuracy of behavioral tracking, a YOLOv5-based model was implemented for high-resolution, automated tracking of subtle swimming alterations. A flow-through system initially characterized 1,228 exo-metabolic features, detecting sublethal shifts at 5 μg/L, which served as early biomarkers identifying toxic stress significantly earlier than traditional reproductive endpoints. Concentration-response analyses identified 12 high-confidence candidates with strict dose-dependent trajectories. Although field validation faced challenges from site-specific matrix effects, several metabolic features maintained consistent, temporally reproducible, and concentration-dependent responses within each site, establishing robust molecular points of departure (PODs) even within complex aquatic matrices.
By integrating these early-warning signals with AI-enhanced phenotyping—achieving 98.1% precision in

adult Daphnia while accurately distinguishing neonates, molts, and debris—this study establishes a mechanistically informative, high-throughput NAM that transcends conventional monitoring. Collectively, these findings provide a robust technological basis for proactive, effect-based regulatory strategies, supporting a paradigm shift in freshwater quality management and chemical safety assessment.

5.01.B.T05 Current Approaches to Prioritise Chemical Contaminants of Emerging Concern in Water

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Contaminants of emerging concern (CEC) pose a significant challenge for the water industry due to their presence in matrices including wastewater, drinking water and biosolids. This is compounded by a lack of knowledge about their occurrence, environmental fate and/or toxicity, making it difficult to assess and mitigate risks. In this paper, we synthesise current tools and approaches used to evaluate and prioritise CEC in matrices relevant to the water industry for research and management. Most approaches were specific to a particular geographic location, with fewer studies considering CEC risk at the national or international level, despite CEC being a global issue. Further, most prioritised CEC in surface water, wastewater and drinking water, with few considering recycled water, groundwater or biosolids. The methods used to identify priority CEC varied from a simple screening based on (predicted) persistent, bioaccumulative and toxic (PBT) properties to automated workflows considering many different criteria. A risk quotient (RQ) or equivalent approach, where measured or predicted occurrence data were compared to toxicity data, was the most common method to identify and rank priority CEC. Overall, this paper identified several limitations when applying existing CEC prioritisation tools for the water industry, and opportunities for prospective prioritisation models are outlined.

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6.01.A.T - Trajectories in Environmental Science & Technology: From Biodiversity and Public Health to Sustainable Solutions

6.01.A.T01 Persistent toxicity as a new unified hazard parameter- why and how?

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Using new approach methodologies (NAMs) to test for a chemical's persistence as well as toxicity provides a rapid way of improving hazard prediction. The assessment of persistence (P), bioaccumulation (B), and toxicity (T) of a chemical is a crucial first step at ensuring chemical safety. Existing methods for PBT assessment are overly complex and cumbersome, have produced incorrect conclusions, and rely heavily on animal-intensive testing. NAMs can overcome the limitations of current PBT assessment. The conventional indicators for PBT are recommended to be replaced by two innovative hazard indicators only, termed cumulative toxicity equivalents (CTE) and persistent toxicity equivalents (PTE). The proposed "toxicity equivalents" can be measured with high throughput in vitro bioassays. CTE refers to the toxic effects measured directly in any given sample, including single chemicals, substitution products, or mixtures. PTE is the equivalent measure of cumulative toxicity equivalents measured after simulated environmental degradation of the sample. With an appropriate panel of animal-free or alternative in vitro bioassays, CTE and PTE comprise key environmental and human health hazard indicators. CTE and PTE do not require analytical identification of transformation products and mixture components but instead

prompt two key questions: is the chemical or mixture toxic, and is this toxicity persistent or can it be attenuated by environmental degradation? The resulting "persistent toxicity" indicator could help to create chemicals that are safe and sustainable by design (SSbD). PTE of environmental mixtures may also be a measure for defining the planetary boundary for chemical pollution. Non-persistent chemicals can be broken down and if their emission stops, they will eventually disappear. Not so the persistent chemicals such as the forever chemicals PFAS. They are here to stay and we need to better understand and manage their impact.

6.01.A.T02 ADME-Informed Mechanistic Prediction of Bioconcentration and Toxicity in a Systems-Based Environmental Risk Framework

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Growing evidence shows substantial discrepancies between predicted bioconcentration factors (BCFs) in fish based on octanol–water partition coefficients and observed values, along with pronounced interspecies variability that cannot be explained by equilibrium partitioning. These limitations highlight the need for mechanistic, systems-based approaches incorporating organism-level processes. In this study, we integrated in vivo exposure experiments, in vitro hepatic S9 metabolic assays, plasma protein binding measurements, high-resolution mass spectrometry (HRMS)-based metabolite profiling, and kinetic BCF models to reassess bioconcentration and toxicity frameworks from an ADME-based perspective. Laboratory bioconcentration experiments revealed more than one order of magnitude variation in BCFs among fish species under identical exposure conditions. Plasma protein–water distribution coefficients (Dpw) showed up to 100-fold interspecies differences for cationic compounds and strongly correlated with species-specific BCFs, indicating that protein binding is a key determinant of internal exposure for certain chemicals. Hepatic S9 assays demonstrated that hepatic metabolic clearance accounts for a major fraction of total elimination, particularly for highly lipophilic chemicals. High-resolution mass spectrometry (HRMS) further identified species-dependent metabolites and revealed differences in metabolic activation between species. Integration of metabolic and protein binding parameters into kinetic fish BCF models significantly improved predictive performance. Overall, bioconcentration was shown to result from interacting processes including gill uptake, gill elimination, plasma protein binding, metabolism, and excretion, with ADME differences identified as primary drivers of interspecies variability in BCF values. These findings support a shift from equilibrium-based to mechanistic, ADME-informed frameworks for environmental risk assessment. The integration of in vivo, in vitro, in silico, and HRMS-based approaches enables improved prediction of chemical exposure and effects across species and reduces uncertainty in ecological risk assessment, highlighting ADME processes as a key biological determinant linking environmental exposure to internal dose and toxicological outcomes.

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6.01.A.T03 Screening Tool or Regulatory Instrument? Positioning Effect-Based Methods in a Forward-Looking Regulatory Context

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Complex mixtures of chemical pollutants are threatening planetary boundaries and both human and

ecosystem health. Effect-based methods (EBMs), including in vitro bioassays, are increasingly recognised as essential tools to capture mixture effects that targeted chemical analysis cannot address. EBMs are particularly powerful in a tiered risk assessment framework, where exceedance of an effect-based trigger value (EBT) activates escalating assessment informed by adverse outcome pathway frameworks that link molecular initiating events to organism- and population-level effects. Understanding the different methods for EBT derivation, including their data requirements, conservatism and applicability domain, is therefore critical.
EBTs have been developed to protect both human health (drinking water EBTs) and aquatic ecosystem health (surface water EBTs). This paper examines the current scientific and regulatory foundations of EBTs, synthesising current derivation approaches and their applicability. These include translation from existing guideline values or tolerable daily intakes, derivation at guideline-equivalent effect levels, and approaches accounting for mixture effects by using bioanalytical equivalent concentrations, specificity ratios, or multiple lines of evidence. A simplified interim approach based on reference compound effect concentration has also been proposed, showing good agreement with more robust methods. The suitability of these approaches varies by assay, endpoint, and regulatory objective, highlighting the need for fit-for-purpose EBTs aligned with protection goal.
By bridging mechanistic toxicology, mixture risk assessment, and applied water management, EBTs represent a critical advancement toward more holistic and protective environmental monitoring and regulation. EBT-informed EBMs can contribute to transdisciplinary solutions that address chemical pollution challenges consistent with emerging global endeavours such as the ISP-CWP and the Stockholm Declaration on Chemistry for the Future.

6.01.A.T04 From Detection to Decision: Water Quality Science for Chemicals of Concern Across Myanmar, India and Australia

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As we approach planetary boundaries for novel entities, water quality science must move beyond detection to decision ready risk assessment and management. Using case studies from Australia, India and Myanmar, we present a transferable, effects-based framework integrating environmental science, toxicology, engineering and governance. It evaluates risks from complex mixtures and chemicals of concern across climates and catchments, and within contrasting regulatory contexts, including differences in guideline maturity, enforcement capacity, and monitoring infrastructure. We propose harmonised principles and tiered decision logic, while tailoring implementation to regional capabilities, resources and infrastructure to enable equitable uptake. Co designed with stakeholders, the approach embeds Indigenous knowledge, traditional practices and socioeconomic realities throughout problem framing, monitoring, interpretation and intervention planning. Designed for phased adoption, it begins with low-cost screening and feasible indicators, then adds analytical and biological resolution as capacity grows.

In India and Myanmar, implementation through the ‘Safe Water’ capacity building program and river scorecards enables risk informed monitoring and community action even where laboratory access and regulatory reach are constrained. In Australia, partnerships with utilities, regulators and industry deliver intervention driven evidence, including cross jurisdiction comparisons of priority chemicals and acceptable risk thresholds. Treatment performance was evaluated using reductions in toxicity (not only chemical removal) to support fit for purpose reuse and defensible discharge decisions. Our systems-based approach combines New Approach Methodologies (NAMs), including rapid bioassays and mechanistic tools, and Adverse Outcome Pathway (AOP) concepts. Together, these improve transparency and enable consistent interpretation across regions, while remaining adaptable to local decision contexts.

The presentation synthesises lessons from the three regions and offers actionable recommendations for:

(1) harmonised, stepwise effects based frameworks; (2) integration of NAM and AOP informed endpoints into guidelines and certification, aligned with regulatory readiness and monitoring capacity; and (3) scalable capacity building strategies, including Indigenous knowledge, to accelerate research to policy and research to practice translation in chemicals and pollution governance.

6.01.A.T05 CRISPR-Based Diagnostics for On-Site Nucleic Acids Detection in Environmental Waters: Application to Pathogenic Cryptosporidium spp.

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PCR-based nucleic acid detection has been a powerful tool for detecting pathogens and other organisms of interest in water samples, but the need for a thermal cycler often limits its use to specialized laboratories and delays the reporting of results. CRISPR-based diagnostics offer a powerful alternative because they can work at a constant temperature (e.g., 37°C), provide rapid results (e.g., < 1 h), and be coupled with intuitive paper-based readouts. However, their application to environmental water samples remains limited, partly because of insufficient sensitivity. Here, we developed a detection platform for the waterborne pathogenic protozoan Cryptosporidium spp. using CONAN, a Cas3-based CRISPR diagnostic system. To improve sensitivity, we developed an enhanced preamplification step, one-pot reverse transcription-nested recombinase polymerase amplification (RT-nested RPA), in which reverse transcription and isothermal RPA were performed sequentially rather than simultaneously. Application of CONAN to RT-nested RPA products enabled detection of C. parvum 18S rRNA molecules within 50 min at 37°C using a paper-based lateral flow assay. The limit of detection was approximately 5–50 copies per reaction, which was equivalent to that of the corresponding qPCR assay. We then applied the assay to 17 river water samples collected in Japan, of which 7 tested positive. Using sequencing of the RPA products as the reference, the assay achieved a positive predictive value of 100% (7/7) and a negative predictive value of 100% (10/10). Together, these results show that RT-nested RPA-CONAN enables rapid, sensitive, and specific detection of Cryptosporidium spp. without requiring a thermal cycler. The CONAN-based nucleic acid detection platform can reduce reliance on centralized laboratory infrastructure and support decentralized environmental DNA/RNA monitoring.

6.01.P - Trajectories in Environmental Science & Technology: From Biodiversity and Public Health to Sustainable Solutions

6.01.P–Mo104 Flexible, Machine Learning-Based Automated Digital Histopathology Increases Throughput and Provides New Insights

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Histopathology is an essential tool for assessing the impact of pollutants at tissue and organism levels and provides a key link between mechanistic and physiological data for adverse outcome pathways. Despite its importance, the use of pathology in environmental studies is diminishing due to heavy workloads and a decreasing trained workforce. Current methods also remain largely qualitative and are prone to observer bias. Recent advances in whole slide scanning technologies and machine learning (ML) based image recognition and segmentation provide opportunities to facilitate the use of histopathology and strengthen experimental outcomes. This research aims to develop a two-step process to a) reduce pathologists' workload; (b) increase sample turnover, and c) provide objective, fully quantitative results to improve the reliability and power of analyses.

Two sets of whole-slide images (WSIs) were used from animals collected during ocean monitoring exercises in 2021: fish liver tissue (268 individuals from 5 North Atlantic species), and blue mussel

(Mytilus edulis, 293 individuals) were graded by 2 trained pathologists for 8 and 6 lesions, respectively. These grades were used to train weakly supervised models using the Clustering-constrained Attention Multiple Instance Learning (CLAM) framework to predict the presence (pathologist grade > 0) or absence (grade = 0) of lesions. Using the output from CLAM models and QuPath-generated annotations, a PyTorch-based segmentation model was trained for each tissue type. Quantification of the segmentation results was obtained based on characteristics of different lesions (e.g., total area coverage or number of cells in large aggregates).
CLAM models were successful for most lesions, with a receiver operating characteristic (ROC) AUC > 0.8, indicating high true-positive-to-false-positive classification performance (e.g., parasites, 0.906; hepatocyte vacuolisation, 0.89). This was also reflected in validation and test errors < 0.25. Heatmaps showing high-attention image areas also suggested that models accurately learned features associated with specific lesions (e.g., steatosis, haemocyte infiltration), but not with others (e.g., necrosis, parasites). Early segmentation results show successful learning and efficient quantification of various lesions. These methods are accessible and require limited expertise and training, paving the way for a more widespread and potent use of histopathology in environmental monitoring.

6.01.P–Mo105 A Multi-Stage Research Framework for Identifying Causal Pathways from Social Media to Supply Chain Emissions

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Consumption-driven greenhouse gas emissions form a major share of global anthropogenic emissions. Current estimation methods, including life cycle assessment (LCA) and multi-regional input-output (MRIO) analyses, are largely sales-based and treat final demand as exogenous. Meanwhile, information diffusion on social media (SNS) has been studied extensively in computational social science, but rarely linked to material environmental outcomes.
The pathway from viral information to environmental impact involves three causal links that are not empirically established: whether SNS diffusion shifts actual consumption, whether such shifts propagate through supply chains, and whether supply chain variability translates into environmental impacts missed by static estimation. Each link is studied in isolation in different fields, with no coherent network framework connecting them.
This study proposes a multi-stage research framework that treats these three links as separate empirical questions. A second objective is to develop new quantitative indicators capturing demand-side, information-driven dynamics not well represented in current environmental assessment. Sectors with high social media engagement and high embodied emissions, such as fashion, food, and digital consumption, are likely entry points.
We propose a three-layer coupled network. Layer 1 is an SNS information diffusion network, explored mainly through simulation on synthetic networks, drawing on diffusion modeling traditions from epidemiology, point processes, and network science. Layer 2 is the physical supply chain network, built from MRIO-based emission accounts. Layer 3 couples the two through product and brand nodes, where candidate indicators of information-induced environmental impact will be developed.
Methods are not fixed in advance. Candidate approaches include community detection, centrality analysis, multilayer network coupling, and graph-based machine learning, alongside techniques from causal inference and time-series analysis. Initial pilot results from simulation-based exploration of Layer 1 will be presented at the conference.
The contribution is methodological. The pathway from information to emissions is treated as testable propositions, not an assumed mechanism. The work aims to show where current environmental assessment can be complemented by demand-side analysis, and where diffusion models may overstate downstream material effects.

6.01.P–Mo106 Lithium Salts as a Novel Tool for Managing Acaricide-Resistant Tetranychus urticae

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The two-spotted spider mite, Tetranychus urticae, is one of the most destructive agricultural pests worldwide and is notorious for its rapid development of resistance to multiple acaricide classes. This resistance threatens effective pest management and highlights the urgent need for alternative compounds with novel modes of action. In this study, we evaluated the acaricidal activity of several commercially available lithium salts against pesticide-susceptible and pesticide-resistant T. urticae populations and compared their efficacy with acequinocyl, a widely used commercial acaricide.
Adult female mite mortality was assessed using standardized leaf-disc spray bioassays, and LC_{50} values were calculated by probit dose–response analysis. In the susceptible population, acequinocyl showed the highest potency, with an LC_{50} of 18.8 mg/L, whereas lithium salts were less active, with LC_{50} values ranging from 425.2 mg/L for LiCl to 4169 mg/L for lithium citrate. However, a strikingly different pattern was observed in the resistant population. LiCl was the most potent compound tested, with an LC_{50} of 514.1 mg/L, comparable to acequinocyl, which showed an LC_{50} of 616.5 mg/L. Importantly, acequinocyl exhibited a 33-fold resistance ratio between the susceptible and resistant populations, while LiCl showed no meaningful resistance shift, with an R_{50} of only 1.2. Even more notably, lithium sulfate, lithium citrate, and lithium lactate displayed resistance ratios below 1, indicating increased susceptibility in the resistant population.
These findings suggest that lithium salts, particularly LiCl, may overcome existing acaricide resistance mechanisms and may even exploit physiological vulnerabilities associated with resistant mite populations. The observed pattern is consistent with negative cross-resistance and supports lithium salts as promising candidates for future resistance-management programs. This work introduces lithium-based compounds as an underexplored and potentially valuable class of acaricidal agents for sustainable crop protection.

6.01.P–Mo103 Evaluating Biochar Filters for Pharmaceutical Removal: A 10-Month Column Study

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Wastewater treatment plants (WWTP) are primarily designed to remove nutrients from influent; however, pharmaceutical residues are typically not eliminated. As a result, contaminated effluent is discharged into receiving waters, posing risks to human and environmental health. In response, the European Wastewater Directive requires the implementation of sustainable advanced (quaternary) treatment technologies. Biochar filters are a promising option for this purpose; however, their long-term performance in wastewater systems remains insufficiently studied. This study evaluated the adsorption performance of five distinct biochar materials derived from different feedstocks, including sewage sludge, seed waste, forest biomass, pine, and spruce, using packed-bed columns. The columns were operated continuously for over 10 months (>630 bed volumes) using real tertiary wastewater effluent from a local WWTP. Two experimental scenarios were investigated: (i) high-load conditions using 16 spiked pharmaceuticals and (ii) normal-load conditions assessing 42 commonly occurring pharmaceuticals. The results identified two biochar materials, sewage sludge and forest biomass biochar, as the most effective, achieving over 99% removal throughout the study period. In contrast, the remaining three biochar materials exhibited significantly earlier breakthrough. These findings highlight the importance of feedstock type, surface properties, and packing density in determining adsorption performance. Fitting of individual pharmaceutical breakthrough curves revealed substantial variability among compounds, strongly

influenced by molecular size and charge. Overall, this study demonstrates the potential of biochar column systems for long-term wastewater remediation and provides important insights into pharmaceutical removal from wastewater effluent.

6.02.P - Tire and Road Wear Particles (TRWP) and Tire-Related Chemicals: Fate, Effects, and Risk Assessment

2.10.P–Tu109 Development of LC–MS/MS Method for Quantitative Analysis of Six Microcystins in Water and Airborne Aerosol Samples

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The occurrence of Harmful Algal Blooms (HABs) in riverine environments involves the production of microcystins (MCs), a type of cyanotoxin produced by cyanobacteria. These toxins consequently cause significant issues of water quality and disruption of aquatic ecosystems. Recently, the aerosolization of these toxins has emerged as a significant issue, as they are released into the atmosphere through natural and anthropogenic mechanisms and subsequent long-distance dispersion. This process creates new health risks for residents and individuals engaged in recreational activities near freshwater bodies. To properly evaluate these risks, it is necessary to develop standardized analytical methods for detecting and measuring these toxins in the air. In this study, we developed a comprehensive method for air sampling, processing, and analysis of six major microcystin congeners (MC-LR, MC-RR, MC-LY, MC-LA, MC-LF, and MC-YR). The method involved a mid-volume sampling strategy using membrane filters to collect airborne particles. For analytical performance validation, we spiked microcystins at known concentrations and performed pretreatment of the samples through mild ultrasonication. This approach allowed us to effectively extract and prepare the microcystin congeners for subsequent analysis. Analytical conditions were optimized using LC-MS/MS to achieve maximum sensitivity for each target compound, and the method's reliability was confirmed through validation of precision, accuracy, recovery, and limit of quantitation (LOQ). This research provides a quantitative analytical method for measuring microcystin concentrations in air samples and helps understand how microcystins disperse in the atmosphere and can be inhaled by humans in areas affected by algal blooms. Furthermore, this research can contribute to the development of public health policies and environmental management strategies to reduce exposure risks. Continued research is needed to further improve these analytical techniques.

6.02.P–Tu104 Effects of Tire Rubber-Derived Chemical 6PPD-Quinone and Its Metabolites on Membrane Potential in Mitochondria Isolated from Japanese Char

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6PPD-quinone (6PPD-Q) is an environmental transformation product of 6PPD, a tire rubber additive, and has long caused mass mortality of coho salmon on the West Coast of North America. 6PPD-Q is highly lethal to some salmonid fish, but its mechanism of action remains poorly understood. Mitochondria dysfunction has been reported as one of the early effects of 6PPD-Q in salmonid cells, but it has not been clarified whether these are direct effects on mitochondria or secondary consequences of other cellular processes. Also, it is not yet clear whether the main cause of toxicity is 6PPD-Q itself or its metabolites. To address these gaps, we investigated the effects of 6PPD-Q, its hydroxylated metabolites (p-OH6PPD-Q and 6PPD-Q-4-OH), and 6PPD on membrane potential in mitochondria isolated from Japanese char (Salvelinus leucomaenis).
Mitochondria were isolated from the liver and brain in Japanese char (wet weight 50 g to 180 g) using a

Dounce homogenizer and centrifugation. The isolated mitochondria were stained with TMRM, a fluorescent dye for measuring mitochondrial membrane potential, at 100 nM. The mitochondria were then exposed to CCCP, a positive control, 6PPD-Q, p-OH6PPD-Q, 6PPD-Q-4-OH or 6PPD in DMSO at 16°C for 40 minutes. Fluorescence intensity was measured using a flow cytometer with an excitation at 488 nm and emission at 585 ± 20 nm, and the values were compared with those of the DMSO control group. The decrease in mitochondrial membrane potential was evaluated by the decrease in fluorescence intensity. p-OH-6PPD-Q, 6PPD-Q-4-OH and 6PPD reduced membrane potential in a concentration-dependent manner. Their EC50 values were 3.8, 6.0, and 4.9 mg/L, respectively, in the brain, and 12, 16, and 10 mg/L, respectively, in the liver, showing no major differences among the chemicals. In contrast, 6PPD-Q didn't significantly reduce membrane potential due to the precipitation at higher concentrations. These results differ from the previous studies where p-OH-6PPD-Q and 6PPD-Q were highly toxic in salmonid cells compared to 6PPD and 6PPD-Q-4-OH. Therefore, the decrease in mitochondrial membrane potential observed in isolated mitochondria wouldn't be directly related to cytotoxicity, indicating that mitochondria dysfunction observed in salmonid cells exposed to 6PPD-Q may be secondary effects of other cellular processes. It is necessary to investigate specific cellular and subcellular targets other than mitochondria to clarify the mechanisms of 6PPD-Q toxicity.

6.02.P–Tu105 Cytotoxicity Assessment of 6PPD-Quinone Using Primary Culture–Derived Cells from Coho Salmon

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6PPD-quinone (6PPD-Q), a transformation product of the tire rubber antioxidant 6-PPD, has recently been identified as a highly toxic compound causing acute mortality in certain salmonid fish species. In addition to in vivo evidence, cytotoxic responses to 6PPD-Q observed in salmonid-derived cultured cells have been reported to be broadly consistent with whole-fish toxicity data, suggesting the potential utility of fish cell–based assays for chemical hazard assessment. However, substantial discrepancies between toxicity values obtained from fish acute toxicity tests and in vitro assays have also been documented. Moreover, no detectable toxicity of 6PPD-Q has been reported in RT-gill cells used in OECD Test Guideline 249, highlighting unresolved differences in sensitivity among fish cell systems.
In this study, primary culture–derived, non-immortalized cells were established from gill and caudal fin tissues of coho salmon (Oncorhynchus kisutch) and maintained by serial passaging for approximately six months.
Cytotoxic effects of 6PPD and 6PPD-Q were evaluated using the developed cells, and the resulting toxicity values were compared with those obtained from a commercially available coho salmon pooled embryo–derived cell line (CSE-119). Differences in sensitivity among cell types and implications for improving fish cell–based toxicity assessment strategies are discussed.

6.02.P–Tu106 Investigation of Test Conditions Affecting the Ecotoxicity of CMTT

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Tire wear particles contain a variety of additives that can be readily leached into the environment. In addition to organic additives, tire particles are known to release substantial amounts of zinc, which is considered one of the major contributors to their toxicity. In the present study, acute toxicity tests were conducted using Daphnia magna (NIES-IV-2 strain) to investigate the test conditions affecting the toxicity of cryo-milled tire tread (CMTT) suspensions. Additionally, we examined the contribution of zinc to the toxicity of CMTT leachates.
Both the CMTT suspension and its filtrate exhibited toxicity toward D. magna, with the 48-h EC_{50} and

95% confidence intervals of 550.37 (149.6-951 mg/L) mg/L and 1414.36 (1178-1651 mg/L) mg/L, respectively. When EDTA was added to the test medium as a chelating agent, the toxicity of CMTT decreased, suggesting that zinc contributes to the toxicity. In the treatments with CMTT addition, the Na^+ concentration decreased to approximately half that of the control medium, whereas the concentrations of dissolved organic carbon and zinc increased in a concentration-dependent manner. The decrease in Na^+ was likely attributable to adsorption onto tire particle surfaces. Given that metal toxicity varies with water chemistry, the reduced Na^+ concentration may have enhanced Zn^{2+} toxicity. These findings indicate that water quality conditions, in addition to the intrinsic toxicity of tire particles, are important in evaluating tire-derived toxicity.

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6.02.P–Tu107 Quantifying Loads and Removal Efficiencies of Elastomeric Particles, Including Tire- and Road-Wear Particles, in Two Municipal Wastewater Treatment Plants in Japan

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Understanding the environmental behavior and pathways of tire and road wear particles (TRWPs) in urban systems is essential for mitigating their discharge to aquatic environments. Previous studies indicate that urban road runoff can contain high concentrations of TRWPs, particularly during rainfall events. In cities with combined sewer networks, such runoff is transported to wastewater treatment plants (WWTPs), whereas in separate systems it may bypass treatment and enter receiving waters directly. In addition, other elastomer-derived particles, including degradation products of 6-N-(1,3-dimethylbutyl)-N′-phenyl-p-phenylenediamine (6PPD), are generated during the use and abrasion of rubber products. These fine particles can enter stormwater, atmospheric dust, and municipal wastewater even under dry conditions, suggesting continuous input to WWTPs irrespective of rainfall. Despite increasing concern, quantitative data on the loads, fate, and removal efficiencies of elastomer particles and TRWPs in WWTPs remain scarce. In particular, time-resolved measurements are lacking, hindering accurate estimation of emission factors and environmental transfer pathways.
In this study, influent and effluent waters from two WWTPs—one operating a combined sewer system and the other a separated system—were sampled hourly during dry weather using automated samplers. Fine particles (>20 μm) belonging to nine elastomer polymer classes, including TRWPs, were identified and quantified using a micro-Fourier transform infrared spectroscopy method developed for this study. Concentrations in sewage sludge were also measured to characterize partitioning behavior and assess retention during treatment. The resulting datasets provide new insights into temporal variability, influent loading trends, and polymer-specific removal efficiencies of elastomeric particles in contrasting wastewater treatment configurations. These findings improve understanding of the role of WWTPs in the urban lifecycle of rubber-derived particulate pollution and contribute essential parameters for predicting their fate in aquatic environments.

6.02.P–Tu108 Development of an Analytical Method for Tire Additive-Related Substances and their Residue Levels in Runoff Water Captured in Expressway-type Catch Basins

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Most tire additives and their transformation products are not chemically bound to the rubber polymers and can be easily released into the environment. Recent studies have started to conduct environmental monitoring of tire additives-related substances (TARSs), however, the recovery rates during the sample

preparation processes and the stability of the substances have not been sufficiently considered, leading to uncertainties in the quantitative results. In this study, we established a quantitative analytical method using high performance liquid chromatography-triple quadrupole Mass Spectrometry (LC-MS/MS) and attempted to determine the levels of TARSs in runoff water captured in expressway-type catch basins. We first established the analytical conditions for 31 TARSs using LC-MS/MS and investigated the stability of these compounds in frozen (-20 °C) reconstituted water based on peak area variations. Next, we conducted spiking recovery tests using river water and evaluated the accuracy of the analytical method based on the spiking recovery rates. Finally, we analyzed TARSs in road runoff water from expressway-type catch basins in Ehime and Toyama Prefectures (Japan) collected in 2026, using the established method. The evaluation of stability revealed that the antioxidant N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD) was significantly degraded in reconstituted water. This compound is too unstable for quantitative analysis. In spiking recovery tests using river water, stable recovery rates were obtained for 14 substances, indicating that quantitative analysis with guaranteed precision is possible. Chemical analysis of runoff water revealed that TARSs were detected at all locations. Among the substances which can be reliably analyzed, the cross-linking agent 2,4,6-tris[bis(methoxymethyl)amino]-1,3,5-triazine (HMMM) and the vulcanization accelerator 1,3-diphenylguanidine (DPG) were detected at high concentrations for all locations. Assessing the environmental risks posed by additive-related substances that leach from tire particles is a pressing research priority for the sustainable use of tires.

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4. Life Cycle Assessment and Sustainability Assessment

4.01.P - Life Cycle Assessment and Sustainability Assessment

4.01.P–Tu092 Comparative Life Cycle Assessment of Soil Remediation Technologies: The Case of Janghang Songrim Forest

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Life Cycle Assessment (LCA), a systematic method of evaluating the environmental impacts of an entire process, will be employed in this study to compare three soil remediation methods. In this study, we apply LCA on the Janghang Songrim Forest in South Korea, a site primarily contaminated by arsenic from historical smelting operations. We examine three soil remediation techniques, soil washing, in-situ stabilization, and phytoremediation. The data used in the assessment is based on actual on-site practices implemented on the site around 2010. This study models and assesses the environmental trade-offs of each remediation scenario from a cradle-to-gate perspective, analyzing every stage from material extraction and transportation to remediation processes. The comparative analysis aims to guide future decisions on sustainable soil remediation by identifying low environmental impact, effective techniques for sites with similar contamination profiles. The goal of this study is to conduct a comparative life cycle assessment of the environmental impacts of widely used soil remediation methods especially focusing on greenhouse gas emissions, resource depletion, and effect on human health. In addition, this study seeks to identify environmental hotspots within each of the three technologies in order to determine the major contributing processes and propose targeted strategies for impact reduction.

4.01.P–Tu093 Life Cycle Assessment of Sustainable Aviation Fuel (SAF) Production from Crude Palm Oil and Palm Fatty Acid Distillate

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Sustainable Aviation Fuel (SAF) is critical for improving energy security, boosting domestic production, and decarbonizing the aviation sector. Among various SAF production technologies, the Hydroprocessed Esters and Fatty Acids (HEFA) is the only commercial way to produce SAF. This study aims to evaluate life cycle greenhouse gas (GHG) reduction and environmental impacts for HEFA SAF production, considering SAF derived from both crude palm oil (CPO) and Palm Fatty Acid Distillate (PFAD). SAF from CPO with 85% methane captured from palm oil mill effluent (POME) included induced land use change reduces GHG emissions by 18% compared to fossil jet fuel. SAF from PFAD achieves a 70% GHG reduction compared to fossil jet fuel. Sustainable farming practices offer limited carbon intensity (CI) reduction when implemented individually but yield cumulative benefits when combined. Achieving low impacts from crude palm oil SAF production requires the integrated implementation of: (i) optimized agricultural inputs, (ii) methane capture and utilization from POME, (iii) adoption of green hydrogen, and (iv) avoidance of high-carbon stock land conversion. Other environmental impact categories are also discussed in the study. These findings highlight the trade-offs between different environmental impact categories while providing insights to optimize SAF production strategies and support the aviation sector's decarbonization goals.

4.01.T - Life Cycle Assessment and Sustainability Assessment

4.01.T01 Evaluating the Usability of Large Language Model–Generated Data for Carbon Footprint Assessment in Activated Sludge Wastewater Treatment Processes

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Recent advances in Large Language Models (LLMs) have increased the use of AI-generated data, highlighting the need to verify the reliability of such data and its applicability to environmental impact assessment. This study aimed to evaluate the performance of LLMs using prompt-based inputs only.

Environmental impact assessment was conducted using Life Cycle Assessment (LCA). LCA is a methodology that quantifies the environmental impacts associated with inputs and outputs throughout the life cycle of a product or system. It enables integrated assessment of interconnected wastewater treatment processes.

The target system was based on the activated sludge process, the most widely used wastewater treatment process in South Korea. The representative treatment train included a grit chamber, primary clarifier, biological reactor, and secondary clarifier. Four LLMs—ChatGPT, Gemini, Perplexity, and Claude—were employed for data generation. To obtain appropriate responses, prompts were iteratively refined and optimized.

To evaluate consistency among LLMs, reproducibility was assessed using text similarity analysis based on Jaccard similarity. Reliability was evaluated by comparing the agreement between LLM-generated data and literature data. In addition, carbon footprint associated with each dataset was quantified using SimaPro.

The results showed that Gemini generated non-existent values, whereas Perplexity failed to provide

extractable data. ChatGPT and Claude extracted values from the literature; however, ChatGPT generated process-specific results, while Claude produced integrated results for the entire treatment process. The data generated by ChatGPT showed approximately 80% agreement with literature values. The estimated carbon footprints of the ChatGPT-generated data and literature data were 0.147 and 0.227 kg CO2 eq., respectively, indicating lower environmental impacts for the ChatGPT-based dataset. This difference appears to be attributable to differences in the structural complexity of literature tables.

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4.01.T02 From Sentiment to Structure: Climate Risk Contagion across Green Assets, Carbon Markets, and Global Equities

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Climate risk is increasingly recognized as a systemic threat to financial stability, yet the mechanisms through which climate-related shocks propagate across environmentally linked financial markets remain poorly understood. This study investigates how financial markets transmit climate-related risks, examining dynamic relationships between novel climate risk indices (transition risk index: TRI and physical risk index: PRI), European Union carbon allowances, green equities, traditional assets (oil, gold), and major equity markets (S&P 500, CSI 300). Analyzing daily data from 2010 to 2023 using standard econometric connectedness measures and frequency-domain spillover analysis, we measure both the magnitude and timescale of financial spillovers. We find three key insights. First, while overall connectedness is moderate (26.88%), it intensifies sharply during global stress, peaking at 50% during COVID-19. Second, green stocks and the US market emerge as primary sources of price shocks, whereas climate risk indices consistently function as net receivers—reacting to, rather than causing, short-term financial movements. This suggests climate news is often overshadowed by broader market sentiment and speculation. Third, frequency-domain analysis reveals spillovers operate on distinct timescales: short-term volatility (1-4 days) is driven by financial assets and investor sentiment (22.17%), while longer-term dynamics (beyond ten days) shift to oil and carbon markets (1.98%), reflecting deeper structural factors like energy policy and macroeconomic trends. This long-term role reversal sees oil and carbon allowances become net transmitters.The climate-finance link operates on two horizons. Investors must distinguish short-term volatility from structural shifts, while policymakers should recognize that noisy market signals are no substitute for direct regulatory action in driving the transition.

Disclaimer/Disclosure: None declared.

4.01.T03 Life Cycle Assessment of the Systemic Effect of Biocides in Paint Waste Reduction and Environmental Impact

Several products placed on the market, such as paints, personal care products, and detergents, do not reach their intended functional aim due to early microbial spoilage. Biocides have been proven effective in controlling microbial growth. However, their effectiveness in reducing waste generation is not fully known, as other variables, particularly those related to consumer behavior, also influence waste generation. Additionally, biocides have the inherent disadvantage of being toxic to humans and the environment; therefore, their use should be limited.
Information on waste generation at storage level can be estimated from retailer data, whereas information at the user level is more difficult to obtain and requires active data collection methods, such as surveys, or passive secondary approaches. Both methods require human and financial resources; therefore, the use of

predictive methods is advisable to reduce the time and cost associated with data collection and processing.
The aim of this study is to present guidelines on how to systematically create scenarios to analyze products containing biocides at both the retail and user levels, assess their environmental impacts, and compare the environmental benefits of using biocides against a baseline scenario without them. For this purpose, a life cycle assessment (LCA) of paint with and without biocide was conducted, considering several waste generation scenarios at both retail and user levels to quantitatively estimate the degree of waste prevention that would justify the use of biocides. The trade-off between reduced resource use due to spoilage prevention and the environmental impacts of biocide production and use was also quantified.
The results show that there are waste generation thresholds below which the addition of biocides is not justified. These thresholds depend largely on the environmental impact category analyzed, highlighting the importance of policy considerations when selecting the most relevant impacts. The uncertainty associated with each impact category was also taken into account to increase the robustness of the study and to demonstrate significant differences in impact between the two products.
The findings of this study can inform policymaking by providing quantitative estimates regarding the use of biocides in the paint sector. In addition, the guideline can support LCA practitioners working with waste prevention models by helping to reduce data collection time and costs.

4.01.T04 Potential of Reclaimed R-32 Refrigerant in Reducing Greenhouse Gas Emissions and Supporting National Climate Change Policy

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Due to the problem of climate change, the demand for air conditioners has increased. The use of R-32 refrigerant in air conditioning systems has significantly increased over the past six years. This refrigerant has a high global warming potential. Reusing refrigerant (known as 'reclaiming') is one approach to help reduce the impact on global warming. However, cooling efficiency must also be considered. This project aims to compare the cooling performance of a vapor-compression system using virgin R-32 refrigerant and reclaimed R-32 refrigerant. The experiment was conducted in a 17.4 m2 room using a 12,100 Btu air conditioner at room temperatures of 24, 25, and 26 degrees Celsius. Temperature data were collected from 10:00 a.m. to 2:00 p.m. at the inlet and outlet of the evaporator coil, compressor, condenser coil, and expansion valve, in order to calculate the Coefficient of Performance (COP) and Energy Efficiency Ratio (EER).
The experimental results showed that the system using reclaimed refrigerant had average COP and EER values approximately 8–10% higher than the system using virgin refrigerant. The reclaimed refrigerant had COP values ranging from 3.26 to 4.05 and EER values ranging from 10.25 to 12.73 Btu per watt-hour, while the virgin refrigerant had COP values ranging from 3.14 to 3.79 and EER values ranging from 9.86 to 11.89 Btu per watt-hour. The life cycle assessment results of refrigerant use, based on a functional unit defined by the amount of refrigerant corresponding to cooling capacity (Btu), indicate that greenhouse gas emissions can be reduced by 11–15 times. Therefore, using reclaimed refrigerant is one approach to help reduce the impact on global warming. However, cooling efficiency must be considered alongside it.

4.01.T05 Integrated LCA and Process Modeling for Critical Raw Materials Recovery from Produced Water

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This study evaluates the environmental and operational feasibility of recovering critical raw materials (CRM) from offshore produced water using an integrated modelling and sustainability assessment

framework. Produced water contains low concentrations of elements such as lithium (Li ~6 ppm), magnesium (Mg ~630 ppm), boron (B ~86 ppm) and silicon (Si ~22 ppm), but very large volumes create a potentially relevant cumulative resource.

The approach combines geochemical modelling, hydrodynamic simulation and life cycle assessment (LCA) to assess the viability of recovery under field-relevant conditions. A thermodynamic model is used to predict precipitation behaviour and identify feasible operating windows, while dynamic flow conditions are evaluated through transport modelling. Experimental validation is performed using a continuous flow laboratory system designed to reproduce temperature, pressure and flow conditions representative of offshore operations.

The study explicitly distinguishes between total removal and recoverable fraction, addressing a key uncertainty in precipitation-based recovery systems. Environmental performance is assessed using LCA with a focus on ecotoxicity, where preliminary results indicate up to 63.7% reduction due to removal of dissolved metals.

A screening-level techno-economic layer is integrated to estimate energy demand, chemical consumption and cost per treated water volume, enabling evaluation of both environmental and economic trade-offs.

The framework is applied to representative produced water compositions and compared conceptually to conventional supply routes for critical raw materials. The objective is not to maximise recovery, but to determine whether combined effects of scaling mitigation and selective recovery can create a viable operational or environmental case.

The results provide decision-relevant insights into the conditions under which CRM recovery from produced water may be beneficial, supporting early-stage screening and reducing uncertainty prior to pilot-scale investment.

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