

IOCTO
3rd Edition
2026
Conference

The 3rd International Online Conference on Toxics

9–11 September 2026 | Online

Program and Abstract Book

Organizers



Media Partners



The 3rd International Online Conference on Toxics

9–11 September 2026 | Online



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Organised by



Conference Secretariat

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Welcome from the Chairs

On behalf of the MDPI journal *Toxics* (ISSN: 2305-6304; Impact Factor: 4.9) and its Scientific Committee, I am pleased to invite you to participate in the **3rd International Online Conference on Toxics (IOCTO2026)**. This meeting will be held **online from 9-11 September 2026**.

The aim of this platform is to bring together students, researchers, and scientists from around the world to present their work and exchange ideas on the exposure, effects, and risks regarding chemicals and materials in terms of humans and the natural environment, as well as on the development of new approaches to assess and/or manage the toxicological and ecotoxicological risks of chemicals and materials.

The topics are organized into five sessions, corresponding to the following journal sections:
S1. Exposure Routes / Exposome of Emerging Contaminants and Materials in the Environment;
S2. Wildlife Ecotoxicology, Sentinel Species, and Ecosystem Health;
S3. Innovating Toxicology: NAMs and Computational Tools for Next-Generation Risk Assessment;
S4. Molecular and Cellular Mechanisms, Comparative Toxicology, and Multi-Omics Integration;
S5. Risk assessment, Policy, and Environmental Justice in Chemical Safety.

Submitted abstracts will be reviewed by the conference committee and, if accepted, authors can choose to submit an extended proceedings paper of their work. All accepted abstracts will be published as one dedicated volume in the *Environmental and Earth Sciences Proceedings* (ISSN: 3042-5743).

The 3rd International Online Conference on Toxics offers you the opportunity to participate in this international, scholarly conference without having the concern or expenditure of travel fees. We would like to invite you to “attend” this conference by presenting your latest work. Abstracts (in English) should be submitted online before **5 June 2026**.



Dr. Natalia Garcia-Reyero
Conference Chair

Institute for Genomics, Biocomputing &
Biotechnology, Mississippi State
University, Starkville, MS, USA



Dr. Carlos Barata
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Institute of Environmental
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Toxics (ISSN 2305-6304) is an international, peer-reviewed, open access journal which provides an advanced forum for studies related to all aspects of toxic chemicals and materials. It publishes reviews and regular research papers. Our aim is to encourage scientists to publish their experimental and theoretical results in detail. There is, therefore, no restriction on the maximum length of the papers, although authors should write their papers in a clear and concise way. The full experimental details must be provided so that the results can be reproduced. Electronic files or software regarding the full details of calculations and experimental procedure can be deposited as supplementary material, if it is not possible to publish them along with the text.

Impact Factor: 4.4 (2024); 5-Year Impact Factor: 5.7 (2024)

Invited Speakers



Prof. Dr. Alesia Ferguson
College of Science and Technology,
North Carolina Agricultural and
Technical State University, Built
Environment Department,
Greensboro, NC, USA



Prof. Dr. Antonella Smeriglio
Department of Chemical,
Biological, Pharmaceutical
and Environmental Sciences
(CHIBIOFARAM), University of
Messina, Messina, Italy



Prof. Dr. Antonia Concetta Elia
Department of Chemistry,
Biology and Biotechnology,
University of Perugia,
Perugia, Italy



Dr. Antonio Peña-Fernández
Department of Surgery, Medical and
Social Sciences, Faculty of
Medicine and Health Sciences,
University of Alcalá, Madrid, Spain



Prof. Dr. Chris Martyniuk
University of Florida,
Gainesville, FL, USA



Dr. Igor V. Tetko
Helmholtz Munich -Research
Center for Environmental Health
(GmbH), Neuherberg, Germany
& BIGCHEM GmbH,
Unterschleißheim, Germany



Dr. Ilaria Guagliardi
National Research Council (CNR) -
Institute for Agricultural and Forestry
Systems in the Mediterranean
(ISAFOM), Rende (CS), Italy



Dr. Ovokeroye Abafe
Brunel University of London,
London, UK



Dr. Sara Tramontini
European Food Safety Authority
(EFSA), Plant Health Unit (PLH),
Parma, Italy



Prof. Dr. Wei Shi

School of Environment, Nanjing
University, Nanjing, Jiangsu, China



Dr. Xiaotao Shen

Nanyang Technological
University, Singapore

Program Overview

Time in CEST	9 September Wednesday	10 September Thursday	11 September Friday
Morning 9:00-12:00	Session 4. Molecular and Cellular Mechanisms, Comparative Toxicology, and Multi-Omics Integration Flash Poster (Session 4)	Session 3. Innovating Toxicology: NAMs and Computational Tools for Next-Generation Risk Assessment Flash Poster (Session 3)	Session 1. Exposure Routes/Exposome of Emerging Contaminants and Materials in the Environment Flash Poster (Session 1)
	Break		
Afternoon 14:00-17:00	Chair Welcome Speech Session 5. Risk Assessment, Policy, and Environmental Justice in Chemical Safety Flash Poster (Session 5)	Session 2. Wildlife Ecotoxicology, Sentinel Species, and Ecosystem Health Flash Poster (Session 2)	

IOCTO2026 Program

9 September 2026 (Wednesday)

Session 4. Molecular and Cellular Mechanisms, Comparative Toxicology, and Multi-Omics Integration

Time: 9:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
9:00–9:05	Prof. Dr. Yankai Xia Session Chair	<i>Welcome from Session Chair</i>
9:05–9:25	Dr. Xiaotao Shen Invited Speaker	MAPA: A Semantic Network Framework For Functional Module Discovery And Interpretation In Multi-Omics Data
9:25–9:45	Prof. Dr. Chris Martyniuk Invited Speaker	New Approach Methods To Study The Toxicity Of Perfluorinated Chemicals
9:45–10:00	Mikhail Novikov Oral Speaker	Comparative Assessment Of Contrast Enhancement Properties Of Gadolinium-Based MRI Contrast Agents
10:00–10:15	Laia Garcia Ferran Oral Speaker	Extracellular Vesicle Release Reflects Dose-Dependent Hepatotoxic Responses In HepG2 Cells
10:15–10:30	Federica Bovio Oral Speaker	Analyzing Cadmium-Driven Biochemical Changes: A Multi-Disciplinary Approach For The Evaluation Of Neuron And Microglia Models
10:30–10:45	Mai Awad Oral Speaker	Oxidative DNA Damage and Repair Disruption Under Pesticide–Metal Co-Exposure
10:45–11:00	Yuting Cheng Oral Speaker	IM-MOTIC: An AI-Assisted Evidence-Driven Framework for Mechanism Mining, Target Exploration, and Validation in Environmental Chemical Toxicity
11:00–11:15	Wei Wu Oral Speaker	Parental-Origin-Divergent m6A Remodeling Mediates Transgenerational Male Reproductive Toxicity Of PFHpA Via PPAR α -Dependent Steroidogenic Disruption
11:15–11:35	Flash Poster Presentations	Austėja Vitkauskaitė Effects of Selenium on Iron Concentration and Catalase Activity in Mouse Liver under Aluminum Exposure Paula Barciela Álvarez Systems-Level Effects Of Plant-Based Cognitive Enhancer Extracts: A Multi-Omics Perspective Maria Inês Monteiro Machado An Inflamed Gut Is Not Always A Leaky Gut: Mycotoxin Permeability In A Co-culture Model Antônio Tonon Bissoli Effects Of Exposure To Tributyltin On Endothelium-Dependent Vasodilation in Mesenteric Resistance Arteries of Wistar Rats
11:35–11:55	Prof. Dr. Antonella Smeriglio Invited Speaker	Misidentification Of Edible And Poisonous Wild Plants In The Mediterranean Area: A Multidisciplinary Approach To Food Safety And Forensic Toxicology
11:55–12:10	Manuela D. Machado Oral Speaker	Toxicological Impacts of Fluoxetine on the Freshwater Microalga <i>Raphidocelis Subcapitata</i> : A Multi-Endpoint Assessment

BREAK

Session 5. Risk Assessment, Policy, and Environmental Justice in Chemical Safety**Time: 14:00 (CEST, Basel) | 8:00 (EDT, New York) | 20:00 (CST Asia, Beijing)**

CEST Time	Speaker	Title
14:00–14:10	Dr. Natalia García-Reyero Dr. Carlos Barata Event Chairs	<i>Welcome from Event Chairs</i>
14:10–14:20	Dr. Gunnar Toft Session Chair	<i>Welcome from Session Chair</i>
14:20–14:40	Dr. Antonio Peña-Fernández Invited Speaker	Linking Chemical And Biological Hazards n Risk Assessment An Interdisciplinary Approach To Evaluating Environmental Contaminants And Emerging Zoonotic Opportunistic Human Pathogens With Relevance For Human Health Protection
14:40–15:00	Prof. Dr. Alesia Ferguson Invited Speaker	Role Of Children's Activities In Their Early Exposures To Chemicals
15:00–15:15	Laura García Cansino Oral Speaker	Enantioselective Determination Of Duvelisib In Wastewater Samples By Electrokinetic Chromatography After μ SPEd Preconcentration
15:15–15:30	Luthando Lukhanyo Tiya Oral Speaker	Distinct Toxicological Profiles Of Pesticide Metabolites Compared To Parent Compounds: Evidence From A Zebrafish Model
15:30–15:45	Ana-Marija Valland Oral Speaker	Genotoxicity Biomarkers In Healthcare Workers Occupationally Exposed To Antineoplastic Drugs: A Systematic Review And Meta-Analysis
15:45–16:00	Vera Vokina Oral Speaker	Methodological Approaches To A Biological Model For Validating Health Damage Criteria Following Wildfire Smoke Exposure
16:00–16:15	Roberto Bava Oral Speaker	Clinical Masking Of Insecticide Toxicity: Pharmacological Antagonism Between Flupyradifurone And Deltamethrin In Honeybees (<i>Apis Mellifera</i>)
16:15–16:30	Ronnel Nolos Oral Speaker	Heavy Metal(Loid) Contamination In A Mining-Impacted Island Province In The Philippines: A Systematic Review
16:30–16:45	Flash Poster Presentations	Daniil N. Malyshev Quantitative Determination Of Toxic Elements In Imidazolium-Based Ionic Liquids By Inductively Coupled Plasma Mass Spectrometry Eduardo Morais Beretta Systematic Review: Does Glyphosate Exposure Cause Cancer? Mirta Milić Spatial Assessment of Environmental Vulnerability Using Multicriteria Geospatial Analysis as a Tool for Integrated Pollution Management in the Grande Tulancingo River, Mexico

END OF DAY 1

10 September 2026 (Thursday)

Session 3. Innovating Toxicology: NAMs and Computational Tools for Next-Generation Risk Assessment**Time: 9:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)**

CEST Time	Speaker	Title
9:00–9:10	Dr. Emilio Benfenati Session Chair	<i>Welcome from Session Chair</i>
9:10–9:30	Dr. Igor V. Tetko Invited Speaker	The Rise Of AI Methods In Computational Toxicology: Limitations, Advantages And Perspectives
9:30–9:50	Prof. Dr. Wei Shi Invited Speaker	NAMs For Screening Of Endocrine Disrupting Chemicals
9:50–10:05	Ibrahim Hamisu Abdul Oral Speaker	GC–MS Characterization, Brine Shrimp Lethality, And In Silico Toxicity Prediction Of Alkaloid Fractions From The Stem Bark Of Nauclea Diderrichii
10:05–10:20	Tithi Paul Oral Speaker	Filling Monitoring Gaps in Freshwater Pesticide Surveillance Using Random Forest Machine Learning
10:20–10:35	Gabriel Pereira Oral Speaker	Combining Explicit Molecular Features And Latent ChemBERTa Embeddings For Ecotoxicological Screening
10:35–10:50	Núria Ferrer-Cortés Oral Speaker	Optimization Of ICP-MS/MS-Based Methodology For Multielemental Analysis In Follicular Fluid: New Approaches In Female Infertility Research
10:50–11:05	Ilse Van Overmeire Oral Speaker	In Silico Assessment Of The Endocrine Disrupting And Genotoxic Potential Of Bisguaiacols As Possible Bisphenol A Alternatives
11:05–11:25	Flash Poster Presentations	Ani Tevosyan Improved Prediction Of Chemical Carcinogenicity Based On Hybrid In Silico/In Vitro Methodology Peihao Wu Multimodal AI Generates Virtual Rats: Predicting Hepatic Burden of Oral Drugs Sezen Yılmaz Sarıaltın Integrated In Silico Assessment Of Environmental And Human Toxicity Of Carbamazepine As A Pseudo-Persistent Emerging Contaminant Bruna De Bessa Alves Human Umbilical Artery as a New Approach Methodology (NAM) to Assess Thyroid-Disruptive Vascular Effects of Emerging Contaminant Mixtures
11:25–11:40	Katherine Virginia Bouchard Oral Speaker	How Optimization Of Skin Sensitization And Photoirritation Assays Are Advancing In Vitro Photoallergy Assessment

BREAK

Session 2. Wildlife Ecotoxicology, Sentinel Species, and Ecosystem Health

Time: 14:00 (CEST, Basel) | 8:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
14:00–14:10	Prof. Dr. Jose V. Tarazona Session Chair	<i>Welcome from Session Chair</i>
14:10–14:30	Prof. Dr. Antonia Concetta Elia Invited Speaker	Expanding The Ecotoxicological Toolbox For Ecosystem Health: Native And Non-Native Wildlife Models
14:30–14:50	Dr. Sara Tramontini Invited Speaker	The Assessment Of Impacts To Ecosystem Services Caused By Invasive Plant Pests In The EU: The New EFSA Approach
14:50–15:05	Winkins Santosh Oral Speaker	Assessment Of Combined Methylparaben And Diethyl Phthalate Exposure On Developmental And Behavioral Toxicity In Zebrafish (Danio Rerio) Embryos And Larvae
15:05–15:20	Leonid Antonov Oral Speaker	Responses Of Water Fleas Against A Complex Mixture Of Pollutants: Using Daphnia Magna To Understand Cocktail Effects
15:20–15:35	Teresa Chianese Oral Speaker	Effects Of Arsenic Exposure On Oxidative And Cellular Stress In Lymnaea Stagnalis
15:35–15:50	Roger Busom Casado Oral Speaker	Coastal To Oceanic Comparison Of Plastic Additive Accumulation In Northeast Atlantic Top Predator Sharks
15:50–16:05	Thimo Groffen Oral Speaker	Comparative stress responses of two freshwater bivalves to emerging PFAS contaminants
16:05–16:20	Paulo Vale Oral Speaker	Retrospective Study Of Seagull Poisonings In Central Portugal: Can Marine Phycotoxins Be Involved?
16:20–16:35	Anne Leung Oral Speaker	The Impact of Cigarette Filters on Aquatic Ecosystems Using Daphnids as Model Organisms
16:35–17:00	Flash Poster Presentations	Sabrina Balsamo Hepatic And Reproductive Toxicity Of Glyphosate Exposure In The Terrestrial Bioindicator Podarcis Siculus Sophia Vidal Occurrence And Bioaccumulation Of PFAS In Bivalve Mollusks: A Systematic Review Clara Naccari Blue Crab Callinectes Sapidus a New Sentinel Species of Metals Pollution in Mediterranean Sea Sebastian Felipe Hidalgo Torres Spatio-Temporal Dynamics of Arsenic and Its Relationship with Physicochemical Parameters in the Tampamachoco Lagoon, Veracruz, Mexico

END OF DAY 2

11 September 2026 (Friday)

Session 1. Exposure Routes/Exposome of Emerging Contaminants and Materials in the Environment**Time: 9:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)**

CEST Time	Speaker	Title
9:00–9:10	Prof. Dr. Rakesh Kanda Session Chair	<i>Welcome from Session Chair</i>
9:10–9:30	Dr. Ilaria Guagliardi Invited Speaker	A Critical Comparative Assessment Of Inductively Coupled Plasma Mass Spectrometry (ICP-MS) And X-Ray Fluorescence (XRF) Methodologies For High-Resolution Determination Of Potentially Toxic Elements In Soil Matrices
9:30–9:50	Dr. Ovokeroye Abafe Invited Speaker	PFAS Exposure In South Africa: Concentrations In Food, Drinking Water And Matched Breast Milk And Serum
9:50–10:05	Ushemegbe Rita Ekhareifo Oral Speaker	Ecological Risk Assessment Of Soils Near Abandoned Pb–Zn Mines In Nigeria
10:05–10:20	Roger Lyrio dos Santos Oral Speaker	Effects Of Tributyltin Exposure On Endothelium-Dependent Coronary Vasodilation In Female Rats
10:20–10:35	Kannalinya Boontee Oral Speaker	Blood And Urine Heavy Metal Level In E-Waste And Non-E-Waste Workers
10:35–10:50	Amir Sapir Oral Speaker	PFOS At Human-Relevant Concentrations Activates A KLF-1–P450 Mitochondrial Protective Axis In Caenorhabditis Elegans
10:50–11:05	Rafael Bertini Simião Oral Speaker	Multispecies Physiological Disruption By Metabolic Contaminants And Sweeteners: Implications For Aquatic Ecosystem Functioning
11:05–11:20	Yu-ting Wei Oral Speaker	Dual-Source Heavy Metal Co-Exposure Impairs Genetic Growth Potential In Preschool Children: A Large Population-Based Mixture Analysis
11:20–11:40	Flash Poster Presentations	Surajit De Mandal Dietary Exposure To Microbial Contaminants And Antibiotic Resistance Genes: Metagenomic Insights From Traditional Fermented Pork Fat Ukam Uno-Ubarei Uno Modulatory Effects Of Vitamin C On Lead Induced Organotoxicity And Histopathology In Male Albino Rats Franciele Domingos Environmental Implications Of Caffeine Exposure On Terrestrial Plant Establishment Ramona Zgavarogea Trace Element Bioaccumulation In Meat And Bone Samples: Environmental Exposure, Nutritional Relevance And Food Chain Transfer
11:40–11:55	Alison K. Bauer Oral Speaker	Polycyclic Aromatic Hydrocarbons And Sugarcane Workers In Guatemalan

END OF IOCTO 2026

Poster List

Submission ID	Authors	Title
Session 1. Exposure Routes/Exposome of Emerging Contaminants and Materials in the Environment		
Sciforum-191216	Tunzeel Iqbal	Tamarix aphylla Leaves Synthesized Biochar Loaded Fe doped MgO Nanocomposites for Dye Pollutants Removal from Water
Sciforum-187310	Maria Carolina Ramirez Hernandez	Chronic diuron exposure alters photosynthetic pigments and antioxidant responses in Eichhornia crassipes
Sciforum-186530	Piotr Kowalczyk	A Simple Method for Quantifying and Characterizing Microplastics at Ultra-Low Concentrations
Sciforum-187060	Anamaria Iulia Török	Comparative evaluation of Chlorella vulgaris and Salvinia natans for the treatment of Mining Wastewaters
Sciforum-194093	Rana Muhammad Mubeen Muhsin	Environmental Monitoring of Perfluoro octane Sulfonate and Perfluorooctanoic Acid in Khanpur Stream, Pakistan: Implications for Human and Ecosystem Health
Sciforum-194240	Ukam Uno-Ubarei Uno	Modulatory effects of vitamin C on lead induced organotoxicity and histopathology in male albino rats.
Sciforum-188296	Ramona Zgavarogea	Trace Element Bioaccumulation in Meat and Bone Samples: Environmental Exposure, Nutritional Relevance and Food Chain Transfer
Sciforum-186528	Franciele Domingos	Environmental Implications of Caffeine Exposure on Terrestrial Plant Establishment.
Sciforum-186531	Anca Becze	Adaptive Monitoring of Climate-Driven Contaminant Pulses: An Integrated Analytical and AI Framework
Sciforum-183762	Abdulwaris Tijani	Assessment Of The Exposome And Exposure Routes Of Antibiotic Residues And Heavy Metals In Birds: Implications For Ecosystem Health-A Systematic Review
Sciforum-186881	Mabel Diaz-Cubilla	Multiparametric Assessment of Microbial Viability in Anaerobic Reactors Exposed to Emerging Contaminants Using Flow Cytometry and Fluorescence Microscopy
Sciforum-186304	Kannalinya Boontee	Blood and Urine Heavy Metal Level in E-Waste and Non-E-Waste Workers
Sciforum-186903	Henrique Costa	Bisphenol F and AF Impair Cerebral Vascular Reactivity via Adrenergic and Nitric Oxide Pathways
Sciforum-193435	Yujie Wang	Preparation of Size-Defined TPU Nano- and Microplastics and Their Cellular Uptake by RAW264.7 Macrophages
Sciforum-187239	Catarina Guimarães	Multiple Drivers of the Spatial Heterogeneity of Microplastics in Dam-Influenced Freshwater Systems
Sciforum-195148	Ukam Uno-Ubarei Uno	Effect of Aflatoxin Contamination on Oxidative Stress, Hematological Indices, and Growth Performance of Broiler Chickens

Sciforum-186541	Katarzyna Jażdżewska	Hidden Losses: Do Isolation Protocols Degrade Microplastics in Food Analysis?
Sciforum-191109	Bukola Obe	Micro-plastics and Nano-plastics as Emerging Contaminants: A Systematic Review of Human Exposure Routes and Epidemiological Evidence of Health Outcomes
Sciforum-187333	Joanna Antos	µSPEED microextraction of veterinary antibiotics in environmental water samples by UPLC
Sciforum-186787	Lacrimioara Senila	PVC, CTA, and PLA-based polymer inclusion membranes for selective removal of metal ions from wastewater
Sciforum-187294	Anna Weronika Sobańska	Organic Sunscreens - infant exposure via breastfeeding
Sciforum-180764	Surajit De Mandal	Dietary Exposure to Microbial Contaminants and Antibiotic Resistance Genes: Metagenomic Insights from Traditional Fermented Pork Fat
Sciforum-186256	Marin Senila	Development of a Passive Sampler Based on Polymer Inclusion Membrane for Uptake of Cu(II) in Wastewater
Sciforum-187316	Raúl Todolí-Carbonell	Bioaccessibility of Metals and Metalloids in Microplastics: In Vitro Digestive Simulation Under Fed Conditions
Sciforum-187076	Marina Bastante-Rabadán	Combined Exposure to Ciprofloxacin and Polystyrene Microplastics: Responses of Aquatic Organisms and Electroactive Bacteria
Sciforum-193412	Emilia Neag	Removal of ammonium from aqueous solutions using low-cost adsorbents
Sciforum-184988	Jun Luo	Combined analysis of microplastic quantification and blood metabolomics for spotted seal mothers and their calves
Sciforum-186534	Natalia Nowak	How Bioavailable Are Polypropylene Microplastics? In Vitro Evidence and Potential Health Relevance
Sciforum-185080	Khaoula Fouzai	Screening and Environmental Safety Assessment of Biosurfactant-Producing Bacteria from Tunisian Soil
Session 2. Wildlife Ecotoxicology, Sentinel Species, and Ecosystem Health		
Sciforum-172292	Edgar Alexander Zapata Vivenes	Autotomy and antioxidant responses as biomarkers of acute and chronic contaminant stress in <i>Eurythoe complanata</i>
Sciforum-187320	Clara Naccari	Blue crab <i>Callinectes sapidus</i> a new sentinel species of metals pollution in Mediterranean Sea
Sciforum-187229	Ivo Pinto	Developmental and biochemical responses of <i>Danio rerio</i> embryos exposed to cyanobacteria
Sciforum-187234	Barbara Caldaroni	Bioaccumulation of trace metals and oxidative stress responses in <i>Apis mellifera</i> across different land use types
Sciforum-187025	Mirta Milić	Optimisation of coelomocyte extrusion for genotoxicity biomonitoring in <i>Eisenia fétida</i>
Sciforum-187163	Rafael Pereira dos Santos	Ecotoxicolipidomics in fish under field conditions: a systematic review of lipid-based responses to environmental contamination
Sciforum-194376	Ali Amini Harandi	Tire Wear Particles and 6PPD-Quinone in Freshwater Ecosystems: Ecotoxicological Effects, Food-Web Transfer, and One Health Implications

Sciforum-187245	Sebastian Felipe Hidalgo Torres	Spatio-temporal dynamics of arsenic and its relationship with physicochemical parameters in the Tampamachoco lagoon, Veracruz, Mexico
Sciforum-193196	Sophia Vidal	Occurrence and Bioaccumulation of Pfas In Bivalve Mollusks: A Systematic Review
Sciforum-186340	Samuel Fernandes Santos	Ecological assessment of two Portuguese estuaries under contrasting urban pressure: Douro vs Lima
Sciforum-180448	Hadia Benhalima	Biomonitoring Soil Health: Ecotoxicological Impact of Multi-Metal Mixtures on the Sentinel Earthworm <i>Aporrectodea giardi</i>
Sciforum-186505	Suzana Žunec	Assessment of Pb neurotoxicity in European brown bears: Evidence from Pb–Ca associations and oxidative stress biomarkers
Sciforum-193616	Sara Futia	Biochemical stress responses in <i>Procambarus clarkii</i> exposed to pristine and aged glitter
Sciforum-187347	Akemi Wiermann Okazaki	Acute toxicity of Nicosulfuron- and S-metolachlor-based herbicides in mixture to <i>Artemia salina</i>
Sciforum-193952	Sabrina Balsamo	Hepatic and Reproductive Toxicity of Glyphosate Exposure in the Terrestrial Bioindicator <i>Podarcis siculus</i>
Sciforum-186933	Ana S. Oliveira	From streets to streams: Insights on the ecotoxicological effects of stormwater runoff on <i>Danio rerio</i> embryos
Sciforum-187021	Mirta Milić	Biomarkers of DNA damage in common carp inhabiting an agriculturally impacted lake in Mexico
Sciforum-194142	Libertad Juárez-Santacruz	Ecotoxicological Risk of Sediments from the Salado River Using Earthworms (<i>Eisenia</i> sp.)
Session 3. Innovating Toxicology: NAMs and Computational Tools for Next-Generation Risk Assessment		
Sciforum-186931	Argel Islas-Robles	Pushing the Limits: Expanding the Applicability Domain of EpiSensA for Skin Sensitization Assessment
Sciforum-187258	Anne Josiele de Lima Vital	Exploring the mechanistic connection between nephrotoxicity and aquatic toxicity: an approach using structure-based computational alerts
Sciforum-186799	Ani Tevosyan	Improved Prediction of Chemical Carcinogenicity Based on Hybrid In Silico/In Vitro Methodology
Sciforum-187232	Argel Islas-Robles	Optimization of the Human Cell Line Activation Test (h-CLAT) for the Identification of Photo-Allergens
Sciforum-191693	Vasanthakannan VM	Theoretical analysis of HCN detection using sumanene-based nanostructures
Sciforum-186263	Margarida Vilaça	Aryl hydrocarbon receptor pathway activation in fish hepatocytes exposed to fire-associated contaminants under elevated temperature
Sciforum-186007	Hung-Lin Kan	ZODDs: A Zebrafish Organ-Specific and Dose-Response Database for Environmental Chemical Mixtures
Sciforum-191485	Peihao Wu	Multimodal AI Generates Virtual Rats: Predicting Hepatic Burden of Oral Drugs
Sciforum-186855	Sezen Yilmaz Sarialtın	Integrated in Silico Assessment of Environmental and Human Toxicity of Carbamazepine as a Pseudo-persistent Emerging Contaminant

Sciforum-187267	Bruna De Bessa Alves	Human Umbilical Artery as a New Approach Methodology (NAM) to assess thyroid-disruptive vascular effects of emerging contaminant mixtures
Sciforum-194377	Ali Amini Harandi	Machine Learning in Environmental Toxicology: Predicting Endocrine Disruption and Cross-Species Toxicity of Emerging Contaminants
Sciforum-187136	Gayathree Thenuwara	Colour-Encoded Gold Nanostructure-Based Lateral Flow Immunoassay with Smartphone-Based Digital Analysis for Rapid Mycotoxin Screening
Session 4. Molecular and Cellular Mechanisms, Comparative Toxicology, and Multi-Omics Integration		
Sciforum-182615	Madson Silveira de Melo	Pyriproxyfen disrupts liver development in <i>Gallus domesticus</i> embryos at environmentally relevant concentrations
Sciforum-187123	Marta Moreno-Torres	Pollutant exposure and pre-existing steatosis sensitize human hepatocytes to drug-induced liver injury
Sciforum-187369	Mónica Gómez-Zamora	Cellular Genotoxicity of Commercial Herbal Products Containing <i>Moringa oleifera</i> and <i>Tecoma stans</i> in Human Lymphocytes
Sciforum-184541	Anum Feroz	Biochemical Disruption of Glutathione-Dependent and Independent Antioxidant Defense Systems under Synergistic Pesticide Exposure in <i>Trogoderma granarium</i>
Sciforum-187031	Levente Levei	Biomonitoring of air pollution in Cluj-Napoca city using tree leaves
Sciforum-193696	Sini Macheri	Investigation of Cellular and Molecular Mechanisms of PFAS-Induced Lung Inflammation in a Human Alveolar Epithelial Cell Line
Sciforum-187217	Antônio Tonon Bissoli	Effects of Exposure to Tributyltin on Endothelium-Dependent Vasodilation in Mesenteric Resistance Arteries of Wistar Rats
Sciforum-187301	Austėja Vitkauskaitė	Effects of Selenium on Iron Concentration and Catalase Activity in Mouse Liver under Aluminum Exposure
Sciforum-179191	Rasa Bernotiene	Attenuation of Cadmium-, Nickel-, and Lead-Induced Oxidative Stress by Green Tea Extract in a Murine In Vivo Model
Sciforum-184899	Marco Aurelio M. Freire	Chronic methylmercury exposure alters astrocytic morphology and NADPH diaphorase reactivity in the rat frontal cortex
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Sciforum-187533	Ana O. S. Jorge	Speciation Uncertainty as the Dominant Driver of Arsenic Risk Characterization in Tuna: A Probabilistic Sensitivity Analysis
Sciforum-186694	Agnieszka Chłopaś-Konowalek	Back to basics – a case of multidrug intoxication involving 6-APB, known on the black market as benzofury
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Session 1. Exposure Routes/Exposome of Emerging Contaminants and Materials in the Environment

sciforum-180764: Dietary Exposure to Microbial Contaminants and Antibiotic Resistance Genes: Metagenomic Insights from Traditional Fermented Pork Fat

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Traditional foods can represent important dietary sources of chemical and microbial exposures, yet their composition and potential health implications remain poorly characterized. This study aimed to comprehensively characterize the nutritional composition, lipid profile, and microbial community of a traditional fermented pork fat from Northeast India. Six samples of fermented pork fat were collected from different regions were analyzed using physicochemical methods, electrospray ionization mass spectrometry (ESI+-MS), and 16S rRNA gene amplicon sequencing with PICRUSt-based functional prediction. Physicochemical analysis showed that sam consisted predominantly of fat (~91% dry weight), with minor amounts of carbohydrates and proteins. Lipid profiling identified diverse mono-, di-, and triacylglycerides, including myristic acid-containing acylglycerides, sterols, and both saturated and unsaturated lipid species, reflecting a complex dietary lipid composition. Metagenomic analysis identified 72 bacterial genera, dominated by the phyla Firmicutes, Proteobacteria, and Bacteroidetes, with *Clostridium* representing the most abundant genus. Functional prediction suggested that the microbial community was primarily associated with energy, carbohydrate, amino acid, and lipid metabolism. PICRUSt analysis also predicted genes related to antibiotic resistance and bacterial components such as flagellin and lipid A biosynthesis, mainly associated with members of Bacillaceae, Bacteroidaceae, Clostridiaceae, Corynebacteriaceae, and Enterobacteriaceae. The analysis suggests that this traditional fermented pork may represent a potential source of microbial hazards; however, further in-depth studies are required to confirm the presence of viable pathogenic microorganisms, expressed virulence factors, and associated health risks. By integrating nutritional profiling, and metagenomic characterization, this study provides the first comprehensive assessment a traditional fermented foods. The findings establish a baseline for future quantitative exposure assessment and risk evaluation of culturally important fermented foods.



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sciforum-183762: Assessment of the Exposome and Exposure Routes of Antibiotic Residues and Heavy Metals in Birds: Implications for Ecosystem Health—A Systematic Review

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Introduction

The widespread use of antibiotics and environmental accumulation of heavy metals have increased contaminant exposure in birds, threatening wildlife, ecosystem integrity, and public health. Birds acquire these contaminants through multiple pathways, contributing to antimicrobial resistance (AMR) dissemination and environmental pollution. Understanding the exposome and major exposure routes is essential for developing effective mitigation strategies. This systematic review synthesized evidence on the occurrence, exposure pathways, and ecological impacts of antibiotic residues and heavy metals in birds.

Methods

A systematic review was conducted following PRISMA 2020 guidelines. Scopus, Web of Science, PubMed, and Google Scholar were searched for studies published between 2000 and 2025 using keywords including “antibiotic residues,” “heavy metals,” “birds,” “exposure routes,” “manure,” and “ecosystem impact.” Out of 182 records, 145 remained after duplicate removal. Following title and abstract screening, 52 full-text articles were assessed, and 25 studies met the inclusion criteria for qualitative synthesis.

Results

Among the 25 included studies, contaminated feed (18 studies), drinking water (16), soil and sediments (15), and environmental deposition (11) were the most frequently reported exposure routes. Cadmium (17), lead (15), mercury (12), and arsenic (10) were the predominant heavy metals detected, while antibiotic residues were commonly identified in feces, muscle, and eggs. Seventeen studies reported that bird droppings facilitated environmental dissemination of antibiotic residues and AMR determinants. Fifteen studies documented heavy metal bioaccumulation with transfer to surrounding soil and aquatic ecosystems. Thirteen studies found that improved feed management, reduced antibiotic use, and better waste management were associated with lower environmental contaminant loads.

Conclusions

Birds are important reservoirs and environmental vectors of antibiotic residues and heavy metals through multiple exposure pathways. Mapping the exposome supports integrated monitoring and sustainable interventions to reduce contaminant release, limit AMR dissemination, and protect ecosystem health.



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sciforum-184988: Combined analysis of microplastic quantification and blood metabolomics for spotted seal mothers and their calves

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The present study set out with the objective of systematically revealing the impact of microplastics transplacental on the metabolic physiology of spotted seal offspring. To this end, microplastics were quantitatively detected in placental tissues from the same batch of spotted seal mothers and their fetuses. Furthermore, peripheral serum samples from mothers and pups were analysed and compared using non-targeted metabolomics techniques. The results demonstrated that PVC was the most prevalent polymer detected in placental tissue, with an average concentration of 4.718 $\mu\text{g/g}$ on the maternal side, while the concentration decreased to 1.105 $\mu\text{g/g}$ on the fetal side, yet still dominated among all detected polymers. Furthermore, PE and PS exhibited a clear "transfer from maternal to fetal side" characteristic; the average concentration of PE on the maternal side was 2.527 $\mu\text{g/g}$, while it decreased to 0.104 $\mu\text{g/g}$ on the fetal side. This finding suggests that, despite the placental barrier's capacity to intercept certain polymers (including PVC, PS, and PE), microplastic particles can nevertheless traverse this barrier and gain entry into the fetus. At the metabolomics level, the study identified 499 differentially expressed metabolites in the serum of mothers and offspring. The analysis revealed that the offspring group exhibited a significant enrichment of metabolites, predominantly comprising small peptides, nucleotides, phospholipids, and metabolites of exogenous compounds. Multivariate statistical analysis demonstrated a clear separation of the metabolomic profiles of offspring and mothers along principal component 1 (PCA1, variance contribution rate 49.1%), and the PLS-DA model ($R^2Y=0.999$, $Q^2=0.855$) confirmed the systematic differences in the metabolomic profiles between mothers and offspring. Pathway enrichment analysis demonstrated significant enrichment in the nucleotide and purine metabolic pathways in offspring, with a high concentration in lysine biosynthesis and degradation pathways. This finding is highly consistent with the physiological state of offspring during rapid growth, active cell division, and tissue construction.



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sciforum-185058: Toxicological Assessment and Biodegradability of a Microbial Glycolipid Biosurfactant for Environmental Applications

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The environmental application of microbial biosurfactants requires a thorough and systematic evaluation of their ecological safety to ensure their suitability for sustainable use. In this study, we investigated the toxicity profile and environmental compatibility of a glycolipid biosurfactant produced by a novel *Pseudomonas fluorescens* strain isolated from Tunisian soil. A series of ecotoxicological assays were conducted to assess its impact on different components of the ecosystem. Phytotoxicity tests performed on *Lepidium sativum* seeds revealed no inhibitory effects on seed germination, root elongation, or overall plant growth, demonstrating excellent compatibility with terrestrial plants and suggesting its safe application in soil environments. Acute toxicity is currently being evaluated using the Microtox® assay with *Vibrio fischeri* to determine EC50 values and further characterize its ecological safety.

In addition, biodegradability assays demonstrated that the biosurfactant is readily biodegradable, with more than 60% degradation achieved within four days under standard conditions. Stability studies indicated that the biosurfactant remains structurally and functionally stable across a wide range of temperatures (30–80 °C) and pH values (2–10), without generating toxic degradation by-products.

Compared to conventional synthetic surfactants, the studied biosurfactant exhibited a significantly lower ecological risk profile, combining low toxicity, rapid biodegradability, and high functional stability. These findings support its potential as a safe, sustainable, and environmentally compatible alternative for large-scale bioremediation applications.



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sciforum-185080: Screening and Environmental Safety Assessment of Biosurfactant-Producing Bacteria from Tunisian Soil

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Biosurfactant-producing bacteria represent a promising and environmentally compatible alternative to synthetic surfactants; however, their large-scale application requires careful assessment of potential ecological toxicity and environmental impact. In this study, several bacterial strains were isolated from Tunisian soil and systematically screened for their ability to produce biosurfactants using standard qualitative and quantitative assays. The most efficient producers were selected for further characterization, and the biosurfactants obtained were evaluated for their environmental safety through a series of toxicity, stability, and biodegradability tests.

Phytotoxicity assays using *Lepidium sativum* seeds at biosurfactant concentrations ranging from 10 to 1000 mg/L showed no inhibitory effects on seed germination or root elongation, with a germination index (GI) exceeding 80% at all tested concentrations, indicating the absence of phytotoxicity. Biodegradability studies demonstrated rapid degradation, with more than 60% degradation achieved within four days, highlighting the biosurfactant's low environmental persistence. Stability assays showed that the emulsification activity (E24) remained stable after exposure to temperatures between 30 and 80°C and within a pH range of 4–10, demonstrating the robustness of the biosurfactant under a wide range of environmental conditions.

Overall, the results confirm that biosurfactants produced by the isolated soil bacteria exhibit a favorable ecotoxicological profile, supporting their potential use as safe, sustainable, and efficient agents in bioremediation and other environmental biotechnological applications.



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sciforum-186127: The Silent Perinatal Passage: A PRISMA 2020 Systematic Review of Transplacental Transfer of PFAS and Microplastics and Fetal Endocrine Disruption

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Introduction

Emerging contaminants (ECs), particularly per- and polyfluoroalkyl substances (PFAS) and microplastics (MPs), are increasingly detected in human biological matrices. During pregnancy, transplacental transfer may expose the fetus to toxic compounds during a critical developmental window. However, this exposure route remains insufficiently integrated into developmental toxicology and One Health risk assessment frameworks.

Methods

A PRISMA 2020-compliant systematic review was conducted using PubMed, Scopus, Web of Science, and Ecotox databases (January 2015–March 2025). Eligible studies included original human research quantifying PFAS or MPs in paired maternal–fetal samples (placenta, cord blood, or meconium) and evaluating endocrine-related outcomes. Two independent reviewers performed study selection and quality assessment.

Results

Among 1,482 screened records, 18 studies met the inclusion criteria. PFAS were detected in 89–100% of placental and cord blood samples, with cord-to-maternal transfer ratios frequently exceeding 0.5 for long-chain compounds. MPs, mainly polypropylene, polyvinyl chloride, and polybutylene succinate, were frequently identified in placental tissues. Higher MP exposure was associated with decreased umbilical cortisol levels ($\beta = -2.20$ ng/mL per IQR increase, $p < 0.01$), increased dehydroepiandrosterone concentrations ($\beta = +0.07$ ng/mL, $p < 0.01$), and a reduced glucocorticoid/androgen ratio ($\beta = -4.37$, $p < 0.01$), suggesting fetal endocrine disruption. To our knowledge, no previous systematic review has jointly evaluated PFAS and MPs transplacental transfer in relation to endocrine outcomes.

Conclusions

Current evidence indicates that transplacental exposure to PFAS and MPs is widespread and associated with alterations in fetal endocrine signaling pathways. These findings support the integration of developmental and transplacental toxicology into One Health risk assessment frameworks and highlight the need for standardized biomonitoring strategies during pregnancy.



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sciforum-186128: Environmental Endocrine Disruptors and Thyroid Dysfunction: A Systematic Review of Mechanisms and Human Evidence

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Introduction

Endocrine-disrupting chemicals (EDCs) are environmental contaminants that interfere with hormone synthesis, metabolism, and receptor signaling, thereby disrupting endocrine homeostasis. The thyroid gland is particularly sensitive to these compounds, and increasing evidence suggests that EDC exposure is associated with thyroid dysfunction and adverse health outcomes.

Methods

A systematic literature review was conducted using electronic databases, including Google Scholar, PubMed, and ScienceDirect. Studies published between 2015 and 2025 were identified using keywords such as “*endocrine-disrupting chemicals*,” “*thyroid function*,” “*thyroid hormones*,” “*bisphenol A*,” “*phthalates*,” “*phenols*,” “*parabens*,” and “*flame retardants*.” Additional filters were applied to identify relevant human, epidemiological, and experimental studies.

Results

Evidence from epidemiological and experimental studies indicates that EDC exposure is associated with alterations in thyroid function. Human studies show that phthalates are linked to thyroid abnormalities, including nodules and disrupted hormone homeostasis. Population-based analyses demonstrate negative associations between exposure to phenols, parabens, and phthalate metabolites and circulating thyroxine (T4) levels, with modifying effects of iodine status and thyroid autoimmunity. Experimental studies further show that bisphenol A (BPA) alters thyroid hormone balance, increasing thyroid-stimulating hormone (TSH) levels and disrupting T3/T4 regulation. In addition, exposure to flame retardants has been associated with an increased risk of papillary thyroid cancer. Mechanistically, contaminants such as perchlorate, nitrate, and thiocyanate impair iodide uptake by inhibiting the sodium-iodide symporter (NIS), thereby reducing thyroid hormone synthesis.

Conclusions

Current evidence suggests that EDC exposure is associated with thyroid dysfunction through multiple biological pathways. Although findings remain heterogeneous, the consistency of epidemiological and experimental data highlights the need for further longitudinal and mechanistic studies to clarify dose–response relationships and inform public health strategies.



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sciforum-186154: Multispecies Physiological Disruption by Metabolic Contaminants and Sweeteners: Implications for Aquatic Ecosystem Functioning

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The continuous release of metabolic pharmaceuticals and artificial sweeteners into aquatic environments has raised concerns due to their persistence and biological activity. Despite their widespread detection, the mechanistic effects of these contaminants on aquatic primary producers and their implications for ecosystem functioning remain insufficiently understood. This study assessed the ecotoxicological responses of three representative aquatic primary producers (*Chlorella vulgaris*, *Nostoc* sp., and *Lemna minor*) exposed to environmentally relevant concentrations of metformin (MET), its transformation product guanyurea (GUA), and the artificial sweeteners sucralose (SUC) and acesulfame-K (ACE-K). Acute (72 h) and subchronic (7 d) exposures were conducted to evaluate growth, photophysiology (Fv/Fm, ETR, NPQ), oxidative stress biomarkers, nitrogen metabolism, and detoxification-related responses. Mixture experiments were performed under subchronic conditions to assess the interaction effects. MET and GUA produced the strongest physiological disturbances across species, including reduced electron transport and nitrogen assimilation, and increased oxidative stress. Artificial sweeteners induced comparatively weaker but significant responses in the participants. Subchronic exposure amplifies physiological disruption relative to acute conditions. Multivariate analysis revealed coordinated responses linking photophysiology, the redox balance, and nitrogen metabolism. Mixture exposure resulted in predominantly additive to moderately synergistic effects, particularly on oxidative stress and photochemical efficiency, with MET and GUA acting as dominant drivers. Metabolic contaminants disrupt interconnected physiological pathways in aquatic primary producers, potentially affecting primary productivity and nutrient cycling. These findings highlight the importance of integrating sublethal and multi-species responses into ecotoxicological risk frameworks, particularly under realistic mixture exposure scenarios.



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sciforum-186256: Development of a Passive Sampler Based on Polymer Inclusion Membrane for Uptake of CU(II) in Wastewater

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For water quality monitoring, conventional sampling methods, like grab sampling, have several shortcomings which have led to the necessity to develop alternative methods, particularly those founded on passive sampling. The passive samplers are deployed *in situ* for a specific period, to accumulate the analytes. Polymer inclusion membranes (PIMs) contain a membrane which comprises an extractant that transports the analyte from the sample into the receiving solution by synchronized extraction and back-extraction. In this study, a membrane produced from polyvinyl chloride as the base polymer in the presence of di-(2-ethylhexyl) phosphoric acid (40%) (D2EHPA) as a carrier was used for passive sampling of Cu(II) from wastewater. 1 M HNO₃ was used as the receiving phase. The influence of feed phase Cu(II) concentration (tested for the range of 10–400 mg L⁻¹) and pH (tested for the range of 3–7 pH) and significantly influence separation characteristics, while membrane thickness has a minor influence. Under the optimum conditions, the system attained 91% extraction and 54% stripping efficiency, when the initial concentration of Cu(II) was 200 mg L⁻¹, and pH = 6. The passive sampling system reaches general transfer coefficients among $7.5 \times 10^{-3} \text{ cm s}^{-1}$ and $4.3 \times 10^{-2} \text{ cm s}^{-1}$. A linear accumulation of Cu(II) was obtained for an exposure time of 5 days. Tests have revealed that D2EHPA ligand is a suitable carrier for the transport of Cu(II) from wastewater. The developed methodology can be applied to provide an average concentration of Cu(II) in the analysed wastewater during the exposure period of passive sampler.



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sciforum-186304: Blood and Urine Heavy Metal Level in E-Waste and Non-E-Waste Workers

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Advances in technology have led to a significant rise in electronic waste. The rapid turnover of devices and improper disposal can pose potential risks to health of waste recycling workers. This cross-sectional study measured heavy metal exposure between informal e-waste dismantling workers in Thailand and compared the exposure with those in non-e-waste workers. Blood samples were collected using a Capitainer B device and analysed for lead (Pb) and cadmium (Cd) using inductively coupled plasma mass spectrometry. In addition, participants provided urine samples which were analysed for arsenic (As), cadmium (Cd), chromium (Cr), lead (Pb), mercury (Hg), and nickel (Ni) using inductively coupled plasma optical emission spectrometry.

176 people took part including 128 e-waste workers and 48 non-e-waste workers. The most dismantled items were fans and refrigerators, and the main tasks involved sorting, taking apart, and separating e-waste materials. Blood lead (Pb), but not cadmium, levels were higher in e-waste workers with median levels (IQR) of 88.9 µg/L (38.2–209.6 µg/L), compared to non-e-waste workers with a median (IQR) of 36.5 µg/L (15.0–70.7 µg/L). This difference was statistically significant ($p < 0.001$). The median level was approximately twofold higher, with increased variability and several elevated values. Approximately 28% of e-waste workers exceeded the ACGIH BEI limit of 200 µg/L. In contrast, there were no statistically significant difference in urine metal levels between e-waste and non-e-waste workers.

These findings suggest that e-waste workers are exposed particularly to Pb and suggest that by raising safety awareness, reducing hazards, and promoting safe practices may help protect informal e-waste communities



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sciforum-186528: Environmental Implications of Caffeine Exposure on Terrestrial Plant Establishment

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Background: The ecotoxicological assessment of caffeine is essential to understand its potential impacts on non-target organisms and to support environmental risk assessment. Caffeine is an emerging contaminant widely detected in aquatic and terrestrial environments due to human consumption and its continuous release via domestic and industrial effluents. Its persistence may affect non-target organisms, including terrestrial plants, by altering physiological and developmental processes. **Objective:** To evaluate the phytotoxic effects of caffeine on four terrestrial plant species (*C. americanus*, *Triticum aestivum*, *Lactuca sativa*, and *Raphanus sativus*) using germination, development, and growth endpoints. **Methods:** Bioassays were conducted following OECD 208 and ISO 18763 guidelines under controlled dark conditions for 72 h. Ten caffeine concentrations (0.0028–97.42 mg/L, ≥99% purity) were tested per species, with six replicates per treatment and ten seeds per replicate. Germination and early seedling development parameters were evaluated after exposure. Effect percentages were calculated and doses classified as non-toxic, moderately toxic, or toxic based on EC₁₀ and EC₅₀ thresholds. A final toxicity index was derived from the integrated response of all endpoints for each species. **Results:** The strongest effects were observed in root and shoot growth. Root inhibition exceeded 50% in *C. americanus* and *T. aestivum* (53.96% and 64.89%), classifying caffeine as toxic for this endpoint. Shoot growth inhibition remained below 50% but showed moderate effects, particularly in *T. aestivum* (27.09%) and *R. sativus* (19.29%). In the GSI endpoint, caffeine showed moderate toxicity for *C. americanus*. Integrated analysis indicated higher sensitivity in *C. americanus*, followed by *R. sativus*, *T. aestivum*, and *L. sativa*. **Conclusions:** Caffeine can impair early plant development, mainly growth-related parameters, potentially affecting establishment and regeneration. These findings support further ecotoxicological studies and its consideration in environmental regulations to protect soil quality and ecosystem functioning.



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sciforum-186530: A Simple Method for Quantifying and Characterizing Microplastics at Ultra-Low Concentrations

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Introduction

Microplastics (MPs) can be defined as synthetic polymer particles ranging in size from 0.1 to 5,000 µm [1]. Currently, a knowledge gap exists in MPs research regarding validation through recovery tests at very low contamination levels (e.g., 0-10 particles) [2–4]. The aim of this study was to develop a simple method for spiking samples with as few as a single particle, while enabling accurate characterization of their size, shape, and morphology.

Methods

Polyethylene MPs (fragments, approximately 30-150 µm in size) were transferred onto filters using an optical microscope and metal tweezers. Particles were then added or removed until the desired number was reached. Counted and photographed MPs were transferred by rinsing the filters with 100 mL of pre-filtered ultrapure water into a separate container. Three particle levels (1, 5, and 10 particles) were prepared in triplicate. Recovery was assessed by filtering the samples and recounting MPs. Characterization was conducted using optical microscopy and scanning electron microscopy.

Results

The recovery testing method was successfully developed, and characterization of MPs was performed. Particle recoveries of 100.00% ± 0.00%, 80.00% ± 20.41%, and 93.33% ± 28.12% were achieved for 1, 5, and 10 particles respectively.

Conclusions

Our method enables sample spiking and full characterization of MPs based on their size, shape, and number, including at the single-particle level. It addresses the current knowledge gap in precise MPs recovery assessment at low contamination levels (e.g., 0-10 particles).

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sciforum-186531: Adaptive Monitoring of Climate-Driven Contaminant Pulses: An Integrated Analytical and AI Framework

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Climate-driven hydrological extremes, such as high-intensity precipitation following drought, rapidly mobilize contaminants from soils and sediments into aquatic ecosystems. These transient "contaminant pulses" frequently escape detection by conventional quarterly monitoring but pose acute risks to ecosystem integrity and human health. Under the One Health framework, capturing these episodic events is critical for accurate risk assessment. This study proposes an adaptive monitoring framework that integrates real-time environmental sensing with event-triggered sampling and artificial intelligence (AI). Continuous sensor data, including conductivity, turbidity, oxidation-reduction potential (ORP), water temperature, and rainfall intensity, serve as proxies to trigger high-resolution analytical characterization using LC-MS/MS, GC-MS/MS, and ICP-MS. The workflow targets diverse contaminants, including pesticides, pharmaceuticals, heavy metals, and antibiotic resistance markers. Preliminary results were obtained from pilot monitoring campaigns conducted at three agricultural catchments with contrasting land-use characteristics. These observations indicate that post-rainfall runoff events can increase pesticide and nutrient concentrations by 3-10 times baseline levels. Nitrate concentrations frequently exceeded 40-60 mg/L, while significant metal mobilization was observed during first-flush events following prolonged dry periods. To manage the resulting high-frequency dataset, a physics-informed Random Forest model was developed to identify contamination patterns and predict short-term exceedance probabilities. Key predictors included cumulative rainfall, rainfall intensity, antecedent dry period duration, turbidity, conductivity, streamflow, and soil moisture. Initial model outputs suggest that rainfall events exceeding 15 mm within 24 hours represent a critical threshold associated with elevated contamination risk. By transitioning from static compliance monitoring to a predictive, climate-responsive framework, this approach enhances early-warning systems for vulnerable catchments. The integration of advanced analytics, real-time sensing, and AI provides the high-resolution data necessary to protect the interconnected health of aquatic ecosystems, wildlife, and human populations in an era of increasing climatic instability.



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sciforum-186534: How Bioavailable Are Polypropylene Microplastics? *In Vitro* Evidence and Potential Health Relevance

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Introduction

Microplastics (MPs) are solid polymer particles of various shapes and sizes, typically ranging from 0.1 to 5,000 µm. Their presence has been widely documented in both the environment and food products. Their occurrence in food suggests that the gastrointestinal tract is one of the primary routes of human exposure to these contaminants. However, their fate within the gastrointestinal tract remains poorly understood. The aim of this study was to develop and evaluate an *in vitro* methodology for assessing the bioavailability of MPs in the human digestive system.

Methods

The bioavailability of polypropylene microparticles was assessed using a three-stage *in vitro* digestion model that simulates the functioning of the human gastrointestinal tract. The particles were subjected to simulated digestion under conditions corresponding to the oral, gastric and intestinal phases, at a temperature of 37°C. Dialysis membranes were used in the model to assess the extent to which the MPs passed into the intestinal lumen. After digestion, the particles were separated by filtration and analyzed using optical microscopy and µ-FTIR spectroscopy.

Results

The results showed that, independent of the type of matrix used, the MPs pass through the dialysis membrane. However, the presence of digestive processes leads to physicochemical changes of the polymer. Surface oxidation and morphological changes were identified using FTIR microspectroscopy (µ-FTIR) and optical microscopy.

Conclusions

The study suggests that polypropylene MPs undergo physicochemical changes in the gastrointestinal tract and may become bioavailable. *In vitro* models are useful tools for preliminary exposure risk assessment; however, they do not fully reflect the complexity of the human body. These findings highlight the need for further research using more advanced biological models and *in vivo* studies to better determine the health relevance of exposure to MPs.

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sciforum-186541: Hidden Losses: Do Isolation Protocols Degrade Microplastics in Food Analysis?

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Introduction

Microplastics (MPs) are defined as plastic particles ranging in size from 0.1 µm to 5 mm. MPs have been found as contaminants in food, including infant and enteral nutrition products. Potassium hydroxide and hydrogen peroxide are frequently used for the isolation of MPs from high-protein matrices. However, methods for the determination of MPs in food have not yet been standardized. Furthermore, it remains unclear whether the isolation conditions may cause degradation of MPs. The aim of this study was to evaluate the effect of reagents and conditions commonly used for the digestion of high-protein food matrices on the stability of polyethylene (PE) and polypropylene (PP) MPs in the absence of the food matrix.

Methods

PE MPs (34–50 µm) and PP MPs (50–80 µm) were exposed to 10% H₂O₂ and 10% KOH at 60 °C for 45 minutes. After filtration, drying, and weighing, the particles were examined for morphological changes and chemical composition. The analyses were performed using scanning electron microscopy (SEM) and Fourier-transform infrared microspectroscopy (µ-FTIR).

Results

SEM images revealed initial signs of PE MPs degradation, manifested as surface cracking, after heating at 60 °C for 45 min. Exposure to 10% H₂O₂ and 10% KOH further intensified PE degradation. In the case of PP MPs, degradation into smaller particles was observed only in the presence of 10% KOH. No changes in the chemical composition of PE and PP MPs were observed under any of the tested conditions.

Conclusions

The applied isolation conditions may induce physical degradation of PE and PP MPs into smaller particles. This may lead to an underestimation of MPs content, as particle size is a major limitation of microspectroscopic techniques used for their determination.

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sciforum-186787: PVC, CTA, and PLA-based polymer inclusion membranes for selective removal of metal ions from wastewater

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In recent years, polymeric inclusion membranes (PIMs) have offered promising solutions to the global concern of heavy metal contamination in water resources. PIMs offer many advantages over traditional separation methods such as ion exchange or reverse osmosis. This study investigates PIMs incorporating polyvinyl chloride (PVC), cellulose triacetate (CTA), and polylactic acid (PLA). The PLA was sustainably produced from lignocellulosic biomass *via* autohydrolysis pretreatment, delignification, simultaneous saccharification and fermentation (SSF) of the resulting cellulose, lactic acid recovery, and polycondensation. Membranes were fabricated by dissolving the polymers in dichloromethane (PVC in tetrahydrofuran), incorporating 2-nitrophenyloctyl ether (NPOE) as a plasticizer and Chelex 100 as a carrier, casting the solutions into thin films, and evaporating the solvents to yield stable, porous structures suitable for heavy metal removal. The membranes were comprehensively characterized using electrospray ionization mass spectrometry (ESI-MS), proton nuclear magnetic resonance (¹H-NMR), ¹³C-NMR, Fourier-transform infrared (FTIR) spectroscopy, thermogravimetric analysis (TGA/DTG), and differential scanning calorimetry (DSC). DSC revealed NPOE's plasticizing effect, which lowered the glass transition temperature. Thermal stability analysis revealed distinct degradation behaviors among the membranes. DSC analysis confirms the differences among the three polymers: PVC, CTA, and PLA. PVC is an amorphous, rigid polymer that degrades before melting, whereas CTA is an amorphous polymer with very high thermal stability. PLA is a semicrystalline polymer that shows well-defined thermal transitions, including the glass transition temperature, crystallization temperature upon cooling, and melting temperature of the crystalline phase, but with limited thermal stability. Thus, PLA displays typical behavior of thermally processable biopolymers. In terms of performance, the membranes demonstrated significant efficiency in cadmium removal, with removal efficiencies of 95% (CTA), 87% (PLA), and 74% (PVC). The maximum adsorption capacities were 42.5 mg/g for CTA, 35.8 mg/g for PLA, and 28.4 mg/g for PVC, indicating the superior performance of the CTA membrane.



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sciforum-186823: Toxicity assessment of the insect repellent nootkatone in developing zebrafish (*Danio rerio*)

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Nootkatone is a naturally occurring sesquiterpenoid found in grapefruit that stands out for its repellent activity. However, its use as a commercial repellent requires a better understanding of its effects on non-target organisms, particularly aquatic species. In this context, this study aimed to evaluate the effects of nootkatone (0.1–10,000 µg/L) on developing zebrafish by assessing a series of endpoints, including survival, deformities, hatching rate, behavior, mitochondrial function, oxidative stress, apoptosis, gene expression, and untargeted lipidomics and metabolomics. Survival remained above 80% at concentrations up to 5,000 µg/L. Complete mortality was observed at 7,500 µg/L, and survival dropped to approximately 10% at 10,000 µg/L. The LC₅₀ for zebrafish larvae at 7 dpf was estimated at 4,900 µg/L. Hatching success and deformity incidence were not affected up to 2,500 µg/L. However, at higher concentrations, hatching decreased while deformities increased. Locomotor activity was significantly impaired at 5,000 µg/L, while no changes were detected at lower concentrations or in anxiety-related behavior. At 10,000 µg/L, nootkatone increased non-mitochondrial respiration and reduced ATP-linked respiration, with no detectable effects at lower concentrations. In addition, reactive oxygen species levels and apoptosis remained unchanged across treatments. Similarly, transcript levels of genes associated with oxidative stress and metabolism were not altered. Lipidomic and metabolomic profiling identified 192 lipid species and 16 polar metabolites. However, none showed significant differences among treatments. Our results indicate that nootkatone exhibits low acute toxicity in developing zebrafish. Further studies should assess its long-term effects across aquatic organisms and other species, contributing to the development of environmentally safer insect repellents.



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sciforum-186842: Short-term treatment with lithium and its effect on the content of elements and fatty acids in aquatic species of *L. minor*

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Lemna minor, a fast-growing aquatic plant with significant potential for phytoremediation and bioenergy production, is considered a sustainable candidate for wastewater treatment and resource recovery. This study evaluated the effects of lithium (Li) exposure (0, 1, 3 and 5mg/L) on *Lemna minor* during a seven-day cultivation period. The investigation included metal accumulation, photosynthetic pigment characterization, lipid extraction, fatty acid profiling, and lipid quality index assessment. Results highlighted the capacity of *Lemna minor* to tolerate Li exposure while changes were observed in the metals-profile. Exposure to 1–5 mg/L Li caused a reduction in chlorophyll a, chlorophyll b, and carotenoid contents, indicating inhibition of the photosynthetic system. Li exposure altered the elemental composition of the plants, particularly causing a significant decrease in Mg and Zn contents. The obtained biomass demonstrated potential for applications in phytoremediation, biofuels, and value-added bioproducts. Palmitic acid (C16:0), α -linolenic acid (C18:3 n-3), and linoleic acid (C18:2 n-6) were the predominant fatty acids identified in *Lemna minor*. Changes in fatty acid profiles indicate adaptive metabolic responses of *Lemna minor* to Li-induced stress conditions. Despite growth inhibition, the antioxidant capacity of the plants was not significantly affected by Li exposure. The study contributes to the understanding of Li-induced stress in aquatic plants and supports the use of *Lemna minor* in sustainable environmental technologies.



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sciforum-186881: Multiparametric Assessment of Microbial Viability in Anaerobic Reactors Exposed to Emerging Contaminants Using Flow Cytometry and Fluorescence Microscopy

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Emerging contaminants (ECs), including sulfamethoxazole, carbamazepine, ibuprofen, and triclosan, are increasingly detected in wastewater treatment systems and may compromise microbial communities involved in anaerobic processes. Conventional culture-based methods provide limited information on the physiological status of these communities, highlighting the need for rapid multiparametric approaches to assess contaminant-induced stress. In this study, anaerobic reactors were exposed to individual ECs and to a combined mixture (MIX) at concentrations ranging from 1 to 10 mg/L for 24–72 h. Microbial viability was evaluated by flow cytometry using Live/Dead staining with SYTO9/propidium iodide (PI), and the results were complemented by fluorescence microscopy. Statistical analyses, including Shapiro–Wilk, Kruskal–Wallis, and Dunn’s post hoc tests, were applied to determine the effects of contaminant concentration and exposure time on microbial viability. Contaminant concentration did not produce statistically significant changes in microbial viability under the tested conditions ($p > 0.05$). In contrast, exposure time emerged as a critical factor affecting microbial health, with triclosan (TCS) and MIX treatments causing the greatest reductions in viable cell populations and alterations in cytometric profiles. Dunn’s post hoc analysis revealed significant differences in reactors exposed to sulfamethoxazole, carbamazepine, and ibuprofen, whereas TCS and MIX showed comparable toxicity patterns. Fluorescence microscopy confirmed a progressive decrease in the viable/non-viable cell ratio over time, particularly in reactors exposed to TCS and MIX. These findings indicate that exposure time, rather than nominal contaminant concentration, was the main driver of microbial viability loss in anaerobic reactors under the tested conditions. The combined use of flow cytometry and fluorescence microscopy provides a robust early-warning framework for monitoring microbial stress in wastewater treatment systems. This approach contributes to a better understanding of the differential toxicity of emerging contaminants and supports the development of advanced monitoring strategies for protecting microbial functions essential to environmental health.



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sciforum-186903: Bisphenol F and AF Impair Cerebral Vascular Reactivity via Adrenergic and Nitric Oxide Pathways

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Bisphenol F (BPF) and Bisphenol AF (BPAF) have been used as substitutes for Bisphenol A (BPA), a compound with estrogenic and androgenic properties. This endocrine disruptor compound was already associated with modifying the middle cerebral artery vascular homeostasis by interfering with the nitric oxide pathway. Although BPA has been banned in several countries, recent data suggest that some of its substitutes, such as BPF and BPAF, may pose a risk to human health. However, the available data on their neurovascular effects remain limited. Therefore, the present study evaluated the effects of BPF and BPAF on smooth muscle cells of the middle cerebral artery (SMC-MCA) of Wistar rats. Pure SMC cultures were performed from MCA explants, and MTT assays were performed to assess viability, proliferation, and cytotoxicity. The concentrations tested ranged from 0.0002 to 1000 μM . Planar Cell Surface Area (PCSA) assays were also performed to assess contractile responses to noradrenaline and relaxation responses to sodium nitroprusside at concentrations of 0.002, 0.02, 0.2, 2, and 20 μM . The results showed dose-dependent effects, and both compounds stimulated cell proliferation at low concentrations (0.02 μM) and induced cytotoxicity at high concentrations (200 and 1000 μM), revealing a non-monotonic profile characteristic of endocrine disruptors. Similar to BPA, these compounds modified the vasoactive activity of SMC-MCA, possibly by modulating α 1-adrenergic receptors, the NO/sGC pathway, and Ca^{2+} channels, suggesting a potential neurovascular-disrupting effect. BPF altered only the vasorelaxant response at concentrations of 0.002 and 0.02 μM , while BPAF affected both the contractile response (0.002 μM) and the vasorelaxant response (2 μM). It was also noted that, at 0.002 μM , BPAF inhibited SNP-induced relaxation, causing a contractile response. Overall, these findings underscore the need for further studies to fully understand the mechanisms by which BPF and BPAF affect vascular function and the risk of developing neurovascular diseases.



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sciforum-186939: Polycyclic Aromatic Hydrocarbons and Sugarcane Workers in Guatemalan

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Introduction

Burning of sugarcane prior to harvesting poses a significant health risk for both workers and the surrounding environment. Mortality from diseases such as kidney disease and lung cancer increase in regions near sugarcane burning. Polycyclic aromatic hydrocarbons (PAHs) are omnipresent environmental pollutants formed primarily through incomplete combustion of carbon. Sixteen PAHs are identified as EPA priority pollutants, and many are known carcinogens. To understand the potential role of PAHs in the negative health effects associated with sugarcane harvesting practices, we aimed to measure PAHs from ash in the sugarcane fields and compare them to PAH metabolites in the urine of Guatemalan workers.

Methods

PAHs were measured in soil and ash samples taken from sugarcane fields using a solvent extraction followed by gas chromatography/mass spectrometry. The PAHs measured were the 16 EPA priority PAHs. Monohydroxylated PAHs are found in the urine, in part as sulfated and glucuronidated conjugates. β -glucuronidase/arylsulfatase incubation releases the metabolites, allowing for quantitative analysis by liquid chromatography/ mass spectrometry.

Results

Fourteen of the 16 PAHs measured are detectable in ash and soil samples taken from sugarcane fields. PAHs are found in considerably higher concentrations in ash samples than in soil samples taken from the same field. Our PAH metabolite method validation studies demonstrate that our lower levels of quantitation are sufficient to detect even baseline levels in non-exposed populations.

Conclusions

Our pilot study demonstrates the necessity to further investigate the health effects of PAHs produced during the burning of sugarcane on the individuals working in and near these fields. Our method allows for the quantification of metabolites of PAHs in urine, providing valuable insight into the degree of exposure. In the near future, our study will evaluate PAH metabolites in urine samples from sugarcane workers to associate with PAHs found in the nearby soil and ash.



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sciforum-186992: Microplastic contamination in *Mytilus galloprovincialis* from the Black Sea, Bulgaria

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Microplastic (MPs) pollution has become an increasing environmental concern in marine ecosystems due to its persistence and potential effects on aquatic organisms and human health. *Mytilus galloprovincialis* is a filter-feeding bivalve widely used as a bioindicator of marine contamination because of its capacity to accumulate pollutants from the surrounding environment. The Black Sea is a semi-enclosed basin particularly vulnerable to anthropogenic pollution, including plastic debris originating from coastal, industrial, and riverine sources. This study investigated MP contamination in *Mytilus galloprovincialis* collected from an aquaculture farm in the southern Bulgarian sector of the Black Sea. Mussel samples were analyzed to determine the abundance, polymer composition, and morphological characteristics of MPs using Laser Direct Infrared (LDIR) spectroscopy. MP particles were identified and classified according to shape and polymer type, providing detailed information on contamination patterns in commercially cultivated mussels. The analysis revealed the presence of diverse MP, with fibers being the predominant forms. Detected polymers included commonly used synthetic materials, such as polyethylene and polypropylene, but also rubber, etc. indicating multiple anthropogenic sources of pollution. The occurrence of MPs in farmed mussels highlights the widespread nature of plastic contamination in the Black Sea marine environment and raises concerns regarding the transfer of MPs through seafood consumption. These findings contribute to the understanding of MP pollution in aquaculture products from the Bulgarian Black Sea and emphasize the importance of continued monitoring and mitigation strategies to reduce marine plastic contamination.



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sciforum-187060: Comparative evaluation of *Chlorella vulgaris* and *Salvinia natans* for the treatment of Mining Wastewaters

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The treatment of mining wastewaters and recovery of critical elements are serious component of a sustainable water management and resource recovery. However, the efficiency of wastewater treatment strongly depends on the physicochemical characteristics of the effluent, particularly its elemental composition and pH. A laboratory-scale bioremediation method using living *Chlorella vulgaris* and *Salvinia natans* species as secondary treatment step for mining wastewater was studied. The removal performance of *Chlorella vulgaris* and *Salvinia natans* was tested separately using synthetic multielement solutions containing regulated and unregulated elements at an initial concentration of 500 µg/L. Both biological systems showed high removal efficiency especially for Al, V, Cr, Ag, Pb, and U, as well as for rare earth elements such as Y, La, Ce, Pr, Nd, Sm, Eu, and Gd. The obtained results indicated element-specific uptake behavior and highlighted the potential of both microalgal and macrophyte-based systems for the simultaneous removal of toxic and critical elements from complex aqueous matrices. The environmental stress induced by multielement exposure was further evaluated through total protein quantification and the analysis, providing insight into the physiological response and tolerance of the studied species during the treatment process. The obtained results recommend the applicability of *Chlorella vulgaris* and *Salvinia natans* as nature-based bioremediation systems, sustainable and low-cost alternatives for the treatment of mining wastewaters and recovery of valuable elements.

Acknowledgement

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sciforum-187076: Combined Exposure to Ciprofloxacin and Polystyrene Microplastics: Responses of Aquatic Organisms and Electroactive Bacteria

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Combined pollution by microplastics and antibiotics is an increasing environmental concern due to their widespread occurrence in aquatic ecosystems and their potential interactions with biological communities. This study evaluated the acute toxicity of individual and combined toxicity of polystyrene microplastics (PS, 2–5 μm) and ciprofloxacin (CPX) on the electroactive bacteria *Geobacter sulfurreducens*, commonly used in bioelectrochemical systems (BES) for wastewater treatment, and three aquatic model organisms representing different trophic levels: *Aliivibrio fischeri*, *Raphidocelis subcapitata* and *Daphnia magna*. Acute ecotoxicological assays were carried out to calculate the Effective Concentration (EC). Combined toxicity was assessed using the combination index (CI)-isobologram method to identify synergistic, additive, or antagonistic interactions.

For *G. sulfurreducens* and *A. fischeri*, EC₅₀ values for mixtures were below 1 mg L⁻¹ and 10 mg L⁻¹, respectively. In *D. magna* the values were also below 1 mg L⁻¹. In *R. subcapitata* the EC₅₀ value was generally higher, below 10 mg L⁻¹, showing lower sensitivity. Synergistic effects were mainly observed in bacterial assays and for *R. subcapitata* the interaction shifted to moderate antagonism as the level of inhibition increased. For *D. magna*, very strong antagonism was observed, while at higher levels of immobilisation the interaction shifted towards moderate antagonism.

Overall, the sensitivity of the tested organisms followed the order: *Aliivibrio fischeri* > *Geobacter sulfurreducens* > *Daphnia magna* > *Raphidocelis subcapitata*. The mixture of CPX with 2 μm PS produced the strongest toxic effects, particularly in bacterial systems, suggesting that smaller microplastics enhance contaminant stress more efficiently than larger particles.



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sciforum-187086: Gold Mining Impacts on Soil Quality: A Comparative Study of Two Sites from the Romanian Apuseni Mountains

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Soil contamination due to gold mining persists in time post-closure, but comparative data contrasting long-closed versus recently suspended operations are scarce. This study aims to compare soil quality between two distinct mining environments located onto Aries River Basin in the Romanian Apuseni Mountains: a closed decades ago gold mining operation (Baia de Arieș) and a recently closed mining site (Roșia Montană).

Eight soil samples were collected in Winter 2021 along the Aries River and its tributary corridors (four per site). Major elements (Fe, Na, Mg, K and Ca) were analysed by Inductively Coupled Plasma Optical Emission Spectrometer (5300 Optima DV, PerkinElmer, MA, USA), while trace elements (Ni, Cr, Cu, Zn, Cd, Pb, Mn, Al, and As) were determined by Inductively Coupled Mass Spectrometer (ELAN DRC II, PerkinElmer, MA, USA). Hg content was measured by cold-vapor atomic fluorescence spectrometry (CV-AFS, Hydra-AF Mercury Analyzer, Teledyne Leeman Labs, Hudson, NY, USA). Soil pollution degree was assessed using individual indices (Contamination Degree, Cd; Geo-accumulation Index, I_{geo}) and complex contamination indices (Contamination factor, CF; Pollution Load Index, PLI).

Cu, Zn, Pb and Ni were the primarily contaminants at both sites, even though the enrichment levels varied. Roșia Montană samples exhibits higher contamination levels than those from Baia de Arieș. Mean CF values were $35,2 \pm 16,7$ (Strong pollution) for Roșia Montană and $18,9 \pm 5,30$ (considerate pollution) for Baia de Arieș, respectively, mean PLI $1,2 \pm 0,6$ (moderate pollution), PLI $1,0 \pm 0,2$ (baseline to moderate pollution).

Despite decades of closure, the historical mining area of Baia de Arieș remains considerably polluted, whereas the more recent exploitation site from Roșia Montană presented severe levels of pollution. These findings highlight the persistence of soil contamination from gold mining and underscore the need for remediation strategies based on element-specific risks and contamination levels.



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sciforum-187155: Single and combined neurotoxic effects of chlorpyrifos and perfluorohexanesulfonic acid (PFHxS) in developing zebrafish (*Danio rerio*)

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Perfluorohexanesulfonic acid (PFHxS), is a per- and polyfluoroalkyl substance (PFAS) and is detected in aquatic ecosystems. Chlorpyrifos (CPF), a widely used organophosphate pesticide, is also frequently detected in surface waters. Although the toxicity of these compounds is well known individually, their combined effects are still poorly understood. In this study, zebrafish embryos were exposed to CPF (0.7–700 µg/L), either alone or combined with PFHxS (10 µg/L), to investigate potential interactive effects. After five days of exposure, endpoints including survival, hatching rate, morphological abnormalities, locomotor behavior, oxidative stress, apoptosis, and transcription of selected genes were analyzed. Survival in the 700 µg/L CPF group was close to 25%, while co-exposure with PFHxS further decreased survival to nearly 5%, suggesting increased toxicity in the combined treatment. A reduction in survival was observed in embryos exposed to 0.7 µg/L CPF alone; however, this effect was not evident in the CPF/PFHxS co-exposure group. Exposure to CPF caused a concentration-related rise in developmental abnormalities, with the highest frequencies detected at 70 and 700 µg/L. Under co-exposure conditions, deformities were detected only at 700 µg/L CPF combined with PFHxS. In general, CPF alone promoted dose-dependent increases in both mortality and malformation rates, whereas the mixture with PFHxS resulted in approximately 30% deformities at 5 dpf. Behavioral analyses demonstrated an overall reduction in locomotor activity depending on both exposure concentration and light/dark phase. No alterations were detected in ROS production or apoptosis levels. However, gene expression assays indicated increased transcription of neurotoxicity-associated genes, including *ache*, *gfap*, *shha*, and *syn2a*, especially at intermediate CPF concentrations and combined exposure. Genes associated with ROS exhibited distinct expression profiles, with *sod1* being upregulated and *cat* downregulated exclusively in the mixture treatment. These findings highlight the importance of mixture toxicity studies to better understand the ecological risks of co-occurring contaminants.



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sciforum-187224: Effects of tributyltin exposure on endothelium-dependent coronary vasodilation in female rats

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Introduction

Tributyltin (TBT) is an environmental contaminant associated with several toxic effects, including cardiovascular alterations. However, its impact on coronary vascular function remains poorly understood. This study investigated the effects of low-dose TBT exposure on coronary endothelial function and vascular morphology in female rats.

Methods

Female rats were treated daily for 15 days with vehicle (control group) or TBT (100 ng/kg/day). Estrous cyclicity was monitored throughout the experimental period. Coronary vascular reactivity was evaluated in isolated hearts using the Langendorff technique by constructing concentration-response curves to bradykinin (0.1–1000 nM, *bolus* injection). Baseline coronary perfusion pressure (CPP) was measured before pharmacological interventions. Bradykinin-induced relaxation was analyzed under control conditions and after infusion of L-NAME, indomethacin, or clotrimazole to investigate the participation of nitric oxide (NO), cyclooxygenase, and cytochrome P450 pathways, respectively. Coronary artery morphology was assessed by hematoxylin and eosin staining.

Results

Exposure to TBT increased the involvement of the NO pathway in endothelium-dependent coronary relaxation. In parallel, coronary arteries from TBT-treated rats exhibited structural alterations characterized by reduced tunica media thickness and signs of smooth muscle cell atrophy. Additionally, TBT exposure disrupted the estrous cycle and promoted histological alterations in reproductive tissues, including changes in endometrial, myometrial, and luminal epithelial thickness.

Conclusion

These findings demonstrate that subacute exposure to low-dose TBT induces important cardiovascular and reproductive alterations in female rats, suggesting that even doses below currently accepted safety limits may represent a potential cardiovascular risk factor.



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sciforum-187239: Multiple Drivers of the Spatial Heterogeneity of Microplastics in Dam-Influenced Freshwater Systems

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Reservoirs are crucial freshwater systems that provide ecological and socio-economic services; however, they are increasingly threatened by anthropogenic pressures, particularly microplastics (MPs) pollution. Beyond MPs' occurrence, it is essential to investigate their sources, spatial distribution, and interaction with hydrodynamic processes to inform effective environmental management. This study aimed to assess the occurrence and spatial distribution (vertical and transversal) of MPs in two reservoir sections between the Portuguese dams of Régua and Carrapatelo. Water samples were collected at marginal and central-channel sampling sites, at three depths per site, and flow conditions were recorded. MPs were quantified and characterized according to type, colour, size, and polymer composition. Surrounding land use, land cover, and anthropogenic pressures, were evaluated. MPs were detected at all sampling sites and depths. Although the dominant MP characteristics-type (fibres), colour (blue) and size category (0.1-0.5 mm)-were consistent across sections, their vertical distribution patterns differed. Régua section exhibited higher MP abundances at greater depths (> 77 %), while for Carrapatelo section this trend was mainly observed in central-channel sites, associated to higher flow conditions (promoting resuspension of MPs deposited in the sediment). Different transversal distribution patterns were also observed: in Régua, MP abundance was relatively similar between marginal and central-channel sites (34 to 55 MPs/L), whereas Carrapatelo showed greater transversal variability (47 to 101 MPs/L), with the highest MP abundance (158 MPs/L) recorded at the greatest depth at one of the central-channel sites. Overall, although the upstream area is more urbanized (Régua), higher MP abundances were observed in the Carrapatelo section, which may reflect the cumulative downstream transport of MPs along the Douro River, compounded by the barrier effect of the dam, as well as the influence of navigation and tourism activities directly affecting the downstream region.



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sciforum-187262: Pharmaceutical Contaminants in Lagos Water Bodies as Cross-Species Toxicological Hazards

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Introduction

Pharmaceutical contamination of urban water bodies poses cross-species toxicological risks to humans, aquatic fauna, and terrestrial animals – a concern central to the One Health framework. In Lagos, Nigeria, inadequate wastewater infrastructure, self-medication, and improper drug disposal drive the accumulation of pharmaceuticals in surface and groundwater systems.

Methods

Water samples were collected from 11 sites across Lagos Mainland, spanning residential and industrial locations. Ten pharmaceutical compounds were quantified by HPLC-MS/MS. Ecological risk was assessed using risk quotients (RQs) based on measured concentrations and predicted no-effect concentrations. Human exposure was evaluated across three routes, oral ingestion, fish consumption, and dermal contact during flooding, using established bioconcentration factors and an acceptable daily intake set at 1% of the lowest therapeutic dose.

Results

Pharmaceuticals were detected at all sampling sites, with artesunate, diclofenac, and amoxicillin showing the highest mean concentrations. All ten compounds exceeded PNEC thresholds for aquatic organisms, with diclofenac posing the greatest ecological risk ($RQ > 29,000$). Oral ingestion produced hazard quotients above 1 for seven compounds, while fish consumption emerged as the most critical human exposure pathway, particularly for chloroquine, diclofenac, and artesunate. Cumulative Hazard Indices exceeded 1 for eight of ten compounds, with diclofenac and chloroquine recording the highest overall risk.

Conclusion

These findings indicate that pharmaceutical contamination of Lagos water bodies poses a measurable cross-species toxicological hazard, with clear relevance to One Health. Findings underscore the urgent need for pharmaceutical surveillance, disposal stewardship, and strengthened ecotoxicological monitoring capacity across West African urban settings.



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sciforum-187263: Spatiotemporal Prediction of PM_{2.5} Pollution in Dhaka District Using Ensemble Machine Learning and Satellite-Derived Indices (2019–2025)

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Dhaka districts suffer from severe air pollution, with PM₂ concentrations averaging 98 µg/m³. annually, nearly 20 times the WHO recommended guideline of 5 µg/m³. However, only three PM_{2.5} sensors covered 1,463 km² of the district. There was no data on PM_{2.5} in a remaining neighbourhood and nowhere to restrain emissions within Dhaka's megacity of 21.8 million people. The study from 2019 to 2025 uses Google Earth Engine, GIS, and machine learning to understand where and when PM_{2.5} is present. It also maps air quality risks across the Dhaka District. The study examines NO₂, CO, SO₂, and CH₄ data from Sentinel-5P/TROPOMI. It also uses the MODIS Aerosol Index and Land Use and Land Cover data. All this data was put together at 119 points in ArcGIS. The Google Earth Engine, GIS and machine learning are used to understand PM_{2.5} distribution. Random Forest outperformed multiple linear regression (MLR) and Extreme Gradient Boosting, with R²=0.8341 vs 0.6449 (p<0.001), RMSE=16.94 µg/m³, and MAE=11.38 µg/m³, confirming that the collective model captures the nonlinear relationship between the predictor variables and PM_{2.5} at different spatial and temporal resolutions that the MLR model fails to. The analysis showed that NO₂ accounted for 66.2% of the PM_{2.5} variability, highly suggesting that emissions from transportation are the primary pollution contributor. Secondly, predicted winter PM_{2.5} concentration reaches 156.70 µg/m³ (31.3 times the WHO guidelines), a peak likely exacerbated by a meteorological thermal reversal. Brick kiln industries, untreated pollutant emissions from industries, and deforestation documented a 12.91% reduction. The study shows an increase in CH₄ plumes in the Matuail area near Jatrabari, Dhaka. The findings of our study aim to show real-time air pollution in Dhaka and the health hazards caused by uncontrolled air pollution. Ultimately, this research provides the AQI risk estimates for Dhaka, offering spatially explicit evidence to support precision emission control and urban afforestation initiatives.



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sciforum-187294: Organic Sunscreens–infant exposure via breastfeeding

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Xenobiotic secretion into breast milk is a concern because it exposes infants to unwanted, potentially harmful compounds. Studying plasma-to-milk transport is challenging due to ethical and technical constraints.

Organic sunscreens are used worldwide to protect skin from the harmful effects of excessive UV exposure. Unfortunately, some of these compounds are absorbed through the skin into the user's blood circulation. This study focused on the ability of organic sunscreens to be released into milk when administered to breastfeeding females.

Initially, a one-class classification methodology was employed. 202 compounds (mostly pesticides, drugs, aromatic hydrocarbons, and cosmetic raw materials) [1] with experimentally demonstrated ability to be secreted into human breast milk were used as reference compounds. Sixteen sunscreens from different chemical families were analyzed, and the key physicochemical properties of the reference compounds and sunscreens were subjected to Principal Component Analysis.

The properties of reference compounds (easily secreted into breast milk) were plotted in the PC2 vs. PC1 coordinate system to form a single cluster. All the studied sunscreens, except for two, fall within the chemical space of 99% of the reference compounds.

We demonstrated that all the sunscreens studied, except for bulky 1,3,5-triazine derivatives, have physicochemical properties that should enable their passage into human breast milk. This conclusion was corroborated by binary classification results obtained using the Classification Tree and Artificial Neural Network methodologies, based on a set of 122 reference compounds [2], which vary in their ability to enter breast milk. Since most of the sunscreens investigated in this study can be absorbed through the skin, infant exposure via the mother's milk seems a possible scenario.

Vijayaraghavan, S. et al. ACS Omega 2024, 9, 13006-13016

Maeshima, T. et al. Pharmaceutical Research 2023, 40, 711-719.



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sciforum-187310: Chronic diuron exposure alters photosynthetic pigments and antioxidant responses in *Eichhornia crassipes*

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Diuron is a persistent photosystem II inhibitor frequently detected in aquatic environments, where it may affect the metabolism of non-target aquatic macrophytes. However, the physiological responses of floating species under chronic exposure are still poorly understood. This study evaluated the physiological and biochemical responses of *Eichhornia crassipes* exposed to diuron in water-sediment microcosms at 2.5, 10, and 25 $\mu\text{g L}^{-1}$ for 45 days. These concentrations were selected to represent an environmentally relevant gradient, ranging from a low concentration close to the reported NOEC and typical environmental levels, to a concentration near the maximum detected in Brazilian aquatic environments, and a higher but plausible critical contamination scenario. Chlorophyll a, chlorophyll b, total chlorophyll, carotenoids, hydrogen peroxide (H_2O_2), malondialdehyde (MDA), and the activities of catalase (CAT), ascorbate peroxidase (APX), and peroxidase (POX) were evaluated at 6, 20, 31, and 45 days after exposure. Higher diuron concentrations reduced chlorophyll levels during the experimental period, indicating a continuous effect on the photosynthetic apparatus. In contrast, carotenoid levels increased in response to the oxidative imbalance caused by the herbicide. Antioxidant enzyme activities varied according to concentration and exposure time, with CAT and APX increasing mainly between 20 and 31 days, suggesting activation of mechanisms related to H_2O_2 detoxification and redox regulation. Although H_2O_2 levels increased under higher concentrations, MDA remained relatively stable throughout the experiment, indicating limited lipid peroxidation under chronic exposure conditions. PCA separated the control from treatments exposed to 10 and 25 $\mu\text{g L}^{-1}$ over time, reinforcing the physiological effects caused by prolonged diuron exposure. Overall, *E. crassipes* showed metabolic acclimation to chronic diuron exposure through antioxidant and photoprotective responses. This acclimation may help maintain plant survival in contaminated aquatic systems and support its potential use in phytoremediation. However, the sustained reduction in chlorophyll levels suggests that prolonged exposure may compromise photosynthetic performance, with possible consequences for macrophyte productivity, ecosystem functioning, and long-term remediation efficiency.



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sciforum-187316: Bioaccessibility of Metals and Metalloids in Microplastics: In Vitro Digestive Simulation Under Fed Conditions

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Introduction: Microplastics, including low-density polyethylene (LDPE), have become a significant environmental concern due to their persistence in ecosystems and their potential to release hazardous metals and metalloids during digestion. This study aimed to evaluate the bioaccessibility of eight elements (As, Br, Cd, Cr, Pb, Sn, Sb, and Zn) from LDPE microplastics, specifically the certified reference material ERM®-EC680m (low-density polyethylene). **Methods:** The Versantvoort method was employed, which simulates human digestion using digestive fluids (saliva, gastric juice, duodenal fluid, and bile). This method allows for the assessment of element release during both the gastric and gastrointestinal phases, with pH control and constant agitation at 37°C. **Results:** A mass study was performed using four different sample amounts (0.2, 0.4, 1, and 2 g) to evaluate the effect of sample mass on bioaccessibility. Bioaccessibility values ranged from 1% to 10%, with some elements showing values below 1%. A trend was observed where bioaccessibility decreased as sample mass increased. The effect of particle size was also studied, dividing the samples into three size intervals: 0.25–0.5 mm, 0.5–0.84 mm, and >0.84 mm. Bioaccessibility values again ranged from 1% to 10%, with no significant effect based on particle size. Three distinct release patterns were observed between the gastric and gastrointestinal phases: 1) elements predominantly solubilized in the gastric phase (As, Cr, Zn, Cd), 2) elements solubilized mainly in the gastrointestinal phase (Br, Sb, Sn), and 3) elements showing reduced bioaccessibility due to precipitation in the gastrointestinal phase (Pb). **Conclusions:** These findings emphasize the complexity of metal release from microplastics, influenced by digestive conditions and metal speciation, and highlight the need for regulation of polymeric materials to prevent human exposure.



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sciforum-187333: μ SPEED microextraction of veterinary antibiotics in environmental water samples by UPLC

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The pharmaceutical industry is one of the fastest-growing sectors. Antibiotics are widely used in human and veterinary medicine. A significant fraction of administered antibiotics is excreted unchanged and enters the environment via manure application, wastewater discharge, and improper disposal. Their presence in aquatic systems is of increasing concern due to ecological risks and the development of antimicrobial resistance. Therefore, there is a strong need for rapid, sensitive, and environmentally friendly analytical methods for their determination in environmental waters [1-4].

A miniaturized and semi-automated solid-phase microextraction procedure based on μ SPEED technology was developed and coupled with ultraperformance liquid chromatography (UPLC) with UV detection. Six veterinary antibiotics were selected for analysis: tetracycline, chlortetracycline, oxytetracycline, doxycycline, sulfamethoxazole, and trimethoprim. The extraction procedure used a PS/DVB-RP sorbent cartridge. The cartridge was conditioned with 250 μ L of MeOH, equilibrated with 250 μ L of H₂O, and then 500 μ L of the sample was loaded three times. The elution step was performed in two cycles using 50 μ L of acidified MeOH. The total extraction time was 6 minutes per sample.

The developed method showed excellent chromatographic performance. Good linearity was obtained for all analytes ($R^2 > 0.99$). Limits of detection ranged from 0.30 to 1.23 μ g/L, while limits of quantification were between 0.92 and 3.73 μ g/L. Recoveries ranged from 46% to 86%. The method was successfully applied to environmental water samples collected from Madeira Island, where no target antibiotics were detected.

The proposed method enables fast, efficient, and environmentally friendly determination of veterinary antibiotics in water samples. The approach significantly reduces solvent consumption and sample volume while maintaining good analytical performance. The semi-automated format improves reproducibility and reduces analyst workload, making it a suitable tool for routine environmental monitoring.



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sciforum-187349: Microplastics Pollution in Selected Groundwater Sources in Ibadan, Nigeria

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Introduction

Groundwater is an important source of freshwater, particularly in developing countries like Nigeria, where it serves as a primary source of drinking water for many households. Microplastics are emerging contaminants of concern in drinking water systems. However, information on their occurrence in groundwater sources and the environmental factors contributing to their presence remains limited in developing countries. This study was conducted to investigate the occurrence and characterization of microplastics in selected groundwater sources in Ibadan, as well as to examine the environmental factors contributing to microplastic contamination.

Methods

Groundwater samples were aseptically collected from sixteen (16) dug wells and eight (8) boreholes. The samples were vacuum-filtered onto 0.45micron membrane filter and visually examined under a dissecting microscope. Microplastics were identified based on shape and colour. An observational checklist was used to collect data on environmental conditions surrounding the groundwater sources, including proximity to pollution sites, surrounding land use and the characteristics of the boreholes and wells.

Results

Microplastics were detected in all twenty-four samples, with abundances ranging from 1-120 particles/litre in dug wells and from 1-90 particles/litre in boreholes. Fragments and fibres were the dominant particle shapes, while the particles were identified in brown, orange, blue and red colours. Findings from the observational checklist indicated that stormwater runoff (62.5%), open dumpsites (25.0%) and improper trash disposal (16.7%) were the likely principal sources of microplastic contamination in the groundwater sources studied.

Conclusion

Microplastics were more abundant in dug wells than in boreholes across the studied locations, likely due to contamination from stormwater runoff and improper waste disposal practices.



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sciforum-188296: Trace Element Bioaccumulation in Meat and Bone Samples: Environmental Exposure, Nutritional Relevance and Food Chain Transfer

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Trace elements present in the environment are transferred through the food chain and may accumulate in animal tissues depending on their biological role, chemical behaviour, and environmental availability. This study investigated the distribution and bioaccumulation of lithium (Li) together with essential and potentially toxic elements (Zn, Cu, Mn, Co, Ni, V, Sr, Pb, Cd, and U) in meat and bone samples collected from different geographical regions of Romania. The research focused on the relationship between environmental exposure, tissue-specific accumulation, and the potential contribution of animal-derived foods to dietary trace element intake. The results demonstrated a distinct tissue-dependent distribution pattern for most analyzed elements. Bone samples exhibited significantly higher concentrations of lithium, strontium, manganese, zinc, and other mineral-associated elements compared to muscle tissue, indicating preferential accumulation within mineralized structures. Lithium concentrations in bone were substantially higher than in meat, suggesting long-term retention and possible incorporation into the hydroxyapatite matrix through ionic substitution mechanisms. Positive associations observed between lithium, strontium, and manganese in bone samples suggest common pathways related to mineral metabolism and skeletal incorporation. In contrast, meat samples showed relatively low and homogeneous lithium concentrations, reflecting systemic exposure and recent dietary intake rather than structural accumulation. Potentially toxic elements, including Pb and Cd, were detected at concentrations below maximum permissible limits, indicating low contamination levels and absence of significant food safety risks. Regional differences in elemental composition highlighted the influence of local geochemical conditions on trace-element transfer through the food chain and tissue bioaccumulation. The findings demonstrate that animal-derived foods contribute to dietary lithium intake and provide valuable information regarding environmental exposure pathways and trace-element accumulation in biological systems.



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sciforum-191109: Micro-plastics and Nano-plastics as Emerging Contaminants: A Systematic Review of Human Exposure Routes and Epidemiological Evidence of Health Outcomes

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Introduction

Global plastic production has surpassed 400 million tonnes annually, with a substantial fraction fragmenting into microplastics (MPs, $<5\text{mm}$) and nanoplastics (NPs, $<1\mu\text{m}$) that persistently contaminate air, water, and food. Continuous human exposure through multiple daily pathways raises urgent public health concerns. This review synthesizes evidence on MP and NP human exposure routes and associated health outcomes.

Methods

A systematic search was conducted across PubMed, Scopus, Web of Science, and Google Scholar for studies published between 2000 and 2024. Following PRISMA 2020 guidelines, 193 records were retrieved, reduced to 149 after deduplication, and screened to 31 studies meeting inclusion criteria. Methodological quality and risk of bias were evaluated using the Newcastle-Ottawa Scale.

Results

MPs were detected in 90% of healthy donors with blood concentrations of $1.84\text{--}4.65\ \mu\text{g/mL}$. Bottled water consumers ingest approximately 90,000 additional MP particles annually versus 4,000 for tap water users. A multicenter observational study detected MPs in carotid artery plaques of 58.4% of patients, with MP-positive individuals showing a 4.5-fold higher risk of myocardial infarction, stroke, or death over 34 months. Brain MP concentrations reached $26,076\ \mu\text{g/g}$ in dementia patients. Most studies were of moderate-to-high quality, though small sample sizes and cross-sectional designs introduced risk of bias.

Conclusions

MPs and NPs are widely detected in human tissues, with epidemiological studies reporting associations, not established causal relationships with cardiovascular disease and neurodegeneration. Standardized biomonitoring methods and strengthened global regulatory frameworks remain urgent priorities.



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sciforum-191216: *Tamarix aphylla* Leaves Synthesized Biochar Loaded Fe doped MgO Nanocomposites for Dye Pollutants Removal from Water

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Water pollution due to the Synthetic dyes is a serious issue now a days. The Chromophoric groups found in dye molecules are the source of color pollution. There are many conventional methods that was adopted to eradicate them. This study examined the synthesis of Fe-doped MgO biochar nanocomposites for the efficient degradation of methyl orange dye from wastewater. Biochar is a solid carbon-rich substance which was obtained from the leaves of *Tamarix aphylla* plant using slow pyrolysis method. After preparation of biochar further synthesis of Fe doped MgO nanocomposites was done by using of iron chloride as a source of iron and then mixed with previously prepared biochar . Afterwards the mixture is stirred for 30 minutes to facilitate reduction and formation of desired material. To settle down the material we allowed the mixture to stand for thirty minutes. Later on the settled material was isolated using decantation and then stored in sealed container. Later on various analytical parameters such as dye concentration, adsorbent dosage, contact time, pH, temperature, photocatalytic degradation, zeta potential and their effect dye on degradation of methyl orange was examined. The evaluation of adsorption rate by changing all the factors one by one helped us to draw valuable conclusions regarding to the efficiency of prepared material .The purity, particle size and morphology of a composite was investigated by using Fourier transform infrared Spectroscopy , X ray diffraction technique , scanning electron microscopy and Transmission electron microscopy respectively.



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sciforum-192374: Ecological Risk Assessment of Soils Near Abandoned Pb–Zn Mines in Nigeria

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Abandoned lead–zinc (Pb–Zn) mining sites are major sources of environmental contamination, particularly in developing countries where post-mining management is often inadequate. In Nigeria, historical Pb–Zn mining within the Benue Trough has left numerous abandoned mine lands (AMLs) that continue to release toxic metals into surrounding soils and water systems. However, few studies have assessed their ecological risks and ecosystem-level impacts. This study evaluates the ecological risks associated with abandoned Pb–Zn mine sites in Nigeria to support remediation and sustainable land management.

A total of 49 soil samples were collected from Gimbi/Rikaya and the Abakaliki sites in Nigeria. Metal, mobility, partitioning, and bioavailability were assessed using the BCR three-step sequential extraction procedure. Risk assessment evaluation was conducted using contamination factor (CF), enrichment factor (EF), geoaccumulation index (I_{geo}), ecological risk index (ERI), and cumulative risk score (CRS). A conceptual site model (CSM) was developed to identify contaminant sources, process and transport mechanisms, exposure pathways, and receptors.

Elevated concentrations of Zn, Pb, Cr, Ni, and Cd were detected in surrounding soils, indicating ongoing dispersion from abandoned mine tailings. Sequential extraction showed that Pb, Cd, and Zn were predominantly associated with exchangeable and reducible fractions, suggesting potential high mobility and bioavailability. Pollution indices classified the sites as strongly polluted with high ecological risks. The CSM identified tailings as the contaminant source, transported via erosion and leaching, ingestion, dermal contact, and inhalation as key exposure pathways affecting terrestrial and domestic receptors.

The study concludes that Abakaliki indicate high metal mobility and ecological risk, with Cd posing the greatest risk in both sites, while cerium was identified as a notable additional contaminant. These results underscore the urgent need for remediation, long-term monitoring, and stronger mine-closure practices to protect ecosystems and nearby communities from exposure to contaminants.



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sciforum-193412: Removal of ammonium from aqueous solutions using low-cost adsorbents

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The excessive release of ammonium into aquatic environments represents a major environmental concern because of its contribution to eutrophication, water quality deterioration, and adverse effects on human and ecosystem health [1]. Natural adsorbents, such as zeolites and microalgae biomass, represent a promising alternative for ammonium removal from aquatic systems. This study aimed to comparatively evaluate the ammonium removal efficiency from synthetic aqueous solutions using low-cost adsorbents.

The experiments were performed under batch conditions, contacting 1 g of adsorbent with 100 mL ammonium solutions at initial concentrations of 25-125 mg/L at room temperature for 24 h. Single adsorbent systems contained 1 g of dried *Chlorella* biomass or natural zeolite, while the hybrid microalgae-zeolite system consisted of 0.5 g of *Chlorella* biomass and 0.5 g of natural zeolite. The ammonium concentrations, before and after treatment, were determined using a PerkinElmer Lambda ultraviolet-visible spectrophotometer. The adsorption capacity and removal efficiency were calculated. Equilibrium data were further analyzed using the Langmuir and Freundlich isotherm models through linear regression analysis.

In the studied range of concentration, the highest ammonium removal efficiency was achieved by natural zeolite (61-81%), followed by the hybrid *Chlorella*-natural zeolite system (32-41%), while the lowest efficiency was observed for the *Chlorella* biomass alone (19-33%). The isotherms parameters indicated favorable adsorption of ammonium onto natural zeolite, suggesting its suitability for ammonium removal.

The obtained results suggest the possibility of using natural zeolite as a low-cost alternative for ammonium removal from aquatic systems and indicate its potential to limit exposure pathways in aquatic environments.

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sciforum-193435: Preparation of Size-Defined TPU Nano- and Microplastics and Their Cellular Uptake by RAW264.7 Macrophages

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The increasing use of thermoplastic polyurethane (TPU)-based clear aligners has raised concerns regarding the potential release of nano- and microplastics during long-term intraoral use. However, systematic biological evaluation of aligner-related plastic particles remains limited, partly due to the lack of well-defined particle fractions suitable for toxicological investigations. In this study, commercial TPU powders were purchased and subjected to mechanical comminution followed by differential centrifugation to obtain particle fractions with distinct size distributions. The morphology and particle size characteristics of the resulting fractions were characterized using scanning electron microscopy (SEM) and dynamic light scattering (DLS), respectively. To investigate particle–cell interactions, TPU particles were incubated with RAW264.7 macrophages, and their localization relative to the cells was examined using confocal microscopy. SEM observations and DLS analyses confirmed the successful preparation of several TPU particle fractions spanning the micro- to nanoscale range, with stable isolation of particle populations down to approximately 200 nm. Confocal microscopy revealed distinct spatial distributions of TPU particles associated with RAW264.7 macrophages. Differences among particle fractions suggested size-dependent interactions between TPU particles and RAW264.7 macrophages. Microscopic observation demonstrated cellular uptake by RAW264.7 cells, while the WST-8 assay revealed a reduction in cell viability. These findings establish a practical size-fractionation platform for TPU-derived nano- and microplastics and provide a foundation for future studies investigating the biological responses and safety assessment of plastic particles associated with oral healthcare materials.



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sciforum-193630: PFOS at human-relevant concentrations activates a KLF-1–P450 mitochondrial protective axis in *Caenorhabditis elegans*

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Background

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants that accumulate in humans and wildlife, yet the cellular mechanisms that protect against PFAS toxicity remain poorly understood.

Results

Using a stress-reporter screen, we identified activation of a p38 MAPK-dependent mitochondrial surveillance pathway in response to PFOS exposure. In parallel, unbiased transcriptomic analysis following chronic exposure to 1.5 ppm PFOS, a concentration comparable to the highest PFOS concentrations reported in human blood, and acute exposure to 12.5 ppm PFOS revealed a detoxification program dominated by cytochrome P450 genes, particularly members of the *cyp-13A* family. We further discovered that the transcription factor KLF-1 is a key regulator of this response. Silencing *klf-1* reduced PFOS-induced P450 expression and increased PFOS sensitivity, demonstrating that the KLF-1–P450 axis is protective. Antioxidant treatments suppressed both MAPK signaling and P450 activation, indicating that mitochondrial ROS act upstream of both pathways. Multi-omics analyses integrating the transcriptomic and metabolomic datasets revealed altered branched-chain amino acid metabolism as an additional major signature of PFOS exposure. We also found that PFOS is more toxic than PFOA in *C. elegans*, whereas the opposite pattern was observed in the related nematode *Pristionchus pacificus*. These findings demonstrate that PFAS toxicity is both compound-specific and species-dependent. Finally, PFOS activated the KLF-1–P450 axis at concentrations as low as 12.5 ppb, highlighting the potential toxicity of PFOS at environmentally and human-relevant concentrations.

Conclusions

Our findings identify a mitochondrial ROS–KLF-1–P450 protective mechanism that mitigates PFOS toxicity and reveal mitochondrial metabolic dysfunction as a central component of PFAS exposure. The conservation of KLF transcription factors and cytochrome P450 pathways raises the possibility that analogous protective responses may be activated in humans exposed to PFOS.



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sciforum-194093: Environmental Monitoring of Perfluoro octane Sulfonate and Perfluorooctanoic Acid in Khanpur Stream, Pakistan: Implications for Human and Ecosystem Health

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PFAS are widely used synthetic chemicals that persist in aquatic environments and can accumulate in biota, raising concerns regarding freshwater quality and ecosystem health. Information on PFAS contamination in Pakistani freshwater systems remains limited despite increasing industrialization. This study evaluated the occurrence, distribution patterns, ecological risk, and human health implications of PFOS and PFOA in Khanpur Stream, Sheikhpura, Pakistan, a freshwater source used for irrigation, fisheries, and domestic purposes.

Sample from 32 locations along a 15 km reach of the stream during February and March 2026 following APHA standard procedures. At each site, triplets' surface and subsurface water samples were collected from depths ranging from 1 to 5 m, resulting in 192 samples. Samples were collected in precleaned glass bottles, concentrated by SPE, and analyzed using LC-MS/MS. Ecological risk was assessed using the risk quotient approach, while noncarcinogenic HHR was evaluated through hazard quotient calculations based on adult drinking water exposure.

PFOS and PFOA were detected in all samples. Surface water concentrations ranged from 10.8 to 36.3 ng/L for PFOS and from 7.8 to 15.2 ng/L for PFOA, whereas subsurface concentrations ranged from 1.7 to 20.4 ng/L and 1.4 to 11.1 ng/L, respectively. Elevated concentrations were consistently observed near paper and pulp industrial zones, while the lowest levels occurred in irrigation dominated areas. ERA indicated that PFOS posed the greatest environmental concern, with risk quotient values ranging from 1.61 to 5.42 in surface waters and from 0.25 to 3.04 in subsurface waters. In contrast, PFOA exhibited low to moderate ER, with RQ values ranging from 0.03 to 0.32. HQ values for both compounds remained below 1, indicating negligible noncarcinogenic risk through direct water consumption. The results identify industrial activities as the primary source of PFAS contamination in Khanpur Stream and highlight PFOS as the dominant contributor to ER within the aquatic environment.



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sciforum-194240: Modulatory effects of vitamin C on lead induced organotoxicity and histopathology in male albino rats.

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Lead (Pb) toxicity remains a major global public health concern, particularly in low-income regions with persistent environmental and occupational exposure. This study evaluated the protective effects of Vitamin C (VC) against Pb-induced organotoxicity and testicular histopathological alterations in male albino rats as a mammalian experimental model. Twenty-four male albino rats were randomly assigned into four groups (n = 6): control, Pb acetate (60 mg/kg body weight), Vitamin C (100 mg/kg body weight), and combined Pb + VC treatment, administered orally for 65 days to simulate prolonged exposure. Lead residues in tissues were quantified using atomic absorption spectrophotometry following acid digestion. Body and organ weights were recorded, and testes were processed for histopathological examination. Statistical analysis was performed using one-way ANOVA, with significance set at $p < 0.05$. Pb exposure significantly increased Pb residues in the brain, kidney, liver, and testes, while Vitamin C co-administration reduced tissue Pb levels by approximately 24–66%, with the greatest reduction observed in the kidney. Pb also caused significant reductions in post-treatment body weight (172.6 g vs 229.0 g in controls) and reproductive organ weights. Vitamin C partially ameliorated these effects, improving body weight (180.9 g) and restoring heart weight to near-control values. Histopathological evaluation revealed severe degeneration and disorganization of seminiferous tubules in Pb-exposed testes, whereas Vitamin C co-treatment markedly preserved spermatogenic architecture and cellular integrity. These findings demonstrate that Vitamin C mitigates Pb-induced organotoxicity and reproductive damage in male albino rats by reducing tissue Pb accumulation and preserving testicular structure. While the results highlight the potential of Vitamin C as an accessible and low-cost protective agent against lead toxicity, further studies are required to validate these effects in human populations before clinical extrapolation.



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sciforum-195148: Effect of Aflatoxin Contamination on Oxidative Stress, Hematological Indices, and Growth Performance of Broiler Chickens

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Aflatoxin B₁ (AFB₁) is among the most potent mycotoxins affecting poultry production. Hence, this study evaluated the dose-dependent effects of AFB₁ exposure on oxidative stress biomarkers, hematological indices, and growth performance in broiler chickens. Ninety healthy broiler chickens were randomly assigned to three groups (n = 30) in a completely randomized design. Group I (control) received basal feed; Group II and Group III received AFB₁-contaminated feed at 40 mg/kg and 80 mg/kg feed, respectively, for 28 days. Aflatoxin B₁ concentrations used in this study are consistent with previously reported models assessing high-dose exposure for mechanistic and dose-dependent toxicological evaluations. AFB₁ (≥98% purity) was sourced commercially and incorporated into feed following standard laboratory protocols. Ethical approval for the use of animals was obtained (Approval No. BIOSC24-12). Growth parameters: body weight gain, feed conversion ratio (FCR), and feed efficiency (FE), were monitored, while blood samples were analyzed for antioxidant enzymes, oxidative damage markers, and hematological indices. Data were analyzed using one-way ANOVA, with differences considered significant at p < 0.05. AFB₁ exposure resulted in a significant, dose-dependent reduction in glutathione, glutathione peroxidase, catalase, and superoxide dismutase activities, alongside marked elevations in malondialdehyde and nitric oxide levels. Hematological assessment revealed significant decreases in red blood cell count, hemoglobin concentration, and packed cell volume. Results showed 13% and 27 % reduction in body weight gain in groups II and III, respectively. FCR increased significantly from 0.18 in the control group to 0.24 in group II and 0.27 in group III, indicating poorer feed utilization. Correspondingly, FE declined from 5.55 in the control to 4.17 and 3.70 in the treated groups, respectively, demonstrating AFB₁-induced growth suppression. These findings provide integrated biochemical, hematological, and performance-based evidence of AFB₁-induced toxicity in broiler chickens, establishing an experimental framework for evaluating mitigation strategies against aflatoxicosis in poultry production systems.



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sciforum-199406: Dual-source heavy metal co-exposure impairs genetic growth potential in preschool children: a large population-based mixture analysis

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Objective

Dual-source heavy metal exposure via diet and industrial take-home pathways impairs children's growth, but population-based evidence on its independent impact on genetic growth potential remains limited. This study aimed to characterize dual-source metal mixtures, identify core toxic components, and examine whether selenium mitigates metal-related growth retardation in preschool children.

Methods

This cross-sectional study enrolled 10,242 children aged 0–7 years. Ten urinary metals (Pb, Cd, Hg, Se, Co, Mo, Cr, Mn, Cu, Ni) were quantified by ICP-MS, with creatinine standardization and Z-score transformation. Three dietary patterns were extracted via principal component analysis (PCA), and industrial/take-home exposure risk was stratified by residential distance to polluting factories and caregivers' occupational hygiene. The primary outcome Adjusted-HAZ was defined as standardized residuals between observed and genetically predicted height-for-age Z-score (HAZ). We applied partial Spearman correlation, generalized linear models (GLM) and three mixture models (WQS, qgcomp, BKMR) to estimate mixture toxicity, with restricted cubic spline (RCS) for nonlinear thresholds, plus stratified and sensitivity analyses with full covariate adjustment and false discovery rate (FDR) correction.

Results

Source apportionment identified two distinct pathways: seafood diet correlated with elevated Hg and Se burdens, while high industrial/take-home exposure increased urinary Pb ($\beta = 0.235$, 95% CI: 0.056–0.414) and Co ($\beta = 0.193$, 95% CI: 0.046–0.340). Seven metals showed significant inverse associations with Adjusted-HAZ after FDR correction. Mixture models consistently revealed a robust overall growth-suppressing effect (WQS $\beta = -0.320$, $P < 0.001$), with Se, Hg, Cd, Cu and Pb as dominant contributors. Hg and Cu exhibited nonlinear inflection points, beyond which growth impairment accelerated sharply. High urinary selenium failed to counteract mixture toxicity, and all findings remained stable in sensitivity tests.

Conclusions

Dual-source heavy metal co-exposure significantly impairs children's genetic growth potential. Selenium supplementation alone cannot alleviate growth damage; source-targeted interventions are critical to protect child growth.



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sciforum-199407: Urinary Nickel Exposure and Growth in Prepubertal Chinese Children: Threshold Effects and Benchmark Dose Analysis

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Introduction

Nickel is a ubiquitous environmental heavy metal, and children are particularly vulnerable to its toxicity. However, nationwide evidence on the association between nickel exposure and growth in prepubertal children remains limited, and benchmark dose (BMD)-based reference values are lacking.

Methods

Based on a nationwide cross-sectional study, 10,008 prepubertal Chinese children were included. Urinary nickel levels were measured and adjusted for creatinine. Height-for-age (HAZ), weight-for-age (WAZ), and BMI-for-age (BAZ) Z-scores were calculated. Multivariable regression, restricted cubic spline (RCS), piecewise regression, and Bayesian BMD modeling were applied to assess associations and estimate the benchmark dose lower confidence limit (BMDL₅).

Results

Urinary nickel concentrations showed a right-skewed distribution, with a geometric mean of 5.68 µg/g creatinine. Significant negative associations were observed between urinary nickel and height, weight, HAZ, and WAZ (all $P < 0.001$), with clear dose-response trends. RCS analyses indicated nonlinear relationships with HAZ and WAZ. Piecewise regression identified thresholds of 3.98 µg/g creatinine for HAZ and 3.80 µg/g creatinine for WAZ and BAZ. Below these levels, growth indicators decreased significantly (all $P < 0.01$), while effects plateaued above them. Bayesian analysis estimated BMDL₅ values of 2.56, 3.08, and 4.77 µg/g creatinine for HAZ, WAZ, and BAZ, respectively.

Conclusions

Urinary nickel exposure was significantly associated with impaired growth in prepubertal children, showing nonlinear dose-response relationships and clear threshold effects. Consistent findings across multiple analytical approaches suggest that even relatively low exposure levels may adversely affect child growth. This study provides important epidemiological evidence for risk assessment of nickel exposure in children.



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sciforum-199409: Association between Urinary Metal Exposure and Child Growth and Development with Dietary Modification Effects

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Objective

To investigate the association between mixed exposure to six urinary metals (aluminum, chromium, iron, zinc, barium, thallium) and growth indicators in children aged 0–9 years, and to evaluate the modifying effects of dietary factors and physical activity on the metal-growth association.

Methods

This cross-sectional study was based on the National Nine-Province Child and Adolescent Cohort, including 10,235 children aged 0–9 years. Urinary metal concentrations were measured by ICP-MS, and height-for-age (HAZ), weight-for-age (WAZ), and BMI-for-age (BAZ) Z-scores were calculated. Linear regression and restricted cubic spline (RCS) were used to assess single-metal effects and non-linear associations; WQS, Qgcomp, and BKMR models were applied to evaluate mixed exposure effects; the CVEK model and additive interaction analysis were used to examine modification by dietary factors and physical activity.

Results

After adjusting for confounders, Tl was significantly negatively associated with HAZ, WAZ, and BAZ; Zn was significantly negatively associated with WAZ and BAZ; Ba was significantly positively associated with BAZ (all $P < 0.01$), while Al, Cr, and Fe showed no statistically significant associations. In mixed exposure models, Tl and Zn were the major negative contributors. RCS revealed non-linear associations for Zn, Tl, Al, and Cr with at least one growth indicator ($P < 0.05$). CVEK models indicated significant modification effects of dietary factors such as milk, freshwater fish/shrimp, cod liver oil, and zinc supplements on metal effects ($P < 0.05$). Additive interaction analysis showed a synergistic effect of zinc supplements combined with summer physical activity on Al-HAZ (RERI=0.18) and Al-WAZ (RERI=0.16), and an antagonistic effect of freshwater fish/shrimp combined with summer physical activity on Ba-BAZ (RERI=-0.28).

Conclusion

Mixed metal exposure in childhood was negatively associated with growth, with Zn and Tl as major contributing metals. Dietary nutrition and physical activity can modify the effects of metals on growth, providing preliminary evidence for comprehensive intervention strategies in children from high-risk areas.



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Session 2. Wildlife Ecotoxicology, Sentinel Species, and Ecosystem Health

sciforum-172292: Autotomy and antioxidant responses as biomarkers of acute and chronic contaminant stress in *Eurythoe complanata*

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The biochemical responses of marine organisms to acute and chronic xenobiotic exposure may vary by tissue. Here, we examined enzymatic and non-enzymatic antioxidant responses in different body regions of the polychaete *Eurythoe complanata* exposed to cadmium (Cd, 200 $\mu\text{g L}^{-1}$), hydrogen peroxide (H_2O_2 , 200 mmol L^{-1}), and a water-soluble fraction of used automobile crankcase oils (WSF-UAO, 3% m/v) in a static aquaria system for 7 and 14 d. Heavy metal concentrations, antioxidant enzyme activities—catalase (CAT), glutathione reductase (GR), glucose-6-phosphate dehydrogenase (G6PDH), and glutathione S-transferase (GST)—, lipid peroxidation, metallothioneins, and soluble thiols were measured in the anterior (A, 20–25 setigers), middle (M, 30–40 setigers), and posterior (P, 20 terminal setigers) regions. Additionally, the number of individuals exhibiting autotomy was recorded. Results showed significantly higher concentrations of Cd and other metals in the posterior region (3.8-fold higher than controls). The M region demonstrated high metabolic activity and antioxidant defense capacity. Thirteen percent of WSF-UAO-exposed polychaetes displayed autotomy in the P region. The increase in antioxidant responses across body regions of Cd- and WSF-UAO-exposed polychaetes suggests compensatory mechanisms against oxidative stress. Autotomy of the P region appears to serve as a detoxification strategy for the accumulation of xenobiotics and reactive oxygen species (ROS) in damaged tissue. These results improve our understanding of how *E. complanata* adapts to both short-term and long-term chemical stress and confirm its potential as a sentinel species for assessing the impact of complex pollutant mixtures in marine environments.



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sciforum-179200: Comparative stress responses of two freshwater bivalves to emerging PFAS contaminants

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Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants, with emerging compounds such as perfluorobutane sulfonate (PFBS) and perfluorobutane sulfonamide (FBSA) increasingly detected in aquatic ecosystems. Effects on aquatic organisms, however, remain poorly understood. We conducted a chronic exposure study to assess species-specific stress responses in *Dreissena polymorpha* and *Corbicula sp.* Bivalves were exposed to PFBS or FBSA across environmentally relevant to extreme concentrations. Mortality, behavioural endpoints (valve movement, burrowing speed and depth, attachment rate), and physiological responses (respiration) were measured. Mortality was low for PFBS (LC50 > 100 mg/L for both species) but higher for FBSA (LC50 = 37.8 mg/L for *Corbicula sp.*; 0.14 mg/L for *D. polymorpha*), indicating greater FBSA potency and higher sensitivity of *D. polymorpha*. Attachment probability of *D. polymorpha* was unaffected by exposure level but lower in PFBS-exposed individuals (40.6%) than in FBSA-exposed ones (62.3%). At the highest PFBS concentration, *Corbicula sp.* burrowed deeper, suggesting a stress response. Burrowing depth was unaffected by FBSA, likely due to 100% mortality at the highest concentration. Valve movement response variables (N = 30) were grouped into principal components to reduce collinearity. Overall, the majority of behavioural variability could be explained by differences between species, whereas PFAS-induced effects were generally subtle, concentration-dependent, and species-specific. Treatment effects were more consistently observed in *Corbicula sp.* than *D. polymorpha*. Oxygen consumption of both species increased significantly with increasing body mass, but there was no significant effect of PFAS type and exposure concentration. Overall, PFBS triggers behavioural responses, whereas FBSA is more lethal. Our findings highlight the value of behavioural and physiological endpoints to detect sub-lethal stress and reveal species-specific responses to emerging PFAS in aquatic ecosystems.



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sciforum-180448: Biomonitoring Soil Health: Ecotoxicological Impact of Multi-Metal Mixtures on the Sentinel Earthworm *Aporrectodea giardi*

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Introduction

Earthworms serve as critical sentinel species for assessing soil health and the ecological impact of chemical stressors. This study investigates the ecotoxicological response of the anecic earthworm *Aporrectodea giardi* to complex environmental mixtures of six heavy metals: cadmium (Cd), chromium (Cr), copper (Cu), nickel (Ni), iron (Fe), and manganese (Mn).

Methods

To simulate realistic soil contamination, four metallic mixtures (M1–M4) were tested over 12 and 24 days. These mixtures, based on agricultural field (Northeast Algeria), contained Cd, Cr, Cu, Ni, Mn, and Fe at specific concentrations (mg/kg): M1 (12, 171, 38, 46, 1110, 30832); M2 (7, 109, 32, 35, 791, 22492); M3 (7, 107, 30, 32, 660, 20722); and M4 (9, 102, 28, 31, 738, 19982). Biological responses were evaluated through oxidative stress biomarkers: total protein content, glutathione (GSH), metallothionein (MT), catalase (CAT), and lipoxigenase (LOX).

Results

Our findings reveal dynamic and concentration-dependent physiological responses. After 24 days, protein levels significantly decreased under the M3 treatment while increasing in all other conditions. Initial fluctuations in GSH and MT contents, marked by a decrease in M1/M4 and an increase in M2/M3 at 12 days, stabilized into a significant enhancement by day 24. CAT was inhibited in nearly all treatments except M3 ($P > 0.05$), while LOX was initially stimulated (M1, M2, M4) before declining across all conditions.

Conclusions

These findings demonstrate that multi-metal mixtures trigger oxidative stress, inducing adaptive responses through MT production and antioxidant defenses (GSH, LOX) to restore redox balance. Overall, the high sensitivity of *A. giardi* underscores its value as a sentinel species for risk assessment and the biomonitoring of metal-polluted soil ecosystems.



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sciforum-184618: Assessment of Combined Methylparaben and Diethyl Phthalate Exposure on Developmental and Behavioral Toxicity in Zebrafish (*Danio rerio*) Embryos and Larvae

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Introduction

Endocrine-disrupting chemicals (EDCs) such as methylparaben (MP), diethyl phthalate (DEP) are widely detected in aquatic environments due to their extensive use in personal care products. Effluent from salon and beauty parlour samples collected from Chennai, India, were characterized by GC-MS analysis, revealing more than 30 compounds and the co-presence of MP and DEP within a complex lipid-enriched matrix, establishing a real-world multi-EDC co-exposure scenario.

Methods

This study evaluated the developmental, physiological, and neurobehavioral toxicity of MP and DEP in zebrafish (*Danio rerio*) embryos using OECD TG 236 guidelines. Embryos were exposed to concentrations of 10, 25, and 50 µg/L for individual compound exposures, and endpoints including mortality, heart rate, hatching success, morphological abnormalities, and behavior were assessed.

Results

Acute toxicity analysis revealed LC₅₀ values of 25.11 µg/L for MP and 36.60 µg/L for DEP, indicating higher toxicity of MP. At 100 µg/L, mortality reached 94% for MP and 71% for DEP. Both compounds induced significant bradycardia, with heart rates declining from 190 bpm (control) to 100 bpm (MP) and 120 bpm (DEP) at 50 µg/L. Hatching success decreased to 18% (MP) and 13% (DEP), accompanied by increased skeletal deformities. Binary mixture exposure (MP:DEP at 1:1, 1:9, and 9:1 ratios) produced enhanced embryotoxicity relative to individual compound groups, with locomotor activity reduced to 40,799 mm in the MP-dominant 9:1 mixture group, indicating synergistic neurobehavioral suppression. Behavioral assays demonstrated anxiogenic responses in DEP-exposed larvae, characterised by elevated light-zone residency and increased upper-tank occupancy consistent with hyperexcitability or anxiety-like phenotype, and non-monotonic alterations in MP-exposed larvae including mild hyperactivity at lower concentrations transitioning to hypoactivity and depression-like behavior at higher concentrations, consistent with hermetic endocrine modulation.

Conclusion

These findings highlight the heightened risk of EDC mixtures and emphasize the need for mixture-based toxicological assessment.



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sciforum-185817: Coastal to Oceanic Comparison of Plastic Additive Accumulation in Northeast Atlantic Top Predator Sharks

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Plastic litter has significantly increased in the last decades due to its excessive production and inefficient waste management, which has led to millions of untreated tons of plastic ending up in the ocean. Over time, plastic waste undergoes degradation and can release various additives into the environment, including plasticisers, flame retardants, and other chemicals. Some have been classified as concerning for human health and environmental safety, such as phthalic acid esters (PAEs), used as plasticizers in plastic materials, and polybrominated diphenyl ethers (PBDEs), historically used as flame retardants. This study aimed to establish a profile of the most prevalent PAEs and PBDEs in the marine environment and to assess spatial differences between coastal and open-ocean areas by evaluating the accumulation patterns of these compounds across different tissues in a top predator, the blue shark (*Prionace glauca*), caught in offshore and coastal waters. A total of 34 blue sharks were opportunistically sampled as bycatch in the North Atlantic, with muscle and liver tissues collected in situ. In total, 8 different phthalates and 26 different PBDE congeners were quantified. The results show differences in PAEs concentrations between coastal and oceanic catches across both tissues analysed ($p < 0.05$), as well as differences in PBDEs in the liver ($p < 0.05$), but not in muscle ($p = 0.084$). Furthermore, both tissues exhibited significant differences in the concentrations of the two plastic additives ($p < 0.001$), with higher levels observed in the liver. This study highlights the complex dynamics of plastic additive accumulation in marine predators, providing important insights into how environmental factors and tissue-specific properties influence contaminant bioaccumulation. These findings contribute to a better understanding of plastic pollution and its potential impacts on marine ecosystems.



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sciforum-185946: The Impact of Cigarette Filters on Aquatic Ecosystems Using Daphnids as Model Organisms

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Cigarettes are the most littered item in the world. 4.5 trillion are discarded annually, and their filters can introduce toxic chemicals and plastics into waterbodies. Therefore, the assessment of the ecotoxicological effects of smoked and non-smoked cigarette filters is necessary. With the freshwater organism, *Daphnia*, this study analyses the toxicity and sublethal effects caused by these two types of filters with New Approach Methodologies, such as effect-based bioassays and enzymatic biomarkers. Toxicity was assessed by measuring mortality following exposure to increasing concentrations of filters. The study also analysed the survival and growth rate, and quantified enzyme activities.

After 48 hours, only smoked cigarette filters were toxic from 100 ml extract/L with an EC₅₀ value of 397 ml/L. In contrast, exposure of 21 days reduced survival at lower concentrations, with smoked filters decreasing median survival to 4 days at 200 ml/L, corresponding to 4 filters per litre of water. Daphnids' growth rate was most affected after 7 days of exposure from concentrations of 5-70 ml/L. Size changes observed at 7 days, were reduced at 14 and 21 days of exposure, suggesting possible acclimation. Enzymatic activity was also altered after 21 days from concentrations of 15-45 ml/L, with significant increases in acid phosphatase and decreases in alkaline phosphatase, peptidase, and β -galactosidase.

Given the observed effects in *Daphnia*, cigarette filters may potentially impact other freshwater organisms. Past literature has shown that daphnids can have similar responses as vertebrae models to other psychoactive substances. Furthermore, negative effects on these primary consumers may lead to cascading effects on higher trophic levels and loss of biodiversity. Lastly, the limited availability of data on environmentally relevant concentrations of filters also underscores the importance of this study, highlighting the need to consider this emerging contaminant in environmental risk assessment frameworks.



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sciforum-186223: Ecotoxicological assessment of the impacts of textile material leachates on the aquatic environment using Protoxkit F

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The textile industry is a major contributor to environmental pollution due to high water consumption and the use of complex chemical substances. During processing, compounds such as dyes, resins, and formaldehyde are applied, posing risks to aquatic ecosystems and human health. Synthetic textiles may additionally release toxic monomers and hazardous finishing agents, highlighting the need for systematic monitoring of their chemical burden. This research aims to assess the ecological and environmental risks associated with textile leachates. The study examines both natural and synthetic textiles in new and used states. Water leachates are prepared under controlled conditions, considering different temperatures and contact times. Ecotoxicity is evaluated using the Protoxkit F microbiotest, which measures 24-hour growth inhibition of the ciliate protozoan *Tetrahymena thermophila*. To ensure a comprehensive assessment, biological results are complemented by physico-chemical analyses, including pH, Chemical Oxygen Demand (COD), and formaldehyde concentrations determined according to relevant ISO standards. The results provide a comparative evaluation of toxic potential across textile types. Statistical analysis identifies the most hazardous materials and the conditions (e.g., temperature) that enhance pollutant release. A correlation is observed between chemical parameters, particularly formaldehyde levels, and reduced protozoan population growth. This study contributes to identifying high-risk textile materials and supports the development of eco-friendly manufacturing practices and stricter regulation of hazardous substances. By integrating biological and chemical monitoring, the research aligns with the One Health approach, emphasizing the interconnectedness of human, animal, and environmental health, and the importance of protecting aquatic ecosystems.

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sciforum-186340: Ecological assessment of two Portuguese estuaries under contrasting urban pressure: Douro vs Lima

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Background

Monitoring estuarine habitats has become an increasing priority, as ongoing urban development in surrounding areas has intensified the pressure already affecting these ecosystems. Therefore, this study aims to assess the ecological status of two estuaries subjected to contrasting levels of urban pressure: the Douro estuary, a highly urbanized ecosystem, and the Lima estuary, a less disturbed ecosystem mainly impacted by port activities.

Methods

The characterization of the surrounding areas of both estuaries was carried out using the Land Occupation Map of Portugal. Three sampling sites were established in each estuary, corresponding to the lower, middle and upper reaches, with sampling campaigns in the Winter and Summer of 2025-2026. At each site, water and sediment samples were collected to evaluate nutrient concentrations, macroinvertebrate communities, organic matter content and sediment granulometry. All data were analysed in accordance with the Water Framework Directive.

Results

Land-use characterization indicated that the Douro basin characterized by agricultural and forest areas (59%), with artificial areas (>5%) being concentrated close to the Douro estuary. The Lima basin is a more heterogeneous landscape, dominated by forest areas (64%), with considerable artificial (16%) and agricultural areas (15%). Nutrient concentrations reached only a good ecological status, primarily constrained by high PO_4^{3-} concentrations exceeding reference values (>0.110). Macroinvertebrate community was more impacted in the Douro estuary, with lower diversity and dominated by tolerant species (e.g. *Peringia ulvae*), while the Lima estuary had sensitive species to polluted conditions (e.g. *Abra tenuis*), especially during Summer. Overall, the Douro estuary had coarser sediments (>55%) than the Lima which was muddier (36%), and both possessed low organic matter content (<5%).

Conclusions

The influence of anthropogenic pressures was more pronounced in the Douro estuary than in the Lima estuary. Nevertheless, the ecological status for the analysed parameters achieved a classification of moderate in both systems.



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sciforum-186505: Assessment of Pb neurotoxicity in European brown bears: Evidence from Pb–Ca associations and oxidative stress biomarkers

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Throughout the last decades, our research group has monitored non-essential trace element levels in brown bears (*Ursus arctos*) from the Dinara-Pindos population to assess exposure to these environmental pollutants, their impact on health, and the risk of chronic toxicity. Lead (Pb) is a high-priority neurotoxicant whose mechanisms of toxicity include molecular mimicry, oxidative stress, mitochondrial dysfunction and neuroinflammation. Given the brain's limited capacity to compensate for toxic damage, this study aimed to investigate the most probable mechanisms by examining the associations between Pb and calcium (Ca) levels as well as biomarkers of oxidative stress. Brain stem samples were collected from 69 free-living brown bears hunted in Croatia between 2022 and 2025 in accordance with the Brown Bear Management Plan. Elements were quantified by inductively coupled plasma-mass spectrometry (ICP-MS). Levels of oxidative stress biomarkers malondialdehyde (MDA), reactive oxygen species (ROS), catalase (CAT) activity and total antioxidant capacity (TAC) were measured in tissue homogenates. Brain Pb levels (mean $\pm$ SD, median, range: 26.8 ± 23.9 , 19.9, 2.11–175 $\mu\text{g/kg}$ dry mass) did not exceed values considered normal for cattle (used as a reference due to the lack of species-specific reference values). A moderate positive association was observed between Pb and the essential Ca (Spearman's $r = 0.45$, $p = 0.000172$, $n = 64$). This correlation may reflect divalent cation mimicry, whereby Pb^{2+} mimics Ca^{2+} by binding to similar sites and entering cells via Ca^{2+} channels. No significant relationships were observed between Pb levels and the investigated oxidative stress biomarkers thereby implying successful maintenance of redox balance in conditions of environmental exposure. This study suggests that Pb levels detected in the bear brain are unlikely to induce oxidative stress, while confirming an association between Pb and Ca, a key essential element involved in brain function.



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sciforum-186888: Retrospective study of seagull poisonings in central Portugal: can marine phycotoxins be involved?

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The Lisbon's Wildlife Rehabilitation Center (LxCRAS) primarily receives birds, with seagulls making up a large share. Most of these were *Larus fuscus* (62%), accounting for 73% of total seagulls showing signs of intoxication (paresias). Admissions of animals originating in the Lisbon and Setúbal districts peaked annually in spring and autumn, coinciding with this species' departure and return from migration, respectively. *Larus michahellis*, a resident species, comprised 21% of admissions and accounted for 16% of seagulls presenting paresias. Fish and shellfish consumed by seabirds can contain marine biotoxins which originated from certain microalgae in their diet. The seasonal occurrence of amnesic shellfish poisoning (ASTs) and paralytic shellfish poisoning (PSTs) toxins was compared with the number of seagulls admitted weekly at LxCRAS with paresias during the last decade (2016-2025). The weekly occurrence of AST neurotoxins was very short-lived and rarely attained concentrations above the human safety level. These episodes did not coincide with admissions above each year's weekly average. The occurrence of PSTs neurotoxins above the human safety level was sporadic, restricted to winter 2016/17 and autumn 2018. There was no evidence that the strong contamination in the Lisbon area during 2018 could have affected seagulls, due to the recurrent autumnal peak in admissions. Paresias incidence increased mainly with the number of *L. fuscus* but not *L. michahellis* admissions, and also with ambient air temperature. Mortality from paresias was higher in autumn than in spring, coinciding also with higher temperatures. As demonstrated earlier in seagulls from the south of Portugal, botulism might be implicated in these intoxications. Seagulls' habits are opportunistic, eating terrestrial prey and human leftovers besides seafood. The high energy expenditure required for migration seems to be driving these animals to seek easily accessible leftovers, which might be spoiled.



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sciforum-186933: From streets to streams: Insights on the ecotoxicological effects of stormwater runoff on *Danio rerio* embryos

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Background

Stormwater runoff from urban areas is an alarming issue to aquatic ecosystems due to its capacity to transport a wide range of contaminants threatening aquatic organisms and compromising the ecosystem integrity. This study aims to evaluate the ecotoxicological effects of stormwater in *Danio rerio* embryos.

Methods

Water samples were collected from three water bodies: Este river, Sousa river and Vale das flores stream. In each site, sampling took place in the upstream, stormwater outlet and downstream locations. Acute fish embryo toxicity assays were performed, evaluating survival, hatching success, and morphological alterations after 96 h in unfiltered water samples. Sub-individual parameters were also evaluated through the analysis of oxidative stress biomarkers (catalase–CAT, and glutathione S-transferases–GSTs activities, and thiobarbituric acid reactive substances–TBARS levels), neurotoxicity (acetylcholinesterase–AChE activity), and cellular energy allocation (CEA).

Results

All sampling sites induced morphological abnormalities in *D. rerio* embryos (e.g., body curvature, hemagglutination and pericardial edema). Higher frequencies were observed in Este and Vale das Flores samples (5-25%). Sousa samples impaired embryo hatching, and caused highest mortality (>95%). Biomarkers responses varied among the studied water bodies. In the Este river, antioxidant system alterations suggest defensive mechanisms activation against oxidative damage, while changes in AChE activity indicate neurotoxic effects. Sousa samples evoked a pronounced toxic response, characterized by enhanced lipid peroxidation alongside alterations in AChE activity and CEA, indicating both oxidative damage and neurotoxicity. Vale das Flores samples caused occasional alterations in TBARS levels and CEA, nonetheless, consistent neurotoxic effects were observed.

Conclusions

The results revealed distinct toxicity profiles among the urban-influenced water bodies. Sousa samples exerted the most severe effects on embryonic development. These findings highlight the sensitivity of early life stages to urban-associated stressors and reinforce the importance of incorporating ecotoxicological bioassays into monitoring strategies, improving the assessment/management of urban freshwater ecosystems.



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sciforum-187021: Biomarkers of DNA damage in common carp inhabiting an agriculturally impacted lake in Mexico

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Aquatic organisms constituted an important food resource for human populations. These are primarily obtained through capture fisheries and aquaculture. However, aquatic ecosystems are increasingly affected by complex mixtures of legacy and emerging contaminants derived from agricultural and urban activities. Many of these compounds are persistent and readily dispersed in aquatic environments, contributing to the deterioration of surface water quality and potentially inducing genotoxic effects in aquatic organisms, which may also represent a risk to consumers. The objective of this study was to determine DNA damage in *Cyprinus carpio* from Atlangatepec Lagoon, Tlaxcala, Mexico, an area characterised by fish production and strong influence from agricultural activities. Blood samples (100 µL) were collected from nine adult organisms in the study area and from organisms obtained from aquaculture production units, which served as the control group. Samples were processed according to the standard alkaline comet assay protocol. Slides were analysed under a fluorescence microscope using Comet Assay IV software. A total of 100 nucleoids per slide (two slides per individual) were analysed to assess tail length, tail intensity, and tail moment parameters as genotoxicity biomarkers. Before statistical analysis, data were log10- and arcsine-transformed to stabilise variances and verify statistical assumptions. Differences between groups were analysed using Welch's t-test in R software (v.4.4.2). Significant differences ($p < 0.05$) were observed between fish from Atlangatepec Lake and the control group for all evaluated parameters, indicating increased DNA damage in exposed organisms. The results indicate the presence of genotoxic agents, likely associated with agricultural runoff and urban discharges. Likewise, these findings confirm the effectiveness of the comet assay as a sensitive biomonitoring tool in ecotoxicology and its value for environmental genotoxicity assessment in aquatic ecosystems of fisheries importance.



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sciforum-187025: Optimisation of coelomocyte extrusion for genotoxicity biomonitoring in *Eisenia fétida*

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Environmental xenobiotics accumulate in terrestrial ecosystems, and some of these compounds can induce cytotoxic and genotoxic effects in exposed organisms. Their toxicity, persistence, and bioaccumulation in food chains have necessitated the use of sensitive methods to assess genetic damage in bioindicator organisms, such as *Eisenia fetida*, which has been recognised as a sentinel species for soil ecotoxicology. However, standardised non-invasive methods for obtaining viable coelomocytes suitable for genotoxicity assays remain limited. The objective of this study was to standardise a methodology for coelomocyte extraction from *Eisenia fetida* for application in micronucleus (MN) and alkaline comet assays. Adult organisms were exposed to an extrusion solution supplemented with guaiacol at concentrations of 0, 25, 50, and 100 mg/mL. Cell viability was determined using the trypan blue exclusion test, while micronucleus frequency and DNA fragmentation parameters were evaluated by optical and fluorescence microscopy, respectively. In the comet assay with software, we measured tail length, tail intensity and tail moment. Statistical analyses were performed using Kruskal-Wallis and one-way ANOVA tests ($p < 0.05$). The extrusion solution, supplemented with 25 mg/mL guaiacol, maintained high cell viability (98%) and DNA integrity while reducing interference from coelomic mucus, thereby improving the visualisation and quantification of coelomocytes. Conversely, exposure to 50 and 100 mg/mL guaiacol resulted in a significant increase in cytoplasmic abnormalities and DNA migration parameters, and a significant decrease in cell viability. This study demonstrates that supplementation with 25 mg/mL guaiacol provides an efficient and non-invasive method for obtaining viable coelomocytes without inducing detectable cytotoxic or genotoxic effects. The optimised protocol represents a useful methodological tool for future biomonitoring and ecotoxicological studies employing MN and comet assays in *E. fetida*.



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sciforum-187163: Ecotoxico-lipidomics in fish under field conditions: a systematic review of lipid-based responses to environmental contamination

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Aquatic organisms are continuously exposed to complex mixtures of environmental contaminants, making it challenging to link exposure to biological effects under realistic conditions. Lipids play central roles in energy metabolism, membrane structure, and cellular signaling, and can act as integrative indicators of environmental stress. Lipidomics has emerged as a powerful tool to capture integrated metabolic responses, supporting the development of ecotoxico-lipidomics as an emerging framework linking environmental exposure to lipid-mediated effects. This study aimed to systematically review lipid-based responses in fish under field conditions and identify consistent patterns across analytical approaches. A systematic literature review was conducted using a structured PECO framework. Searches were performed in Web of Science, PubMed, ScienceDirect, and Wiley Online Library using keywords related to lipidomics, fish, and contamination (last updated in April 2026). Studies were included if they assessed lipid profiles (fatty acids, lipid classes, or molecular species) in wild-caught or in situ exposed fish and examined associations with environmental contamination. Following screening and eligibility assessment, 25 studies were included. Most studies (84%) employed targeted approaches, primarily focusing on fatty acids or bulk lipid classes, whereas only a few applied untargeted lipidomics. Consistent patterns across studies included reductions in long-chain polyunsaturated fatty acids and increases in saturated and monounsaturated fatty acids, along with alterations in membrane and storage lipids. These responses were associated with metals, persistent organic pollutants, and wastewater-derived compounds. Most studies provided associative or functional interpretations, while mechanistic insights remained limited. Nevertheless, these patterns can be interpreted within an ecotoxico-lipidomics perspective. Lipid-based approaches provide robust insights into the effects of environmental contamination in fish under field conditions, but current evidence is dominated by targeted strategies with limited molecular resolution. Integrating untargeted lipidomics with exposomic and multi-omics data will be essential to advance ecotoxico-lipidomics as an emerging comprehensive and integrative approach.



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sciforum-187229: Developmental and biochemical responses of *Danio rerio* embryos exposed to cyanobacteria

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Freshwater ecosystems are increasingly threatened by cyanobacteria blooms, which degrade water quality and affect aquatic organisms. Early life stages of fish are sensitive to environmental stressors and are therefore well suitable for ecotoxicological assessment. This study evaluated the effects of cyanobacteria on early developmental stages of *Danio rerio* embryos. Fish Embryo Acute Toxicity tests were conducted using the cyanobacteria *Aphanizomenon flos-aquae* and *Microcystis aeruginosa* to assess developmental endpoints and physiological responses, including oxidative stress, neurotoxicity, and energy metabolism. Embryos were exposed to cyanobacterial cell concentrations of 1.9×10^4 (low risk), 7.5×10^4 (medium risk), 1.5×10^5 (high risk), 3.0×10^5 (high risk), and 1.2×10^6 (very high risk), according to World Health Organization. No mortality or effects on embryo size were observed across the treatments. Hatching was first recorded at 72 h, in agreement with standard guidelines, and after 96 h complete hatching occurred in all treatments except at the highest *M. aeruginosa* concentration (95%). Morphological abnormalities were absent at early stages and remained generally low throughout the assay. *A. flos-aquae* induced only minor and transient alterations, such as hemagglutination and spinal curvatures, whereas *M. aeruginosa* caused a higher frequency and diversity of abnormalities, including hypopigmentation, pericardial oedema, hemagglutination, spinal curvature, and absence of pectoral fins. *A. flos-aquae* exposure resulted in decreased catalase and glutathione S-transferases activities, while *M. aeruginosa* induced increases, suggesting activation of antioxidant and detoxification pathways. Lipid peroxidation levels and acetylcholinesterase activity remained largely unchanged, indicating limited oxidative damage and no clear neurotoxicity effects. Electron transport system activity increased under both exposures, reflecting elevated metabolic demand. Overall, both cyanobacteria elicited organism-level effects, while sub-individual responses revealed clear species-specific patterns, with *M. aeruginosa* causing stronger embryotoxic and physiological stress responses. These findings support the integration of sub-lethal endpoints into environmental monitoring, improving cyanobacteria risk assessment and ecosystem health evaluation.



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sciforum-187234: Bioaccumulation of trace metals and oxidative stress responses in *Apis mellifera* across different land use types

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Bees are vital pollinators that play a crucial role in sustaining ecosystem structure and function and serve as valuable indicators of local environmental quality. Trace metals can bioaccumulate in their tissues and hive products, potentially affecting both insect health and the safety of bee-derived products. Although honeybees have been widely used as bioindicators of environmental contamination, integrated assessments combining trace metal accumulation with oxidative stress biomarker responses across different land use contexts remain limited, particularly at the regional scale. This study evaluated oxidative stress biomarkers and trace metal accumulation in honeybee (*Apis mellifera*) tissues collected from rural, industrial and urban sites in the Umbria region, Italy, using a total of 30 (trace metals) and 75 (biomarkers) individuals per site. Specimens showed site-specific patterns of metal accumulation in their tissues. In the rural site, higher Cu concentrations were detected, likely associated with agricultural activities. Conversely, the urban site was characterized by elevated Cd and Pb levels, probably related to vehicular traffic, while the industrial site exhibited higher Tl concentrations, potentially linked to metallurgical processing. The influences of trace metal concentrations on oxidative stress biomarkers were investigated in the abdomen-thorax tissues and in the heads. Oxidative stress biomarkers showed site-specific modulation, with variations in superoxide dismutase, catalase, glutathione peroxidase, glutathione reductase and cholinesterase activities reflecting different patterns of trace metal exposure across rural, urban and industrial sites. Overall, the integration of tissue metal burdens with biomarker responses allowed the identification of site-specific biological signatures in honeybees, reflecting the influence of rural, urban and industrial pressures. This evidence supports the use of honeybees not only as indicators of contaminant presence, but also as responsive biological sentinels capable of revealing early physiological effects of environmental metal exposure.



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sciforum-187245: Spatio-temporal dynamics of arsenic and its relationship with physicochemical parameters in the Tampamachoco lagoon, Veracruz, Mexico

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Coastal lagoons are commonly regarded as critical sinks for hazardous chemical agents (HCAs) due to their unique hydrodynamics and significant anthropogenic pressures. Among these agents, arsenic (As) is of particular concern due to its environmental persistence, high toxicity, and ability to mimic essential elements like phosphorus (P) in cellular processes, making it a highly polluting agent and a multisystemic disruptor. In estuarine-lagoon systems such as Tampamachoco, the environmental kinetics of As are considered high, as they depend on physicochemical variables that influence speciation and bioavailability, posing a risk to food security and public health. This study analyzed the spatio-temporal dynamics of this metalloid and its correlation with physicochemical parameters including pH, salinity, temperature, dissolved oxygen, electrical conductivity, and total dissolved solids over an annual cycle from January to December 2025. The dry season (June and August) yielded the highest peak concentrations of As (0.013 mg/L and 0.018 mg/L, respectively), in contrast to the cold fronts and rainy seasons. Although the reported concentrations did not exceed the maximum permissible limits established by Mexican regulatory frameworks (NOM-001-SEMARNAT-2021) of 0.1 mg/L, low inverse correlations were observed with electrical conductivity ($\rho=-0.386$), salinity ($\rho=-0.276$), and total dissolved solids ($\rho=-0.381$), alongside a low positive correlation with temperature ($\rho=0.326$). These data suggest that As does not follow the general ionic load of the matrix; rather, its presence appears to be governed by temperature-dependent processes rather than evaporation or salt concentration mechanisms.



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sciforum-187298: Integrated Ecotoxicological Assessment of Hematological, Oxidative Stress, Genotoxic, and Histopathological Biomarkers in Bighead Carp (*Aristichthys nobilis*) Exposed to Bisphenol A

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Background

Bisphenol A (BPA) is a pervasive endocrine-disrupting chemical frequently detected in aquatic ecosystems due to extensive industrial and domestic applications. Continuous discharge of BPA into freshwater environments poses serious ecological risks to aquatic organisms, particularly fish species used as environmental sentinels. This study aimed to evaluate the ecotoxicological effects of BPA in bighead carp (*Aristichthys nobilis*) using an integrated biomarker approach.

Methods

Bighead carp were exposed under controlled laboratory conditions to different concentrations of BPA for 60 days alongside an untreated control group. Multiple biomarkers were assessed, including hematological indices, serum biochemical parameters, oxidative stress markers, antioxidant enzyme activities, genotoxic responses, and histopathological alterations in liver, kidney, brain, and heart tissues.

Results

BPA exposure caused significant physiological and biochemical disturbances in exposed fish. Hematological analysis revealed decreased erythrocyte count, hemoglobin concentration, lymphocytes, and monocytes, whereas leukocyte and neutrophil counts increased significantly. Serum biochemical profiling demonstrated elevated ALT, AST, ALP, urea, creatinine, glucose, cholesterol, and LDH levels, accompanied by reduced total protein and albumin. Oxidative stress biomarkers, including ROS and TBARS, were significantly increased, while antioxidant enzymes such as catalase, superoxide dismutase, and peroxidase were markedly reduced. Genotoxic effects were evidenced by increased nuclear abnormalities and DNA damage. Histopathological observations revealed necrosis, hemorrhage, inflammatory infiltration, and cellular degeneration in multiple organs.

Conclusion

The findings demonstrate that chronic BPA exposure induces multi-organ toxicity and oxidative stress-mediated damage in *A. nobilis*. Integrated biomarker responses highlight the ecological threat of BPA contamination and support the utility of freshwater fish as sentinel species for aquatic ecosystem health assessment.



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sciforum-187320: Blue crab *Callinectes sapidus* a new sentinel species of metals pollution in Mediterranean Sea

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Introduction

Blue crab is an aline species spreading in Mediterranean and Adriatic Sea, able to accumulate trace metals in tissues. This study evaluated the use of the blue crab as sentinel species for metal pollution in the Sacca di Goro, lagoon at the mouth of the Po River flowing into the Adriatic Sea, vulnerable to industrial, riverine and maritime contamination.

Methods

The study was carried out on bronchial muscle, carapace, claws, gills and related pulps of *Callinectes sapidus* samples (n=12) collected from Sacca of Goro, Adriatic Sea (Italy). All samples were digested and analyzed by ICP-MS for the determination of toxic metals and metalloids Hg, Pb, Cd, Cr, Ni and As [1].

Results

The results confirmed the presence of highest concentration of As, intermediate for Ni, Pb, Cr and Hg, lowest of Cd. However, the Metal Pollution Index (MPI), related to metals accumulation in each tissue, was <1 (safety level). Considering the different parts analyzed, the highest metal levels were found in carapace, followed by gills, claws and bronchial muscle. The lowest concentrations were present in the pulps of carapace, claw and gill (the edible parts) but As was upper the MRL (0.10 mg/kg), established by EU Regulation 2025/1891 for crustaceans [2].

Conclusions

The presence of toxic metals and metalloids in tissues of blue crabs is correlated to the exposure in the marine environment of Sacca di Goro, showing that *Callinectes sapidus* could be a valid sentinel species of Adriatic Sea. The MPI values suggested a low contamination of this marine ecosystem; however, the residual levels of As in edible pulps (> MRL) highlight potential toxicological risks for consumer of this seafood.

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sciforum-187341: Responses of water fleas against a complex mixture of pollutants: Using *Daphnia magna* to understand cocktail effects

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Natural freshwater systems rarely contain a single contaminant, yet regulatory ecotoxicology continues to rely heavily on single-chemical tests conducted in defined laboratory media. This discrepancy between how pollutants are tested and how organisms actually encounter them limits our ability to understand real, possibly synergistic, effects in the wild. In this study, the model organism, sentinel *Daphnia magna*, was exposed to a six-component cocktail spanning three contaminant classes: the pharmaceuticals, propranolol, diltiazem and metformin; the metals, nickel and lithium; and the herbicide, glyphosate. Exposures were conducted under standardised conditions, with acute and chronic toxicity characterised using dose-response curves and survival plots, respectively. To capture sub-lethal responses of the mixture alone, additional endpoints were measured: filtration activity, growth, a panel of key enzymatic markers, and untargeted metabolomic fingerprints. The toxicity of the mixture exceeded what individual-compound data would predict, pointing to non-additive interactions among components. Concentration-dependent changes were observed across every endpoint, with a clear decline in growth at 7, 14 and 21 days, and with feeding rate together with enzyme activities responding in a dose-dependent manner. These findings highlight the limitations of traditional risk assessment frameworks in predicting the toxicity of complex mixtures. Ongoing work aims to target two complementary goals: further parallel single-chemical assays on each of the six constituents, run under matched conditions to quantify the magnitude of synergism within the mixture; and exposures conducted in natural river water matrices, to test whether laboratory-derived biomarkers remain informative in field-relevant, realistic conditions. This broader integrative approach promotes the development of daphnid-based New Approach Methodologies (NAMs) as practical tools for improved early-warning systems in freshwater monitoring.



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sciforum-187347: Acute toxicity of Nicosulfuron- and S-metolachlor-based herbicides in mixture to *Artemia salina*

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Introduction

The combined use of two or more pesticides in the field has become an increasingly common practice. Herbicides based on Nicosulfuron and S-metolachlor are an example as they have complementary modes of action. However, mixing these substances can cause environmental problems and may pose a threat to aquatic ecosystems. The objective of this study was to evaluate the acute ecotoxicological effects of the mixture of Nicosulfuron- and S-metolachlor-based herbicides to *Artemia salina*.

Methods

The bioassay was conducted in accordance with ABNT NBR 16530:2021. Assessments were performed at 24 h and 48 h. For each treatment, four replicates were performed, consisting of ten nauplii in 10 mL of solution. Five treatments were tested. Concentrations were established based on previous research, in which the NOEC of Nicosulfuron (2.67 mg/L) and S-Metolachlor (29.7 mg/L) were determined. Thus, the treatments consisted of mixtures of the herbicides in proportional amounts (100%, 75%, 50%, and 25%). The interaction of the mixtures was analyzed using the Colby model (1967).

Results

Nauplii immobilization was observed only at 48 h. Values ranged from 5% to 35%, but none of the concentrations differed statistically from the control (Tukey, $p > 0.05$). Furthermore, application of Colby's model (1967) revealed an additive interaction among the mixtures. This indicates that the effects of the mixtures are equivalent to the effects of the individual compounds.

Conclusions

The purpose of using the NOEC was to determine whether combining two concentrations that had no effect when tested alone could produce an effect when mixed. However, the absence of a significant difference demonstrates that the results are positive from the perspective of developing safe mixtures. Thus, this mixture may not pose a danger to other aquatic organisms such as *A. salina*. However, the behavior of mixtures is not fixed, and a case-by-case evaluation is necessary.



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sciforum-193196: Occurrence and Bioaccumulation of PFAS in Bivalve Mollusks: A Systematic Review

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Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants that have been widely detected in aquatic ecosystems and seafood. Due to their filter-feeding behavior and bioaccumulation capacity, bivalve mollusks are considered important bioindicators of environmental contamination. This systematic review aimed to evaluate the occurrence and distribution of PFAS in bivalve mollusks and identify recent trends in contamination profiles. A systematic literature search was conducted in the Scopus and ScienceDirect databases, including original articles published between 2019 and 2025. After screening and eligibility assessment, 34 studies were included in the review. Most studies were conducted in North America, Europe, and China, revealing a significant geographic bias and limited information from developing regions. Legacy PFAS compounds, especially perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS), were the most frequently reported contaminants, while an increasing number of recent investigations reported emerging compounds such as including trifluoroacetic acid (TFA), FHxSA, PFBS and C6O4. PFOA concentrations ranged from 0.185 to 111.57 ng/g wet weight (ww), while PFOS concentrations ranged from 0.002 to 1137 ng/g ww, demonstrating substantial variability among species and locations. The most frequently investigated species were, *Mytilus galloprovincialis*, *Crassostrea virginica*, and *Ruditapes philippinarum*. The findings confirm the widespread occurrence of PFAS in bivalves and highlight concerns regarding environmental persistence and food safety. The increasing detection of replacement compounds emphasizes the need for continued monitoring and further investigation of their ecological and toxicological implications under a One Health perspective.



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sciforum-193616: Biochemical stress responses in *Procambarus clarkii* exposed to pristine and aged glitter

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Glitter is a primary microplastic typically composed of a polyethylene terephthalate or polyvinyl chloride core coated with a reflective metallic layer, usually containing aluminium, titanium, iron or bismuth. Despite its widespread use and direct release into aquatic environments, its biological effects on freshwater organisms remain poorly understood. This study investigated sub-lethal biochemical responses to glitter exposure in the non-native crayfish *Procambarus clarkii*. Adult males and females were exposed for 30 days to pristine or lake-aged glitter at 0.067, 0.134 and 0.268 g/L, with an unexposed control group. Tested concentrations were selected from previous microplastic exposure studies, due to the limited availability of environmental concentration data for glitter. Lake-aged particles were obtained through *in situ* conditioning in a lacustrine environment to simulate environmental weathering. A multi-biomarker approach was applied to the hepatopancreas. Catalase, glutathione peroxidase, glutathione reductase and glutathione S-transferase were analysed as oxidative stress-related biomarkers, while carboxylesterases, lipase and N-acetyl- β -D-glucosaminidase were assessed as hydrolase activities. The electron transport system was included as a marker of energy metabolism. Gamma generalized linear models were used to evaluate the effects of glitter type, concentration and type-specific dose-response patterns. After false discovery rate correction, significant responses were mainly restricted to carboxylesterase activity. The interaction between glitter type and concentration was significant for carboxylesterase measurements with three substrates tested: p-nitrophenyl butyrate, α -naphthyl acetate and α -naphthyl butyrate. Pristine glitter generally increased carboxylesterase activity with concentration, whereas lake-aged glitter induced stable or slightly decreasing responses. Oxidative stress biomarkers did not show robust generalized effects. Overall, these findings indicate that glitter may induce targeted biochemical alterations rather than broad oxidative stress activation. Carboxylesterase activity appears to be a sensitive endpoint for detecting exposure to synthetic particulate materials, while the contrasting effects of pristine and aged glitter highlight the importance of environmental weathering in modulating biological responses.



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sciforum-193682: Transgenerational impacts of TBBPA on the freshwater snail *Lymnaea stagnalis*

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Tetrabromobisphenol A (TBBPA), a widely used brominated flame retardant, raises concern due to its endocrine-disrupting properties similar to BPA. Yet its long-term and transgenerational effects remain poorly understood, especially in freshwater organisms like the snail *Lymnaea stagnalis*, which plays a role in nutrient cycling and ecosystem stability. Although there is growing evidence that chemically induced effects can be transgenerational, ecotoxicological studies beyond one generation remain limited. This study investigated whether parental TBBPA exposure influences the vitality of exposed snails and the development of unexposed F1 and F2 offspring, addressing potential carryover and transgenerational effects.

Adults were exposed for up to 28 days at TBBPA nominal concentrations of 75 and 2000 µg/L. Egg masses from exposed parents (F1 embryos) were transferred to clean medium to isolate carry-over effects from direct exposure. Some F1s were raised to reproductive age in clean water, with resulting F2s raised similarly. For comparison, embryos from unexposed parents were directly exposed to 50–1,000 µg/L TBBPA and monitored for 14 days.

Parental exposure resulted in impaired reproduction (cumulative EC₅₀ 798 µg/L) from day 3. F1 reproduction was more sensitive (EC₅₀ 392 µg/L), suggesting transgenerational effects in the absence of direct exposure. F1 embryos also showed various abnormalities, including small shells, delayed hatching, reduced pigmentation, and malformations (EC₅₀ ~404 µg/L). Directly exposed embryos from unexposed parents showed similar abnormalities but greater sensitivity (EC₅₀ 294 µg/L at 14 days), with 100% mortality at 1000 µg/L.

Neither F1 nor F2 recovered from these effects (e.g. decrease in shell size) over the 5-month observation period. This suggests that TBBPA can affect the viability of the offspring even in the absence of exposure, which may have long-term consequences for population stability and biodiversity. The results emphasize the need for multigenerational assessment beyond early life stages.



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sciforum-193945: Effects of Arsenic Exposure on Oxidative and Cellular Stress in *Lymnaea stagnalis*

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Arsenic is confirmed as one of the most persistent and threatening environmental contaminants to the integrity of aquatic ecosystems, frequently originating from industrial discharges related to microelectronics, textiles, and glass production. In order to gain deeper insights into toxicity pathways in macroinvertebrates, this study analyzed the biological responses of the freshwater gastropod *Lymnaea stagnalis*, an established bioindicator model. Adult specimens were subjected to a 7-day exposure to arsenic concentrations ecologically representative of contaminated sites.

The investigation focused on the digestive gland, which represents the primary organ involved in metabolic detoxification processes. The results highlighted severe structural and histological damage, characterized by tissue disorganization, intense cytoplasmic vacuolization, and marked inflammatory infiltration phenomena. At the biochemical level, the sub-lethal exposure triggered a massive production of reactive oxygen species (ROS) in the target tissues, providing clear evidence of severe oxidative stress. This altered redox status promoted a significant up-regulation of the molecular chaperone protein HSP70, confirming the activation of cellular defense and protein protection systems.

Furthermore, the concomitant modulation of key apoptotic biomarkers suggested that arsenic exposure can successfully trigger the early stages of programmed cell death pathways. Overall, this research elucidates the complex molecular networks and tissue alterations underlying metalloid toxicity in freshwater invertebrates. The findings reaffirm the high sensitivity and effectiveness of *L. stagnalis* as an ideal biological sentinel for environmental risk assessment and water quality monitoring programs.



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sciforum-193952: Hepatic and Reproductive Toxicity of Glyphosate Exposure in the Terrestrial Bioindicator *Podarcis siculus*

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Soil contamination represents a critical threat to terrestrial biodiversity, yet wild vertebrates remain underutilized in environmental risk assessments. This study evaluates the field lizard *Podarcis siculus* as a resilient wild model organism to investigate the hepatic and reproductive toxicity of the widely used herbicide glyphosate (Gly). Sexually mature specimens of both sexes were orally exposed to two environmentally relevant concentrations of Gly (0.05 and 0.5 µg/kg body weight) for three weeks on alternate days. Following euthanasia, the liver and gonads were processed for multidisciplinary morphological, histochemical, and biomolecular analyses. The results revealed severe tissue impairment and cellular stress across all treated groups, starting from the lowest concentration tested. Histological observations highlighted a marked disorganization of the tissue architecture. Extensive collagen deposition was recorded between hepatocytes and sinusoids in the liver, as well as between ovarian follicles and seminiferous tubules, indicating a generalized fibrotic process. In the liver, a distinct increase in granules of glycogen, melanin, and lipofuscin was observed. Reproductive tissues showed dramatic alterations; males exhibited impaired spermatogenesis, characterized by a reduction in spermatozoa along with thinning and gaps in the seminiferous tubule walls. In females, a severe disorganization of the follicular theca, granulosa, and zona pellucida occurred, accompanied by the proliferation of small follicular stem cells and apoptosis of pyriform cells. Biochemically, cellular stress was confirmed by the overexpression of superoxide dismutase 1, glutathione peroxidase 1, and metallothionein. Furthermore, Gly acted as a potent endocrine disruptor, altering the expression and localization of estrogen receptors alpha and beta in all examined tissues. This xenoestrogenic effect was confirmed by the aberrant induction of vitellogenin synthesis in the male liver. In conclusion, sublethal glyphosate exposure severely compromises tissue integrity, glucose metabolism, and fertility in *P. siculus*, validating this species as a sensitive sentinel for terrestrial ecotoxicology.



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sciforum-193985: Testicular CNR1 and CNR2 expression in stray dogs from Campania Region, Italy: insights from a One Health sentinel model

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In Campania Region (Italy), illicit drug residues, including cocaine, have been detected in surface waters, highlighting the occurrence of emerging anthropogenic contaminants. Within a One Health perspective, stray dogs represent useful sentinels for tracking environmental risks. In this context, the endocannabinoid system contributes to male reproductive homeostasis and inflammatory regulation, making cannabinoid receptor 1 (CNR1) and cannabinoid receptor 2 (CNR2) relevant candidates for investigating testicular remodelling. This study investigated changes in CNR1 and CNR2 expression during progressive spermatogenic impairment in canine testes. To this aim, twenty male stray dogs from the Campania Region were enrolled and classified according to spermatogenic status as follows: normal spermatogenesis (Group A), altered spermatogenesis (Group B), severely impaired spermatogenesis (Group C), and intratubular seminoma (Group D). CNR1 and CNR2 were assessed by immunohistochemistry and Western blot. CNR1 showed weak to moderate diffuse cytoplasmic immunopositivity in spermatogonia and primary spermatocytes in Group A. Group B displayed reduced positivity confined to scattered residual germ cells and peritubular areas. Group C exhibited the highest immunoreactivity across all groups, with markedly increased staining in residual germ cells and peritubular compartments. Group D showed heterogeneous staining in tumour and stromal cells. CNR2 displayed scattered positivity in spermatogonia, primary spermatocytes and interstitial cells in Group A, reduced germ cell signal in Groups B and C, and stromal positivity in Group D, including cells morphologically compatible with macrophage-like elements and mesenchymal components. Western blot analysis showed reduced CNR1/CNR2 protein signal in Group B compared with Group A, followed by increased expression in Groups C and D. Overall, these findings suggest that CNR1 and CNR2 expression changes during progressive impairment of spermatogenesis and neoplastic remodelling. However, further studies integrating environmental exposure assessment and cell specific co-localization are needed to clarify the biological significance of these receptors in canine testicular damage.



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sciforum-194142: Ecotoxicological Risk of Sediments from the Salado River Using Earthworms (*Eisenia* sp.)

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Introduction

The Salado River is located in the Mezquital Valley, Mexico. Along its course, it receives large volumes of wastewater from industrial, agricultural, and mining activities, as well as effluents originating from Mexico City through the Grand Drainage Canal. These discharges contain toxic substances that, due to their physicochemical properties, accumulate in river sediments, posing a potential risk to organisms inhabiting this ecosystem. The aim of this study was to evaluate the genotoxic effects of contaminants accumulated in the sediments on the coelomocytes of earthworms (*Eisenia* sp.) collected from the river.

Methods

Ten earthworms (*Eisenia* sp.) were collected from each of five sampling sites distributed along the Salado River. In the laboratory, the organisms were placed in an extrusion solution to obtain coelomocytes. Genotoxicity was assessed using the micronucleus and comet assays. Cell viability was determined by the trypan blue exclusion test, and cytotoxicity was evaluated using the neutral red uptake assay. Statistical analyses were performed by comparing each sampling site with a reference site and a negative control using analysis of variance (ANOVA) followed by Tukey's post hoc test, with a significance level of $p < 0.05$.

Results

Earthworms collected from the Salado River exhibited cell viability greater than 80%, with no evidence of cytotoxic effects among sampling sites. DNA damage was detected through a statistically significant increase ($p < 0.05$) in both micronucleus frequency and DNA fragmentation compared with the reference site and the negative control.

Conclusions

The results indicate the presence of compounds with genotoxic potential in the river sediments, representing a risk to aquatic and terrestrial biota and potentially affecting overall ecosystem health.



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sciforum-194376: Tire Wear Particles and 6PPD-Quinone in Freshwater Ecosystems: Ecotoxicological Effects, Food-Web Transfer, and One Health Implications

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Introduction

The rapid growth of motor vehicle use has intensified non-exhaust emissions, particularly tire and road wear particles (TRWPs). Among these, the tire antioxidant 6PPD and its atmospheric transformation product, 6PPD-quinone (6PPD-Q), are emerging environmental contaminants. Recent studies link 6PPD-Q to Urban Runoff Mortality Syndrome (URMS) in coho salmon, raising concerns about cross-species vulnerability and One Health implications.

Methods

A systematic review was conducted following the PRISMA guidelines for abstracts. We systematically searched peer-reviewed literature and regulatory reports across major academic databases from January 2020 to mid-2026. Studies were screened based on predefined eligibility criteria, and risk of bias was formally assessed. Data were extracted regarding environmental occurrence, species-specific toxicity (LC50/EC50), molecular mechanisms, and exposure biomarkers.

Results

The systematic search yielded 200 initial records, of which 129 studies met the final inclusion criteria after rigorous screening. Of these, 14 studies evaluated environmental occurrence, demonstrating that 6PPD-Q is widely distributed in urban freshwater networks and sediments. Acute toxicity was analyzed in multiple studies, confirming extreme sensitivity in coho salmon (LC50 ~0.04 to 0.095 µg/L). Furthermore, numerous included studies reported sublethal effects in other aquatic species, highlighting blood-brain barrier disruption, oxidative stress, and lipid metabolism dysregulation. Human and veterinary biomonitoring studies (n=12) indicate systemic exposure, with 6PPD-Q detected in human matrices such as urine, blood, placental tissues, and cerebrospinal fluid.

Conclusions

Based on the systematic synthesis of the 129 included studies, 6PPD and 6PPD-Q constitute significant transboundary pollutants linking aquatic ecotoxicity to human systemic exposure. Current stormwater mitigation strategies may be insufficient, underscoring the urgent need for integrated One Health strategies, green chemistry alternatives, and coordinated cross-disciplinary biomonitoring to safeguard environmental and public health.



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Session 3. Innovating Toxicology: NAMs and Computational Tools for Next-Generation Risk Assessment

sciforum-186007: ZODDs: A Zebrafish Organ-Specific and Dose-Response Database for Environmental Chemical Mixtures

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Introduction

Environmental contaminants typically exist as complex mixtures, yet their combined effects and dose-response relationships remain poorly characterized. To address this gap, we constructed ZODDs, a Zebrafish Organ-Specific and Omics Dose-Response Database that integrates chemical, anatomical, and dose-response information with high-throughput omics data.

Methods

The database is organized into two components. The first component comprises a curated list of chemicals sourced from the STITCH database, which has been integrated with zebrafish gene expression datasets obtained from the Gene Expression Omnibus (GEO). The second component comprises a comprehensive collection of gene expression datasets specifically related to the anatomical systems of zebrafish, sourced from the Expression Atlas. For each study, the exposure design, concentration range, duration, or developmental stage was harmonized and mapped to standardized identifiers. Differentially expressed genes were recalculated using an in-house R script.

Results

The current version of ZODDs comprises over 300 zebrafish exposure experiments and 14 organ-specific transcriptomic datasets, organized into structured tables containing differentially expressed genes and associated metadata.

Conclusions

This resource enables integration with the ZFinfer-Mixture inference system for the exploration of organ-specific chemical exposure inferences, mixture interactions, and dose-response trends under environmentally relevant chemical exposure scenarios. In this study, we present a representative PFNA case study demonstrating how dose-related transcriptomic data can be applied within the zebrafish inference model. The case study illustrates how ZODDs can support dose-dependent interpretation of chemical-induced biological responses. Collectively, this zebrafish-centered mixture and omics platform provides a reusable data foundation to enhance our understanding of how environmental chemical mixtures affect different organs and potentially support the development of new approaches for regulatory chemical risk assessment.



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sciforum-186263: Aryl hydrocarbon receptor pathway activation in fish hepatocytes exposed to fire-associated contaminants under elevated temperature

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Global warming has increased wildfire frequency, contributing to the accumulation of pollutants such as polycyclic aromatic hydrocarbons (PAHs) and dioxins. Firefighting activities further contribute to the release of harmful substances, including perfluoroalkyl substances (PFAS) used in fire suppression. Such compounds reach aquatic ecosystems and can disrupt hepatic metabolism in fish. Rising water temperatures due to global warming may also affect detoxification processes. In vitro fish liver models have been used to assess pollutant effects, but are seldom used to investigate the combined effects of temperature and contaminants. This study evaluated whether increased temperature modulates cytochrome P450 1A (CYP1A) activation induced by the aryl hydrocarbon receptor (AhR) ligands tetrachlorodibenzo-*p*-dioxin (TCDD) and benzo[*k*]fluoranthene (B[*k*]F). Effects of the PFAS perfluorooctane sulfonic acid (PFOS) were also assessed. Monolayer cultures of primary brown trout (*Salmo trutta*) hepatocytes (n = 5) were exposed (48 h) to B[*k*]F (1, 10, 20 µM), TCDD (1, 10 nM) and PFOS (10, 30 µM) at 18 °C and 22 °C, simulating a 4 °C increase during heat waves. Trypan blue, alamarBlue, and lactate dehydrogenase (LDH) viability assays were performed to assess exposure effects. RT-qPCR evaluated CYP1A and AhR expression. The two-way ANOVA revealed that B[*k*]F (10 and 20 µM), but not TCDD or PFOS, increased LDH leakage. Furthermore, higher temperature enhanced LDH release, with no differences in the other viability tests. All TCDD and B[*k*]F concentrations significantly increased CYP1A expression relative to controls, whereas AhR mRNA levels increased after TCDD and B[*k*]F (10 and 20 µM). PFOS did not change CYP1A or AhR expression. No temperature or interaction effects were detected. Overall, the model was responsive to B[*k*]F and TCDD but not to PFOS, and temperature only impacted LDH leakage under the tested conditions. These results highlight the need to explore combined exposures under more environmentally realistic scenarios.



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sciforum-186464: Optimization of ICP-MS/MS-based methodology for multielemental analysis in follicular fluid: new approaches in female infertility research

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Introduction

Heavy metals are recognized as potential endocrine disruptors associated with female infertility. Their determination in follicular fluid (FF), a biologically relevant matrix reflecting the ovarian microenvironment, may improve the assessment of environmental exposure and support studies on reproductive toxicity as it offers valuable insights into its multielemental composition. However, FF remains poorly characterized, and standardized analytical methodologies are lacking. This study aimed to optimize ICP-MS/MS conditions for multielemental determination in FF, providing a robust analytical basis for future toxicological and risk assessment studies.

Methods

Five FF samples from patients undergoing in vitro fertilization were pooled, aliquoted, and processed according to each type of analytical test. Different dilution factors were evaluated, and half of the aliquots were spiked for recovery assessment. Continuous ICP-MS/MS acquisition was performed using helium (He) as collision gas. Additionally, strategies to reduce spectral interferences for arsenic (⁷⁵As) and selenium (⁷⁴Se) were assessed using oxygen (O) as reaction gas.

Results

Continuous analysis in He mode achieved recoveries within the optimal range (100–120%) for all aliquots, including undiluted samples, supporting reliable multielemental determination. In continuous O mode, spectral interferences persisted under most conditions. The best performance for ⁷⁵As and ⁷⁴Se was obtained using a 1:2 dilution with 5–10% oxygen, yielding recoveries close to 100%. The optimized method enabled the determination of heavy metals and rare earth elements relevant to environmental exposure assessment and reproductive toxicology.

Conclusions

Continuous ICP-MS/MS analysis in He mode was identified as the most suitable approach for multielemental analysis of FF, while O reaction mode may improve the determination of selected elements after further optimization. Although biological validation requires larger cohorts, this standardized analytical workflow provides a reproducible platform for high-quality exposure assessment, facilitating future integration with multivariate statistical analyses, mechanistic studies on endocrine disruption, and next-generation risk assessment within NAM-based reproductive toxicology.



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sciforum-186799: Improved Prediction of Chemical Carcinogenicity Based on Hybrid In Silico/In Vitro Methodology

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Introduction

In silico methods such as quantitative structure–activity relationship (QSAR) modeling and read-across are widely used for rapid and cost-effective carcinogenicity assessment. However, their predictive reliability is often restricted by applicability-domain (AD) limitations, particularly for structurally diverse compounds.

Methods

We developed a hybrid framework integrating multi-source in silico and in vitro-derived data to improve human carcinogenicity prediction and reduce AD limitations. A graph neural network (GNN) was pretrained on mouse carcinogenicity data using multitask learning with rat carcinogenicity as an auxiliary task. The model was enriched with graph-level features derived from supporting bioassay endpoints and compound-induced gene expression embeddings. It was then fine-tuned on a human carcinogenicity dataset while excluding an independent test set of 166 compounds absent from the animal datasets. The test set included 28 carcinogens and 138 non-carcinogens. An ensemble combining GNNs with descriptor-based gradient boosting models was constructed. Applicability-domain assessment was performed through confidence estimation, where prediction probabilities between 0.4 and 0.6 were considered outside the AD.

Results

The baseline mouse-trained GNN showed limited transferability to human data, achieving a Matthews correlation coefficient (MCC) of 0.19, with an average of 49.3 compounds outside the AD. The integrated and fine-tuned ensemble improved the MCC to 0.50 while reducing out-of-domain compounds to an average of 6.8, substantially increasing chemical-space coverage. For comparison, extrapolation of conventional 2-year rodent carcinogenicity assays to humans on the same dataset achieved an MCC of 0.62 and 82% accuracy.

Conclusions

Our hybrid in silico/in vitro method improved prediction accuracy and significantly reduced applicability-domain limitations. Combining biologically relevant bioassay and gene expression features allows for broader and more cost-effective carcinogenicity assessments while decreasing dependence on animal testing, highlighting its promise as a New Approach Methodology.

Funding

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sciforum-186855: Integrated in Silico Assessment of Environmental and Human Toxicity of Carbamazepine as a Pseudo-persistent Emerging Contaminant

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Introduction

Carbamazepine is one of the most frequently detected pharmaceutical residues in aquatic environments due to its extensive use, incomplete removal in wastewater treatment plants, and resistance to biodegradation. Therefore, it is considered a pseudo-persistent emerging contaminant. This study aimed to provide an integrated *in silico* evaluation of its environmental persistence, bioaccumulation, and potential human toxicity.

Methods

Carbamazepine and its metabolites/degradation products ($n = 16$ compounds) were evaluated using VEGA QSAR (v1.2.4) and EPA TEST (v5.1.2). Environmental persistence was assessed through water and sediment persistence and ready biodegradability models. Bioaccumulation potential was evaluated using bioconcentration factor (BCF), logKow, and logKoc. Toxicity assessment focused on mutagenicity, developmental toxicity, carcinogenicity, hepatotoxicity, and endocrine-disrupting activity involving estrogen and androgen receptor pathways.

Results

Persistence predictions generally showed low reliability, limiting confidence in water- and sediment-persistence estimates. However, 9,10-dihydro-9-oxoacridine was identified as a reliably non-biodegradable compound with good reliability (GR), whereas iminodibenzyl showed moderate reliability. Hydrophobic derivatives, particularly acridine and iminodibenzyl, demonstrated the highest bioaccumulation potential, and *in silico* physicochemical predictions were consistent with experimental LogP and solubility data. Most compounds were predicted to be non-mutagenic; however, acridine exhibited the strongest genotoxic profile, supported by experimental evidence. Additionally, 10,11-epoxycarbamazepine, 2-hydroxycarbamazepine, and 3-hydroxycarbamazepine showed predicted mutagenic potential. Almost all investigated derivatives triggered alerts in the carcinogenicity and developmental toxicity models. Ten compounds, including carbamazepine, oxcarbazepine, eslicarbazepine, licarbazepine, and 10,11-epoxycarbamazepine, were identified as developmental toxicants with GR. Hepatotoxicity was experimentally confirmed for carbamazepine and oxcarbazepine and predicted for most derivatives. Endocrine-disrupting activity was generally absent; however, 2- and 3-hydroxycarbamazepine exhibited possible estrogen receptor interaction signals with GR.

Conclusions

Carbamazepine and several transformation products may pose human health concerns, particularly through persistence, genotoxicity, and developmental toxicity-related signals. These findings demonstrate the utility of integrated in silico approaches for prioritizing pharmaceutical contaminants and their metabolites.



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sciforum-186862: How Optimization of Skin Sensitization and Photoirritation Assays are Advancing *in vitro* Photoallergy Assessment

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The development of reliable *in vitro* methods to assess photoallergy is critical as global regulatory agencies move toward reducing, refining, and replacing animal testing. Currently, no validated OECD Test Guidelines exist for the evaluation of photoallergy; however, advances in New Approach Methodologies (NAMs) for skin sensitization and photoirritation provide a strong foundation for progress. This original research consists of case studies exploring optimization and evaluation of photo-adapted versions of three established skin sensitization assays (OECD Test Guideline series 442)—the photo-Direct Peptide Reactivity Assay (photo-DPRA), photo-KeratinoSens™, and photo-Human Cell Line Activation Test (photo-h-CLAT)—for their applicability in assessing photoallergic potential. Each assay was modified to include irradiation exposure based on existing literature. The case studies consist of assessing irradiation exposure on the three test systems in absence of reference chemicals, impacts of seeding density on controls and reference chemical prediction in the photo-KeratinoSens™ assay, and evaluation of cell surface marker expression in photo-h-CLAT. Results demonstrated irradiation conditions, reference chemical selection, evaluation of test system sensitivity, and evaluation of data are essential components for successful assay predictivity and reproducibility. Assessment of individual assay components prior to a validation study is critical to ensure reliable results. Historical experience performing traditional skin sensitization and photoirritation assays will facilitate transfer of the methods to laboratories seeking to develop or optimize these assays. Continued refinement and validation of these assays will be pivotal for establishing a comprehensive, tiered testing strategy for *in vitro* photoallergy evaluation.



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sciforum-186891: GC–MS Characterization, Brine Shrimp Lethality, and In Silico Toxicity Prediction of Alkaloid Fractions from the Stem Bark of *Nauclea diderrichii*

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Introduction

Alkaloids remain an important source of bioactive compounds with therapeutic potential; however, the toxicological characterization of many ethnomedicinal plants remains limited. *Nauclea diderrichii* is widely utilized in West African traditional medicine for the management of various ailments, yet the toxicity profile of its alkaloid constituents is poorly understood. This study investigated the chemical composition, preliminary cytotoxicity, and predicted toxicological properties of alkaloid-rich fractions obtained from the stem bark of *N. diderrichii* using integrated analytical, biological, and computational approaches.

Methods

Alkaloid-rich fractions were obtained through solvent extraction and chromatographic separation of powdered stem bark material. Chemical profiling was performed using gas chromatography–mass spectrometry (GC–MS), and compounds were identified through comparison with mass spectral databases and retention index data. Preliminary toxicity screening was conducted using the *Artemia salina* brine shrimp lethality assay across graded concentrations of each fraction, with mortality assessed after 24 hours of exposure. Median lethal concentration (LC₅₀) values were estimated from dose–response relationships. Major identified compounds were further subjected to in silico toxicity prediction using ProTox-II to evaluate predicted acute toxicity and organ toxicity endpoints.

Results

GC–MS analysis revealed the presence of structurally diverse alkaloidal and heterocyclic constituents, including indole- and quinoline-related compounds, with compositional variability observed among fractions. Brine shrimp lethality assays demonstrated concentration-dependent toxicity, with selected fractions exhibiting moderate to high cytotoxic activity based on LC₅₀ values. In silico prediction suggested varying toxicity classes and organ toxicity liabilities for several major constituents, supporting the observed bioactivity patterns in the biological assay.

Conclusion

The combined GC–MS, brine shrimp lethality, and computational toxicity findings provide preliminary evidence that alkaloid fractions from *N. diderrichii* possess biologically active constituents with measurable toxicological effects. This integrated approach contributes baseline toxicological data for the plant and supports further mechanistic, pharmacological, and safety investigations of its alkaloid components.



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sciforum-186931: Pushing the Limits: Expanding the Applicability Domain of EpiSensA for Skin Sensitization Assessment

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Introduction

Skin sensitization is an immune-mediated process leading to allergic contact dermatitis following dermal exposure to chemicals. The Epidermal Skin Sensitization Assay (EpiSensA) is an *in vitro* assay adopted in 2024 by OECD to assess skin sensitization potential. The assay evaluates keratinocyte activation, which is the second key event in the skin sensitization adverse outcome pathway. The current applicability of the assay is limited by a minimum solubility requirement ($\geq 0.0122\%$ w/v) in validated vehicles such as 4:1 acetone:olive oil (AOO), distilled water, or 50% ethanol. Chemicals not meeting this criterion are considered incompatible with the test system.

Methods

The EpiSensA quantifies changes of expression in marker genes (*ATF3*, *GCLM*, *DNAJB4*, and *IL-8*) following topical chemical exposure to a reconstructed human epidermis (RhE) model. Our experiments assessed strategies to expand the applicability domain of EpiSensA by evaluating alternative solvents, conducting testing of neat materials (to mimic consumer exposure), and assessing the skin sensitization potential of medical device extracts.

Results

Alternative solvents including mineral oil, olive oil, dimethyl sulfoxide (DMSO), saline, and acetonitrile were evaluated. Of these, mineral oil and olive oil were identified as compatible with the EpiSensA, maintaining tissue viability $>95\%$ and gene induction below established positivity thresholds (*ATF3* <15 -fold; *GCLM* and *DNAJB4* <2 -fold; *IL-8* <4 -fold). A body lotion and a perfume were tested neat and predicted to be positive, based on increased expression of *ATF3* and *IL-8* in both products, and *DNAJB4* in the lotion. Olive oil-based extracts of latex gloves and non-latex condoms, prepared according to ISO 10993-12, did not exceed classification thresholds and thus were classified as negative in the assay.

Conclusion

These findings suggest the potential to expand the EpiSensA applicability domain to include alternative solvents, neat materials, and medical device extracts, while highlighting key considerations and the need for further evaluation for regulatory application.



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***sciforum-187104: In silico* assessment of the endocrine disrupting and genotoxic potential of bisguaiacols as possible bisphenol A alternatives**

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Introduction

Bisguaiacols (BGs) are proposed as safer and more sustainable alternatives to bisphenol A (BPA), largely due to structural modifications like methoxy substituents on the benzene ring of bisphenols (as in BGs) resulting in reduced estrogenic potential. However, the full toxicological profile of BGs remains insufficiently characterised. This study focuses on genotoxicity and endocrine disruption (ED) as key endpoints. The aim is to provide *in silico* predictions for seven BGs and compare these with three bisphenols (BPs), and to integrate these predictions with New Approach Methodologies (NAMs) to support hazard identification.

Methods

ED was evaluated using QSAR models and molecular docking. Genotoxicity was assessed using QSAR models. Selected BGs were further evaluated using NAM-based assays, including CALUX assays targeting nuclear receptors and an integrated genotoxicity battery.

Results

QSAR results for estrogen receptor binding were variable, while androgen receptor predictions were consistent. Docking indicated receptor-specific binding preferences and thyroid receptor interactions not captured by QSAR models. CALUX assays confirmed lower or absent endocrine activity for selected BGs compared to BPA across multiple receptors, supporting *in silico* trends.

QSAR models predicted BPs and corresponding BGs non-mutagenic. Two models for predicting micronucleus activity yielded conflicting results both for BPs (with good reliability) and BGs (with moderate reliability). The model for chromosomal aberration indicated limited activity, with only BGP acid predicted active with low reliability. *In vitro* NAM-based genotoxicity assays supported these predictions, showing ROS, DNA lesions, clastogenic activity and secondary genotoxicity for BPA and at reduced level for BGs.

Conclusions

BGs show a lower or comparable receptor-dependent ED potential as BPs. QSAR models for genotoxicity are unable to distinguish BGs from BPs. The integration of QSAR tools, docking, and NAMs provides complementary evidence, reduces uncertainty in early hazard assessment, and enables prioritisation of candidate substances as safer BPA alternatives.



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sciforum-187136: Colour-Encoded Gold Nanostructure-Based Lateral Flow Immunoassay with Smartphone-Based Digital Analysis for Rapid Mycotoxin Screening

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Mycotoxin contamination in food and feed remains a major challenge, particularly because multiple toxins can co-occur and complicate monitoring. Rapid screening methods are required to complement laboratory analysis and support timely on-site decision-making. In this work, a colour-encoded lateral flow immunoassay (LFIA) platform was developed using zearalenone (ZEN), aflatoxin B1 (AFB1), and fumonisin B1 (FB1), with the longer-term objective of enabling multiplex detection on a single test strip. To provide distinguishable optical signals for future multi-analyte detection, gold nanostructures with different morphologies were synthesised, including spherical gold nanoparticles with diameters of 20–40 nm, gold nanostars with overall sizes of ~88–140 nm, and gold nanoflowers with an overall size of ~100 nm. These nanomaterials were characterised by UV-Vis spectroscopy, dynamic light scattering (DLS), and scanning electron microscopy (SEM) to assess their optical behaviour, size distribution, morphology, and colloidal properties. Mycotoxin-specific hapten-protein conjugates were prepared and immobilised on LFIA test lines, while antibody-nanoparticle conjugation conditions were optimised through pH adjustment, antibody loading, and blocking strategies to obtain stable detection probes. Individual competitive LFIA strips were fabricated for ZEN, AFB1, and FB1 and evaluated as single-analyte systems. The assays produced clear visual responses, with toxin-dependent changes in test line intensity, confirming effective competitive binding and qualitative detection. To support objective interpretation, a prototype smartphone-based application was developed in Flutter for on-device digital analysis. The application allows users to select and display LFIA images alongside a reference image, automatically detect horizontal colour bands, extract average colour information, and analyse band signals using RGB/Hex values and HSV colour space. Detected bands are labelled by assigned line position, and test validity is assessed from control line presence. Overall, this work supports future multiplex LFIA development by integrating colour-encoded gold nanostructures, competitive immunoassay formats, and prototype digital analysis for rapid, on-site multi-mycotoxin screening in food safety applications.



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sciforum-187232: Optimization of the Human Cell Line Activation Test (h-CLAT) for the Identification of Photo-Allergens

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Photosensitization refers to light-induced adverse tissue effects resulting from exposure to photoreactive chemicals in combination with ultraviolet (UV) or visible light. Unlike phototoxicity, photoallergy is an immune-mediated delayed hypersensitivity reaction in which light transforms a chemical into a sensitizer capable of activating dendritic cells and inducing allergic contact dermatitis. To support the development of new approach methodologies (NAMs) for photoallergy assessment, this study optimized the human Cell Line Activation Test (h-CLAT) for use with UVA exposure.

The photo-h-CLAT was established by incorporating UVA irradiation (1.7 ± 0.2 mW/cm²; total dose 5 J/cm²) into the standard h-CLAT framework (OECD TG 442E) using THP-1 cells. Four sequential method iterations were evaluated to optimize assay performance and reproducibility. Modifications included changes to pre- and post-exposure incubation periods, rinsing procedures, antibody incubation time, and preparation of test chemicals in either DPBS or phenol red-free medium. Chlorpromazine hydrochloride (CPZ) was tested at multiple concentrations to monitor assay sensitivity and consistency. Following treatment, cells were stained for CD54 and CD86 expression and analyzed by flow cytometry. Compounds were classified as positive when the light-to-dark relative fluorescence intensity ratio was ≥ 2.0 for CD54 or ≥ 1.5 for CD86.

CPZ consistently exceeded the CD54 threshold under UVA exposure and was established as a reliable positive control. Following optimization, the photo-h-CLAT correctly identified 9 of 10 reference chemicals with compelling evidence of photoallergenicity. These findings highlight the potential of the photo-h-CLAT as a NAM for identifying photoallergens and support its further refinement and evaluation.



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sciforum-187258: Exploring the mechanistic connection between nephrotoxicity and aquatic toxicity: an approach using structure-based computational alerts

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Toxicogenomics investigates molecular changes induced by toxic agents to understand and predict adverse effects on human and environmental health. The toxicity of chemical compounds may transcend the biological specificity of isolated organisms, aligning with the One Health concept. Because chemically driven processes are broadly conserved across taxa, compounds associated with human nephrotoxicity may also represent environmental hazards, supporting a One Health perspective for hazard prioritization. Therefore, this study aimed to computationally screen the potential aquatic hazard of a toxicogenomic dataset associated with nephrotoxicity using structure-based alert systems. Sixty-six compounds associated with acute renal tubular necrosis were retrieved from the Comparative Toxicogenomics Database (CTD), an integrated resource of toxicological, toxicogenomic, and pathway data, and submitted to the OECD QSAR Toolbox (v4.8) using four alert systems: Verhaar scheme (Modified); OASIS mechanism of action-based aquatic toxicity classification (MOA-OASIS); Cramer Rules; and HESS repeated-dose alerts, parsed for renal and hepatic structural indicators. All compounds received a MOA-OASIS assignment, with 67% falling into the "Reactive unspecified" category, indicating limited mechanistic resolution for this class of electrophilic nephrotoxicants. Narcotic modes of action accounted for 29%, consistent with potential mechanisms involving nonspecific membrane interactions. Under the Verhaar scheme, 44% were assigned to defined classes, while 56% remained unclassifiable. The Cramer Rules classified 76% as high hazard. HESS alerts identified 41 compounds with explicit renal toxicity indicators, of which 25 also received a "Reactive unspecified" aquatic MOA. The results suggest that structural features associated with nephrotoxicity may also be relevant to aquatic hazard assessment and provide mechanistic hypotheses based on shared structure-derived indicators. Given that the analysis relied exclusively on structure-based alerts, these findings should be regarded as hypothesis-generating rather than evidence of shared biological mechanisms. These findings support the use of toxicogenomic resources and computational screening for One Health-oriented hazard prioritization.



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sciforum-187267: Human Umbilical Artery as a New Approach Methodology (NAM) to assess thyroid-disruptive vascular effects of emerging contaminant mixtures

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Thyroid hormone system disruption (THSD) is a significant public health concern and an EU research priority. Currently, no New Approach Methodologies (NAMs) are available in the OECD TG to assess THSD. Pregnant women are exposed daily to personal care products containing emerging contaminants, while contaminant interactions may further complicate chemical risk assessment. This work investigated the vascular effects of a mixture of UV filter octylmethoxycinnamate (OMC, 50µmol/L) and antimicrobial agent triclosan (TCS, 10µmol/L), under simulated hyperthyroidism conditions (T3, 6nmol/L). Human umbilical artery (HUA, n=4) was used for ex vivo organ bath experiments. Vascular homeostasis was assessed by serotonin (5-HT, 1µmol/L)-induced contraction and nifedipine (Nif, 1µmol/L)-induced relaxation. Results showed a significant increase ($p=0.009$) in Nif-induced relaxation in T3-exposed HUA ($83.88 \pm 2.33\%$) compared with the control group ($62.73 \pm 2.25\%$). Further, T3-exposed HUA treated with TCS exhibited a significant decrease in Nif-induced relaxation ($55.52 \pm 2.22\%$) compared with arteries exposed to a single T3- ($83.88 \pm 2.33\%$, $p=0.005$) and OMC-exposure ($82.74 \pm 2.76\%$, $p=0.005$) or OMC+TCS mixture ($77.32 \pm 3.11\%$, $p=0.018$). These findings highlight the T3-role in vascular tone modulation and vasorelaxation, suggesting signaling pathways beyond Ca^{2+} channels inhibition. Under simulated hyperthyroidism, vascular responses suggest differential modulation by TCS and OMC: OMC appear consistent with those elicited by T3, whereas TCS effects are compatible with predominant Ca^{2+} channel inhibition. In the mixture, vascular effects resemble those observed in OMC- and T3-exposed HUA, suggesting a possible contribution of OMC to the overall response. These hypotheses require further investigation. Overall, these proof-of-concept findings support the relevance of HUA as a NAM for THSD research. By preserving key physiological features and enabling ex vivo assessment of vascular responses, HUA represents a valuable tool for supporting human risk assessment of thyroid-disrupting chemicals.



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sciforum-187287: Combining Explicit Molecular Features and Latent ChemBERTa Embeddings for Ecotoxicological Screening

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Introduction

Evaluating the environmental impact of cosmetic ingredients requires robust alternatives to in vivo testing. This study proposes an in silico workflow to predict fish toxicity by integrating bioconcentration factor (BCF; toxicokinetics) and Aryl Hydrocarbon Receptor (AhR) activation (toxicodynamics) models.

Methods

Structures were standardized (cleanup, salt removal, charge neutralization and tautomeric canonicalization with RDkit), retaining canonical SMILES with ≥ 2 carbon atoms and specific organic elements. A hybrid descriptor pipeline combined six physicochemical properties, 166 MACCS keys, and 384 transformer ChemBERTa-77M-MLM embeddings. Dimensionality reduction incorporated low-variance filtering, principal component analysis (PCA) for ChemBERTa embeddings, and Random Forest (RF) feature selection. The BCF dataset (N=1,046, from three public sources) trained an RF regressor. Duplicated SMILES were excluded or merged by the mean of logBCF if standard deviation ≤ 0.25 . The AhR dataset (PubChem AID 2845; N=948 actives after removing discordant duplicates) trained an XGBoost classifier using undersampling for class imbalance and a 70/20/10 split.

Results

The BCF model achieved a Leave-One-Cluster-Out Cross-Validation (LOCO-CV) R^2 of 0.48 (RMSE=0.88). On an external validation set (N=77), it yielded $R^2=0.54$ and RMSE=0.66, outperforming existing literature models for the same molecules with minimal overfitting (Y-scramble $R^2=-0.05$). The AhR activation model achieved a cross-validation Q^2 of 0.89 (Y-scramble ROC-AUC=0.49). The validation set metrics were: accuracy 0.86, sensitivity 0.74, specificity 0.88, F1-score 0.56, and ROC-AUC 0.88.

Conclusions

Integrating explicit features with Transformer-based embeddings generates robust predictive models. Despite improving predictive performance, dense embeddings lack the mechanistic transparency of OECD QSAR Principle 5, hindering regulatory acceptance. Addressing this gap requires coupling explainable AI (e.g., SHAP and similarity maps) with established frameworks like AOP 150 (AhR Activation) to provide mechanistic weight-of-evidence.



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sciforum-187370: Mechanistic Convergence of the Chemical Exposome in Nephrotoxicity: A Systems Toxicology Network Approach

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Introduction

The chemical exposome comprises the cumulative environmental and pharmacological exposures that shape biological systems over time. In the kidney, these exposures may influence inflammatory and metabolic pathways that contribute to renal injury. Nevertheless, nephrotoxicity assessment still predominantly evaluates substances individually, which may overlook shared mechanistic patterns. This study investigates whether different nephrotoxic agents converge on common molecular pathways within renal interaction networks.

Methods

The approach is entirely computational and aligned with New Approach Methodologies (NAMs). Substances associated with nephrotoxicity were retrieved from CTD, GeneCards, and UniProt. Genes linked to these exposures were integrated to construct protein–protein interaction networks using STRING (Homo sapiens; confidence ≥ 0.700). Network topology was evaluated in Cytoscape through degree distribution, centrality measures, and modular organization. Functional enrichment analysis was conducted in Reactome to identify recurrent biological pathways.

Results

Preliminary network integration suggests the presence of overlapping interaction modules across chemically distinct exposures. Shared highly connected nodes are observed within pathways related to inflammation, oxidative stress, mitochondrial dysfunction, and immune signaling. Ongoing topological evaluation is being conducted to further characterize recurrent structural patterns within the renal interaction network.

Conclusions

The results support the hypothesis that nephrotoxicity in the context of the chemical exposome involves shared molecular architectures rather than isolated effects. A systems-level network perspective may contribute to more integrative and mechanistically grounded renal risk assessment models.



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sciforum-191485: Multimodal AI Generates Virtual Rats: Predicting Hepatic Burden of Oral Drugs

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Background & Aims

Drug-induced liver injury (DILI) remains a major cause of drug attrition, boxed warnings, and post-marketing withdrawal. However, its low incidence and high inter-individual variability limit the sensitivity of preclinical animal studies. We aimed to develop a multimodal virtual toxicology framework capable for simulating rat hepatic responses and improving detection of rare hepatotoxicity signals.

Methods

We developed Virtual Rat Experiment Model (VREM), a multimodal conditional generative adversarial network integrating chemical structure descriptors, bioactivity and network toxicology-informed pathway perturbation features. A modality-aware mixture-of-experts architecture adaptively fused heterogeneous biological information under different dose and exposure-duration conditions. The model was trained using 10,205 rat experimental records and externally validated using 1,453 records. Performance was evaluated using Pearson correlation, cosine similarity, root mean square error (RMSE), and Experimental Consistency Score (ECS).

Results

VREM faithfully reproduced biomarker distributions and consistently outperformed QSAR models. Key liver-injury biomarkers showed strong agreement between predicted and observed values, including ALT (adjusted $R^2 = 0.9803$), AST (adjusted $R^2 = 0.9740$), and ALP (adjusted $R^2 = 0.9612$). ECS values exceeded 0.90 for ALT, AST, and ALP across 10 independent generation runs. External validation demonstrated robust generalization despite substantial dataset distribution shifts, with significantly higher cosine similarity ($P = 3.36 \times 10^{-31}$) and lower RMSE ($P = 4.71 \times 10^{-58}$) than background distributions. Large-scale virtual experiments on 30 boxed-warning oral drugs identified potential DILI signals in 22 compounds, compared with only one compound detected in preclinical toxicology studies.

Conclusions

VREM provides a scalable multimodal digital twin framework for virtual hepatotoxicity experimentation. The model enables high-fidelity simulation of hepatic responses and substantially improves detection of low-frequency hepatotoxicity signals difficult to capture in conventional preclinical studies.



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sciforum-191693: Theoretical analysis of HCN detection using sumanene-based nanostructures

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Hydrogen cyanide, HCN is a highly toxic and dangerous gas molecule widely used in industries including mining, electroplating, chemical synthesis and polymer manufacturing. The detection of HCN gas molecule is important because even low concentrations can cause severe health problems, respiratory failure, nervous system damage, unconsciousness and death. In addition to its harm-ful effects on human health, HCN can also cause serious environmental pollution and poses significant risks in industrial workplaces and accidental leak situations. However, the detection of HCN at very low concentrations remains a challenging task. Therefore, the development of highly sensitive and selective sensing materials for efficient HCN detection has become an important research area in gas sensing applications. In this work, I performed density functional theory calculations using the B3LYP exchange–correlation functional and the 6-31G(d,p) basis set to investigate the HCN sensing performance of sumanene and nitrogen-substituted sumanene. The reliability of the theoretical results was further supported by performing vibrational frequency analyses to make sure that the optimized adsorption geometries correspond to stable local minima without any imaginary frequencies. Based on the electronic structure calculations, the adsorption configurations, adsorption energies, and electronic properties were systematically investigated and compared to the adsorption of HCN on pristine sumanene and nitrogen-substituted sumanene systems. The obtained results reveal that HCN interacts more strongly with nitrogen-substituted sumanene than with pristine sumanene. This investigation provides the theoretical predictions and also highlights the novelty of employing nitrogen-substituted sumanene as an efficient HCN sensing material, offering valuable insights for the rational design of the high-performance gas sensors for toxic gas detection.



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sciforum-193991: Filling Monitoring Gaps in Freshwater Pesticide Surveillance Using Random Forest Machine Learning

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Pesticide contamination of surface waters represents a persistent environmental challenge, particularly in agriculturally intensive regions where runoff and spray drift continuously introduce compounds into freshwater systems. Despite growing regulatory attention, routine monitoring programs remain limited in both spatial coverage and the number of substances analyzed, resulting in significant blind spots regarding actual contamination levels. This study explored whether Random Forest machine learning models could help bridge these gaps using monitoring data from Bretagne, France, a region where roughly 65% of land is under agricultural use.

Two models were developed, one predicting pesticide occurrence and one predicting concentrations, trained on predictors including land use, seasonality, chemical identity, and pesticide class. Both models showed strong predictive performance, with the concentration model accounting for over 99% of variance in independent test data. Compound-specific variables, particularly chemical identity and pesticide class, proved far more informative than spatial predictors like land use, though seasonal and landscape factors still contributed meaningfully. Applying the models to an expanded dataset covering unmonitored site-pesticide combinations suggested that actual contamination levels may be nearly three times higher than what conventional monitoring programs currently detect.

These results point to a substantial underestimation of pesticide presence in freshwater and support the use of data-driven approaches as a practical complement to field monitoring in environmental risk assessment.



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sciforum-194377: Machine Learning in Environmental Toxicology: Predicting Endocrine Disruption and Cross-Species Toxicity of Emerging Contaminants

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Introduction

The rapid proliferation of synthetic chemicals, pharmaceuticals, and agrochemicals has transformed global ecosystems, raising concerns about endocrine-disrupting chemicals (EDCs) and cross-species toxicity. Traditional *in vivo* toxicological testing is increasingly inadequate to evaluate the growing volume of emerging contaminants (ECs), necessitating computational approaches.

Methods

This systematic review evaluates the application of artificial intelligence (AI) and machine learning (ML) in environmental and veterinary toxicology within a One Health framework. Databases spanning 2000–2026 were analyzed to assess predictive modeling of EDCs, including PFAS, phthalates, bisphenols, and pharmaceutical mixtures. Classical ensemble algorithms (Random Forest, GPBoost) were compared with deep learning architectures such as Communicative Message Passing Neural Networks (CMPNN) and 3D-structure-based models (3DMol-Tox). Cross-species toxicity prediction was examined by juxtaposing Interspecies Correlation Estimation (ICE) models with multi-feature ML algorithms.

Results

AI-driven models demonstrated superior accuracy in predicting endocrine disruption and extrapolating toxicity across taxonomic boundaries. Advanced deep learning approaches outperformed traditional methods in handling complex chemical structures and mixture effects. Critical methodological challenges were identified, including information leakage in train-test splitting, which can inflate predictive performance. Integrating AI with ecotoxicological data enables more reliable risk assessment, linking molecular initiating events to sentinel species, veterinary health, and ecosystem resilience.

Conclusions

Machine learning provides a transformative framework for predictive toxicology, bridging gaps between molecular mechanisms and ecosystem-level outcomes. These approaches enhance cross-species risk assessment, accelerate screening of emerging contaminants, and support One Health strategies for safeguarding environmental and animal health.



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Session 4. Molecular and Cellular Mechanisms, Comparative Toxicology, and Multi-Omics Integration

sciforum-179016: Zinc modulates nickel-induced oxidative stress in the liver of murine model

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Background

Chronic nickel exposure is increasingly recognized for its potential to disrupt liver function and metabolic homeostasis. Zinc, an essential trace element, plays key roles in enzymatic activity, metal binding, and antioxidant defence, with evidence suggesting competitive interactions with nickel. Investigating their combined effects may clarify the interactions between toxic and protective metals in the liver and provide insight into potential interventions.

Aim

This study evaluated the impact of zinc on oxidative stress biomarkers in the livers of nickel-exposed mice.

Methods

Animals were divided into control, nickel-exposed, zinc-exposed, and zinc-plus-nickel exposure groups. The oxidative status of the liver was assessed by measuring the levels of reduced glutathione (GSH), malondialdehyde (MDA) and metallothionein (MT) expression.

Results

A single NiCl₂ injection decreased hepatic GSH by 28%, while zinc alone caused no significant change. Zinc pre-treatment (20 min prior to NiCl₂) led to a further 40% decrease. After 14 days, GSH levels were comparable across groups and remained at control level. MDA increased by 282% after a single NiCl₂ dose and by 87% after repeated exposure. Zinc alone reduced MDA by 20% after a single dose but had no effect after prolonged exposure. Pre-treatment with zinc attenuated Ni-induced MDA elevation by 146% after a single exposure and by 50% after repeated exposure. MT expression increased by 35% after a single NiCl₂ injection and by 57% after 14 days. Zinc alone elevated MT by 20% (single dose) and 48% (14 days). Combined exposure resulted in greater MT induction, reaching 41% after a single treatment and 70% after repeated exposure.

Conclusion

These findings indicate that nickel induces hepatic oxidative stress, while zinc modulates this response in a time-dependent manner. The protective effect of zinc against lipid peroxidation may be linked to its ability to induce metallothionein expression.



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sciforum-179191: Attenuation of Cadmium-, Nickel-, and Lead-Induced Oxidative Stress by Green Tea Extract in a Murine In Vivo Model

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Introduction

Heavy metal toxicity is a significant environmental and public health concern, with continual exposure to cadmium (Cd), nickel (Ni), and lead (Pb) occurring through contaminated air, water, soil, and food. These metals are known to induce oxidative stress, leading to increased lipid peroxidation in biological tissues.

Methods

This study aimed to evaluate the protective antioxidant effects of green tea extract (GTE) against lipid peroxidation induced by Cd, Ni, and Pb in mice. Outbred white laboratory mice were administered intraperitoneal injections of CdCl₂, NiCl₂, and Pb(CH₃COO)₂, with or without GTE, over a 14-day period. Lipid peroxidation levels were assessed in red blood cells, liver, and brain tissues by measuring thiobarbituric acid reactive substances (TBARS), expressed as malondialdehyde (MDA) equivalents.

Results

Exposure to all metals significantly increased lipid peroxidation levels in all examined tissues, confirming their pro-oxidant effects. Co-administration of GTE significantly reduced lipid peroxidation levels in both liver and blood, with complete normalization of oxidative status observed in brain tissue.

Conclusions

These findings demonstrate that green tea extract exerts significant protective effects against heavy metal-induced oxidative damage. This study underscores the potential of green tea as a natural antioxidant agent in mitigating heavy metal toxicity, highlighting its relevance in toxicological risk assessment and prevention strategies.



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sciforum-182615: Pyriproxyfen disrupts liver development in *Gallus domesticus* embryos at environmentally relevant concentrations

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Introduction

Extensively used in vector-control programs across public health and agriculture, pyriproxyfen (PPF) is an insect growth regulator considered to pose minimal risk to non-target organisms. However, growing evidence indicates that it can cross biological barriers and interfere with conserved molecular pathways. Although its neurotoxicity in vertebrates has been described, their hepatotoxic potential during embryogenesis remains poorly understood. Thus, the aim of this study was to investigate the PPF effects on liver development of *Gallus domesticus*.

Methods

Fertilized eggs were exposed at embryonic day 1 (E1) to vehicle control (1% DMSO), the WHO-recommended PPF concentration (0.01 mg/L), or a worst-case scenario concentration (10 mg/L). Embryos were incubated until E10, when liver were collected for biometric, histological, histochemical, and cellular analyses. All experimental procedures were approved by the Animal Use Ethics Committee of the Federal University of Santa Catarina (5843231018).

Results/Discussion

Embryos exposed to PPF exhibited increased hepatosomatic index along with marked histoarchitectural disruption, including reduced hepatocyte density and increased vacuolization at both PPF concentrations. The combined histopathological index was significantly elevated in PPF-exposed groups. Histochemical analyses further demonstrated metabolic impairment, whereas toluidine blue O reaction showed increased metachromasia at both PPF concentrations, suggesting accumulation of acidic components associated with cellular stress. Conversely, Periodic Acid-Schiff reaction revealed reduced neutral polysaccharides only at 10 mg/L, suggesting glycogen depletion. Reduced Coomassie Brilliant Blue reaction suggested loss of protein integrity or synthesis. Moreover, cellular markers confirmed disrupted hepatic development, in which proliferation (PHH3) was significantly reduced, while apoptosis (cleaved caspase-3) increased even at PPF environmentally relevant concentration (0.01 mg/L).

Conclusion

Together, these results demonstrate that PPF compromises liver homeostasis, metabolism, and cellular turnover during early development, establishing its potential as an embryonic hepatotoxicant. These findings underscore the need for ecotoxicological monitoring and stricter evaluation of PPF use in environments shared with non-target vertebrates.



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sciforum-183454: Toxicological impacts of fluoxetine on the freshwater microalga *Raphidocelis subcapitata*: a multi-endpoint assessment

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Introduction

Pharmaceuticals are increasingly recognised as active stressors in aquatic systems. Among them, the antidepressant fluoxetine (FLX) is frequently detected in freshwater systems. Despite its widespread occurrence, FLX mode of action, at the cellular level, remains poorly understood. This study aimed to investigate how FLX interferes with the physiology of the freshwater microalga *Raphidocelis subcapitata* at environmentally relevant concentrations.

Methods

Algal cultures were exposed to FLX (15–30 $\mu\text{g L}^{-1}$) in OECD medium for 72 h. Growth, metabolic activity, mitochondrial function, photosynthetic pigments content, photosynthetic performance, oxidative stress (via reactive oxygen species, ROS, accumulation and lipid peroxidation, LPO), and membrane integrity were evaluated.

Results

Exposure to 20–30 $\mu\text{g L}^{-1}$ FLX resulted in a pronounced inhibition of algal growth, likely associated with disruption of nuclear division. At 15–30 $\mu\text{g L}^{-1}$, FLX induced significant metabolic alterations, mitochondrial dysfunction (characterized by inner membrane hyperpolarization), and reduction in chlorophyll *a* (Chl*a*), and carotenoids (CAR) content. Photosynthetic performance was severely impaired by decreases in maximum photochemical quantum yield (F_v/F_m), effective quantum yield (Φ_{PSII}), and electron transport rate (ETR) of photosystem II. At 30 $\mu\text{g L}^{-1}$, oxidative stress was evident through ROS accumulation and increased LPO, while membrane integrity showed only minor disruption.

Conclusions

FLX acts as a multi-target disruptor in *R. subcapitata*, affecting cell division, metabolism, and photosynthesis in an integrated way. These findings highlight the ecological relevance of pharmaceutical contamination and emphasize the need to consider sublethal mechanistic effects when assessing risks in freshwater environments.



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sciforum-184541: Biochemical Disruption of Glutathione-Dependent and Independent Antioxidant Defense Systems under Synergistic Pesticide Exposure in *Trogoderma granarium*

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Introduction

Trogoderma granarium is a major stored-grain pest with increasing resistance to commonly used insecticides deltamethrin and phosphine. Bifenthrin and chlorpyrifos are effective alternatives at low concentrations (Feroz et al. 2020). Sublethal exposures, particularly at LC₂₀ levels, are environmentally relevant as they allow survival while inducing physiological stress. This study investigates how these insecticides and their synergistic combinations disrupt antioxidant defense systems, revealing secondary toxicity mechanisms and alterations in cellular redox homeostasis.

Methods

Fourth- and sixth-instar larvae from susceptible (Lab-S) and resistant (GUW) populations were exposed for 48 h to LC₂₀ concentrations of bifenthrin, chlorpyrifos, and their combinations (3:1 and 1:3). The activities of glutathione-dependent (glutathione-S-transferase, glutathione reductase, glutathione peroxidase) and non-glutathione antioxidant enzymes (superoxide dismutase, catalase, peroxidase, polyphenol oxidase) were quantified spectrophotometrically.

Results

LC₂₀ values demonstrated strong synergistic interactions, with mixtures showing markedly lower toxicity thresholds than individual insecticides. For example, in sixth instar susceptible larvae, LC₂₀ values decreased from 131.34 ppm (bifenthrin) and 46.31 ppm (chlorpyrifos) to 8.88 ppm (3:1 mixture) and 0.16 ppm (1:3 mixture). Resistant populations exhibited higher LC₂₀ values (e.g., 51.81 ppm at 1:3), though combinations partially overcame resistance. Enzymatic analyses revealed significant reductions ($p \leq 0.05$, Tukey's test) in antioxidant activities across all treatments compared to untreated controls. Combined exposures produced stronger inhibitory effects than individual treatments, indicating synergistic disruption of antioxidant defense systems.

Conclusion

These results demonstrate that insecticide mixtures induce oxidative stress by disrupting both glutathione-dependent and independent antioxidant systems. Even at sublethal (LC₂₀) levels, these exposures compromise cellular homeostasis without causing immediate mortality. Although combined treatments may reduce required chemical doses, the ecological risks of chronic low-dose mixture exposure require further investigation.

Feroz, A., Shakoori, F.R. and Riaz, T., Shakoori, A.R., 2020. Development of resistance in stored grain pest, *Trogoderma granarium* (Everts) against deltamethrin and its effective control by synergistic toxicity of bifenthrin and chlorpyrifos. *Journal of Stored Products Research*, **88**: 101673.



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sciforum-184776: Chronic Dual-Band Radiofrequency Exposure Selectively Affects Spatial Memory Retention Without Altering Anxiety-Like Behavior in Rats

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Background: Radiofrequency electromagnetic fields (RF-EMFs) are increasingly recognized as widespread environmental exposures associated with wireless communication technologies. Although these fields are non-ionizing, their possible neurobehavioral effects remain debated, particularly during growth and under repeated multi-band exposure conditions. **Objective:** This study evaluated whether chronic exposure to single- and dual-band RF signals affects anxiety-like behavior, spatial learning, and memory retention in growing male rats. **Methods:** Forty male Wistar rats were randomly assigned to four groups: sham-exposed controls, 800 MHz-exposed rats, 900 MHz-exposed rats, and sequential 800/900 MHz-exposed rats. Single-band groups were exposed for 3 h/day, whereas the dual-band group received 3 h/day at 800 MHz followed by 3 h/day at 900 MHz. Exposures were conducted 6 days/week for approximately four months. Anxiety-like behavior was assessed using the elevated plus maze. Spatial learning and memory were evaluated using the Morris water maze. **Results:** RF exposure did not significantly affect elevated plus maze outcomes, including open-arm latency, time spent in open or closed arms, and arm-entry indices, suggesting no measurable effect on anxiety-like behavior or locomotor activity. In the Morris water maze, escape latency decreased significantly across training days in all groups, indicating preserved spatial learning. No significant Exposure effect or Exposure × Day interaction was observed during acquisition. However, the probe trial showed a significant reduction in target-quadrant time in the sequential 800/900 MHz group, while platform-site crossings did not differ significantly. **Conclusion:** These findings indicate a complex neurobehavioral profile: chronic RF exposure did not alter anxiety-like behavior or acquisition learning, but sequential dual-band exposure was associated with a selective reduction in spatial memory retention. Because this effect was endpoint-dependent and occurred under a longer dual-exposure schedule, interpretation remains cautious. The cellular and molecular mechanisms through which RF-EMFs may influence living cells are still not fully understood, highlighting the need for integrated behavioral, histological, oxidative-stress, and mechanistic investigations.



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sciforum-184899: Chronic methylmercury exposure alters astrocytic morphology and NADPH diaphorase reactivity in the rat frontal cortex

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Introduction: Mercury (Hg) remains a persistent environmental pollutant with well-documented neurotoxic potential. Despite global awareness of its hazards, Hg continues to be extensively employed in artisanal gold mining, particularly in developing regions, contributing to environmental contamination and human exposure. In aquatic environments, inorganic Hg can be converted into methylmercury (MeHg) through microbial biomethylation, facilitating its bioaccumulation along the food chain and increasing the risk of human exposure. The central nervous system is particularly vulnerable to MeHg toxicity due to its high metabolic demand and sensitivity to oxidative and metabolic disturbances. Here, we assessed the effects of chronic MeHg exposure on NADPH-diaphorase (NADPH-d) activity and astrocytic responses in the frontal cortex of rats. **Methods:** Adult rats were randomly assigned to control and MeHg-exposed groups (n = 6 per group). The MeHg group received the compound by oral gavage (0.04 mg/kg/day) for 60 days, while control animals received the vehicle following the same schedule, in accordance with a protocol approved by the UFPA's Ethics Committee for Animal Experimentation (ID# BIO 225-14-CEPAE-UFPA). After the exposure period, brain tissue samples were analyzed to determine Hg concentration, NADPH-d histochemical reactivity, and astrocytic morphology using glial fibrillary acidic protein (GFAP) immunohistochemistry. **Results:** Chronic MeHg exposure resulted in significant accumulation of Hg in cortical tissue and a reduction in NADPH-d neuropil optical density ($p < 0.05$). Morphometric analysis indicated that NADPH-d-positive neurons were relatively preserved, suggesting resistance to chronic toxic exposure. In contrast, astrocytes exhibited marked morphological alterations, including cellular swelling and hypertrophy. **Discussion/Conclusions:** These findings suggest that prolonged exposure to MeHg induces selective neurochemical and glial changes in the frontal cortex. The reduction in NADPH-d neuropil reactivity may reflect impaired synthesis or intracellular transport of the enzyme, whereas the apparent resistance of NADPH-d-positive neurons could be related to metabolic adaptations or potential protective mechanisms involving nitric oxide signaling.



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sciforum-185654: “Oxidative DNA Damage and Repair Disruption Under Pesticide–Metal Co-Exposure”

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Piperonyl butoxide (PBO) is an organic compound widely used as a pesticide synergist to enhance the efficacy of active ingredients like pyrethrins. While traditionally considered low-risk for mammals, recent evidence suggests its genotoxic potential may be underestimated, particularly in individuals with compromised DNA repair. This study investigated the DNA damage response triggered by PBO in a mammalian Chinese hamster ovary (CHO) cell model.

Immunofluorescent microscopy was used to track γ H2AX foci, a sensitive marker for DNA double-strand breaks. To determine the mechanism of damage, EdU (5-ethynyl-2'-deoxyuridine) labeling was used to identify cells in the S-phase of the cell cycle. The study specifically compared standard CHO cells with PARP-deficient PADR9 cells to observe the effects of impaired repair mechanisms.

PBO treatment resulted in a significant, dose-dependent increase in γ H2AX foci. These genotoxic effects were profoundly exacerbated in PARP-deficient PADR9 cells, which exhibited extensive pan-nuclear γ H2AX signaling and widespread genomic instability. EdU incorporation confirmed that the observed DNA damage was predominantly S-phase dependent, identifying replication stress as the primary mechanism of PBO-induced toxicity. **Conclusions** These results reveal a previously underappreciated genotoxic pathway for PBO, demonstrating that substances labeled as low-risk can cause substantial genomic damage under compromised biological conditions. The specificity of this damage to DNA replication highlights a critical need to reassess the safety of PBO exposure, particularly for populations with genetic predispositions to impaired DNA repair.



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sciforum-186131: “Comparative neurotoxic effects of conventional and alternative plasticizers on microglia”

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Plasticizers are widely incorporated into plastics to enhance their flexibility, yet their non-covalent binding to the polymer matrix enables continuous human exposure through multiple routes. Increasing evidence suggests that some of these compounds can reach the central nervous system. One of the most commercially produced, di(2-ethylhexyl) phthalate (DEHP), is currently restricted due to documented toxicological effects, including endocrine disruption and neurotoxicity. This has driven its progressive substitution with alternative compounds considered safer such as acetyl tributyl citrate (ATBC) and acetyl triethyl citrate (ATEC), although accumulating evidence suggests that these substitutes may induce similar neurobiological effects. More recently, bio-based plasticizers such as thymol:menthol (TY-ME), a natural deep eutectic solvent (NADES), have been proposed as next-generation alternatives. These systems are considered biodegradable and potentially biocompatible and may even exert intrinsic bioactive properties; however, their impact on neural cells remains largely unexplored.

In this study, we evaluated the effects of these plasticizers on human microglial HMC3 cells, focusing on cell viability and molecular responses associated with neuroinflammation and oxidative stress. Cytotoxicity was assessed using the MTT assay, while gene expression levels of *TGF- β 1*, *IL-6*, *IL-1 β* , and *HMOX1* were quantified by RT-qPCR. DEHP exposure resulted in pronounced cytotoxicity together with strong induction of pro-inflammatory and oxidative stress markers. ATBC elicited a comparable response profile, suggesting that its biological impact may resemble that of the phthalate it replaces. In contrast, TY-ME exhibited moderate cytotoxic effects and minimal modulation of gene expression, indicating a comparatively attenuated impact on microglial activation. ATEC showed the lowest overall toxicity, although it was associated with a detectable oxidative stress response.

Overall, these findings highlight that phthalate-free alternatives are not necessarily devoid of biological activity and underscore the importance of systematically evaluating both conventional and emerging plasticizers in relevant human cell models to support the development of safer materials.



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sciforum-186321: Hemin drives transcriptional remodeling in intestinal epithelial cells.

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Diet plays a critical role in human health, and high consumption of red and processed meats is associated with increased colorectal cancer risk. Although hemin is required at physiological concentrations, excessive intestinal exposure induces pro-oxidant effects, disrupts tissue homeostasis, and compromises barrier integrity, thereby establishing a pro-inflammatory and oxidative microenvironment that may promote epithelial injury and contribute to colorectal carcinogenesis.

Methods

We exposed rat intestinal epithelial cells (IEC-6) to 10 μ M hemin and characterized transcriptomic changes using bulk RNA sequencing. KEGG and Gene Ontology analyses identified enriched pathways. Key biological processes were validated through targeted functional assays: ROS production (H_2O_2 , NO, O_2^-) by flow cytometry, NRF2 nuclear translocation by immunofluorescence, DNA damage by γ H2AX staining, anchorage-independent growth by soft agar colony formation, and inflammatory mediators using a multiplex cytokine assay.

Results

Transcriptomic analysis revealed a distinct gene expression profile, with enrichment in pathways related to oxidative stress, inflammation, and cell proliferation, and downregulation of cell cycle-associated pathways, particularly WNT and BMP signaling. Functionally, hemin increased ROS production and induced NRF2 nuclear translocation. Hemin exposure also increased γ H2AX staining, indicating genotoxicity, and enhanced colony formation in soft agar assays lead to carcinogenic potential. Moreover, hemin fails to modulate the secretion of inflammatory factors, despite a significant change in the expression of pro-inflammatory genes.

Discussion/Conclusions

These results link hemin-induced transcriptomic changes to oxidative stress and genotoxicity in intestinal epithelial cells, while revealing a dissociation between pro-inflammatory gene expression and cytokine secretion. Overall, excess hemin may promote early colorectal carcinogenesis mainly through oxidative damage, cell cycle dysregulation, and genotoxicity, highlighting potential targets for dietary interventions.



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sciforum-186618: An Inflamed Gut is Not Always a Leaky Gut: Mycotoxin Permeability in a Co-culture Model

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Inflammation can impair intestinal barrier function by disrupting tight junctions, altering immune signalling, and increasing epithelial permeability [1]. Mycotoxins like ochratoxin A (OTA), zearalenone (ZEN), and aflatoxin B1 (AFB1) are common food contaminants that can aggravate intestinal damage and oxidative stress [2]. Although inflammation is assumed to enhance xenobiotic uptake, evidence remains inconsistent [3]. Therefore, this study aimed to evaluate whether acute inflammation affects the toxicity and permeability of a mycotoxin mixture.

Caco-2/HT29-MTX (90:10) intestinal coculture model was differentiated for 21 days to establish a functional intestinal barrier. Inflammation was induced with a cytokine cocktail (IFN- γ , IL-1 β , and TNF- α) [4]. Intestinal monolayers, either inflamed or normal, were subsequently exposed apically to a mixture of OTA, ZEN and AFB1 (500 μ g/L each, non-cytotoxicity assured by preliminary assays, level possible in foods[5]). Barrier integrity was monitored by real-time TEER, gene expression was analysed by qPCR, and mycotoxin transport (180 min) was quantified by HPLC-FLD.

Inflammation significantly reduced TEER and increased inflammatory (IL-1 β , 5-fold) and oxidative stress (SOD2, 15-fold) markers, confirming successful induction. However, barrier-related gene expression remained unchanged, consistent with previous studies [6,7]. Mycotoxin exposure did not affect TEER or gene expression in either normal or inflamed monolayers. All three mycotoxins crossed the barrier, with AFB1 showing the highest permeability (3.81×10^{-6} cm/s), followed by ZEN (2.66×10^{-6}) and OTA (7.70×10^{-6}), consistent with previous reports [8]. Transport profiles were comparable under both conditions.

These findings indicate that acute inflammation induces inflammatory and oxidative responses without increasing mycotoxin permeability. This shows that reduced barrier integrity does not necessarily translate to enhanced xenobiotic transport, thereby emphasising the importance of functional and mechanistic permeability assessments beyond TEER measurements alone.

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[2] doi.org/10.1111/1541-4337.13242

[3] doi.org/10.1080/10717540490280345

[4] doi.org/10.1038/s41598-024-74802-w

[5] doi.org/10.1002/jsfa.70686

[6] doi.org/10.1016/j.foodres.2025.115907

[7] doi.org/10.1016/S0002-9440(10)62264-X

[8] doi.org/10.1016/j.fct.2019.110595



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sciforum-186659: Low-Dose Tributyltin Exposure Induces Vascular Dysfunction and Oxidative Stress in Resistance Mesenteric Arteries of Wistar Rats

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Introduction: Tributyltin (TBT) is a persistent organic pollutant with bioaccumulative potential. Although the tolerable daily intake is 250 ng/kg/day (WHO), recent evidence suggests cardiovascular toxicity at lower doses. This study investigated the functional and histomorphometric effects of low-dose TBT exposure on resistance mesenteric arteries in rats. **Methods:** Female Wistar rats were exposed orogastrically for 15 days to vehicle (CT) or TBT (100 ng/kg/day). Protocols were approved by the Ethics Committee (#19/2022). Vascular reactivity to phenylephrine (PE, 10^{-9} – 10^{-4} M) was assessed via wire myography before and after L-NAME (300 μ M) incubation. Collagen area fractions and morphology were quantified via ImageJ/Fiji software after *picrosirius* red and H&E staining. Oxygen reactive species (ROS) were evaluated by DHE fluorescence. Data were analyzed using two-way ANOVA (vascular reactivity), Student's t-test (histomorphometry), and one-way ANOVA (ROS), with Sidak's/Tukey's post-tests ($p < 0.05$). **Results:** TBT induced a leftward shift in the PE contraction curve (pEC_{50} CT: 5.8 ± 0.1 ; TBT: 6.2 ± 0.05), indicating increased vascular hypersensitivity. While L-NAME reduced EC_{50} in the CT group, the TBT group did not show a shift (EC_{50} 6.2 ± 0.05 vs. 6.0 ± 0.14), suggesting impairment in the nitric oxide (NO) pathway. TBT exposure elevated basal ROS levels and increased pro-oxidant responsiveness to angiotensin II (CT: 25.33 ± 4.03 a.u.; TBT: 42.29 ± 3.21 a.u.). Histologically, TBT increased collagen deposition (15.33 ± 1.97 % vs. CT 10.33 ± 0.91 %), although lumen and tunica media dimensions remained unchanged. **Conclusion:** Exposure to TBT below established safety limits triggers early vascular dysfunction characterized by hypersensitivity, impaired NO signaling, and increased oxidative stress and fibrosis. These findings highlight important microvascular alterations, even at levels currently considered safe by international agencies.



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sciforum-186725: Efficacy-Toxicity Trade-Offs in Surfactant Formulation: Quantifying Irritation Synergy and Functional Performance in SLS/LDAO Binary Mixtures

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Surfactant-induced skin irritation remains a major toxicological concern in cosmetic and cleansing formulations, particularly those based on anionic surfactants such as sodium lauryl sulfate (SLS). In this study, the irritation-mitigating potential of binary mixtures of SLS and the amphoteric surfactant lauryl dimethylamine oxide (LDAO) was systematically evaluated, with special emphasis on the quantitative assessment of synergistic effects related to protein denaturation and skin compatibility.

Binary SLS/LDAO mixtures at different ratios were characterized in terms of critical micelle concentration (CMC), surface tension, foam generation and irritant potential using the Zein protein denaturation test. In addition, interaction parameters associated with mixed micellization and interfacial adsorption were calculated to quantify the degree of physicochemical synergy. All mixtures exhibited a marked reduction in CMC and minimum surface tension compared to the individual surfactants, indicating the formation of thermodynamically stable mixed micelles. Negative interaction parameters confirmed strong attractive interactions between SLS and LDAO in both micellar (b^M) and interfacial domains (b^S).

From a toxicological perspective, the Zein test revealed a pronounced decrease in protein denaturation with increasing LDAO content. Importantly, the experimentally determined Zein values of the mixtures were significantly lower than the cumulative values calculated from the individual surfactants at equivalent concentrations, demonstrating a clear synergistic reduction of irritant potential. This effect was especially pronounced in mixtures rich in LDAO (60:40 and 50:50), which shifted the classification from irritant or moderately irritant to non-irritant systems.



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sciforum-187031: Biomonitoring of air pollution in Cluj-Napoca city using tree leaves

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Air pollution associated with urbanization and traffic emissions represents a major environmental concern in urban areas. Urban vegetation can accumulate airborne particulate matter and associated metals, providing valuable information on the spatial distribution of atmospheric pollution. Tree species with different leaf morphologies have distinct accumulation capacities, making them useful indicators of local environmental quality. This study aimed to assess the accumulation of Cu, Pb, Zn, Cd, Cr and Ni in white cedar (*Thuja occidentalis*) and black poplar (*Populus nigra*) leaves collected from Cluj-Napoca city characterized by different anthropogenic influences. White cedar and poplar leaf samples were collected from 6 different sites in Cluj-Napoca influenced by road traffic and residential activities were collected. The concentrations of metals were determined using inductively coupled plasma mass spectrometry after microwave-assisted acid digestion. The results showed that Pb and Cr concentrations in white cedar leaves, were relatively uniform among sampling sites, whereas Cu, Zn, and Ni concentrations were significantly higher with intense traffic, indicating the influence of vehicular emissions. In contrast, metal concentrations in poplar leaves exhibited showed higher spatial variability, Zn being accumulated dominantly. For both species, none of the metals reached phytotoxic levels. The obtained results suggests that the leaves of white cedar and black poplar are effective biomonitoring tools for assessing urban air quality and traffic-related pollution.

Acknowledgement

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sciforum-187033: Comparative Assessment of Contrast Enhancement Properties of Gadolinium-Based MRI Contrast Agents

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Background

Limitations of the use of gadolinium-containing radiocontrast agents, caused by the development of acute and long-term complications, stimulate the search for new, safer, and more effective forms based on gadolinium nanoparticles. Objective: comparative assessment of the magnetic contrast properties of a gadolinium nanocomposite and a gadolinium-containing diagnostic agent.

Methods

The dynamics of organ accumulation and visual MRI patterns were studied in 5 healthy female Wistar rats using a Siemens Avanto 1.5 T MRI scanner. For MRI, anesthetized animals were placed in the ventral position in a head coil; a preliminary MRI examination was performed, after which a solution of the gadolinium nanocomposite or the reference agent (Omniscan) was administered at equivalent gadolinium doses via a catheter into the lateral tail vein or into the abdominal cavity, followed by repeat MRI scanning with images acquired every 2–3 minutes. The center of the imaging region was the abdominal cavity and retroperitoneal space, with the chest included in the field of view.

Results

The comparative analysis showed that arabinogalactan-stabilized gadolinium nanoparticles possess magnetic contrast properties, evidenced by enhancement of T1-weighted images of the liver parenchyma upon intravenous administration and of the abdominal cavity upon intraperitoneal administration. Magnetic contrast imaging of the kidneys and urinary bladder was greater with Omniscan than with the gadolinium nanocomposite. However, the maximum contrast enhancement coefficient of the gadolinium nanocomposite in the liver parenchyma increased by 20% compared to baseline, whereas Omniscan administration resulted in only a 13% increase in T1-weighted signal intensity of the liver parenchyma.

Conclusion

The use of the gadolinium nanocomposite holds promise for MRI diagnostics. At this stage, it is still premature to discuss the potential clinical application of the studied gadolinium nanocomposite; a more detailed investigation of its effects on relaxation processes in both normal and pathologically altered tissues is required.



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sciforum-187123: Pollutant exposure and pre-existing steatosis sensitize human hepatocytes to drug-induced liver injury

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Introduction

Drug-induced liver injury (DILI) is a major cause of acute liver failure. Unlike intrinsic DILI, which is dose-dependent, idiosyncratic DILI (iDILI) occurs unpredictably at therapeutic doses and remains difficult to predict in standard preclinical models. Emerging evidence suggests that acquired conditions, including exposure to persistent organic pollutants (POPs) and pre-existing hepatic steatosis may increase susceptibility by enhancing drug toxicity.

Methods

Human Upcyte hepatocytes were exposed to perfluorooctanoic acid (PFOA) or bisphenol A (BPA), alone or in combination with azathioprine (AZA), amoxicillin/clavulanic acid (AMOX/CLAV) or clavulanic acid (CLAV). Cell injury was assessed by MTT, neutral red uptake or LDH release. Metabolic steatosis was induced by oleate/palmitate (O/P, 2:1), and the impact of AZA and valproic acid (VPA) on intracellular triglycerides was quantified by AdipoRed. Gene expression was analyzed by RT-qPCR.

Results

Environmental pollutants potentiated drug hepatotoxicity. A synergistic loss of viability was observed with PFOA+AMOX/CLAV and after acute co-exposure to PFOA +AZA when compared to PFOA. Co-treatment with PFOA and CLAV also increased expression of the NRF2-related genes and FGF19, when compared to CLAV alone, consistent with activation of oxidative stress-adaptive pathways. In parallel, supporting a synergistic interaction, co-exposure to AZA and BPA caused a greater-than-expected decrease in cell viability, increased ROS levels, promoted glutathione metabolism and a lipogenic gene expression profile, and induced triglyceride accumulation.

Preloading hepatocytes with O/P markedly modified their response to steatogenic drugs. In AZA-treated cells, O/P slightly enhanced cytotoxicity and strongly potentiated triglyceride accumulation. RT-qPCR analysis showed increased expression of several lipogenesis-related genes, particularly PLIN2, CIDEA, ACC2 and AGPAT5. O/P also potentiated VPA-induced triglyceride accumulation.

Conclusions

These preliminary findings suggest that environmental and metabolic context modulate hepatocyte susceptibility to drug toxicity. Incorporating pollutant exposure and steatotic background into in vitro testing may improve mechanistic understanding of iDILI.



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sciforum-187217: Effects of Exposure to Tributyltin on Endothelium-Dependent Vasodilation in Mesenteric Resistance Arteries of Wistar Rats

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Tributyltin (TBT) is a persistent organic pollutant and endocrine disruptor associated with cardiovascular damage. Although the World Health Organization established an acceptable daily intake (ADI) of 250 ng/kg/day, evidence suggests that even low doses may induce vascular dysfunction. However, the effects of TBT on mesenteric resistance arteries (MRA) remain unclear. This study evaluated the effects of low-dose TBT exposure (100 ng/kg/day) on MRA vascular reactivity. Female Wistar rats (12 weeks old) were divided into two groups: CT – receiving vehicle solution (0.4 % ethanol), and TBT – receiving TBT (100 ng/kg/day), both administered via oral gavage. All experimental protocols were approved by the Institutional Ethics Committee (#19/2022). Mesenteric resistance arteries were isolated and mounted on a wire myograph for vascular reactivity analysis. Concentration-response curves to acetylcholine (ACh, 1 nM–10 μ M) were obtained in vessels precontracted with phenylephrine (PE, 3 μ M), as well as curves to PE (1 nM–100 μ M), before and after incubation with L-NAME (300 μ M), indomethacin (10 μ M), or clotrimazole (0.75 μ M). Data were analyzed using two-way ANOVA followed by Sidak's post hoc test and Student's t-test ($p < 0.05$). TBT exposure did not alter vasodilation (CT: 90.5 ± 2.9 %; TBT: 93.2 ± 3.1 %), but promoted changes in the epoxyeicosatrienoic acid (EET)-mediated relaxation pathway, reducing the maximum response (CT EET: 62.5 ± 6.3 %; TBT EET: 6.7 ± 2.5 %). In the nitric oxide pathway, the presence of TBT modified the maximum response (TBT: 93.2 ± 3.1 %; TBT L-NAME: 74.26 ± 5.5 %), unlike the CT group (CT: 90.6 ± 2.9 %; CT L-NAME: 80.4 ± 6.67 %). The remaining relaxation pathways remained similar. In conclusion, TBT alters vascular mechanisms even at doses below the ADI value.



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sciforum-187301: Effects of Selenium on Iron Concentration and Catalase Activity in Mouse Liver under Aluminum Exposure

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Introduction

Aluminum exposure induces oxidative stress and disrupts iron homeostasis. Selenium exerts its biological functions mainly through selenoproteins containing the amino acid selenocysteine and may indirectly modulate the activity of antioxidant enzymes, including catalase. However, depending on its chemical form, Se can also exert pro-oxidant effects. The liver plays a key role in Fe and Se homeostasis. The aim of this study was to evaluate the effects of different selenium forms on Fe homeostasis and catalase activity in mouse liver exposed to aluminum.

Methods

Experiments were performed on 4–6-week-old BALB/c mice, which were orally administered sodium selenite or selenomethionine (0.2 mg Se/kg bw), aluminum (100 mg Al/kg bw), or their combinations in tap water (License No. G2-80) for 8 weeks. Fe concentration was determined by inductively coupled mass spectrometry, and catalase activity was measured spectrophotometrically.

Results

Subacute aluminum administration increased Fe concentration in the liver of mice by 45% compared to control ($p < 0.05$). Selenomethionine increased Fe concentration by 30%, and sodium selenite by 17% ($p < 0.05$). Selenomethionine and sodium selenite in combination with aluminum significantly increased Fe concentration to 127% and 139% of control, respectively. Aluminum had no effect on catalase activity. Selenomethionine and sodium selenite increased catalase activity, but these changes were not statistically significant. Co-exposure to aluminum and selenomethionine increased catalase activity by 58% ($p < 0.05$), whereas co-exposure with sodium selenite did not alter catalase activity.

Conclusions

Subacute aluminum exposure most strongly disrupted hepatic Fe homeostasis, increasing its concentration. Both organic selenomethionine and inorganic sodium selenite also increased Fe levels, but the effect of selenomethionine was approximately two-fold greater than that of sodium selenite. Selenomethionine significantly reduced Fe concentration and increased catalase activity under aluminum exposure, whereas sodium selenite did not produce statistically significant changes in either parameter.



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sciforum-187345: Toxicological Assessment of the Herbicide Tebuthiuron: Elucidating Behavioral and Transcriptomic Responses in Developing Zebrafish.

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Tebuthiuron is a phenylurea herbicide extensively used as an agrochemical to control weeds in various crops, which often leads to contamination of aquatic environments. Despite its high-water solubility and relatively long half-life in soil, studies on tebuthiuron toxicity in fishes at environmental concentrations are limited. This study aimed to unravel the toxicity mechanisms of tebuthiuron using the zebrafish model. Zebrafish embryos were exposed to tebuthiuron at 0.1, 10, 1000 or 5000 µg/L for 5 days to assess hatchability, heart rate, locomotor activity, apoptosis and gene expression. Results revealed insignificant effects on hatchability, heart rate, and apoptosis (as measured using Acridine Orange stain). However, behavioral changes were noted with hyperactivity of zebrafish larvae during the 1st light period (at 10 µg/L), the 2nd light period (at 10 & 1000 µg/L), and the 3rd dark period (at 1000 µg/L) of the visual motor response assay. At the molecular level, downregulation of oxidative stress related genes (cat, sod1, and sod2) was observed at 10 and 5000 µg/L tebuthiuron. Furthermore, the neurotoxicity related gene acetylcholinesterase (ache) was downregulated while microtubule-associated protein tau (maptb) and synapsin 2 alpha (syn2a) were upregulated at 5000 µg/L tebuthiuron. These findings indicate that while hatchability and heart rate remained unaffected, tebuthiuron exposure induced significant motor responses alongside alterations in oxidative stress and neurotoxicity at molecular levels at higher concentration. This suggests potential cellular vulnerability particularly at higher doses that need further future investigation.



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sciforum-187361: Dose-Dependent Toxicity Assessment of Metronidazole in Developing Zebrafish (*Danio rerio*)

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Antibiotics are extensively used in human and veterinary medicine and livestock production. Antibiotics are considered as pseudo-persistent compounds, and a significant portion is excreted in original form and enters the aquatic environment. Persistence of these chemicals in aquatic environments poses a significant risk to aquatic organisms. Metronidazole is used to treat various protozoal and bacterial infections in humans and animals. In this study, larval zebrafish were exposed to environmentally relevant concentrations of metronidazole to assess its potential toxic impacts. The primary objectives were to assess the effects of metronidazole on the survival rate, oxidative stress and transcriptome of zebrafish embryos. Larval zebrafish were exposed to 0.1, 1.0, 10, 100 and 1000 µg/L metronidazole continuously for five days. There were no significant effects on survival rate, however metronidazole exposure induced antioxidant and redox-regulatory pathways, particularly at higher concentrations, as evidenced by significant upregulation of *nrf*, *cat*, *sod1*, and *sod2* due to activation of oxidative stress against high exposure concentration whereas lower exposure concentrations (0.1 µg/L) have caused minimal response showing no transcriptional changes in zebrafish. Locomotor activity was also observed as embryos showed hypoactivity during 1st dark period at 0.1 and 1000 µg/L. In the transcriptome analysis, 1000µg/L metronidazole caused upregulation of pathways related to circadian rhythm, fat digestion and absorption whereas, 0.1µg/L altered fat digestion and absorption and caused downregulation of *il1b* (Interleukin-1 beta), *klf4*, *chia*, *ela2* and *arg2*. Furthermore, Transcriptomics analysis also revealed significant perturbations in processes involved with cholesterol and lipid homeostasis, inflammatory response and cytoskeletal processes which provide plausible mechanistic explanation for the observed induced deformities in embryos including pericardial edema and yolk sac edema. Overall, metronidazole exposure altered locomotor activity, gene expression and biological pathways in larval zebrafish. This study contributes to improved understanding of antibiotic-related toxicity in non-target species.



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sciforum-187364: Di-n-butyl Phthalate-Induced Cardiovascular Effects Following Long-Term In Vitro Exposure

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Introduction

Plasticizers used in polymers are closely linked to cellular toxicity and, more recently, to cardiovascular health risks. Among these, di-n-butyl phthalate (DBP)—a low-molecular-weight phthalic acid ester used in adhesives—poses a significant concern. While DBP toxicity is documented, most in vitro studies focus on short-term effects, leaving the consequences of chronic, prolonged exposure poorly understood. This study aimed to optimize a long-term in vitro methodology to evaluate DBP's impact on the cardiovascular system by simulating exposure periods in vascular smooth muscle cells (A7r5) ranging from 1 to 10 days.

Methods

Cells were cultured in 96-well microplates and exposed to ten DBP concentrations (0.001 to 1000 μM). The experimental design included two control groups (culture medium and an ethanol vehicle) to ensure baseline accuracy. Cell viability was assessed using MTT assays, followed by ANOVA statistical analysis.

Results

Results revealed a significant toxicity peak 96 hours post-exposure. This effect was most prominent at the highest dosages (500–1000 μM) and, notably, at the lowest concentration (0.001 μM)—a value 10^5 times lower than the maximum—suggesting a complex concentration-response relationship. Between 96 and 240 hours, cellular recovery was limited, indicating persistent cytotoxic effects throughout the observation period. Furthermore, physical changes were observed in both the culture appearance and the plastic surface of the plates.

Discussion/Conclusions

These structural impacts will be further investigated using scanning electron microscopy (SEM). In conclusion, DBP exposure induces time and dose-dependent responses that may contribute to vascular dysfunction following prolonged exposure. These findings underscore the necessity of long-term models to accurately assess the persistent risks posed by phthalate exposure.



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sciforum-187369: Cellular Genotoxicity of Commercial Herbal Products Containing *Moringa oleifera* and *Tecoma stans* in Human Lymphocytes

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Introduction

Medicinal plants are widely used because of their accessibility and perceived therapeutic benefits; however, the genomic safety of many commercial herbal products remains poorly characterized. *Moringa oleifera* and *Tecoma stans* are species commonly used in traditional medicine and frequently marketed as natural health-promoting products. This study aimed to evaluate the genotoxic potential of commercial products containing extracts of these species using the Comet assay as a sensitive screening tool for detecting DNA damage in human lymphocytes.

Methods

An exploratory in vitro study was conducted using lymphocytes obtained from five healthy volunteers. Two commercial products labeled as mainly containing *M. oleifera* and *T. stans* were tested at concentrations based on the manufacturer-recommended daily doses (*M. oleifera*, 0.02 mg/mL; *T. stans*, 0.54 mg/mL). For each donor and treatment, duplicate slides were prepared, and 100 cells per slide were scored, using negative and positive controls for comparison. DNA damage was quantified using comet frequency (%) and the DNA Damage Index from the Comet Assay (DICA). Statistical analyses included one-way ANOVA, Dunnett's post hoc test, and Cohen's d effect size estimation.

Results

Both commercial products produced significantly higher DNA damage than the negative control. Increased comet frequency and DICA values indicated increased DNA fragmentation following exposure. ANOVA and Dunnett's test confirmed significant treatment-related effects. Cohen's d values ranged from moderate to very large, supporting the biological relevance of the observed genotoxic response.

Conclusions

Under the evaluated experimental conditions, the tested commercial products induced detectable genotoxic effects in human lymphocytes. Although these findings are based on a single genotoxicity endpoint, they provide preliminary evidence supporting further toxicological investigation. Because commercial formulations may contain additional ingredients, the observed effects cannot be attributed exclusively to *M. oleifera* or *T. stans*. Further studies are needed to identify the compounds responsible for the observed genotoxicity.



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sciforum-187372: Integrated Occupational Biomonitoring of Formaldehyde Exposure Using Buccal Cytome Biomarkers and Cognitive Screening in Hospital Pathology Workers

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Introduction

Formaldehyde is a recognized human carcinogen used in pathology laboratories. Occupational exposure has been associated with genotoxic and neurocognitive effects; however, evidence regarding early biological alterations in healthcare workers remains limited. This study evaluated environmental formaldehyde exposure, buccal cytome biomarkers, and cognitive **performance** in pathology laboratory workers from a hospital in Mexico.

Methods

An observational, cross-sectional comparative study included 22 formaldehyde-exposed workers and 4 hospital workers without occupational exposure (reference-group). Demographic, occupational, and clinical information was obtained from questionnaires and clinical records. Exposed workers were categorized into tertiles according to years of occupational exposure for subgroup analyses. Cognitive performance was assessed using the digital Spanish version of MoCA Xpress. Buccal epithelial cells were collected, duplicate slides prepared, and 1,000 differentiated cells per slide scored for micronuclei and cytotoxicity endpoints. Personal formaldehyde concentrations were measured in seven representative workers using the NIOSH 2016 method. Statistical analyses were performed in R 4.6.1.

Results

Personal monitoring showed formaldehyde concentrations of 1.33 ± 1.01 ppm, exceeding the INSST (Spain) occupational exposure limit (0.3ppm) and the NIOSH recommended exposure limit (0.45ppm). Median micronucleus frequency was 0 (IQR 0.12) MN/1000 cells in the reference group and 0.12 (IQR 0.25) in exposed workers ($p=0.532$). Cytotoxicity markers were consistently elevated, highlighting mean karyorrhexis frequencies of 166.0 cells/1000 in the reference group and 121.0-158.0 cells/1000 across exposure tertiles, suggesting marked cytotoxicity that may have masked potential genotoxic effects. No significant group differences were observed, although cognitive scores tended to decline with exposure duration ($p=0.068$).

Conclusions

Despite formaldehyde concentrations exceeding recommended occupational exposure limits, no statistically significant differences were detected among study groups in buccal cytome biomarkers. Nevertheless, the marked cytotoxicity observed should be considered a relevant adverse biological effect and may have masked potential genotoxic effects. Larger studies integrating complementary biomarkers are warranted to clarify early occupational effects.



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sciforum-187428: Systems-level effects of plant-based cognitive enhancer extracts: A multi-omics perspective

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Introduction

Plant-based cognitive enhancers act via multimodal neurobiological pathways and have demonstrated moderate efficacy in executive function in preclinical and clinical studies, with minimal occurrence of clinically adverse neurobehavior effects ¹⁻³. Among these, *Centella asiatica* is one of the most extensively investigated botanical extracts. While multi-omics tools are advancing our understanding of the metabolic profiling and biosynthetic pathways, systemic-level mechanisms and long-term safety remain incompletely mapped ⁴.

Aim and Methodology

A systematic PRISMA-guided review was conducted in Scopus, and Web of Science to identify *in vitro* and *in silico* studies reporting transcriptomic and metabolomic analyses of plant-derived cognitive enhancers. A total of 38 studies met the inclusion criteria. Transcriptomic (RNA-seq and microarray) and metabolomic (LC-qTOF-MS and NMR) data were qualitatively synthesized. The following biological pathways were considered: neurotrophic signaling (BDNF and CREB), oxidative stress (Nrf2), inflammation (NF-κB), apoptosis, and energy metabolism.

Results

Evidence supports plant-based cognitive enhancers as polypharmacological, multitarget systems that over sustained dosing can upregulate BDNF and pathways associated with synaptic plasticity, modulate mitochondrial/Krebs cycle flux, enhance antioxidant responses, and influence inflammatory signaling pathways ⁵⁻⁷. Recurrent transcriptomic and metabolomic signatures involved BDNF/CREB signaling, while *C. asiatica*-related studies reported positive and negative triterpene interactions with the neuronal transcriptome and metabolome of mouse cortical neurons ⁸. An integrated omics perspective could help resolve the networks of metabolites driving synergistic and antagonistic effects ⁹. Regardless of dose, standardization and diversity of the plant metabolomic pool, as well as rigorous long-term safety evaluations, remain essential for the responsible long-term use of these enhancers ^{7,10}.

Conclusions

The metabolic reprogramming and neuroprotective activities of plant-derived cognitive enhancers in the CNS are mechanistically complex and exhibit distinct multi-omics signatures. Integrating orthogonal analytical techniques, such as metabolomics and transcriptomics, may inform the rational design of safe and efficacious neuro-nutraceuticals for food applications.



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sciforum-191884: Transcriptome and behavioral effects of afidopyropen, a novel pesticide, in zebrafish embryos/larvae

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Introduction: Afidopyropen is a novel Group 9D insecticide with a chordotonal organ Transient Receptor Potential Vanilloid-type (TRPV) channel modulator mode of action on crop-destroying insects like aphids and other plant-parasitic insects. There is currently little information to date regarding potential off-target effects of afidopyropen on aquatic species. **Methods:** To address this knowledge gap, we quantified several sub-lethal endpoints including developmental toxicity, oxidative stress, transcriptomics, and locomotor behavior in early staged zebrafish following low concentration exposure to afidopyropen. **Results:** Survival rates of larval fish were slightly reduced by 10% following exposure to either 10 or 100 µg/L afidopyropen over 7 days. There was no difference in reactive oxygen species (ROS) in fish among treatments; however, there was an up-regulation of both *sod1* and *sod2* mRNA levels at 0.1 and 1 µg/L, suggesting an oxidative stress response and mitigation of ROS. There was a significant increase in apoptosis based on acridine range staining across all treatments tested. RNA-seq revealed 380 transcripts differentially expressed in zebrafish exposed to 100 ng/L (P-value < 0.05) and 9 after FDR correction. There were 1555 transcripts differentially expressed (P-value < 0.05) and 15 after an FDR correction in zebrafish exposed to 1 µg/L. Biological processes altered by afidopyropen included proteasome, cardiac muscle contraction, oxidative phosphorylation, and ribosomes. These processes were consistently altered in zebrafish at both concentrations tested. Pathway analysis identified processes related to ion channels as up-regulated with afidopyropen exposure in larval fish, including sensory transduction, synaptic transmission, and long-term synaptic potentiation. Evidence for both hypoactivity (dark period) and hyperactivity (light period) of larval zebrafish were observed following afidopyropen exposure, potentially associated with dopamine-related gene networks and ion channels identified in transcriptomics. **Discussion/Conclusion:** This study improves mechanistic understanding of potential toxicity for a novel pesticide class in early fish embryogenesis.



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sciforum-192394: IM-MOTIC: An AI-Assisted Evidence-Driven Framework for Mechanism Mining, Target Exploration, and Validation in Environmental Chemical Toxicity

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Introduction

The rapid emergence of environmental chemicals has increased the need for efficient approaches to characterize their mechanisms of toxicity. However, mechanistic evidence is often dispersed across toxicological databases, pathway annotations, experimental models, and published studies, making it difficult to identify biologically plausible and testable mechanisms. We developed Intelligent Mining-Mechanisms of Toxicity in Chemicals (IM-MOTIC) as an evidence-driven framework for mechanism inference, target exploration, and experimental validation.

Methods

IM-MOTIC integrates evidence from toxicity and chemical-disease databases (CTD), chemical bioactivity and target databases (ToxCast, ChEMBL), pathway and functional annotation resources (KEGG, GO, Reactome), and protein-protein interaction databases (STRING), supplemented by curated literature evidence. The framework includes five steps: defining the chemical or chemical group and toxicity endpoint; standardizing and integrating evidence; organizing weighted mechanism relationships; inferring candidate toxicity pathways; and prioritizing mechanisms using a Mechanism Confidence Score. Evidence weights are assigned according to evidence type, biological relevance, directness, species support, and literature reliability. IM-MOTIC was further used to extend prioritized mechanism networks, identify underexplored mechanism-associated targets, and guide molecular and cellular validation. Pesticide-associated neurotoxicity was used as a proof-of-concept case.

Results

IM-MOTIC generated evidence-linked mechanism maps connecting pesticides, molecular targets, biological pathways, neurotoxic phenotypes, and disease-related outcomes. In the pesticide neurotoxicity case, the framework prioritized mechanisms involving neuroinflammatory signaling, oxidative stress, mitochondrial and metabolic dysfunction, and epigenetic regulation. Network extension further highlighted molecular nodes and underexplored targets for experimental investigation. Subsequent validation supported the involvement of selected predicted targets and pathways in pesticide-induced neurotoxic responses, demonstrating the feasibility of using IM-MOTIC to infer, extend, prioritize, and validate mechanistic targets.

Conclusions

IM-MOTIC provides a practical framework for integrating heterogeneous toxicological evidence, prioritizing and extending candidate mechanisms, identifying potential molecular targets, and guiding experimental validation. This approach may support mechanism-oriented toxicology research and next-generation risk assessment of environmental chemicals.



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sciforum-193194: The Protective Effects of N-Acetylcysteine on Di-Ethyl Phthalate Exposed Uterus of Wistar Rats

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Diethyl Phthalate (DEP) is a chemical widely used industrially as a plasticizer to improve the flexibility of plastics. DEP leaches from plastic products and enters body tissues because it does not bind to plastic polymers and have been reported to have endocrine disrupting effects. The aim of this study was to investigate the protective effects of N-acetylcysteine (NAC) in the uterus of female wistar rats exposed to DEP. Uterine dysfunction was evaluated by histopathological, biochemical and hormonal assays. Twenty female adult Albino rats were divided into four groups of five rats per group as follows: Group A rats (were given 0.5ml of olive oil orally to serving as control), Group B rats (were orally administered 100mg/kg bwt NAC), Group C Rats (orally received 500 mg/kg bwt of DEP suspended in 0.5ml of olive oil), and Group D Rats (were orally administered 100mg/kg bwt NAC and 500 mg/kg body weight of DEP concomitantly) for seven days. Histopathological results showed that DEP induces mild inflammation in the endometrial stroma of the uterus, while the endometrium and myometrium of the NAC co-treatment group were normal. Biochemical assays revealed that DEP reduced Glutathione reductase (GSH), Superoxide dismutase (SOD), and Catalase levels, while they were increased in the NAC co-treatment group. DEP also increased levels of Nitric oxide, Lipid peroxidation marker, Hydrogen peroxide, and Myeloperoxidase levels while they were decreased in the NAC co-treatment group. The hormonal assay results showed a slight decrease in the levels of Follicle-Stimulating Hormone(FSH) and Estrogen in Group C, which was improved in Group D. Conclusion: Exposure to Diethyl phthalate (DEP) at the administered dose for (7) days induced mild inflammatory, and oxidative stress in the uterus while co-treatment with NAC produced a modest, and short-term protective effect. Further studies in exploring longer exposure duration should be considered.



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sciforum-193281: Parental-origin-divergent m⁶A remodeling mediates transgenerational male reproductive toxicity of PFHpA via PPAR α -dependent steroidogenic disruption

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Short-chain per- and polyfluoroalkyl substances (PFAS), including perfluoroheptanoic acid (PFHpA), are increasingly used as alternatives to legacy PFAS, yet their heritable reproductive toxicity and underlying epitranscriptomic mechanisms remain unclear. We established complementary maternal and paternal PFHpA exposure mouse models and evaluated male reproductive outcomes across generations. Testicular histology, computer-assisted sperm analysis, hormone measurements, MeRIP-seq/RNA-seq, qRT-PCR, Leydig-cell assays, gene perturbation, molecular docking, surface plasmon resonance and PPAR α antagonism were integrated to define lineage-specific mechanisms. The results indicated that PFHpA exposure induced testicular structural abnormalities, impaired sperm-related parameters and reduced testosterone production in directly exposed males and unexposed descendants. Maternal and paternal lineages displayed distinct global and transcript-specific m⁶A remodeling patterns, but both converged on lipid metabolism, PPAR signaling and steroidogenic disruption. In the maternal lineage, reduced *Mettl3* expression was associated with decreased m⁶A modification and expression of *Lpl*, and *Lpl* overexpression partly restored testosterone synthesis in TM3 Leydig cells. In the paternal lineage, increased *Rbm15*-related m⁶A remodeling was linked to reduced *Fabp1* expression in testes and Leydig cells. PFHpA interacted with PPAR α in silico and by surface plasmon resonance, and pharmacological PPAR α antagonism attenuated PFHpA-induced testosterone reduction. In conclusion, Parental PFHpA exposure produces parental-origin-divergent epitranscriptomic responses that persist across generations but converge on a PPAR α -dependent lipid-steroidogenic axis. These findings identify m⁶A remodeling as a mechanistic mediator of short-chain PFAS-induced transgenerational male reproductive toxicity and support stronger consideration of parental origin in PFAS reproductive risk assessment.



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sciforum-193337: Transcriptional Landscape of Metal Transporter Genes And Potentially Toxic Elements Exposure in Ckdu

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Background and Aims

Toxic metals, widely derived from diverse industries, insidiously build up in the body. It remains unclear whether these increased levels are a cause or a consequence. This study probed the influence of toxic metals and associated transporter genes on the etiology of chronic kidney disease of unknown etiology (CKDu), with a particular emphasis on the function of metal transporters.

Methods

The study encompassed 211 CKDu patients and 214 controls, matched for age and sex. We analyzed blood samples for toxic metals, gene expressions, and kidney function tests. The quantification of toxic metals was performed using Inductively Coupled Plasma-Mass Spectrometry (ICP-MS). We assessed the gene expressions of biomarkers (MT2 and DMT1) via qRT-PCR. The quantification was executed using the $2^{-\Delta CT}$ method. For the analysis of toxic metals in urine, urine samples were adjusted with urinary creatinine.

Results

In our study, we observed elevated levels of toxic metals in patients with CKDu. Specifically, the median levels in CKDu patients were significantly increased as follows: aluminum (32.32 vs 13.44), nickel (5.04 vs 1.26), arsenic (4.04 vs 0.79), cadmium (3.17 vs 0.1), mercury (16.17 vs 7.55), and lead (1.58 vs 0.24). Similarly, CKDu patients had significantly higher levels of creatinine-adjusted urinary metal median levels as follows: aluminum (2.96 vs 1.92), nickel (0.35 vs 0.22), arsenic (1.32 vs 0.39), cadmium (0.59 vs 0.19), mercury (0.06 vs 0.07), and lead (0.09 vs 0.07).

The metal transporter genes including DMT gene (2.50-fold, $p=0.01$) and MT2 (1.54-fold, $p=0.02$) genes were overexpressed among CKDu patients. Multivariate analysis revealed only DMT along with three toxic metals i.e. Al, Hg and Pb were independently associated with eGFR.

Conclusion

Out of seven, screened toxic metals (Al, Hg, Pb, Ni, Cd and As), only Cd, Hg and Pb along with DMT gene expression were independently associated with eGFR as revealed from multivariate analysis. Their increased serum concentration is leading to high urinary concentration, supported by enhanced gene expression of DMT and MT2 genes.



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sciforum-193415: Extracellular vesicle release reflects dose-dependent hepatotoxic responses in HepG2 cells

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Introduction

Drug-induced liver injury (DILI) is a leading cause of acute liver failure and a major challenge in clinical practice and drug development. Extracellular vesicles (EVs) are membrane-bound nanoparticles emerging as sensitive biomarkers of cellular stress and damage. While most studies have focused on EV cargo, quantitative changes in particle number as a function of drug dose remain poorly characterized. Here, we evaluated whether EV concentration is modulated dose-dependently in HepG2 hepatocytes exposed to two hepatotoxic drugs affecting mitochondrial disruption.

Methods

HepG2 cells (1×10^6 /well) were treated with valproic acid (VPA) or amiodarone (AMI) at IC₁₀ and IC₅₀, as previously determined by Martínez-Sena et al. Conditioned medium was sequentially centrifuged to remove cells and debris, then EVs isolated by SEC yielding a vesicle-enriched (F1) and protein-enriched (F2) fraction. F1 particle concentration was quantified by TRPS and both fractions analysed by ATR-FTIR to estimate protein concentration based on amide I band absorbance. Comparisons used an unpaired t-test ($n=1$) between treated and untreated control cells. EV identity will be confirmed by Western blot using positive and negative markers and morphological characterization will be performed by TEM.

Results

Both drugs induced a dose-dependent increase in EV concentration versus untreated controls. No significant differences were observed at IC₁₀ (VPA: 1.12-fold, $p=0.778$; AMI: 2.74-fold, $p=0.093$). At IC₅₀, VPA showed a 2.5-fold increase ($p=0.0183$) and AMI a nearly 5-fold increase ($p=0.0014$). ATR-FTIR revealed higher protein in F2 of treated samples, while F1 remained low (~ 0.48 – 0.91 mg/mL), confirming effective SEC-based separation. EV counts will be normalized to viable cell number in subsequent analyses.

Conclusions

EV concentration increases dose-dependently in HepG2 cells at IC₅₀ for both VPA and AMI, suggesting EV release reflects hepatocellular stress. Further validation including EV marker profiling, morphological characterization, and analysis of patient samples will be required to establish EVs as non-invasive DILI biomarkers.



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sciforum-193696: Investigation of Cellular and Molecular Mechanisms of PFAS-Induced Lung Inflammation in a Human Alveolar Epithelial Cell Line

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Per- and polyfluorinated alkyl substances (PFAS) are a large group of environmentally persistent chemicals widely used in products like non-stick cookware, firefighting foams, textiles, and waterproof coatings. Their high stability and tendency to bioaccumulate have raised health concerns, linked to immune, thyroid, liver, kidney, and pancreatic issues. Although the health effects of oral exposure through contaminated water and food are well-documented, the risks of inhalation and their impact on lung health remain largely unexplored. This study examined how perfluorooctane sulfonic acid (PFOS), a long-chain legacy PFAS, and perfluorobutane sulfonate (PFBS), a short-chain alternative, influence oxidative stress, hypoxia signaling, and inflammasome activation in human alveolar epithelial (A549) cells. Cells were exposed for 24 hours to increasing concentrations (10–200 μM) of PFOS or PFBS. Cytotoxicity was assessed using an MTT assay, reactive oxygen species (ROS) levels were measured with the DCFH-DA assay, and protein levels of HIF-1 α and NLRP3 were analyzed via Western blotting and immunocytochemistry. PFOS had an IC_{50} of 179 μM , while PFBS was non-cytotoxic at all tested doses. PFOS exposure significantly elevated intracellular ROS, caused a temporary nuclear stabilization of HIF-1 α at lower concentrations, and dose-dependently increased NLRP3 expression—peaking at 100 μM and slightly decreasing at 150 μM . Immunocytochemistry showed increased cytoplasmic and perinuclear localization of NLRP3 following PFOS treatment. Overall, these results suggest that PFOS, even at non-cytotoxic levels, can induce oxidative stress and inflammatory pathways in lung epithelial cells through activation of the ROS–HIF-1 α –NLRP3 axis, whereas PFBS exhibits minimal cellular effects. The study highlights oxidative and hypoxia-driven inflammasome activation as a key mechanism behind PFOS-related lung inflammation and potential injury.



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sciforum-193698: Exposure assessment of N-Nitroso-compound levels in GC patients and explored the potential core genes of Nitrosamine-induced GC carcinogenesis

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Background

Exposure to N-nitroso compounds (NNCs) is closely correlated with the pathogenesis of gastric cancer (GC). This study aimed to investigate the internal levels of N-nitrosamines in GC patients and further explore the potential key triggers underlying NNCs-induced GC carcinogenesis by combining network toxicology approaches with experimental verification.

Methods

Solid-phase extraction coupled with gas chromatography-mass spectrometry (SPE-GC-MS) was applied to determine the concentrations of nine N-nitrosamines in 24 pairs of urine samples from GC patients and healthy controls. Potential N-nitrosamine-associated target genes related to GC were retrieved from the Comparative Toxicogenomics Database (CTD) and GeneCards database. Core hub genes were screened via topological analysis and functional enrichment analysis. Molecular docking simulations were performed to evaluate the binding interactions between N-nitrosamines and target proteins. RT-qPCR was used to validate the expression levels of key genes.

Results

Nine N-nitrosamines were successfully detected in urine samples. Among them, the levels of NMor (18.67 ± 14.94 ng/mL), NPyr (7.03 ± 12.49 ng/mL), NDPA (6.11 ± 6.50 ng/mL), and NDphA (5.52 ± 2.86 ng/mL) were significantly elevated in urine samples from 24 paired GC patients. Six genes, including BUB1B, FANCI, PLK1, TOP2A, CDK1, and CCNB1, were identified as the core genes involved in N-nitrosamine-induced GC tumorigenesis. Functional enrichment results revealed that the apoptotic process, G2/M transition were the vital biological mechanisms mediating the carcinogenic effect of N-nitrosamines. Furthermore, RT-qPCR validation confirmed that BUB1B, FANCI, PLK1, TOP2A, and CCNB1 were significantly upregulated in GC tissues and cell samples.

Conclusion

A total of nine were detected in urine samples of GC patients. BUB1B, FANCI, PLK1, TOP2A, CDK1, and CCNB1 are key regulatory genes involved in N-nitrosamine-induced gastric cancer, suggesting their potential value as biomarkers for gastric cancer. Limitations: The sample size for gastric cancer patients is relatively small; we will continue to expand the study population for further validation.



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sciforum-193930: Analyzing Cadmium-Driven Biochemical Changes: a Multi-Disciplinary Approach for the Evaluation of Neuron and Microglia Models

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Introduction

Cadmium is a highly toxic, non-essential heavy metal that accumulates in the human body, leading to severe neurotoxicity. It enters the central nervous system through the olfactory nerves or by increasing blood brain barrier permeability. Cadmium bioaccumulation triggers oxidative stress, which fuels neuroinflammatory pathways linked to neurodegenerative disorders. Understanding these metal-driven molecular alterations is critical for clarifying the mechanisms of cellular harm.

Methods

Human neuroblastoma SH-SY5Y cells have been used to investigate the impacts of cadmium on both the process of neuronal differentiation as well as on fully differentiated neuronal-like cells. In this study biochemical approaches were coupled with Fourier Transform Infrared (FTIR) microspectroscopy as a marker-free, non-destructive method to obtain an unbiased look at the cellular biochemical profile.

Results

By merging biochemical data and micro-FTIR spectroscopic data with advanced machine learning algorithms, the study shows the modifications in physicochemical properties of lipids induced by cadmium exposure during the differentiation process; in fact cadmium alters membrane lipid composition, which leads to alteration in neurite outgrowth. Moreover there is a reduction in carnitin and cardiolipin content paired with a lower mitochondrial respiration and ATP production in cadmium-differentiating cells.

Conclusions

Pairing non-destructive spectroscopic insights with supportive biochemical and omics analyses clarified cadmium impact on neuronal differentiation, also this multi-disciplinary approach allows to understand the molecular pathways responsible for cadmium-induced cellular damage.



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Session 5. Risk Assessment, Policy, and Environmental Justice in Chemical Safety

sciforum-179577: Chemical Pollution by Potentially Toxic Elements in the Mubuku Irrigation Scheme, Uganda: A Stochastic Human Exposure-Risk Modeling and Environmental Health Implications

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Anthropogenic activities in sub-Saharan Africa have increasingly contaminated agro-ecosystems with potentially toxic elements (PTEs), posing risks to food safety and public health. Study assessed the concentration, sources, and dietary health risks of 14 PTEs (As, Pb, Cd, Co, Cr, Hg, Ni, Cu, Fe, Mn, Se, Zn, Th, and V) in a point-source irrigation water ($n = 1$), agricultural soils ($n = 9$ composite samples), and commonly consumed vegetables (onion, cabbage, and amaranth; $n = 24$ composite samples) collected from the Mubuku Irrigation Scheme, western Uganda. Concentrations were determined using inductively coupled plasma-optical emission spectroscopy. Health risks were evaluated using deterministic non-carcinogenic (hazard quotient (HQ) and index (HI)) and carcinogenic (total cancer risk, TCR) assessments, complemented by Monte Carlo simulation (MCS; 10,000 iterations). More than 20% of detected PTEs in vegetables exceeded WHO/FAO limits. Arsenic (2.22–3.57 mg/kg), Pb (2.02–3.66 mg/kg), and Hg (0.42–0.61 mg/kg) consistently exceeded guideline values (0.1, 0.3, and 0.001 mg/kg, respectively), with the highest accumulation observed in amaranth. Irrigation water contained elevated As (1.56 mg/L) and Pb (2.73 mg/L). Estimated HI of PTEs indicated considerable non-carcinogenic risk ($HI > 1$) for all vegetables, driven primarily by Pb ($HQ = 3.21$ – 5.06) and As ($HQ = 0.85$ – 2.70) for adults (65–70 kg) and geriatrics (60 kg). Carcinogenic risk estimates ($TCR = 5.72 \times 10^{-4}$ – 2.99×10^{-3}), including 50th (5.97×10^{-4} – 7.51×10^{-2}) and upper-bound (95th) percentile (7.71×10^{-4} – 1.49×10^{-1}) stochastic outcomes, surpassed acceptable thresholds (10^{-6} – 10^{-4}), indicating probable high lifetime cancer risks, exposure uncertainty and potential risk amplification among high-end consumers. Principal component analysis explained 83.2% of total variance, identifying mixed geogenic and anthropogenic sources, with soils and amaranth as dominant exposure pathways. This study provides the first integrated deterministic–probabilistic–multivariate assessment of PTE risks in a Ugandan irrigation scheme. The findings underscore urgent public health concerns and offer critical baseline evidence to support risk-informed management, targeted remediation, and sustainable agricultural policy interventions.



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sciforum-182518: Systematic Review: Does Glyphosate Exposure Cause Cancer?

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Introduction

Glyphosate is the active ingredient in more than 750 herbicides, marketed for over 40 years. The IARC was the only authority to classify glyphosate as probably carcinogenic to humans. The aim of this study was to evaluate whether exposure to the herbicide glyphosate causes cancer.

Methods

Approved by the Institutional Research Advisory Committee of the proposing institution (Protocol 6681). A systematic literature review of observational studies was conducted, with the inclusion criteria being: studies that assessed cancer incidence and exposure to the herbicide glyphosate; cohort studies; case-control studies; case series or case reports; experimental studies with animals; and *in vitro* studies. The systematic review question was: Can exposure to the herbicide glyphosate cause cancer? The research period was from 1983 to 2026. The generic search strategies were: (glyphosate OR roundup) AND (Neoplasms OR cancer OR "carcinogenicity tests" OR Carcinogenicity).

Results

737 articles were found, of which 245 duplicate were excluded, 79 were subsequently excluded for not being object of study, and finally, 33 complete articles evaluated were excluded because they were review articles, conference abstracts, or were out scope. Of 46 articles included for qualitative analysis, 8 were *in vitro* studies, 5 were experimental studies with animals, and 33 were observational studies with humans. All the studies evaluated showed some relationship between glyphosate and cancer. *In vitro* studies showed a relationship between glyphosate exposure and breast, skin, and prostate cancer. Experimental studies with animals showed a relationship with breast, skin, liver, kidney, and lymphoid neoplasms. Observational studies with humans showed a stronger relationship with lymphoid neoplasms, breast, pancreas, and bladder cancer.

Conclusion

Exposure to glyphosate is a risk factor for the development of cancer, and not only for lymphoid neoplasms. However, more studies are needed to establish this relationship properly.

Keywords

roundup; glyphosate; neoplasms; cancer; carcinogenicity



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sciforum-184592: Accounting for Non-Additive Effects in Multicomponent Aquatic Systems: Implications for Environmental Risk Assessment of Chemical Mixtures

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Introduction

Environmental risk assessment of chemical mixtures in aquatic systems is often based on additive assumptions. However, trace metals and coexisting ligands, mineral particles, dissolved organic matter, and anthropogenic surfaces may interact through coupled equilibria, producing responses that differ from the sum of individual effects. Special attention is given to environmentally relevant metal ions such as Pb(II), Cu(II), Cd(II), and Zn(II), together with common complexing or competing components, including humic substances, phosphate, carbonate, chloride, iron and aluminum oxides, and microplastic-associated surfaces.

Methods

This study introduces a thermodynamic interpretation of non-additive effects in multicomponent aquatic systems. A coupled or observed equilibrium response is compared with an additive reference state defined under comparable conditions. Deviations are expressed using dimensionless ratios of equilibrium, solubility, adsorption, or distribution parameters and converted into apparent Gibbs free-energy terms. This provides a common energetic criterion for classifying additive, synergistic, and antagonistic behavior.

Results

The proposed approach shows that synergistic effects correspond to stabilization of the coupled system relative to the additive reference state, whereas antagonistic effects indicate destabilization or reduced retention. The same logic can be applied to metal complexation, precipitation-boundary displacement, adsorption on mineral or organic surfaces, and retention by microplastic-associated phases. These processes may alter dissolved metal concentrations, apparent bioavailability, and toxicity under realistic mixture conditions.

Conclusions

Non-additive interactions should be considered in aquatic mixture assessment when coupled chemical equilibria control contaminant speciation and mobility. The proposed criterion does not replace toxicological testing but provides a quantitative chemical basis for identifying mixture conditions that may increase or decrease environmental risk.



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sciforum-185533: Human Health Risk Assessment of Metal Exposure through Consumption of Various Fish Species in the Local Market, Muscat, Oman

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Fish is an important dietary source of high-quality protein and essential micronutrients; however, metal contamination poses significant food safety and public health concerns. This study investigated the concentrations of six metals (Pb, Cu, Cd, Ni, Zn, and Fe) in the edible tissues of eight important fish species: Tuna (*Thunnus tonggol*), Sheri (*Lethrinus spp.*), King fish (*Scomberomorus commerson*), Trevally fish (*Caranx ignobilis*), Catfish (*Arius spp.*), Leather (*Oligoplites spp.*), Kofer (*Argyrops spinifer*), and Dhala (*Rastrelliger kanagurta*). A total of 16 samples were collected from local markets in Oman and analyzed using Atomic Absorption Spectroscopy. Human health risks were assessed through Estimated Daily Intake (EDI), Hazard Index (HI), and Carcinogenic Risk (CR).

The mean metal concentrations (mg kg^{-1} , wet weight) were found to be Zn (16.478), Fe (5.165), Ni (0.501), Cu (0.419), Pb (0.341), and Cd (0.048), following the decreasing order $\text{Zn} > \text{Fe} > \text{Ni} > \text{Cu} > \text{Pb} > \text{Cd}$. Zinc was the most abundant, whereas cadmium was present at the lowest level. A statistically significant positive correlation between Pb and Cd ($r = 0.58$) suggests a possible common anthropogenic source. The calculated EDI values ($\text{mg kg}^{-1} \text{ body weight day}^{-1}$) showed a similar trend, with Zn contributing the highest intake. The overall hazard index ($\text{HI} = 0.6027$) remained below the safety threshold ($\text{HI} < 1$), indicating negligible non-carcinogenic risk. Additionally, carcinogenic risk values for Pb and Ni were below the acceptable limit (1×10^{-4}), suggesting minimal cancer risk.

Statistical evaluation demonstrated that variation in metal concentration was significantly influenced by metal type ($p < 0.001$), whereas differences among fish species were not statistically significant ($p = 0.462$). The findings suggest that fish sold in Oman markets are generally safe for consumption regarding the analyzed metals. However, regular monitoring remains essential to protect public health and support long-term environmental sustainability.



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sciforum-186694: Back to basics—a case of multidrug intoxication involving 6-APB, known on the black market as *benzofury*

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Introduction

The misuse of new psychoactive substances poses a threat to public health. Although new compounds are constantly emerging, substances that have been known for years should not be overlooked in routine toxicological analyses, as users often return to using them. Benzofurans, known as *benzofury*, are synthetic phenethylamines that exhibit structural and functional similarities to MDMA and MDA. Concurrent use of benzofury with, among others, synthetic cathinones may trigger a sympathomimetic syndrome characterized by serious and severe somatic and CNS symptoms. The first benzofurans to appear on the drug market were 5-APB and 6-APB. The authors present a case of a fatal multi-substance overdose involving 6-APB in a young man.

Methods

Post-mortem biological matrices were subjected to analysis using a LC-MS/MS and HS-GC-FID/FID. This comprehensive approach covered a broad spectrum of substances, encompassing drugs, illicit substances, NPS, volatile compounds. Information pertaining to the circumstances of death was obtained from prosecutor.

Results

The authors analyze this case of death in terms of the composition, mechanism of action, toxicity, and concentrations of substances identified in samples collected during the autopsy. The materials confirmed the presence of 6-APB, 6-APDB, MDMA, amphetamine, methamphetamine were detected. No ethyl alcohol was detected. The results obtained may indicate poisoning by multiple substances. These results correlate with information regarding the symptoms the man exhibited prior to death, which may suggest the occurrence of a sympathomimetic syndrome.

Conclusions

In cases of suspected death following simultaneous ingestion of multiple xenobiotics, the authors recommend conducting extensive toxicological analyses using various analytical techniques. Detection of a toxic substance in biological material, combined with a detailed history of poisoning symptoms and an investigation into the circumstances of the incident, is helpful in compiling a report on the investigation, including an interpretation of the toxicological analysis results.



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sciforum-186705: Risk Communication and Household Water Source Switching in Arsenic-Affected Rural Cambodia

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Introduction

Chronic exposure to arsenic-contaminated groundwater remains a major environmental health concern in rural Cambodia. While testing and notification programs can inform households about unsafe drinking water, risk information alone may not lead to exposure reduction when alternative sources are costly, distant, or socially constrained. This study examines how arsenic risk communication can be evaluated as a behavioral intervention in household water source choice.

Methods

The study focuses on arsenic testing and education activities in Kandal Province, Cambodia, where households were informed about high arsenic levels in their drinking water and advised to switch to safer sources. Using existing household-level evidence and program documentation, the study develops a quasi-experimental evaluation framework for assessing changes in water source switching, new source choice, water expenditure, collection time, and water treatment behavior. Particular attention is given to treatment definition, counterfactual construction, and threats to identification.

Results

Preliminary evidence suggests that high-arsenic notifications were associated with substantial household switching to alternative drinking water sources. However, the absence of a contemporaneous untreated control group limits direct causal interpretation. The proposed framework identifies feasible comparison strategies and highlights key empirical challenges, including selective testing, spillovers between households, baseline heterogeneity, and constraints on access to safe water.

Conclusions

The study contributes to environmental health policy by linking toxicological risk information with household adaptation behavior. It also clarifies how arsenic testing programs can be evaluated more rigorously in low-resource settings, where equitable access to safer water remains central to chemical risk reduction.



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sciforum-186813: Integrated mycological and HPLC analysis of aflatoxins in wheat caryopses under storage conditions

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Introduction

Aflatoxins are among the most hazardous mycotoxins contaminating cereals, representing a major concern for food safety due to their potent hepatotoxic and carcinogenic effects. Their occurrence in wheat is strongly influenced by environmental factors and post-harvest storage conditions, highlighting the need for sensitive and reliable analytical methods for contamination monitoring, risk assessment, and compliance with food safety regulations.

Methods

This study assessed fungal contamination and aflatoxin presence in wheat caryopses from four cultivars grown in north-central Romania. A standardized analytical method was applied, including methanol-water extraction, immunoaffinity column clean-up, and quantification of aflatoxins B1, B2, G1, and G2 by reversed-phase HPLC with fluorescence detection and post-column derivatization. Chromatographic separation was carried out under isocratic conditions using a water-acetonitrile-methanol mobile phase at 30°C and a flow rate of 0.7 ml/min, with fluorescence detection at 360/440 nm.

Results

Optimized chromatographic conditions (water-acetonitrile-methanol 60:20:20, v/v/v; 0.25 ml/min; 40 µl injection) ensured efficient separation of aflatoxins, with retention times of 13.3, 11.4, 10.3, and 8.9 min for B1, B2, G1, and G2, respectively. Microscopic analysis identified *Alternaria* and *Fusarium* species. Aflatoxins were detected in only one sample, with concentrations of 0.11 µg/kg (B1), 0.02 µg/kg (B2), and 0.10 µg/kg (G1), while G2 was not detected, resulting in a total level of 0.22 µg/kg, below the EU maximum limit for cereals. Recovery rates ranged from 77.1% to 87.9%, confirming adequate method performance.

Conclusions

The study confirms the presence of *Alternaria* and *Fusarium* spp. in wheat caryopses, while aflatoxins were detected only in one sample at low levels. These findings indicate a low contamination risk and full compliance with food safety standards. The validated HPLC method proved robust and reliable for routine aflatoxin monitoring, supporting its use in food control programs. Continued surveillance and improved post-harvest practices remain essential to ensure long-term mycotoxin risk mitigation.



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sciforum-186946: Genotoxicity Biomarkers in Healthcare Workers Occupationally Exposed to Antineoplastic Drugs: A Systematic Review and Meta-Analysis

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Introduction

Healthcare workers involved in preparation and administration of antineoplastic drugs face chronic low-level exposure to human carcinogens as classified by the International Agency for Research on Cancer. Despite established safety protocols including personal protective equipment and closed-system drug transfer devices, studies confirm that ongoing exposure persists. Although genotoxic effects in this occupational field are biologically possible, the evidence is still inconsistent and not completely synthesized across various contexts, protection levels, and biomarker endpoints.

Methods

This systematic review and meta-analysis is being conducted following PRISMA 2020 guidelines. The basis of this review is formed by literature searches of PubMed and Scopus from 2015 to 2026, combining terms for antineoplastic drug exposure, healthcare workers, and genotoxicity biomarkers. Eligibility of studies report on micronucleus frequency, chromosomal aberrations, or DNA strand breaks measured by comet assay in occupationally exposed workers. Risk of bias is assessed using the Newcastle-Ottawa Scale. Heterogeneous outcome formats across studies are converted to a common scale and pooled using a random-effects model.

Results

Preliminary search identified studies reporting elevated genotoxicity biomarker frequencies in exposed workers compared to controls across genotoxicity endpoints including micronucleus frequency, chromosomal aberrations, and DNA strand breaks. Effect magnitude varied substantially across settings, with studies reporting high compliance with personal protective equipment and closed-system drug transfer devices consistently showing attenuated or absent genotoxic effects. Differences in protective equipment use and handled drug mixtures appear to contribute substantially to heterogeneity across studies.

Conclusions

Healthcare workers who handle antineoplastic medications are consistently at risk for genotoxicity. The degree of preventative measures in place is inversely correlated with the effect magnitude. These findings highlight a critical gap between existing safety guidelines and real-world protection, contributing to the evidence base for mandatory implementation of closed-system drug transfer devices and standardised biological monitoring in oncology settings.



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sciforum-186996: Heavy Metal(loid) Contamination in a Mining-Impacted Island Province in the Philippines: A Systematic Review

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Introduction

Marinduque, Philippines, has faced persistent heavy metal(loid) contamination following catastrophic mining disasters in the 1990s, including the Boac River spill that released over 1.6 million metric tons of mine tailings. Despite nearly three decades of documented environmental impact, no comprehensive synthesis of the existing literature had been conducted.

Methods

This systematic review followed the PRISMA framework, searching the Scopus database using the keywords "Philippines," "Marinduque," and "metal." From 625 initially identified records, 31 studies met the inclusion criteria. Bibliometric analysis was performed using VOSviewer, including co-occurrence and co-authorship analyses to map thematic clusters and research networks.

Results

Heavy metal(loid) concentrations, particularly Cu, Cr, Mn, Pb, and Zn, consistently exceeded regulatory standards across surface water, groundwater, sediments, soil, agricultural crops, and biota. Bibliometric analysis identified six thematic clusters, with dominant research foci on health risk assessment, machine learning-based prediction, and bioremediation. Publication activity peaked in 2021-2022, driven largely by a government-funded health and vulnerability project. Critical gaps remain in sediment monitoring and long-term ecological impact studies.

Conclusions

Mining-related heavy metal(loid) contamination in Marinduque remains an ongoing environmental and public health concern. Key priorities include continuous monitoring, rehabilitation of abandoned mine infrastructure, phytoremediation and bioremediation strategies, and the integration of findings into provincial environmental policy.



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sciforum-187042: Methodological Approaches to a Biological Model for Validating Health Damage Criteria Following Wildfire Smoke Exposure

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Introduction

Prolonged exposure to smoke from wildland fires causes various health impairments, primarily affecting the respiratory, cardiovascular, and nervous systems. To substantiate safe exposure levels to landscape fire smoke, a biological model closely mimicking natural conditions has been developed.

Materials and Methods

Experiments were conducted on adult Wistar rats. Mean CO concentrations ranged from 20 to 30 mg/m³, and PM_{2.5} concentrations from 0.37 to 0.93 mg/m³. The total duration of biomass smoke exposure in the experiment was 1, 4, 8, 20 (4 h/day, 5 days), and 80 (4 h/day, 5 days/week, 4 weeks) hours. The cumulative exposure loads for CO and PM_{2.5} were calculated. Behaviour was assessed using the open-field test; EEG recordings, histological analysis of the cerebral cortex and testes, and DNA fragmentation and DNA methylation levels in testicular and blood cells were evaluated. First-generation offspring were examined immediately after birth and at maturity.

Results

A biphasic relationship was observed: lower exposure levels were associated with activation of CNS parameters, whereas further increases in duration or intensity led to significant inhibition of these parameters. Regarding the reproductive system, an adverse response in the form of impaired postnatal development of offspring, in the absence of a pronounced gonadotoxic effect in the parental generation, was detected at cumulative exposure loads ranging from 0.22 to 4 mg. Prolonged exposure to wildland fire smoke for one month was accompanied by marked impairment of spermatogenic function in the testes and increased neonatal mortality in offspring.

Conclusion

Safe smoke exposure levels (based on PM_{2.5} and CO indicators) were established with regard to the functional state of the central nervous and reproductive systems, genotoxicity parameters, DNA methylation, and offspring health.



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sciforum-187220: Spatial Assessment of Environmental Vulnerability Using Multicriteria Geospatial Analysis as a Tool for Integrated Pollution Management in the Grande Tulancingo River, Mexico

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The deterioration of fluvial systems represents an environmental problem associated with urban growth, agricultural activities, and industrial development, which promote the dispersion of contaminants within hydrographic watersheds. In this context, identifying environmentally vulnerable areas is a useful tool for strengthening integrated pollution management strategies. This study aimed to assess the environmental vulnerability of the Grande Tulancingo River watershed using a multicriteria geospatial analysis that integrates biophysical and anthropogenic variables. The hydrographic delimitation of the watershed was carried out by processing an INEGI Digital Elevation Model using the SIATL simulator, allowing the definition of the drainage network, the main channel, and the catchment area. Biophysical and anthropogenic variables were integrated and processed using Geographic Information Systems (ArcGIS 10.8). Criteria selection, standardisation, reclassification, and weighting were conducted in accordance with specialised scientific literature. Subsequently, the criteria were integrated using the Weighted Overlay method to generate an environmental vulnerability map classified into five categories. The results indicated that the watershed covers an area of 1,887.623 km² and exhibits distinct hydrographic dynamics among the upper, middle, and lower zones, favouring contaminant transport toward accumulation areas. Agricultural activities cover approximately 58.2% of the watershed and were identified as the primary potential source of diffuse pollution from fertilisers and pesticides. The multicriteria analysis showed that 16.6% of the watershed exhibits moderate to very high environmental vulnerability, primarily in areas near the main channel and in zones with high hydrological connectivity. The multicriteria geospatial approach allowed the identification of priority areas for environmental monitoring and management, strengthening decision-making processes aimed at protecting aquatic ecosystems.



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sciforum-187269: Enantioselective Determination of Duvelisib in Wastewater Samples by Electrokinetic Chromatography after μ SPEed Preconcentration

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The development of sensitive and selective analytical methodologies for the determination of chiral drugs in complex matrices is of increasing importance in pharmaceutical, clinical, and environmental analysis. Duvelisib is a chiral anticancer drug marketed as the pure S-enantiomer [1], and its determination in environmental samples requires efficient preconcentration due to the low concentration levels expected in these matrices. In this work, a miniaturized solid-phase extraction procedure based on μ SPEed technology was developed and combined with Electrokinetic Chromatography (EKC) for the enantioselective determination of duvelisib in wastewater samples.

The extraction procedure, based on previous works of our research group [2,3], was optimized using PS/DVB-RP μ SPEed cartridges. The cartridges were conditioned with methanol and equilibrated with water before sample loading. Wastewater samples were then extracted, followed by elution with methanol, solvent evaporation, and reconstitution in the background electrolyte (BGE) prior to EKC analysis. The enantiomeric separation was achieved using sulfobutylated- β -cyclodextrin as chiral selector in 25 mM formate buffer (pH 3.0) at 30 °C and an applied voltage of -30 kV, allowing the rapid and efficient separation of both duvelisib enantiomers in 5.1 min and with an enantiomeric resolution of 3.1.

The proposed methodology showed satisfactory analytical performance. Extraction recoveries that included 100% for both enantiomers were obtained. Good linearity was achieved, with correlation coefficients higher than 99.3%, while precision values were satisfactory in terms of migration times and corrected peak areas (lower than 1.5% and 6.9%, respectively). Detection limits were in the low $\mu\text{g L}^{-1}$ range. In addition, no significant matrix interferences were observed after the μ SPEed procedure.

The developed μ SPEed-chiral EKC methodology provides a rapid, efficient, semiautomatic, and environmentally friendly strategy for the enantioselective determination of duvelisib in wastewater samples, improving sensitivity while reducing solvent consumption and sample handling according to the principles of green analytical chemistry.



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sciforum-187275: Clinical Masking of Insecticide Toxicity: Pharmacological Antagonism Between Flupyradifurone and Deltamethrin in Honeybees (*Apis mellifera*)

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Introduction

In veterinary apiculture, diagnosing pesticide poisoning is challenging because current toxicological frameworks are based on single-agent acute lethality (LD₅₀), which does not account for pharmacological interactions. Flupyradifurone (FL) and deltamethrin (DM) have overlapping agricultural use, but their combined clinical effects are unknown. This study characterized their acute oral toxicity alone and in combination.

Methods

Caged honeybees (20 per group, 10 replicates) received oral administration of: DM 21.6 mg/L; FL 50 mg/L; FL 100 mg/L; DM+FL50; DM+FL100; or sugar solution (control). Clinical monitoring over 72 hours included survival (Kaplan-Meier), daily food consumption, and abnormal behavior (incoordination, decreased movement, moribundity).

Results

DM alone caused significant mortality vs. controls ($p < 0.001$). FL 50 mg/L allowed 46% survival at day 3. FL 100 mg/L caused 100% mortality by day 2. DM+FL50 significantly improved survival vs. DM alone ($p < 0.001$) and vs. FL50 alone ($p < 0.001$). DM+FL100 significantly improved survival vs. FL100 alone ($p < 0.001$), with bees surviving up to day 3, while no significant improvement was observed vs. DM alone ($p > 0.05$). Food consumption and abnormal behavior confirmed antagonism.

Conclusions

Antagonism between FL and DM can mask toxicity severity, leading to clinical underestimation of pesticide exposure in honeybees. By pharmacological extrapolation, similar antagonistic interactions may occur in livestock species (e.g., sheep, cattle, pigs) exposed to contaminated feed or pastures, potentially concealing subacute or chronic poisoning. From a veterinary clinical perspective, this challenges the assumption that single-agent toxicity data predict real-world outcomes across species. Diagnostic protocols should include multi-residue screening, and risk assessment frameworks must integrate mixture toxicity testing for both pollinators and production animals.



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sciforum-187533: Speciation Uncertainty as the Dominant Driver of Arsenic Risk Characterization in Tuna: A Probabilistic Sensitivity Analysis

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Arsenic (As) is common in marine fish, predominantly as arsenobetaine and other organic forms of negligible toxicological concern. Inorganic arsenic, the species of regulatory relevance, typically constitutes only a minor fraction of total arsenic in pelagic fish such as tuna, yet speciation data are frequently unavailable in occurrence monitoring programmes, forcing risk assessors to rely on assumed inorganic fractions. The magnitude of uncertainty introduced by this assumption, and its influence on risk conclusions, remains poorly characterised. This study quantified the impact of speciation uncertainty on probabilistic inorganic arsenic risk characterisation in Portuguese and Spanish adult tuna consumers. Total arsenic concentrations were determined by ICP-MS/OES in 37 yellowfin tuna samples collected at the Port of Vigo and fitted to a log-normal distribution. Consumption data from IAN-AF 2015 (Portugal) and ENALIA2 2016 (Spain) were modelled as gamma distributions fitted by percentile matching to national dietary survey summary statistics. Monte Carlo simulation ($n = 10,000$ iterations) was performed independently under three inorganic arsenic fraction assumptions: 100% (fully conservative), 10%, and 5%, the latter two reflecting values reported in the literature for marine fish. Under the fully conservative scenario, median margins of exposure (MOE) against the upper $BMDL_{0.1}$ were 21 and 37 for Portugal and Spain respectively, with no iterations exceeding the low-concern threshold of $MOE = 10,000$. Even under the most realistic assumption of 5%, median MOEs of 432 and 742 remained far below 10,000, with fewer than 2% of simulated exposures classified as low concern in either population. Speciation assumption drives substantial variation in absolute MOE values but does not alter the fundamental risk conclusion: inorganic arsenic exposure from tuna consumption warrants concern across the full consumer distribution regardless of the fraction applied.



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sciforum-189229: Quantitative determination of toxic elements in imidazolium-based ionic liquids by inductively coupled plasma mass spectrometry

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Introduction

Ionic liquids (ILs) represent a large class of compounds, among which imidazolium-based ILs are the most studied and commercially available solvents. Due to their high thermal stability, low volatility and incombustibility, they are classified as green solvents. Recently, the scientists have questioned their ecological compatibility. Nowadays, open data on the research of ionic liquids for, according to the WHO report, probably essential (Si, V, Ni, Sn) and potentially hazardous (Pb, Hg, Cd, As, Tl, Ba, Sb) elements to the environment and human health are absent. Ionic liquids were studied for these elements by inductively coupled plasma mass spectrometry (ICP-MS).

Methods

Ionic liquids [BMIM]BF₄, [BMIM]TFA and [BMIM]TCF were examined within the research. Microwave acid digestion was carried out in the «Ethos Up» system («Milestone», Italy). Quantitative analysis was performed on ICP-MS «iCAP MTX» («Thermo Scientific», USA).

Results

[BMIM]BF₄ contained Si (113 mg/kg), Pb (0.036 mg/kg), [BMIM]TFA-Si (34.2 mg/kg), V (0.18 mg/kg), Ni (2.0 mg/kg), Sn (0.018 mg/kg), Sb (0.035 mg/kg), [BMIM]TSF-Si (5.3 mg/kg), V (0.87 mg/kg), Ni (27.7 mg/kg), Pb (1.4 mg/kg), Cd (0.88 mg/kg), Sb (0.16 mg/kg), which contradicts principle № 5 (Safer Solvents and Auxiliaries) of Green Chemistry. For comparison, here are the maximum limits of toxic elements in soils (LEX-FAOC097999): Si, Sb–n/d, V, Ni, Pb–50 mg/kg, Sn–10 mg/kg, Hg–0.5 mg/kg, Cd, Tl–1 mg/kg, As–20 mg/kg, Ba–500 mg/kg.

Conclusions

As of today, ATSDR, FAO and WHO only provide the MRLs of trace elements for humans and in the environment, but not their toxicity within ILs. Despite detecting potentially hazardous elements in imidazolium-based ILs, an objective assessment of their toxicity to the environment and human health remains difficult. Due to the lack of experimental data, further research is extremely promising and requires detailed analysis to ensure environmental safety.



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sciforum-191926: Microplastics in the muscle of marine fish from coastal China: occurrence and characteristics

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Introduction

Microplastics in fish muscle are relevant to seafood-related human exposure, but data on their occurrence and characteristics remain limited, particularly across coastal regions of China. This study investigated microplastic contamination in the muscle of marine fish and estimated dietary exposure in the Chinese population.

Methods

A total of 131 marine fish representing 19 species were collected from the Bohai Sea, East China Sea, and South China Sea. Microplastics in muscle within the 10–500 µm size range were extracted and identified using laser direct infrared imaging. Dietary exposure was estimated using the mean microplastic concentration in muscle combined with individual marine fish consumption data from Chinese food consumption surveys.

Results

Microplastics were detected in the muscle of 125 of 131 fish (95.4%). The mean, median, and range of microplastic abundance in muscle were 19.31, 12.96, and 0.00–97.83 items/g, respectively. Particles <100 µm accounted for 90.7% of detected microplastics, with the 20–50 µm fraction being predominant. Fragments were the most abundant shape category (48.2%), and polyvinyl chloride was the dominant polymer (42.7%). For the 10–500 µm fraction, the mean and 95th percentile dietary exposures were 2.78 and 19.54 items/kg body weight/day in the general population, and 20.25 and 53.64 items/kg body weight/day in marine fish consumers, respectively.

Conclusions

Microplastics were prevalent in the muscle of marine fish from coastal China, and the marine fish consumption constituted a source for dietary microplastics exposure. The data on microplastics contamination characteristics and dietary exposure may support the future seafood-related microplastic assessment.



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sciforum-193649: Environmental and Health Risk Assessment of Heavy Metal Soil Contamination: A Pilot Study of the El-Karma Industrial Site (Annaba, Algeria)

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Introduction

Contamination of agricultural soil by hazardous environmental toxins from industrial activities is a major concern. In Algeria, Annaba's municipality faces severe environmental degradation driven by the El-Hadjar steel complex, posing critical public health risks through soil and groundwater pollution.

Methods

To characterize individual exposure risks, soil samples collected from four agricultural plots (S1 to S4) in El-Karma, a site highly exposed due to its proximity to the steel complex, were analyzed to quantify the concentrations of potentially toxic elements (PTEs). Concurrently, a questionnaire-based toxicological survey was conducted in the study area among 75 residents and 25 farmers operating at the site. The survey evaluated health effects from inhaling or ingesting suspended particulate matter, dermal contact with toxic soil, and consuming contaminated groundwater.

Results

Soil analyses confirmed significant PTE contamination. Spectrometry quantified concentrations (mg/kg) of Cd, Cr, Cu, Ni, Mn, and Fe, respectively, showing higher levels in parcel S1 closer to the source: S1 (12, 171, 38, 46, 1110, 30832); S2 (7, 109, 32, 35, 791, 22492); S3 (7, 107, 30, 32, 660, 20722); and S4 (9, 102, 28, 31, 738, 19982). The survey revealed that 71% of residents experience foul odors from volatile organic compounds, forcing 72% to close windows, while 76% report high indoor humidity. Participants reported health problems like respiratory diseases, cancers, hypertension, and diabetes, indicating that continuous inhalation of industrial emissions acts as a direct chronic stressor. Among farmers, 64% work eight hours daily and 100% rely on well water for irrigation, though all use protective equipment.

Conclusions

Spectrometric and survey data confirm that the El-Hadjar complex is a critical source of PTE contamination, exposing populations through direct inhalation/dermal contact and indirect food/water consumption. Vulnerable rural populations and young children require strict, targeted protective strategies based on source-pathway-ecosystem relationships to safeguard this economic agricultural zone.



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sciforum-193771: Distinct Toxicological Profiles of Pesticide Metabolites Compared to Parent Compounds: Evidence from a Zebrafish Model

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Background

South Africa's extensive pesticide use presents significant health risks via direct exposure and environmental residues in food and water. Limited data on human metabolism and toxicity of pesticide metabolites hinder accurate risk assessments. This study investigated the toxicity of glyphosate, imidacloprid, chlorpyrifos, mancozeb, and their metabolites using a larval zebrafish model to provide insights into potential human health risks associated with low-level pesticide exposure.

Methods

A dose range for the pesticides was determined by translating internationally acknowledged human acceptable operator exposure levels to zebrafish-relevant doses and estimating metabolite doses to account for unknown pesticide metabolism. Zebrafish larvae at 94 hours post-fertilization (hpf) were exposed to pesticides or metabolites until 118 hpf. Acute toxicity endpoints, including survival and morphological abnormalities (e.g., pericardial edema, spinal curvature), were assessed. A 5-day exposure protocol also evaluated neurobehavioral effects via larval locomotion using the light-dark transition test (LDTT), with activity tracked via automated systems (Daniovision and Ethovision, Noldus).

Results

Metabolites frequently exhibited greater toxicity than parent compounds. Desnitro-imidacloprid and 6-chloronicotinic acid, both imidacloprid metabolites, were more toxic than the parent compound at slightly elevated doses, inducing reduced locomotion, developmental delays, and severe malformations. Chlorpyrifos oxon caused 100% mortality at all tested levels, unlike chlorpyrifos and chlorpyrifos-methyl, which were tolerated at AOEL levels. However, chlorpyrifos oxon and chlorpyrifos-methyl caused significant motor deficits and deformities, likely due to acetylcholinesterase inhibition. Glyphosate showed low acute toxicity, but its metabolite methylphosphonic acid induced developmental defects and yolk sac edema, while increased basal activity suggested neurotoxic stress. Mancozeb resulted in complete mortality and severe malformations, with its metabolite ethylenethiourea also reducing locomotion and inducing deformities.

Conclusion

These findings reveal significant toxic effects of both pesticides and their metabolites at or near accepted exposure levels. Including metabolites in toxicity assessments is crucial to accurately evaluate potential human health risks.



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