BOOK OF ABSTRACTS
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Institute of Environmental Assessment and Water Research

1ST SESSION

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ORAL PRESENTATIONS

YRD 2025

IDAEA Young Researcher´s Day

December 2nd, 2025

Enhancing the risk assessment of pesticides on bats

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ABSTRACT

The intensification of agricultural practices, driven by the growing global demand for food, has caused a marked decline in landscape heterogeneity and a ubiquitous presence of pesticides. As a result, many wild species inhabiting agricultural environments are at risk due to habitat loss and chemicals exposure. Among them, bats play a key role because they provide ecosystem services such as pest control or seed dispersal.

This study aims to evaluate the exposure levels and potential physiological effects of pesticides used in the rice fields of the Ebro Delta on the bat species Soprano pipistrellus (*Pipistrellus pygmaeus).*

To study how pesticides are distributed within this habitat and transferred from their application to the bats, water and sediment samples were collected throughout the rice-growing season in rice fields (organic and conventional) and natural areas, in 3 periods corresponding to the main pesticide treatments. Insects that constitute the bats' diet were sampled using emergence and light traps. To further assess exposure, bat fur and faces were sampled. All samples will be analyzed by HPLC–MS/MS at IDAEA.

To investigate the potential effects of pesticides on bats, body condition of each specimen has been assessed. Blood samples have been collected for metabolomic analyses. To determine potential genotoxic effects, micronucleus tests will be performed. Finally, the effects on bats behavior will be evaluated by comparing their relative activity before and after pesticide application.

The proposed case study will provide some necessary knowledge to conduct an improved Environmental Risk Assessment (ERA) for bats in agricultural environments.

Keywords: bats, pesticides, risk assessment, rice fields, Ebro Delta

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Comprehensive screening of emerging contaminants in Antarctic Peninsula waters using ion mobility-enabled HRMS

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ABSTRACT

The Antarctic Peninsula is among the most remote and least populated regions on Earth. Despite the protective measures to safeguard its fragile ecosystem and geographic isolation, anthropogenic pressures are increasing. Early research focused on persistent organic pollutants capable of long-range environmental transport, allowing them to reach remote areas. More recently, additional pollutants originating from nearby regions have been identified, largely linked to human activity. These last findings are based on targeted studies examining a limited range of compounds, leaving a significant gap in the comprehensive characterization of ice chemistry pollution.

To address this, advanced analytical techniques, such as wide-scope screening and non-target analysis (NTA) using liquid chromatography coupled with ion mobility-mass spectrometry were applied to samples from Deception, King George, and Livingston Islands. Ion mobility adds a complementary dimension to compound identification, enhancing confidence in NTA results. A semi-quantitative approach was also employed to assess environmental risk. In total, 88 compounds were detected in at least one sample, among 53 confirmed with reference standards (Level 1), 28 matched with spectral libraries (Level 2A), and 7 annotated with Level 3 confidence following Celma et al. Ion mobility data enabled the identification of several isomers of the same compound, such as adenosine, and differentiate isobaric compounds like paraxanthine and theobromine. Most concentrations were in the ng/L range (91.8%), with a few reaching µg/L. Industrial chemicals, personal care products, and naturally occurring substances showed the highest levels. Diethyl phthalate, currently listed for endocrine disruptor assessment, was the most abundant and widespread compound.

Keywords: Antarctic region, water samples, Non-target analysis, ion mobility, semi-quantification

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Calibration of ceramic passive samplers and their use in measuring contamination in river- and groundwater

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ABSTRACT

Conventional grab sampling provides only a snapshot of water quality, often missing short-term fluctuations in contaminant levels. Passive samplers, by contrast, integrate pollutant uptake over time and deliver time-weighted average concentrations, offering a more realistic picture of the contamination status in aquatic systems. The objective of this study was to optimize a methodology based on CPS to determine groundwater pollution. Ceramic Passive Samplers (CPS) are 5 cm × 1 cm porous ceramic tubes containing sorbent, and they offer a cheap and easy way to sample river- and groundwater. However, to enable their quantitative use, the sampling rate (Rs) must first be determined through calibration to convert accumulated mass in CPS into water-equivalent concentrations. In this work, Rs values for 60 common contaminants of emerging concern (CECs) were established under controlled laboratory using spiked water and during a period of 20 days under slight agitation, to simulate water flow in a piezometer. Finally, CPS were deployed in river- and groundwater along the river Besòs (Barcelona, Spain) to assess contamination levels. In parallel, grab samples were collected to validate the CPS technology.

Time-weighted concentrations of Acetaminophen measured with CPSs reached up to 688 ng/L, revealing contamination that grab samples failed to detect. Contaminants such as Diclofenac and O-desmethylvenlafaxine showed good agreement between CPS and grab sampling. The findings confirm that CPS provides a robust, low-maintenance approach for monitoring trace CECs in groundwater and rivers. The work also creates a database of Rs values, facilitating future field applications and interstudy comparisons.

Keywords: groundwater, contamination, passive sampler, water quality

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Transcriptomics to unravel different modes of action of organophosphate flame retardants

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ABSTRACT

Organophosphate flame retardants (OPFRs) are a diverse group of chemicals used to make materials less flammable. Because of their structural and physicochemical diversity, including differences in polarity, solubility and persistence, they can cause a wide range of toxic effects, such as neurotoxicity, hepatotoxicity, metabolic disorders, and alterations in reproductive pathways, among others.

In this study, we investigated the effects of three OPFRs, triphenyl phosphate (TPhP), tri(2-butoxyethyl) phosphate (TBOEP) and tris(1-chloro-2-propyl) phosphate (TCIPP), in zebrafish embryos. Exposures were performed from 4 to 5 days post-fertilisation, and effects on developmental parameters and survival rates were evaluated. Samples were collected for a dose-response analysis (0, 8.23, 28.27, 100.6, 351, 1230 µg/L) using a high-throughput microfluidic qPCR platform to quantify 96 genes previously selected. Based on these results, a concentration of 351 µg/L was chosen for a deeper transcriptomic analysis using RNA sequencing.

Our results show that each compound triggers a distinct transcriptional profile. TPhP mainly affects pathways related to drug, lipid, and glucose metabolism; TBOEP alters developmental processes, particularly eye development; and TCPP modulates a smaller set of genes, mostly linked to ferroptosis and apoptosis.

Overall, our findings highlight that OPFRs act through compound-specific mechanisms and that their molecular diversity plays a key role in their toxicity. In future work, we aim to characterise a list of ten OPFRs to gain a wider understanding of their modes of action and to select candidates for more detailed studies using single-cell technologies and fluorescence-activated cell sorting (FACS).

Keywords: flame-retardants, zebrafish, transcriptomics

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Abstract title

Polycyclic Aromatic Hydrocarbon and Black Carbon Concentrations and Sources: A Case Study in Primary Schools and Homes in Barcelona

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ABSTRACT

Indoor air quality in schools and homes is a growing concern for children's health[1,2].This study assessed the concentrations of polycyclic aromatic hydrocarbons (PAHs) and black carbon (BC) in indoor and outdoor environments and investigated their possible sources. Sampling campaigns were conducted in five primary schools and seven homes in urban Barcelona during both cold and warm seasons, along with an additional campaign at a rural school. Air samples were collected using low-volume samplers connected with SPE cartridges for PAH analysis in both gas and particle phase. $PM_{2.5}$ filter samples were collected for organic carbon and organic molecular tracer analysis in particulate matter, and continuous BC particle concentrations were obtained with portable micro-aethalometers. Total average PAH concentrations were generally higher indoors (12.8 ± 7.9 ng/m³) than outdoors (6.9 ± 2.9 ng/m³), mainly due to more volatile PAHs associated with indoor activities especially at homes, while less volatile, and more toxic PAHs were strongly correlated with BC. The average indoor-outdoor concentration ratio of 1.1 ± 0.4 indicated traffic as dominant contributor to indoor BC and less volatile PAHs in the urban areas, whereas biomass burning was a major source at the rural site. These sources also contributed to the organic matter identified in indoor samples, along with soil dust inputs, cooking activities, and personal care products. The PAH and BC levels observed in this study are lower than those reported in Barcelona a decade ago, reflecting the positive impact of the city's mitigation measures which have improved outdoor air and consequently benefited indoor environments.

References :
[1] Almeida et al,2011.https://doi.org/10.1016/j.atmosenv.2010.11.052
[2] Gignac, F et al, 2021. https://doi.org/10.1016/j.envint.2021.106614

Keywords: Indoor Air quality, Children´s exposure, PAH, BC, Organic aerosol

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Urinary Biomonitoring and Statistical Evaluation of Lifestyle Trends in Children Exposed to Endocrine Disruptors

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ABSTRACT

Children are daily exposed to contaminants through diet, inhalation, or skin contact, which may affect their health. Human biomonitoring (HBM) enables the assessment of this exposure by analyzing biological samples such as urine, a non-invasive matrix widely used in large population studies. Endocrine disruptors (EDCs) are a group of chemical substances that are ubiquitous in the environment, as they can be found in the form of pesticides, industrial products and plasticizers, among others. Their harmful effects can alter estrogenic regulation, which can cause adverse health effects, such as alterations in reproductive function and proper development in children.

In this study, 100 prioritized EDCs were analyzed in urine samples from 350 eight-year-old children belonging to the INMA cohort in Asturias, Spain. Low-resolution mass spectrometry combined with tandem mass spectrometry was used for the analysis (Agilent 6475 LC/TQ).

Nine compounds were detected in more than 40% of samples, including parabens, bisphenols and benzophenones. Different statistical tests were conducted on these compounds to identify exposure patterns related to diet, socioeconomic status, and other characteristics. It was determined that compounds such as ethyl paraben, benzophenone-1, and benzophenone-3 were more frequently detected in girls. Furthermore, for the first time, a direct correlation was established between fish and meat consumption and the presence of bisphenol S.

In conclusion, this study highlights the need for continuous biomonitoring to assess the potential health risks of contaminants, as well as the importance of conducting statistical analyses to establish links between the presence of EDCs and different everyday habits.

Keywords: Human biomonitoring, Endocrine disruptors, Children

Impact of the Superblock Model on the Urban Water Cycle: Trace Metals and Dissolved Organic Matter Dynamics across the Built Environment

ABSTRACT

Traditional water sources are struggling to meet rising urban demands, highlighting the need for alternatives such as rainwater, stormwater, or aquifers. The Barcelona Superblock provides a novel urban model integrating green infrastructure, like sustainable urban drainage systems (SUDS), to capture, treat, and recharge stormwater while enhancing local supplies. Yet stormwater remains a major contributor to diffuse urban pollution. To overcome current limitations on stormwater harvesting practices, we evaluated stormwater quality with emphasis on dissolved metals and organic matter (DOM) at the small catchment scale. Seven sampling campaigns were conducted across three Barcelona districts, targeting rain, stormwater from roads and pedestrianized streets (i.e., conventional vs. Superblock), and SUDS effluent. Results showed that both superblocks and SUDS reduced pollutant loads and mitigated ecotoxicological risks. Trace metal and DOM concentrations followed the trend: Rain < SUDS effluent < Pedestrian Street runoff < Road runoff, highlighting traffic-related impacts and SUDS treatment capacity (ranging from 23 to 70%). Risk characterization ratios indicated episodic ecotoxicological risk in stormwater, especially in road runoff due to elevated concentrations of Cu and Zn, while SUDS consistently remained below risk thresholds. SUDS also acted as biogeochemical filters, transforming DOM into more stable, humic-like forms and reducing its concentration by up to 65%. Trace metals and DOM emerged as biogeochemical tracers and proxies for stormwater quality, enabling more effective and sustainable urban water management. These findings support the integration of Superblock-like strategies into urban planning to reduce contaminant urban discharge.

KEYWORDS: urban stormwater, DOM, trace metals, SUDS, MCR-ALS chemometrics, ecotoxicological risk assessment.

HIGHLIGHTS

- Ancillary positive effects of superblock model: less pollution in urban water cycle
- Pollution sequence followed: rain<SUDS effluent<pedestrian street runoff<road runoff
- DOM shifted to more humic and less protein-like forms across the built environment
- SUDS acted as pollution sinks and enriched the aromaticity of DOM (higher $SUVA_{254}$)
- SUDS reduce episodic ecotoxicological risk in runoff from urban catchments

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High-throughput effect-directed analysis of thyroid hormone-disrupting compounds in Swedish stormwater ponds

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ABSTRACT

Stormwater is a diffuse source of a wide variety of organic micropollutants originating from urban activities into the aquatic environment. Because many of these micropollutants have high solubility in water, stormwater ponds, commonly installed for flood control and water treatment, can accumulate and release complex contaminant mixtures that degrade the quality of receiving freshwater systems. High-throughput effect-directed analysis (HT-EDA) combined with suspect and non-target screening provides a powerful approach for prioritization of unmonitored endocrine-disrupting compounds in urban stormwater. In this study, grab samples of eleven outdoor stormwater ponds across urban and remote areas of Uppsala, Sweden were collected and concentrated using solid-phase extraction (SPE). The extracts were assessed for their capacity to compete with thyroid hormone (TH) for binding to the TH distributor protein transthyretin (TTR), a key molecular initiating event of TH system disruption. Extracts with higher binding affinity to TTR were selected for fractionation into 96-well plates using two orthogonal separation modes: hydrophilic interaction chromatography (HILIC) and reverse-phase chromatography (RP). The resulting fractions were screened on a competitive TTR-binding assay using a fluorescent conjugate of TH, and subsequent chemical analysis of the same extracts was performed using trapped ion mobility-quadrupole time-of-flight mass spectrometry. Data processing using suspect and non-target screening was focused on those fractions with high TTR-binding activity. This approach enabled the identification of several chemical features as potential drivers of TH disrupting activity in stormwater. This study demonstrates how HT-EDA-based feature prioritization can support routine detection of contaminants of emerging concern in complex environmental mixtures.

Keywords: stormwater, effect-directed analysis, thyroid-hormone disruption, ion mobility, hydrophilic interaction liquid chromatography

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FLASH PRESENTATIONS

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Modeling redox dynamics an urban aquifer located at the Besòs River Delta

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ABSTRACT

Urban aquifers are polluted by a wide range of organic substances such as pharmaceutical compounds, personal care products, industrial substances or per- and polyfluoroalkyl substances (PFAS), which are artificial organic substances widely used across various industrial sectors. As long as the use of urban aquifers is being considered as a source of freshwater in the coming years to face water scarcity periods and cover the growing freshwater demand, the investigation of the hydrochemical processes controlling the natural attenuation of these organic substances is crucial.

The main objective of the study is the evaluation, quantification and modelling of the redox processes that control the evolution of organic substances (or CECs) at the field scale, since in a previous investigation about the presence of PFAS in an urban aquifer in Barcelona it was identified the influence of groundwater redox dynamics on their evolution.

A field campaign was conducted in the Besòs River delta in 2024. Over the course of one month and a half we collected 2 river and 9 groundwater samples each week in a site that behaves as a river bank filtration system, where the water status can be monitored at different times after its infiltration. These data are being used to develop and calibrate a reactive transport model with the PHT3D code. The final aim is to derive the kinetic parameters controlling the behavior of organic substances under different groundwater redox states. These parameters will be able to use at other places to predict the behavior of these substances once they reach the environment. While the results are not yet available, we will present the research process in detail.

Keywords: CECs, degradation rates, reactive transport, urban groundwater

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Establishing *Tetraselmis suecica* as a Marine Bioindicator: Growth Dynamics, Spectrophotometric Calibration, and Standard Toxicity Assays

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ABSTRACT

Microalgae are key organisms found in aquatic environments at the base of the trophic chain. Their relatively simple cultivation, achieved with the use of laboratory equipment such as incubators, makes them ideal model organisms for assessing the effects of water pollution by various chemical contaminant classes, including Contaminants of Emerging Concern (CECs).

The most used bioassay to evaluate lethal effects on microalgae is the OECD 201 growth inhibition test, which measures cell density in a culture over 72 hours at increasing contaminant concentrations. While cell counting is normally achieved by optical microscopy, this method can be time-consuming and lacks precision. To overcome this limitation, we linked spectrophotometric measurements of Absorbance at 680 nm with *T. suecica* optical density measurements, and then we used them to assess the growth phases of the cultures. Toxicological tests were then developed to determine EC50 values of inhibition for the standard compounds Potassium dichromate ($K_2Cr_2O_7$) and 3,5-Dichlorophenol (3,5-DCP), and for a model synthetic mixture of 14 CECs commonly detected in marine waters.

The EC50 values obtained with standard contaminants (7.61 mg/L for 3,5-DCP and 28.29 mg/L for $K_2Cr_2O_7$) aligned with literature data, proving the bioassay using *T. suecica* as a model organism and spectrophotometric measurement of growth inhibition a bioanalytical tool for the evaluation of marine contamination. However, exposure to the CECs mixture up to 32 times the environmental concentration showed no significant inhibition. Future work will investigate more sensitive tests that can detect sublethal changes and early effects of contamination.

Keywords: Microalgae, Bioassay, Growth Inhibition, CECs, marine waters

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Olive Leaves as Silent Witnesses of Atmospheric Mercury Pollution

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ABSTRACT

The chlor-alkali plant in Flix (Tarragona, Catalonia, Spain) was a major mercury emission source for decades. To evaluate the evolution of atmospheric mercury contamination after the cessation of industrial activity and the removal of dumped residues from the Ebro River bed, olive leaves were used as bioindicators.

In 2006, when the plant was still operational, 39 olive leaf samples were collected in the surroundings of the industrial site. Mercury concentrations showed a clear spatial gradient, with the highest levels near the plant, reaching up to 1.94 ppm. In 2024, a new sampling campaign was carried out at the same locations, analyzing 50 samples to assess the long-term changes after remediation. Mercury concentrations markedly decreased, with a maximum of 262.10 ppb. All mercury determinations were performed on whole leaves using a direct mercury analyzer (DMA-80), allowing precise quantification without chemical digestion. The data correspond to total mercury concentrations.

The comparison between 2006 and 2024 reveals a substantial decline in mercury accumulation in olive leaves, indicating a significant reduction of atmospheric mercury inputs in the area after the shutdown of the chlor-alkali plant and the removal of contaminated sediments. These results confirm that olive leaves are effective bioindicators for monitoring atmospheric mercury pollution and reflect the environmental benefits derived from remediation actions.

Keywords: Mercury, Olive leaves, Chlor-alkali plant, Industrial emissions, Environmental monitoring

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How porous media heterogeneity controls stirring and dispersion

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ABSTRACT

We study stirring and dispersion in steady flow through two-dimensional heterogeneous porous media. A fluid is stirred by the porous medium structure that leads to spatial flow variability and the deformation of fluid elements. While dispersion measures the extension of a solute distribution, stretching underpins solute mixing, chemical reactions and biological activity. Despite this, much less is known about fluid stretching in porous media. Its relation to the dispersion process on the one hand and the flow and medium properties on the other remain open questions. To close this gap, we probe the heterogeneity mechanisms that are at the origin of stretching and dispersion of fluid elements, and quantify the upscaled laws that govern their dynamics. Thus we perform detailed numerical simulations of Darcy flow in two-dimensional porous media characterised by a spatially varying hydraulic conductivity. Dispersion is analysed in terms of first-passage time distributions of fluid elements and the temporal evolution of their displacement mean and variance, while deformation is studied in terms of the probability density function and average elongation of fluid elements. We find that the dispersion and stretching behaviours are closely related. The exponents that govern the decay of the first-passage time distributions and evolution of the displacement variances also determine the evolution of the mean elongation. These dynamics are quantified in a single upscaled theoretical framework that bridges between Eulerian flow structure, large scale dispersion and stretching of fluid elements.

Keywords: Stirring, Disperson, Upscaling method

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Development and validation of an analytical method for the quantification of polyethylene micro and nanoplastics in human faeces

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ABSTRACT

Human exposure to micro- and nanoplastics (MNPLs) occurs through ingestion, inhalation, and dermal contact. Recent studies indicate that MNPLs may induce inflammatory lesions, increasing internalisation, tissue translocation, and disrupt cellular processes, potentially leading to oxidative stress. To assess human exposure to MNPLs, this study aimed to develop and validate an analytical method for the detection and quantification of MNPLs in human faeces.

Nanoscale polyethylene (PE) standards (~50 nm) were first synthesised following a procedure adapted from Merdy et al. [1], involving polymer dissolution in an organic solvent, formation of O/W emulsions, and controlled cooling to induce precipitation within emulsion droplets. Particle size and aggregation were assessed by transmission electron microscopy (TEM), and hydrodynamic diameter was measured by dynamic light scattering (DLS). The resulting polydisperse material was then used to fortify synthetic faeces prepared according to the protocol by Penn et al. [2] at five concentrations (3–143 ppb).
Two digestion protocols were evaluated for the analytical method development and validation: (1) Fenton's reagent followed by strong acid digestion, and (2) alkaline digestion with KOH, prior to polymer extraction and analysis. Detection was performed using size-exclusion chromatography coupled with high-resolution mass spectrometry and atmospheric pressure photoionization (SEC-APPI-HRMS). Polymer identification relied on characteristic monomer losses and Kendrick mass defect analysis.
Fenton-based digestion presented the best performance, yielding recoveries of 49–64% for PE. The validated method showed detection and quantification limits of 0.34 and 1.03 µg/kg for PE, respectively. Precision, expressed as %RSD, ranged from 7.8–25%. Overall, this work provides a robust analytical framework for the study of MNPLs in human faeces and supports future research on their occurrence and potential health implications.

Keywords: Micro and nanoplastics, Faeces, High-resolution mass spectrometry

References

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[2] R. Penn, et al., Water Res. 132 (2018) 222–240

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Assessing Methodological and Physiological Drivers of Tree Water Isotopic Variability

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ABSTRACT

Water stable isotopes are valuable proxies for tracing water fluxes within the critical zone. This technique has helped to develop conceptual models of water distribution across scales, making it essential to understand how trees regulate water stored within their internal compartments. We sampled a representative *Pinus sylvestris* tree within an ecohydrologically monitored forest plot in the Vallcebre research catchments (NE Spain). The aim of this sampling was to assess potential variability in the isotopic signatures across different parts of the tree to enhance understanding of soil-root-tree water uptake processes. Samples were collected from various soil depths (0–100 cm), woody tissues of twigs and branches, the stem (cores at 3 different heights), and roots in all four cardinal directions during two sampling periods (July and September 2023). Water from soil and wood samples was extracted using both cryogenic and cavitron methods and analyzed for stable isotope ratios. Additional data included long-term meteorological records, throughfall volumes and isotopic signatures, soil moisture content, and sap flow rates. Preliminary findings showed consistent patterns across both sampling dates: twigs and branches displayed isotopic values close to those of soil and throughfall, whereas roots and stem tissues exhibited more depleted values, clearly distinct from soil, twig, and branch signatures. To determine whether these isotopic observed differences arise from methodological factors or reveal intrinsic processes within the tree. These additional analyses promise new insights into the internal water dynamics of trees, with implications for understanding their role in critical zone water fluxes.

Keywords: deuterium, oxygen-18, ecohydrology, cavitron, cryogen

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Photolysis and Transformation of Octocrylene and Its Metabolites in Aquatic Matrices

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ABSTRACT

Octocrylene (OC) is a commonly used UV filter that has recently been identified by the European Chemicals Agency (ECHA) and ANSES as a contaminant of concern due to its persistence, bioaccumulation, and ecotoxicity in aquatic environments, leading to a 2025 REACH restriction proposal for its use. This growing regulatory scrutiny underscores the need to elucidate OC environmental behavior, transformation products, and long-term impacts across aquatic ecosystems. Benzophenone (BP) is reported as one of its major photodegradation products, and 2-cyano-3,3-diphenylacrylic acid (CPAA) is recognized as a major human metabolite. Understanding the transformation of these compounds under UV exposure is important to understand their environmental behaviour and the potential formation of photo-transformation products.

This study investigates the photolysis of OC, BP, and CPAA under simulated sunlight. Each compound was prepared at controlled concentrations in four aqueous matrices: HPLC water, river water, seawater, and wastewater and irradiated in a SUNTEST chamber for up to 10 hours, alongside dark controls to distinguish photolytic transformation from other processes. UV–Vis spectroscopy and semiquantitative analysis using UHPLC-HRMS were used to track degradation kinetics and identify transformation products. The distinct behaviors observed across matrices highlight the interplay of processes driven by variations in dissolved organic matter, pH, and ionic strength, leading to differentiated impacts among aquatic environments. Further, evaluation of HRMS data to identify photoproducts and species formation profiles were performed and will be presented. This approach will help clarify transformation pathways and assess whether environmentally relevant photoproducts emerge across the different water matrices.

Keywords: Octocrylene, CPAA, Benzophenone, Photolysis, HRMS, UV filters

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Drivers of Contaminants of Emerging Concern (CECs) concentration in aquifers and rivers of the Besòs basin (Catalunya, Spain)

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Keywords: groundwater, rivers, CECs, catchment, pollution

ABSTRACT

Contaminants of emerging concern (CECs) are increasingly detected in European waters, yet they are rarely studied jointly across different water matrices at basin scale. To understand processes driving CECs concentration at such scale, we investigated the occurrence of 120 CECs in wastewater treatments plants (WWTPs), surface water, and groundwater (GW, wells and springs) across the Besòs catchment. We combined non-parametric correlation analysis with grouping strategies to infer whether basin compartments shared pollution sources and attenuation mechanisms. CECs above LOD were classified based on detection frequency into *Group 1* (35 river-ubiquitous compounds) and *Group 2* (61 more spatially-variable CECs). Contaminants were further classed regarding maximum concentration as "*Peak"* when exceeding 200 ng/L (i.e.: P-90 concentration in rivers) in at least one river stretch and as *noPeak* otherwise. Sucralose concentration (a conservative marker for mixing with domestic wastewater) correlated well with several *Group 1* CECs but poorly with most *Group 2* CECs. In 70% of river stretches and 62% of GW, most of total CECs concentration was explained by *Group 1 Peak* CECs (like hydrochlorothiazide, naphthalene-1-sulfonic acid or melamine), mainly industrial and domestic. In other GW samples (38%), *Group 2 noPeak* CECs (e.g., gabapentin, venlafaxine, propranolol or triphenyl phosphate) were more prevalent. Those sites also had a high concentration of CECs which were <LOD in WWTPs and in most rivers (e.g., propranolol), suggesting release from subsurface sinks rather than recent inflow from WWTPs or losing river stretches. Lower CECs concentration in GW with respect to rivers was attributed to mixing, sorption to organic matter and biotransformation.

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Ecotoxicological Assessment of UV Filters in Zebrafish Embryos (*Danio rerio*)

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ABSTRACT

The increasing release of ultraviolet (UV) filters into aquatic systems due to the massive use of cosmetic and sunscreen products has raised environmental concerns because of their persistence, bioaccumulation, and toxic potential to aquatic organisms. Their main entry into aquatic environments occurs either through recreational water activities or wastewater discharges. The presence of these emerging contaminants has been reported in water bodies worldwide, where they can affect the embryonic development of fish and other organisms. In this context, the present study aims to compare acute toxicity of the synthetic UV filter Octocrylene with its main photodegradation product benzophenone, and the derivative 2-cyano-3,3-diphenylacrylic acid (CPAA), and two natural compounds with photoprotective properties, the flavonoids Rutin and Quercetin, which could potentially substitute it in environmentally friendly formulations. The comparison was performed through *in vivo* assay using zebrafish (Danio rerio) embryos, applying the standardized OECD 236 methodology (Fish Embryo Acute Toxicity Test, FET). Embryos were exposed to increasing concentrations of each compound during the first 96 h post-fertilization. Lethality, malformations, and delayed hatching and development were evaluated, allowing the calculation of EC50 and the establishment of dose-response curves. The results showed that benzophenone exhibited the highest acute toxicity, followed by CPAA, quercetin, and rutin, whereas octocrylene did not cause adverse effects at the tested concentrations. These findings highlight the relevance of prioritizing photoprotective alternatives with lower ecological risk and provide a solid scientific basis to support regulatory decisions aimed at reducing the environmental impact of sunscreen agents.

Keywords: ultraviolet filters, acute toxicity, embryo zebrafish, emerging contaminants, ecotoxicology

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Methodological approach for a simultaneous determination of persistent and non-persistent organic pollutants in human blood. Results from birth cohort studies.

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ABSTRACT

An experimental and analytical protocol for the detection and quantitation of 47 persistent and non-persistent pollutants (POPs) in serum samples has been developed. The analysed compounds included POPs such as organochlorine pesticides (OCs), polychlorinated biphenyls (PCBs), and polybrominated diphenyl ethers (PBDEs), and vinclozolin (VIN), tecnazene and quintozene. Serum samples (0.5 mL) were mixed with a methanol:H_2O solution (1 mL, 1:3) and hexane (3 mL). Samples were further shacked (1 hour) and centrifuged (30 min). Non-polar phase (hexane) was transferred into conic tubes, evaporated to dryness under N_2 and reconstituted in isooctane. OCs and PCBs were measured by GC-ECD, and PBDEs by GC-MS-NICI (Bustamante et al, 2025). A total of 219 serum samples were analysed. Results at 8 years were compared with those already determined in these participants at 4 years. Sixteen compounds showed detection frequencies > 50 %, with DFs reaching 100% for 4,4'-DDE, hexachlorobenzene (HCB), PCB-180, Aldrin and Endrin. Aldrin was the compound showing the highest median concentration (0.76 ng/mL), followed by VIN (0.31 ng/mL), 2,4'-DDE (0.28 ng/mL) and 4,4'-DDE (0.23 ng/mL). The concentrations at 8 years of age were lower than those found at 4 years or in pregnant women for HCB, 4,4'-DDE, PCB-153 and PCB-180. However, in the case of β-HCH and PCB-138, the concentrations at age 8 were higher than at age 4. Child's gain vs. maternal transfer correlations showed that at age 4, children's OCs levels strongly correlated due to breastfeeding (Garí et al, 2019). At age 8, the slopes for HCB, 4,4'-DDE, PCB-153 and PCB-180 decreased, nevertheless, correlations still remain significant (R^2 > 0.26), indicating a continued maternal influence. For some compounds (β-HCH and PBC-138) with higher exposure levels at age 8, slopes are ≈ 0, suggesting additional environmental exposure to these compounds.

Keywords: OCs, PCBs, PBDEs, mothers, 4-year-old children, 8-year-old children

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Flow and Mixing in Unsaturated Heterogeneous Soils Under Infiltration-Evaporation cycles

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ABSTRACT

Water infiltration in the vadose zone is a transient and unstable process influenced by several factors, including the non-linearity of soil properties, rapidly changing boundary conditions, hysteresis, macroscopic surface tension, and soil heterogeneity. Understanding and characterizing these processes is crucial for managing water resources and assessing pollutant transport in the context of climate change. In this work, we aim to evaluate the impact of these factors on water flow, solute transport, and mixing during infiltration–evaporation cycles.

We use the FEniCS software to numerically solve flow and transport equations, modeling flow with the dimensionless Richards equation and solute transport with the advection–dispersion equation. Simulations were performed for three soil types (fine sand, loam, and clay), incorporating Gaussian random permeability fields to represent heterogeneity by varying correlation lengths (isotropic and anisotropic) and variance. We also explored a range of Péclet numbers to assess their impact on transport. Flow was evaluated via volumetric water content, and solute transport was characterized using breakthrough curves, center-of-mass displacement, solute front width, dispersion coefficients, and segregation intensity.

Our findings indicate that soil heterogeneity and dynamic boundary conditions significantly influence flow and solute transport. Vertically anisotropic heterogeneity promotes deeper infiltration and earlier solute arrival, while isotropic heterogeneity enhances multidirectional mixing and tailing in breakthrough curves. High Péclet numbers intensify advective transport, leading to faster solute displacement and broader dispersion fronts, whereas low Péclet conditions favor mixing and reduce segregation. These effects are more pronounced in sandy soils, and less evident in clay soils.

Keywords: unsaturated flow, solute transport, isotropic and anisotropic heterogeneity, FEniCS, finite element methods, infiltration-evaporation cycles.

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Meta-analysis of zebrafish gene expression to uncover toxicity biomarkers

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ABSTRACT

The zebrafish (*Danio rerio*) is widely used in toxicology because it combines the biological complexity of a vertebrate with the practicality of a high-throughput model [1]. Its genome shares strong similarity with humans, and its rapid development and transparent embryos allow the assessment of chemical effects at the molecular, cellular, and organismal levels [2]. These features make zebrafish particularly suitable for detecting early transcriptional changes that occur before visible toxic effects appear. Identifying such molecular responses can reveal sensitive biomarkers of exposure and effect, improving the prediction of chemical risks. This is especially important for contaminants of emerging concern (CECs), which may trigger adverse responses at environmentally concentrations.

To identify transcriptome-level biomarkers linked to CECs exposure, a comprehensive literature review was conducted to compile RNA sequencing datasets from zebrafish embryos exposed during the first five days post-fertilization. Seventy-nine studies were selected from public repositories (e.g., GEO, SRA, ArrayExpress) selecting 2739 datasets involving 201 compounds. These datasets were standardized for gene annotation and classified based on compound class, physicochemical properties, concentration, exposure duration, developmental stage, and mode of action. The *association plot* tool in R was applied to explore gene–response relationships across exposure categories.

The results showed comparable transcriptional trends across diverse contaminants, indicating common biological responses to chemical stress in zebrafish embryos. These shared expression patterns offer valuable molecular indicators for assessing the combined effects of contaminants of emerging concern and may support future efforts to predict mixture toxicity in aquatic ecosystems.

Keywords: *Transcriptomics, Zebrafish, Biomarker, Gene Expression, CECs.*

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FLASH PRESENTATIONS

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Multi-Suspect Screening of Polar and Nonpolar Marine Biotoxins Using a Tandem SPE and Dual-Column LC-HRMS Approach

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ABSTRACT

Marine biotoxins are a diverse group of compounds produced by harmful algae, representing a major concern for marine ecosystems, seafood safety, and public health. Their wide range of physicochemical properties, from highly polar to strongly nonpolar, makes their simultaneous extraction and analysis particularly challenging.

In this work, we optimized a novel sample preparation method capable of extracting from seawater both polar and nonpolar marine biotoxins, including the following groups: Azaspiracids, Okadaic acid, and Saxitoxins .

The method is based on a tandem solid-phase extraction (SPE) approach that combines two cartridges (HLB and Envi-Carb) with complementary selectivity. After sample loading, sequential elution allows the recovery of biotoxins across a broad polarity spectrum. The extracts were subsequently analyzed by liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS) using two distinct chromatographic columns: 1) Synergi C18 reversed-phase column for the separation of nonpolar toxins and 2) BEH Amide column for the polar fraction. This dual-column configuration ensures optimal retention and resolution of compounds with markedly different properties.

The qualitative screening data independent acquisition all ion fragmentation mode tool (DIA-AIF) using a Q Exactive Orbitrap was employed based on the previous reported by Picardo et al, [1]. Both targeted and suspect screening have been combined with online in-house database and suspect list to retrieve candidates as suspect biotoxins and their metabolites or degradation products. The in-silico analysis of mass spectrums allowed a fast structural characterization.

The developed method has demonstrated high reproducibility, efficient matrix clean-up, and broad analyte coverage, enabling a comprehensive assessment of marine toxins in complex environmental samples.

Keywords: Marine Biotoxins, Tandem SPE, Multi-suspect screening.

References:

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MethodsX, vol. 8, Jan. 2021, doi: 10.1016/j.mex.2021.101286.

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Spectral Analysis of Fourier Neural Operator Limitations in Advection-Dominated Geothermal Systems

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ABSTRACT

FNOs work well for geothermal modeling but fail when advection dominates. We investigated this by analyzing how Péclet number affects FNO accuracy through spectral methods. We simulated heat transport across diverse permeability fields and flow regimes, then trained FNOs for each case. The key finding: increasing advection shifts solutions toward high-frequency content that standard FNOs can't handle. Errors grow substantially with Péclet number and correlate strongly with spectral characteristics. Permeability heterogeneity amplifies this effect. We identified critical flow regimes where FNO performance breaks down, showing that diffusion-dominated systems suit standard FNOs while advection-dominated cases need better architectures. This connects physical parameters directly to ML performance for practical applications.

Keywords: Fourier neural operators, Péclet number, geothermal modeling, spectral analysis, advection-diffusion, surrogate modeling.

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Abstract title: Modelling the Impact of Insect Herbivory on CO_2 Fluxes in a Subarctic Mountain Birch Forest

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ABSTRACT

Subarctic forests act as important carbon sinks whose balance can be rapidly altered by biotic and abiotic stressors. Using four years (2021–2024) of eddy covariance CO_2 flux data from a mountain birch forest (*Betula pubescens*) near Abisko, northern Sweden, we examined the impact of a severe caterpillar outbreak that caused complete defoliation in 2023. Observed data revealed a strong reduction of the Net Ecosystem Exchange (NEE) of the forest during defoliation. To estimate fluxes under undisturbed conditions, we applied a Machine Learning RandomForest model and the LPJ-GUESS vegetation model. The annual cumulative carbon balance of the herbivory year (2023) shows the forest as a strong source of carbon (with an annual C balance of 150.147 gC/m²), compared to the predicted annual results of 0.195 gC/m² and -102.637 gC/m² estimated by the RandomForest and LPJ-GUESS models, respectively. In the recovery year (2024), the observed C balance returned to 5.168 gC/m², indicating a rapid restoration of sink strength. These results provide complementary insights into biosphere–atmosphere interactions and emphasize the need to integrate herbivory-driven disturbances into carbon cycle models for northern ecosystems under climate change.

Keywords: *Carbon fluxes, Eddy Covariance, RandomForest*, LPJ-GUESS model.

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ORAL PRESENTATIONS

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Uncovering the Chemical Burden of Mediterranean Seafood: Multi-class Contaminant Assessment to Support Future Regulation

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ABSTRACT

Persistent organic pollutants (POPs) and contaminants of emerging concern (CECs) are getting attention due to their persistence, bioaccumulation, and potential adverse effects on human and environmental health [1,2]. The European Chemicals Agency (ECHA) emphasizes the need for robust biomonitoring and occurrence data to identify and regulate hazardous substances. However, information on many non-regulated emerging pollutants in seafood remains scarce [3].

This study addresses this gap by characterizing a broad range of contaminants in fishery products from the Catalan coast. Ten pollutant families, including organophosphate esters (OPEs), phthalates (PAEs), non-phthalates plasticizers (NPPs), bisphenols, UV-filters, flame retardants such as polybrominated diphenyl ethers (PBDEs) and short-chained chlorinated paraffins (SCCPs), were analyzed in the muscle tissue of 13 wild-caught species collected from five coastal locations (91 individuals). Human dietary exposure was also evaluated.

SCCPs contributed the most to the total contaminant load across most species, followed by PAEs and NPPs. Median concentrations were highest for SCCPs (750 ng/g ww) and PAEs (1.29 ng/g ww). The compound families with the highest detection frequencies were PBDEs (93% of samples), SCCPs (90%), OPEs (82%), and PAEs (73%).

Estimated daily intakes for fish consumption were below established safety thresholds. However, the simultaneous detection of multiple emerging pollutants in seafood intended for human consumption underscores potential cumulative risks.

By providing occurrence data for underregulated and understudied substances, this study provides scientific evidence to support future prioritization and regulation of contaminants at the European level. These findings reinforce the importance of expanding monitoring programs to capture the evolving chemical landscape of the marine environment.

Keywords: seafood, biomonitoring, risk assessment, regulation

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Assessment of the neurotoxic potential of PM_{10} extracts from rural Bellver de Cerdanya (Catalonia) using cell-based models

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ABSTRACT

Air pollution contributes to 4.2 million premature deaths yearly, primarily from cardiovascular, respiratory, and cancers[1]. Fine particulate matter ($PM_{2.5}$ and PM_{10}) can translocate to the brain via systemic circulation or olfactory routes, triggering oxidative stress, neuronal injury, and neurodegenerative conditions like Alzheimer's and Parkinson's[2]; yet, its neurotoxic mechanisms are poorly characterized. This study aims to evaluate the neurotoxic potential of PM_{10} extracts from a rural background site in Bellver de Cerdanya (Catalonia) through integrated chemical and biological approaches.

Organic extracts were obtained from PM_{10} filters collected seasonally at Bellver de Cerdanya. Chemical composition was determined by GC-MS targeting thirty organic compounds including biomass-burning tracers (levoglucosan, mannosan) and polycyclic aromatic hydrocarbons. Neurotoxicity was assessed in SH-SY5Y neuroblastoma cells using viability assays, ROS quantification, XRE, ARE, and p53 reporter gene activation, and acetylcholinesterase (AChE) activity measurement. Lipidomic profiling was conducted in human neurocortical organoids to characterize membrane lipid alterations.

Winter samples exhibited elevated pollutant concentrations due to intensified biomass combustion and reduced atmospheric dispersion. Cold-season extracts induced significant cytotoxicity, oxidative stress, and xenobiotic response activation in SH-SY5Y neuroblastoma cells, while warm-season samples primarily inhibited AChE, indicating disrupted cholinergic signaling. Lipidomic analysis revealed seasonal remodeling of membrane lipids, particularly gangliosides critical for neuroprotection and synaptic function. Correlation of chemical profiles with biological endpoints linked specific emission sources to distinct neurotoxic outcomes, highlighting the value of multidisciplinary strategies in elucidating air pollution's neurological impacts.

Keywords: Air pollution, Neurotoxicity, Particulate Matter, Bellver, Oxidative stress, Lipidomics

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Photolytic Behavior and Environmental Stability of Plant-Derived UV Filters: Rutin and Quercetin as Sustainable Alternatives to Octocrylene

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ABSTRACT

Millions of people apply sunscreen every summer, but the same products that protect human skin from the sun can pose risk to aquatic environments. This year, the European Chemicals Agency (ECHA) has issued a restriction proposal for the widely used UV filter octocrylene in personal care products due to its persistence, bioaccumulation, and ecotoxicity in. This regulatory context highlights the urgent need for alternative UV filters with effective photoprotection and improved environmental performance. Rutin and quercetin, two plant-derived flavonoids, are being investigated within the ECOSUN project as potential eco-friendly UV absorbers. Both substances are promising options for next-generation sustainable sunscreen formulations due to their strong UV absorption (280–400 nm) and antioxidant properties.

This study uses a SUNTEST chamber to simulate sunlight and assess the photolytic degradation kinetics of quercetin and rutin in four aqueous matrices: wastewater, river water, salt water, and HPLC-grade water. UHPLC-HRMS and UV-Vis's spectroscopy were used to monitor concentration decay and identify transformation products. Quercetin exceeded 90% degradation in HPLC-grade water but was undetectable in the other matrices, probably as a result of matrix-dependent instability and low persistence. In contrast, rutin exhibited nearly complete degradation across all tested matrices.

These results reveal the high flavonoids' inherent photo-reactivity and non-accumulative nature, supporting their potential as effective UV absorbers. This study constitutes one of the first experimental comparisons of synthetic and natural UV filters suggesting that in the future, ecosystem safety and human photoprotection may be combined in a single formulation.

Keywords: Rutin · Quercetin · Photolysis · UHPLC-HRMS · Natural UV Filters · Environmental Sustainability

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Iberian Climate Change palaeoarchives at the highest temporal resolution for addressing the thermo-hydro-climate unknowns ahead (extreme events)

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ABSTRACT

The Mediterranean Sea is expected to be one of the regions most severely impacted by current and future climate change, already experiencing more frequent hydro-extremes and thermal-extremes, which are to be exacerbated in the near future, together with thermal-extremes (heat and cold waves) as yet to be evaluated in seasonality and predictability.

While past centennial-scale climate fluctuations have been investigated, little is known about higher-frequency variability at human timescales. This study aims to investigate hydroclimate dynamics and Sea Surface Temperature (SST) variability over the past ~2,000 years at unprecedented temporal resolution using high-resolution biomarker analyses.

We integrate Mass Spectrometry Imaging (MSI) and conventional alkenone analysis to achieve sub-annual to decadal resolution in SST reconstructions from marine sediments collected in the Western Mediterranean and Tagus areas. MSI is further combined with elemental proxies from µXRF mapping, including indicators of continental input and marine productivity.

Pilot analyses of sediment cores from the Alboran, Balearic and Tagus areas show that MSI can effectively detect alkenones even in non-laminated sediments with low organic concentrations. Balearic values remain below detection limits, consistent with previous Gas Chromatography (GC) analysis, though ongoing analyses are as yet to confirm. Preliminary results also reveal climate variability over the past ~2,000 years, including periods such as the Late Little Ice Age, the Little Ice Age and the Post-Industrial period.

This high-resolution approach offers a more detailed perspective of past oceanographic conditions and climate dynamics and points to advanced statistical modelling, essential when addressing the regional impacts of climate change.

Keywords: MSI, alkenones, biomarkers, Mediterranean, palaeoclimatology

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Simulated Riverine Biodegradation of Bioplastics: Additive Leaching and Dissolved Organic Matter Characterization

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ABSTRACT

Bioplastics have emerged as promising alternatives to fossil-based plastics products due to their higher biodegradability and renewable origin. However, a key challenge is that bioplastics often require larger amounts of plastic additives to achieve mechanical and functional properties comparable to those of conventional plastics, raising concerns about their potential environmental impact.

Among the different environments where biodegradation have been investigated, riverine systems are particularly relevant due to their dynamic physical and chemical conditions. Ultraviolet (UV) radiation promotes photooxidative degradation, leading to polymer chain scission, while hydrodynamic forces and interactions with sediments enhance mechanical fragmentation. Together with microbial biodegradation and hydrolysis, these processes play a crucial role in the degradation of plastics and the release of associated additives.

In this study, we simulated riverine biodegradation conditions using continuous water recirculation channels to investigate the leaching behavior of plastic additives from four different materials: a polyethylene (PE) trash bag and three commercial bio-based materials used for single use applications: trash bags, single use glasses and plates. Released additives were analyzed using liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS) via suspect screening analysis. Additionally, dissolved organic matter (DOM) was characterized through high resolution mass spectrometry (HRMS) to assess the extent and nature of the biodegradation processes occurring during the experiment. Among all the materials, the bio-based glass showed the highest number of leached additives (162 over the month-long experiment), while the bio-based plate exhibited the lowest (129). The most leached compound families were plasticizers and polymer-production-related compounds. In terms of biodegradation and in every material, lignin-type compounds increased over the course of the experiment due to their lower biodegradability compared to the other compounds studied.

Keywords: bioplastics, biodegradation, riverine, suspect screening analysis, lixiviation, additives

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Flow-rate distribution in 2D disordered porous media

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Current field work: Flow, transport and mixing in porous media
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ABSTRACT

We study steady Stokes flow through a two-dimensional packing of circular beads. We build a minimal statistical model for the flow-rate distribution based on a mapping of the pore space to a network of Poiseuille-flow tubes. We show that the flow rates at the pores follow a Gamma distribution, and that the flow-rate distribution at throats is fully determined in terms of it. The predictions agree closely with computational fluid dynamics simulations and show better agreement than prior mean-field models. The study clarifies how local splitting and merging shape flow in disordered porous networks.

Keywords: flow rate, porous media, bead packing, distribution

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Communicating Science on Natural Hazards: Managing Uncertainty in Multi-Risk Assessment

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ABSTRACT

Scientific communication is a strategic tool in natural risk management, enhancing mitigation strategies and supporting informed decision-making. It also contributes to building a society that is more aware of potential risks and better prepared to face them. Effective communication must consider the target audience (general public, scientists, decision-makers, first responders, media), the timing (before, during, and after an event), the type of message derived from risk assessment, the communication channels, and the overall objective.

Risk perception is another key factor influencing how information is received and acted upon. Therefore, understanding the social, cultural, and economic contexts that shape perception is essential.

A major challenge remains the communication of multi-hazard concepts, acknowledging that natural hazards rarely occur in isolation, and of scientific uncertainty, which often involves complex numerical expressions and limited public understanding. Addressing these challenges is crucial to maintaining trust and fostering effective responses throughout the risk management cycle.

This doctoral research examines these issues through the case of volcanic risk communication in the Canary Islands, where volcanic eruptions are treated as multi-hazard events. The study aims to identify gaps in current communication practices, develop a case study on the quantification and communication of uncertainties, and propose a new framework for scientific communication integrating uncertainty and multi-hazard perspectives.

The methodology combines social and geoscientific approaches, including literature review, risk perception surveys, stakeholder mapping, interviews, hazard modeling, uncertainty quantification, and participatory workshops.

Keywords: Scientific communication; Uncertainties; Multi-hazard; Multi-risk; Risk perception.

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Human Exposure Assessment to Tire-Related Chemicals through Citizen Science and Multi-Matrix Biomonitoring

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ABSTRACT

Tire-Related Chemicals (TRCs) are emerging environmental contaminants of concern due to their widespread presence and potential toxicity. These compounds, including manufacturing additives and transformation products released through tire wear, enter human systems via inhalation, ingestion, and dermal absorption. Assessing human exposure to TRCs is essential for understanding their health impacts and informing risk mitigation strategies. However, adolescents remain underrepresented in this research despite being highly vulnerable to traffic-related pollution.

The CIRCULATE study used an Urban Health Laboratory methodology, co-creating research with secondary-school students in Barcelona's Metropolitan Area through three phases: participatory diagnosis of environmental health issues, co-creation of research questions, and collaborative protocol development. Students defined their research questions, focusing on exposure pathways relevant to their living and learning environments. They actively participated by using fixed and portable air quality sensors, deploying silicone patches as environmental passive samplers, and providing biological samples.

We assessed individual exposure to 26 TRCs using complementary matrices: urine samples and silicone wristbands. Samples from the students and their families underwent optimized extraction and liquid chromatography-tandem mass spectrometry target analysis. Detection frequencies above 50% were registered for 12 and 23 compounds in urine and wristbands, respectively. The transformation product 6PPD-q showed 88% and 96% detection in urine and wristbands, respectively. Silicone patches presented detection frequencies over 50% for 19 compounds, with 6PPD-q being detected in 78% of the samples.

This citizen-science approach increased environmental literacy and ownership and consolidated a replicable protocol for neighborhoods with varying traffic characteristics, supporting the effort to characterize general population exposure.

Keywords: #tirechemicals #tirewearparticles #microplastics #humanexposure #exposome

3RD SESSION

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FLASH PRESENTATIONS

Abstract - Tobias Grundhöfer

Karst aquifers are complex and highly heterogeneous groundwater systems where water and solutes can move rapidly through interconnected conduit networks. This leads to fast breakthrough responses at springs but also to prolonged tailing caused by storage and slow release from immobile zones. Understanding and predicting solute transport in such systems is difficult because of their multiscale structure and strongly variable flow dynamics. In this work, we investigate solute transport using both synthetic and real karst networks. The synthetic networks allow us to test how network structure and flow variability influence transport under controlled conditions, while real karst systems provide natural examples for comparison. Flow is simulated using a graph-based approach capable of representing both laminar and turbulent conditions, while solute movement is modeled with a particle-tracking method based on Time-Domain Random Walks (TDRW). This framework allows us to systematically explore the relationships between network topology, flow heterogeneity, and large-scale transport behavior. Our results show that network connectivity and flow variability strongly affect solute spreading and breakthrough characteristics. Despite the complexity of individual flow paths, ensemble transport metrics such as breakthrough curves reveal consistent scaling behaviors across different network types. These findings highlight the value of synthetic models for isolating key physical controls on transport in karst systems and contribute to the development of improved models for predicting contaminant dynamics in real aquifers.

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Multiple Stressors in a Mediterranean Lagoon: An Integrated Chemical, Ecotoxicological and Molecular Approach

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The combined effects of chemical pollution, eutrophication and climate change pose a significant threat to coastal lagoons. The Orbetello Lagoon (Tuscany, Italy) is exposed to multiple anthropogenic pressures, including urban and aquaculture effluents, legacy contamination, and inputs of emerging pollutants. This complex setting provides an ideal case study to investigate how chemicals and physical factors can affect ecosystem health and its biodiversity. Within the E-TRACE project, a multidisciplinary approach was adopted to assess the ecotoxicological status of the area and to identify potential sources of contamination and ecological risk factors. Ecotoxicological investigations include biomarker analyses on bioindicator species (*Chelon labrosus* and *Mytilus galloprovincialis*), focusing on detoxification and biotransformation pathways, oxidative stress, neurotoxicity, genotoxicity, immune and metabolic alterations. Additional assessments involve acute and chronic toxicity bioassays on sediment elutriates to evaluate organismal responses to environmental stressors. Chemical analyses are carried out on water, sediment, and bioindicator species to assess the occurrence and distribution of contaminants such as organophosphate esters, non-phthalate plasticizers, UV filters, and fragrances. Moreover, environmental DNA metagenomic and metabarcoding analysis being performed on sediment and water samples to provide a high-resolution assessment of microbial and metazoan biodiversity, and to detect species of community interest, as well as invasive or non-indigenous taxa. The integration of ecotoxicological, chemical, and molecular data will provide a comprehensive understanding of ecosystem responses to multiple stressors and contribute to developing a transferable model for evaluating and managing the ecological health of Mediterranean transitional environments affected by anthropogenic pressures and climate changes.

Keywords: Lagoon ecosystems; Ecotoxicology; Biodiversity; Biomarkers; Chemical pollution; Environmental risk assessment.

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Analysis of heat transport in rough rock fractures under multiple surface roughness

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ABSTRACT

This study focuses on the influence of fracture surface geometry on heat transfer in saturated rocks, a key aspect for the development and management of deep geothermal energy. We study the response to a cold temperature pulse injection under different roughness scenarios, by means of analytical solutions and numerical simulations on synthetic and real fractures aperture fields. Results reveal that fracture roughness considerably influences heat transport and that the behavior is sensitive to variations of the fracture aperture field due to the activation of relative sliding between the fractures surfaces. Analytical results estimated on synthetic fractures with sinusoidal profiles exhibit distinct breakthrough curves depending on the relative sliding between surfaces. Larger slips lead to aperture fields with larger averages and distributed over a wider range of values, which results in earlier peak temperatures due to a dominant advective behavior. The tailing of the breakthrough curves shows a transient slope value of -1.4, which evolves toward an asymptotic behavior with a characteristic -1.5 slope over long timescales, confirming that diffusive exchange governs in the long term. In the final phase of this work, this behavior will be compared against results from numerical simulations on real aperture fields generated from scanned rough granite surface.

Keywords: heat transfer, rock fracture, surface roughness, numerical model, fluid flow.

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Effect Directed Analysis on Microbial Communities as Indicators of Chemical and Ecotoxicological Quality Status of the Aquatic Environment

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ABSTRACT

In aquatic environments, emerging contaminants rarely occur as single compounds. Rather, they exist as complex mixtures that may pose significant ecological and human health risks, even at trace concentrations. Traditional monitoring approaches often fail to capture the combined effects of these mixtures or to identify the key chemicals responsible for ecosystem impairment. Effect-Directed Analysis (EDA) is a cutting-edge approach that has been successfully used in environmental monitoring. Biofilms, consisting of autotrophic and heterotrophic microorganisms, are highly sensitive to environmental stressors, excellent indicators of ecosystem health, and often considered the smallest functioning unit of aquatic ecosystems. This doctoral research aims to introduces a novel ecologically relevant EDA framework using natural freshwater biofilms as model communities and integrating early responses at the molecular level (metabolomics) to identify toxic chemical contaminants from complex environmental mixtures. The biofilm-based EDA approach incorporates: (i) sample preparation, including extraction of chemical mixtures from environmental samples and fractionation to progressively reduce mixture complexity; (ii) bioassays to evaluate the toxicity of whole extracts and their corresponding fractions; and (iii) advanced chemical analysis to identify toxicants within the whole extract and toxic fractions. By linking bioassay responses with chemical composition, this study seeks to identify key chemical drivers of toxicity, explain observed mixture effects, and prioritize hazardous contaminants contributing to freshwater ecosystem impairment. The project is conducted within the Pharm-ERA Marie Skłodowska-Curie Actions Doctoral Network, which develops innovative concepts and methods to assess the environmental risks of pharmaceuticals, transformation products, antimicrobial resistance, and pathogens across the soil–water–sediment continuum.

Keywords: Biofilms, Effect-Directed Analysis, Complex Chemical Mixtures, Pharmaceuticals, Metabolomics

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Method development for the analysis of per- and polyfluorinated chemicals (PFAS) in human blood. Preliminary results from cohort studies

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ABSTRACT

Per- and polyfluoroalkyl substances (PFASs) have been widely used as surfactants and surface protectors in various industrial products. Their extensive manufacture and usage have caused worldwide occurrence of these compounds in various environmental matrices. Several human biomonitoring studies have confirmed the PFAS presence in human tissues and fluids. This study aims to develop and optimize an analytical method for the analysis of 24 PFASs in human blood samples from cohort studies, and to characterize internal exposure profiles to PFASs in an adult population of Barcelona (Catalonia, Spain) and a birth cohort from Poland.

Keywords: PFAS, internal exposure, human blood, cohort study, birth cohort

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Integrating 3D geological modelling as the foundation for hydrogeological analysis

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ABSTRACT

Climate change and population growth are increasing the pressure on groundwater resources, making their sustainable management more challenging. To build reliable hydrogeological models and guide effective decision-making, it is essential to first establish a solid geological framework. However, numerical hydrogeological models rely on simplified structural assumptions when the structural framework is poorly constrained, leading to significant uncertainties in flow simulations and resource estimations.

Developing a 3D geological model at the basin scale is therefore a fundamental step before numerical modelling. Such models allow a detailed characterization of subsurface geometry, defining aquifers and confining layers, structural controls, and spatial heterogeneity that influence groundwater dynamics. In this study, the geological model will be built using GemPy, an open-source Python-based library for implicit structural geomodelling, supported by GemGIS for geospatial data processing. The model integrates publicly available datasets, including geological maps, borehole lithological records, and complementary data from previous studies.

GemPy applies an implicit potential-field interpolation method, enabling the reconstruction of complex structures such as folds, faults, and unconformities, while ensuring transparency and reproducibility. The resulting 3D geological model will serve as the structural foundation for subsequent hydrogeological modelling, enhancing conceptual reliability and numerical consistency. This open-access and data-driven workflow supports better understanding and management of groundwater systems under increasing climatic and anthropogenic stress.

Keywords: 3D geological modelling, geological framework, groundwater modelling

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Non-target screening and physicochemical profiling of infiltrated chemicals in stormwater biofilters.

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ABSTRACT

Sustainable Urban Drainage Systems (SUDS) are engineered infrastructures developed to mitigate the impacts of urbanization on natural hydrological cycles. Their relevance has increased under climate change conditions, where extreme rainfall events are becoming more frequent, often leading to pollutant mobilization and sewer overflows that degrade surface water quality. While SUDS have shown efficiency in retaining hydrophobic contaminants such as polycyclic aromatic hydrocarbons (PAHs), understanding of their behavior toward more polar, LC-amenable compounds remains limited. In this study, stormwater samples were collected upstream and downstream of a SUDS installation to assess its performance in removing a wide spectrum of contaminants. A non-target analysis (NTA) was conducted following sample pre-concentration via Vacuum-Assisted Extraction (VAE) and analysis using an Orbitrap Eclipse™ Tribrid™ Mass Spectrometer. More than 12,000 molecular features were detected through high-resolution mass spectrometry. Roughly half of these features showed statistically significant reductions in the effluent, demonstrating effective retention by the SUDS. In contrast, approximately 1,500 features increased in intensity, suggesting release from the substrate or formation of transformation products (TPs). Compounds exhibiting no significant change were primarily polar analytes, indicating limited removal. Using mass spectral libraries and in silico fragmentation, over 200 contaminants were tentatively identified. This work highlights the potential of NTA to elucidate contaminant dynamics in SUDS, providing insight into both parent compound removal and transformation processes, and emphasizing the need for long-term evaluations of SUDS performance in mitigating emerging contaminants.

Keywords: Sustainable Urban Drainage Systems (SUDS); stormwater runoff; non-target analysis (NTA); high-resolution mass spectrometry (HRMS)