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SESSION 1

Oral communications





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Beyond yield: soil microbial and metabolic responses to biosolid-based fertilization across contrasting soil textures

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ABSTRACT

Biosolid-derived amendments offer a strategy for nutrient recycling in agriculture, but their effects on soil microbial communities and crop performance may vary with soil properties. This study investigated wheat (*Triticum aestivum* cv. Jabalcón) responses to biosolid-based fertilization in sandy and silty clay loam (SCL) soils over a 140-day greenhouse experiment. Five treatments were compared: raw biosolid, biosolid amended with 10% biochar, biosolid-derived compost, inorganic fertilizer, and an unfertilized control. Plant growth, chlorophyll content, grain and straw yield, and seed protein concentration were assessed alongside soil bacterial community composition and flag-leaf metabolomic profiles.

Soil texture strongly influenced treatment responses. In sandy soil, all fertilized treatments showed similar grain and straw yields, chlorophyll content, and seed protein concentrations, with relatively limited differences in bacterial community composition among amendments, although microbial shifts were more pronounced compared with the unfertilized control. In SCL soil, microbial restructuring was more pronounced, particularly under compost, which increased the relative abundance of *Bacillota* and *Bacteroidota*. However, stronger microbial shifts did not translate into proportionally greater crop productivity: compost and inorganic fertilizer achieved similar mean grain yields, while raw biosolid produced the highest mean seed protein concentration. Metabolomic profiles also differed between soil types, revealing distinct plant responses despite comparable yields under some treatments.

These findings indicate that microbial community composition, plant physiology, metabolism, and crop productivity are only partially coupled, with soil texture shaping their relationships. Integrating soil microbial and plant responses may therefore provide a more comprehensive assessment of biosolid-derived amendments than crop yield alone, supporting soil-specific approaches to sustainable nutrient recycling.

Keywords: Biosolid-derived amendments; soil texture; wheat; soil microbiome; metabolomics; circular economy.

Modelling and characterization of Groundwater Resources in Densely Populated Urban Areas

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Groundwater plays a key role as an alternative drinking water resource, especially in urban areas facing water scarcity issues and where existing supplies are threatened by discharges from anthropogenic sources. In this context, the combination of numerical models with groundwater-monitoring sensors provides powerful tools for predicting the behaviour of contaminants in urban aquifers, determining when and how groundwater can be safely used to meet growing demands. Previous studies typically develop models based on historical data and do not integrate real-time sensor data for model validation and improvement.

In this research, we develop and apply monitoring techniques to characterise aquifer conditions in Sant Adrià del Besòs, deploying multiple sensor types across approximately twenty (20) observation wells. Through a cross-sectional study, we explore the potential of using this sensor data for the early detection of contaminants in the studied water body.

This study aims to: (i) develop a detailed three-dimensional model of specific contaminants, incorporating the main processes controlling their evolution in the aquifer; and (ii) establish a workflow to integrate measured data into the numerical model, improving its realism. A combined qualitative and quantitative approach will enhance the model's representativeness via detailed hydrogeological characterisation. For the numerical groundwater model, flow processes will be simulated by MODFLOW, while the PHT3D (or PHAST) code will simulate chemical evolution and reactive transport processes.

Finally, this research will significantly enhance our comprehension of contaminant transport dynamics in urban groundwater. Evaluating these dispersion patterns contributes fundamentally to broader environmental impact assessments.

Keywords: Groundwater Monitoring, Hydrogeological Characterization, Real-time Sensor Data, Three-dimensional Transport Model, Urban Water Quality.

Acknowledgements: This research is part of the UrbanM2O project, which is funded by the Horizon Europe research and innovation program (grant no. 101180710) and by the Swiss State Secretariat for Education, Research, and Innovation (SERI).

Elemental Characterization of Food-Smoking Materials and Their Particulate Emissions: Towards an Integrated Assessment of Exposure and Toxicity

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ABSTRACT

Biomass burning contaminants are a major concern for environmental quality and human health. Indoor emissions from household biomass combustion are classified by the International Agency for Research on Cancer (IARC) as probably carcinogenic (Group 2A), and outdoor air particulate matter (PM) as carcinogenic (Group 1). This research develops integrated analytical approaches to characterize biomass combustion emissions and assess exposure, focusing on scarcely investigated sources such as food smoking.

The elemental composition of 50 food-smoking materials and of their emissions was determined by ICP-MS targeting 40 elements. Emitted PM was collected on filters and monitored in real time by size fraction; morphology was assessed by HR-SEM. Emissions consisted mainly of respirable fine particles. The starting materials displayed a typical biomass-derived elemental signature enriched with Ca, Mg and K, whereas emitted PM showed a markedly different profile driven by volatilization and subsequent condensation processes. Significant fuel-to-PM correlations were found for Li, K, Rb, Cs, Tl and Pb, with K, Rb and Cs acting as established tracers of biomass burning. Potentially toxic elements (Cd, Cr, Pb) were also quantified.

Because elemental characterization alone cannot capture the full potential health hazards of combustion emissions, ongoing work investigates the organic fraction of PM, particularly polycyclic aromatic hydrocarbons (PAHs) and related compounds, alongside cytotoxicity testing in A549 human lung epithelial cells. Integrating inorganic and organic chemical signatures with cellular responses will provide a more comprehensive basis for exposure evaluation and risk assessment.

Acknowledgements: Funded by Sapienza University of Rome (projects 2023 and 2025; grants RM123188F73F6255, AR125199C0876C2A).

Keywords: Biomass burning; Food smoking; Particulate matter; Toxic elements; ICP-MS

Potential human exposure to heavy metals by users of installations with crumb rubber flooring

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ABSTRACT

The production of ground tire rubber (GTR) is one of the most relevant industries of rubber reclamation worldwide, and a common use of GTR is the creation of crumb rubber flooring, typically found in infant playgrounds and sport facilities. The degradation of these surfaces produces rubber particles, some of which are small enough to enter the respiratory tract if resuspended (PM_{10}).

Samples of surface and airborne PM_{10} were taken from different installations with crumb rubber flooring in the city of Barcelona. Concentrations of 57 different inorganic components were tested, including several heavy metals present in GTR, like Co, Cu, or Zn, with concentrations up to 2.63 mg/g found of the latter in surface dust, comparable to levels found in Barcelona road dust.

An oxidative potential (OP) test was performed to check the ability of the samples studied to oxidize relevant antioxidant molecules present in respiratory tract lining fluid. The best correlation was found between Zn concentration and OP, indicating that this metal is redox active in this matrix and could damage the lungs if inhaled.

Although heavy metal concentrations found in airborne PM_{10} were much lower than in surface dust, their resuspension can follow complicated patterns, as user activity can generate events of high resuspension that cannot be monitored accurately with routine air sampling. Further studies are required to determine the severity of this exposure route to heavy metals in these urban areas with high physical activity, and other exposure pathways like ingestion or dermal contact.

Keywords: heavy metals, playgrounds, tire rubber, PM_{10}, zinc, oxidative potential

Stream-level prioritisation of critical raw material recovery opportunities under different recycling conditions in an industrial copper smelter

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ABSTRACT

Internal recycling in copper smelting maximises metal recovery and minimises waste generation but may also modify the circulation of valuable and deleterious elements. This study develops a stream-level methodology to prioritise secondary streams for Critical Raw Material (CRM) recovery using industrial data from Flash Smelting Furnace (FSF), Electric Furnace (EF), and converting operations. Sampling campaigns at an industrial Cu smelter covered three sustained operating regimes defined by converter electrostatic precipitator (ESP) dust recycling: S0, without recycling (January–December 2019); SP, with 60–70% recycling (February 2020–January 2021); and S100, with 100% recycling (February 2021–January 2022). Six secondary streams were evaluated using the FSF feed composition as the reference for calculating element-specific enrichment factors (EF), which were subsequently log-transformed and min–max normalised.

Two dimensions were defined: recovery valorisation potential (V_{rec}), based on Cu, Co, Sb, and Bi, and metallurgical burden (P_{met}), based on As and Pb. Both were integrated into a stream-level criticality index (IC), while mass-flow data provided independent evidence. Robustness was evaluated through 567 weighting scenarios. Converter ESP dust showed the highest baseline IC (0.750) and ranked first in 92.4% of sensitivity scenarios. Under S100 conditions, this stream showed strong enrichment in Bi (EF_{Bi} = 286), As (EF_{As} = 35), and Sb (EF_{Sb} = 4.2). Its annual generation (1240 $t \cdot y^{-1}$) corresponds to estimated loads of 41.6 $t \cdot y^{-1}$ Bi and 37.0 $t \cdot y^{-1}$ As. Integration of valorisation potential and metallurgical burden into IC, supported by ranking robustness, identified converter ESP dust as the priority stream for subsequent CRM recovery studies.

Keywords: Copper smelting; Critical raw materials; ESP dust; Internal recycling; Enrichment factor; Stream prioritization.

Atmospheric inputs of persistent organic pollutants from a former chlor-alkali plant in the Ebro River after completion of remediation activities

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ABSTRACT

Persistent organic pollutants (POPs), including polychlorinated biphenyls (PCBs) and organochlorine pesticides, were extensively synthesized in most of the 20th century. In Spain, one of the largest manufacturing facilities was located in Flix, a town along the lower Ebro River. During the years of manufacture, the chlor-alkali plant discharged more than 5×10^5 t of industrial waste into the Flix Reservoir, resulting in extensive contamination of the reservoir and downstream river reaches. An environmental remediation programme for the removal of the industrial waste was implemented in 2010, with dredging of the polluted sediments completed in 2023.

In this study, current atmospheric concentrations of organochlorine compounds (OCs) from the former industrial site were assessed using olive tree (Olea europaea) leaves, as a passive air sampler, collected along concentric transects up to 40 km from the facility. Strong evidence of contamination associated with the former chlor-alkali plant was found for hexachlorobenzene (HCB), octachlorostyrene, p,p'-DDT, o,p'-DDE, p,p'-DDE, and PCB congeners 101, 138, 153, and 180. Results were compared with those from a similar study conducted in 2006, before polluted sediment dredging. Notably, HCB concentrations decreased by approximately one order of magnitude in 20 years. The estimated area of influence contracted from around 15 km to 5 km. A potential secondary emission source was also identified 4 km north of the facility, coinciding with a historical industrial waste disposal site.

Overall, the results indicate a substantial decline in atmospheric inputs of OCs following remediation of the Flix Reservoir. However, legacy contamination associated with the former chlor-alkali plant remain a source of atmospheric POPs in the area.

Keywords: PCBs, OCPs, Leaves, Air

Reactive Barriers Modulate Contaminant Remobilization Under Abrupt Conductivity Changes in Soil Aquifer Treatment

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ABSTRACT

Soil Aquifer Treatment (SAT) improves reclaimed-water quality through contaminant attenuation during infiltration. However, contaminants retained in the porous medium may be remobilized when influent hydrochemistry changes. This study investigated how abrupt shifts in electrical conductivity affect contaminant retention and whether reactive materials modify the response of SAT systems to these perturbations.

Six columns were operated for five weeks with secondary effluent from the Sant Feliu de Llobregat WWTP (Barcelona, Spain). Three columns contained sand, whereas three were filled with a reactive mixture of compost, biochar, woodchips, clay, zeolite and sand. After this baseline phase, one sand/reactive-barrier pair continued receiving untreated effluent as a control, a second pair received effluent mixed with Milli-Q water to decrease ionic strength, and the third received effluent mixed with seawater to increase it. Physicochemical parameters, contaminants of emerging concern (CECs), culturable and molecular *Escherichia coli*, somatic coliphages, sulfite-reducing *Clostridium* spores, and antibiotic resistance genes (*blaTEM*, *sul1*, and *tetW*) were monitored. At the end of the experiment, the filling materials were extracted and analyzed to assess contaminant retention.

Abrupt conductivity changes caused transient declines in treatment performance and promoted the remobilization of previously retained contaminants, particularly when conductivity decreased. The response varied with contaminant type and porous-medium composition, showing that retention under stable operation does not necessarily imply permanent removal. These findings demonstrate that both reactive-barrier design and influent hydrochemical variability must be considered to ensure robust SAT performance and minimize transient contaminant breakthrough.

Keywords: Managed aquifer recharge, contaminant remobilization; electrical conductivity; transient breakthrough



SESSION 2

Oral communications





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Single-pore representation of coupling between evaporation and salt precipitation

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ABSTRACT

Drying of brine in porous materials is a fascinating nonlinear problem involving evaporation, solute and vapor transport, and precipitation reaction which alters the pore geometry, affecting further evaporation, transport and reactions. It has crucial implications on soils, carbon subsurface storage, and building materials. How precipitation affects evaporation remains unknown, impeding our ability to model brine drying. To bridge this gap, I aim to establish a constitutive relationship between salt precipitation and evaporation rate (E), which will then allow me to upscale (using pore-network modeling). This is achieved by an idealized, highly-controlled microfluidic experiment using time-lapse imaging: brine is dried (by nitrogen purging) in a single-channel ("pore") from a pinned meniscus (where crystallization occurs), causing a second meniscus to recede (where we measure E).

Before precipitation, we observe a gradual decrease in E, explained by an osmotic effect. Precipitation occurs at high supersaturation, triggering nucleation away from the evaporating meniscus, followed by rapid crystal growth. During this period, E increases abruptly, probably due to rapid consumption of salt by the growing crystal. Subsequent salt growth progressively limits liquid transport, eventually causing the recession of the evaporating meniscus and a substantial decrease in drying rate due to increased vapor diffusion length. After this point, E decreases linearly with salt thickness, noting the slope differs as the salt morphology changes from large crystals with well-defined surfaces to smaller crystal aggregates. Our promising findings point to the strength of this approach in elucidating the underlying physics required for modeling evaporation-induced salt precipitation.

Keywords: evaporation, salt precipitation, microfluidics, pore scale, reactive transport

Application of CPxplorer: An Open-Source Quantification Tool for Polychlorinated Alkanes and Chlorinated Paraffins Compounds

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ABSTRACT

Polychlorinated alkanes (PCAs) are the main component of Chlorinated Paraffins (CPs), commonly classified by chain length into short-chain (SCCPs, ∑PCAs-C_{10-13}), medium-chain (MCCPs, ∑PCAs-C_{14-17}) and long-chain (LCCPs, ∑PCAs-$C_{>18}$). Due to their persistence and toxicity, SCCPs and MCCPs were listed under Annex A of the Stockholm Convention in 2017 and 2025, respectively [1]. However, PCA analysis faces substantial analytical challenges. CP mixtures contain thousands of chromatographically unseparated isomers with overlapping m/z ratios and co-eluting interferences unresolved by low-resolution mass spectrometry. Furthermore, environmental sample accumulation patterns do not match those of commercial standards, heavily impacting quantification accuracy [2]. While deconvolution-based strategies using high-resolution mass spectrometry resolve these issues by reconstructing sample-matched patterns from congener response factors [3], [4], the underlying method complexity continues to deter many laboratories from undertaking PCA analysis. Moreover, different laboratories choose different quantification strategies and the standardization and comparison of results is a major challenge. To lower this technical barrier, we present CPxplorer [5]: an open-source, user-friendly software toolbox for the rapid deconvolution-based quantification of PCAs. CPxplorer allows processessing raw data from multiple instrument vendors without requiring prior file conversion, and features an interactive graphical interface to assess patterns and quantification quality. By presenting how this software simplifies complex HRMS data processing for PCA quantification, we encourage other research groups to utilize CPxplorer to overcome historical analytical hurdles and routinely integrate PCA analysis into their workflows.

Keywords: Chlorinated paraffins (CPs), Polychlorinated alkanes (PCAs), Open-source tools, High-resolution mass spectrometry (HRMS), Persistent organic pollutants (POPs), CPxplorer.

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Organic pollutants in diverse types of sediments from a tropical Reef System of the Southern Gulf of Mexico

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ABSTRACT

The Veracruz Reef System is located off the coast of Veracruz in the southern Gulf of Mexico. It is a Ramsar site and biosphere reserve with significant biological, tourism, and economic importance. Anthropogenic activities (port activity and agriculture), river discharges, and marine and coastal currents introduce several pollutants. Polycyclic Aromatic Hydrocarbons (PAHs) enter the environment from both natural sources and anthropogenic activities (oil industry or the burning of fossil fuels). Plasticizers include bisphenols (BPs) and phthalates (PAES), used as plastic additives to provide strength, transparency, and flexibility (e.g., plastic bottles, food containers, and toys). These pollutants are toxic and endocrine disruptors to organisms and humans; they tend to accumulate in sediments and aquatic organisms due to their affinity for organic matrices. Therefore, it is important to determine their presence in matrices such as sediments. Using GC-MS/MS, concentrations of PAHs, BPs, and PAES were determined in surface and trap sediments and sediment cores. The concentrations ranged from <detection limit (DL) to 836 ng/g, 7.0 × 10^{-2} to 1.35 ng/g, and 0.18 to 4.59×10^{3} ng/g for surface sediments, <DL and 78 ng $g^{-1}$and 0.12 to 3.17 × 103 ng/g for trap sediments, and <DL and 60 ng g^{-1}, not detected to 1.19 µg/g for sediment cores for HAP, BPs and PAES respectively; BPs are not included for trap sediments and sediments core. Likewise, mean hazard risk (M-HQ) for benthic organisms for each contaminant family was calculated, finding low risk for BPs, medium to high risk for PAEs, and medium risk for PAHs.

Maximum 250 words.

Keywords: PAHs, Bisphenols, PAES, reef sediments, Gulf of Mexico, hazard risk.

Towards ecologically relevant effect-directed analysis: a periphytic biofilm bioassay for complex contaminant mixtures

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ABSTRACT

Complex mixtures of organic contaminants in surface waters may pose ecological risks even at trace levels, yet conventional monitoring rarely captures mixture effects or identifies their drivers. Effect-Directed Analysis (EDA) links observed effects to causative chemicals but relies mainly on in vitro or single-species bioassays. This doctoral work develops an ecologically relevant EDA approach using freshwater periphytic biofilms as the biological screening tool. Initially, sample preparation was optimized using a model mixture of 81 compounds, with CHROMABOND® HR-X selected as the preferred solid-phase extraction sorbent based on its broad compound coverage and high extraction recovery performance. A UHPLC-HRMS/MS method was optimized for target and future suspect screening, detecting all 81 compounds. A UHPLC fractionation method was also developed to separate extracts into 40 fractions of same volume. Next, river biofilms grown in natural condition at artificial channels were exposed to a simplified 9-compound mixture and to the 81-compound mixture (eight nominal concentrations, 0–100 µg/L; 4–72 h). To capture community responses at different levels, structural (phototroph community composition), functional (photosynthetic efficiency, extracellular enzymes, community respiration) and molecular (meta-metabolomics) endpoints were measured. Photosynthetic efficiency was the most sensitive endpoint, with EC10 values of 0.07–0.49 µg/L for the simplified mixture and 18.2–1.1 µg/L over 4–72 h for the 81-compound mixture, suggesting mixture interactions that EDA can help resolve. Leucine-aminopeptidase was inhibited at 30 and 100 µg/L after 4 h, while other enzymes and phototroph community composition showed no significant concentration-dependent response within 72 h. These findings suggest the potential of functional endpoints, supporting their further evaluation through the integration of bioassays coupled with fractionation, and LC-HRMS/MS to identify potential drivers of mixture toxicity.

Keywords:

Effect-Directed Analysis; Periphytic biofilms; Bioassay, Chemical mixtures; Ecological relevance

Hydrochemical source apportionment and contaminant transfer pathways in a Mediterranean urban aquifer under drought recovery conditions

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ABSTRACT

Groundwater is an increasingly strategic resource in drought-prone Mediterranean regions, yet recharge pathways and contaminant transport in urban aquifers remain poorly constrained because natural and anthropogenic sources exhibit overlapping hydrochemical signatures. We applied an enhanced open-source mixing framework (SOUPY) integrating hydrochemical and isotopic tracers to quantify recharge-source contributions across the Besòs Delta aquifer (Barcelona, Spain) during the transition from prolonged drought to hydrological recovery. SOUPY explicitly incorporates end-member uncertainty and quantifies uncertainty in the inferred mixing proportions through stochastic ensemble optimization. River-derived recharge was identified as the dominant inferred recharge source contributing to groundwater composition (59 ± 7%), followed by natural recharge (26 ± 7%), whereas the remaining sources contributed only minor fractions. Although direct urban runoff represented only a minor recharge component, the inclusion of the semi-conservative tracers Zn and Cu enabled the model to resolve hydroclimatically driven changes in recharge-source composition, revealing a marked shift from dry-season to wet-season river recharge following drought recovery. Ecotoxicological assesment identified urban runoff as the principal Zn source and river–aquifer interactions as its dominant transfer pathway to groundwater, making Zn the primary ecological risk driver. Overall, the results demonstrate that river–aquifer interactions control both recharge dynamics and contaminant transport under changing hydroclimatic conditions. The proposed framework provides a transferable, uncertainty-aware approach for investigating recharge dynamics and contaminant pathways in complex urban aquifers across Mediterranean settings.

Keywords: Urban groundwater, SOUPY, source apportionment, uncertainty analysis, ecotoxicological risk.



SESSION 3

Oral communications





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Abstract title

Quantitative evaluation of governance options for groundwater-quality improvement in an urban coastal multilayer aquifer: the Besòs River Delta case study

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ABSTRACT

Groundwater is an increasingly strategic resource for water security, particularly under growing water demand and more frequent droughts associated with climate change. However, many aquifer systems are affected by significant water-quality degradation. The multilayer aquifer of the Besòs River delta (Barcelona) is a representative example, having been historically subjected to intense urban and industrial pressures and affected by a range of contaminants, including contaminants of emerging concern.

To evaluate potential recovery strategies, a calibrated three-dimensional groundwater flow and transport model was used to represent the multilayer aquifer system and river–aquifer interactions. Six Governance and Policy Options were implemented by modifying recharge, groundwater abstraction, river–aquifer exchange and the quality of the introduced water. The strategies combined managed aquifer recharge through infiltration wells, direct infiltration, advanced oxidation processes, nature-based solutions based on constructed wetlands, and groundwater abstraction control. Their performance was evaluated using a normalised groundwater-quality improvement indicator.

The results show that strategies combining Managed Aquifer Recharge with advanced treatment or nature-based solutions produced the greatest groundwater-quality

improvements, whereas strategies based mainly on improving river discharges produced more limited effects. The spatial analysis further showed that the hydraulic configuration of recharge and the pathway through which higher-quality water enters the aquifer strongly influence the groundwater response.

This study provides a quantitative and transferable methodological framework for prioritising recovery interventions in complex aquifer systems subjected to anthropogenic pressure.

Keywords: Managed aquifer recharge; groundwater quality; numerical modelling; nature-based solutions; river–aquifer interactions; urban aquifers.

Biomonitoring of Bisphenols in Canine Hair from the Land of Fires (Southern Italy) Using LC-MS/MS within a One Health Framework

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ABSTRACT

Environmental exposure to endocrine-disrupting chemicals (EDCs) represents an emerging concern within the One Health framework, highlighting the interconnectedness of environmental, animal, and human health. Among these contaminants, bisphenols are widely used in industrial and consumer products and are ubiquitously distributed in the environment. Domestic and stray dogs (*Canis familiaris*), sharing environmental conditions with humans, may serve as sentinel species for assessing exposure to these compounds.

This study investigates the occurrence of bisphenols in canine hair collected from the *Land of Fires*, a highly anthropized area in Southern Italy affected by longstanding environmental contamination. Unlike conventional biological matrices, such as blood and urine, hair offers a non-invasive sampling approach and the potential to reflect cumulative exposure over extended periods, providing complementary information on environmental contaminant exposure.

Hair samples from 25 dogs are processed using an adapted extraction procedure involving sequential washing with ultrapure water and sodium dodecyl sulfate (0.1%), followed by methanol/acetic acid extraction and ultrasonic treatment with acetone.[1]

Bisphenols are determined by liquid chromatography coupled with triple quadrupole

tandem mass spectrometry (LC-MS/MS), operating in Multiple Reaction Monitoring (MRM) mode, enabling highly sensitive and selective detection of the target compounds. By exploring canine hair as a biomonitoring matrix, this investigation aims to contribute to the assessment of environmental exposure to EDCs and support the potential role of dogs as sentinel organisms within a One Health perspective, providing a basis for future integrated environmental and health monitoring strategies.

Keywords: Canine hair, Environmental biomonitoring, Bisphenols, LC-MS/MS

Reference:

1. Makowska, K., et al. (2022). Hair sample analysis as a method of monitoring exposure to bisphenol A in dogs. International Journal of Environmental Research and Public Health, 19(8), 4600. https://doi.org/10.3390/ijerph19084600

Neural Operators for Thermal Front Propagation in Heterogeneous Geothermal Reservoirs

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Current field work: Geostorage and geoenergy. Surrogate modelling of heat transport in deep geothermal reservoirs with neural operators (scientific machine learning).
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ABSTRACT

Deep geothermal systems inject cold water into hot rock and recover it heated at a production well. In heterogeneous reservoirs the flow concentrates along high-permeability paths, and the cooled region advances as a sharp, irregular thermal front whose arrival at the production well limits the system's lifetime. Forecasting it under uncertainty requires many simulations, motivating fast surrogate models. We evaluate Fourier and wavelet neural operators and DeepONet as surrogates of finite-element simulations of heat transport over stochastic permeability fields in three Péclet regimes. The models predict the temperature field from one snapshot to the next and are applied recursively, each prediction becoming the next input. We test three modifications, each acting on a different model component: a basis localised in space and frequency, a Sobolev penalty on spatial gradients in the loss, and the pressure field as an additional input. Since global error norms cannot distinguish a blurred front from a displaced one, we introduce metrics that separate front sharpness, oscillation and position. The prediction splits into two phases. With exact inputs, the models form the front accurately and the localised basis resolves it best. Once they consume their own outputs, errors compound, the ranking of architectures reverses and none of the modifications helps. Training each step on the previous prediction instead of the reference field (pushforward training) reduces the final error an order of magnitude more than any modification. The limiting factor is not how the front is formed but how it is propagated.

Keywords: neural operators; surrogate modelling; autoregressive prediction; geothermal reservoirs; thermal front; heterogeneous porous media

Contribution of sources to the oxidative potential (OP) of particulate matter (PM) in Barcelona: 2018-2024

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ABSTRACT

This study quantified the contribution of sources to the oxidative potential (OP) of particulate matter (PM) in Barcelona over 2018-2024. More than 2,000 PM_{10}, $PM_{2.5}$ and PM_1 filters, collected every three days at an urban background station, were chemically characterized. Source apportionment was performed with Positive Matrix Factorization (PMF) for PM_{10}, $PM_{2.5}$, PM_1 and PM_{Coarse} (PM_{1-10}). OP was measured using ascorbic acid (AA) and dithiothreitol (DTT) assays, and source contributions to OP were estimated using the University Grenoble Alps regression toolbox, which selects the optimal model. OP of PM_{10} was also used to derive contributions for the coarse and fine fractions. The results showed that PM_{10} and $PM_{2.5}$ had very similar source contributions to OP. Separating PM_{10} into a fine fraction (PM_1) and a coarse fraction (PM_{Coarse}) allowed for a more precise identification of the sources driving OP. Anthropogenic sources were the main contributors, namely traffic, industrial emissions, and anthropogenic mineral dust. Within traffic, non-exhaust emissions contributed more to OP than exhaust emissions, making them the leading source overall. Cement plants were the second most important source of OP, as measured using DTT. These findings confirm that the sources driving OP differ from those driving PM mass, which supports OP as a complementary metric for air quality assessment and future epidemiological studies.

Keywords: Air quality, particulate matter, geochemistry, oxidative potential, source apportionment



SESSION 1

Flash presentations





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Hydrogeological controls on PFAS distribution in an urban-industrial alluvial aquifer: insights from the Ripoll River basin, northeastern Spain

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ABSTRACT

Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants of increasing concern in groundwater systems affected by urban and industrial activities. Understanding their distribution and mobility in heterogeneous alluvial aquifers requires considering both contaminant composition and transient hydrogeological conditions. This study investigates PFAS occurrence and potential hydrogeological controls in an urban-industrial sector of the Ripoll River basin, northeastern Spain. The study integrates two sampling campaigns (October 2025 and March 2026) at nine groundwater wells, the Ripoll River and an adjacent drainage channel, with hydrochemical analyses, stable isotopes and continuous groundwater-level monitoring.

Preliminary results reveal a consistent hydrogeological differentiation among wells. Isotopic compositions identify a group with characteristics similar to those of the river; the groundwater levels in these wells are particularly sensitive to river-stage fluctuations. This differentiation is also reflected in major-ion composition. Principal Component Analysis (PCA) of the detected PFAS provides complementary evidence: principal component analysis identifies compositional patterns dominated by short-chain carboxylates and by PFPeS and PFHxS, while the river-associated group exhibits higher PC1 scores during the October campaign. Exploratory correlations also suggest associations between short-chain PFAS and dissolved Na and K.

Together, these preliminary findings support the hypothesis that hydrogeological connectivity and groundwater dynamics influence PFAS distribution across the study area. Further integration of hydraulic and chemical data will help refine this conceptual model and guide future groundwater flow and contaminant transport modelling.

Keywords: PFAS; alluvial aquifer; hydrogeological connectivity; groundwater–surface water interaction; contaminant transport.

Assessing Benzodiazepine Consumption in Two Catalan Cities by Integrating Wastewater Analysis and Health Data

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ABSTRACT

Benzodiazepines (BZDs) are among the most prescribed psychoactive medications worldwide and are extensively used for the treatment of anxiety disorders, insomnia, epilepsy, and alcohol withdrawal. Spain remains one of the European countries with the highest levels of BZD consumption, highlighting the need for monitoring approaches beyond prescription data. In this context, wastewater-based epidemiology (WBE) represents a promising tool for assessing population-level drug consumption.

This study evaluated BZD use in the metropolitan area of Barcelona and the city of Lleida between 2014 and 2022 by integrating WBE data with conventional public health indicators. Wastewater samples from three WWTPs (Prat, Besòs, and Lleida) were analyzed for selected benzodiazepines: alprazolam, diazepam, lorazepam, oxazepam, and temazepam. Wastewater-derived loads were compared with prescription data (DHD), hospital emergency admissions related to psychoactive substances, mortality from acute reactions to psychoactive substances, and population survey data on hypnosedative use.

Overall, wastewater results indicated an increasing trend in BZD consumption over the study period, with a pronounced decline during the COVID-19 period followed by recovery in subsequent years. Lorazepam was the dominant compound in both wastewater and prescription datasets and showed particularly high consumption among women and older adults. Hospital emergencies related to hypnosedative use increased during the study period, whereas BZD-related mortality showed a declining trend. Correlation analyses revealed stronger associations between wastewater-derived loads and emergency admissions, while stronger associations were observed with mortality and prescription-based consumption indicators.

These findings support the value of WBE as a complementary approach for monitoring benzodiazepine use and improving the assessment of its public health impact.

Keywords: Benzodiazepines (BZDs), Wastewater-Based Epidemiology (WBE), Drug consumption, Public health indicators.

Experimental Analysis of Dispersion and Mixing in 3d Darcy scale Porous Media

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ABSTRACT

We study the impact of heterogeneity on dispersion and mixing in darcy scale porous media. Mixing in porous media is the process from which the homogenization of an initially segregated system is done. It is a key process for a vast type of applications, from ground remediation methods to numerous engineering applications where the facilitation of chemical reactions is needed. This process is the result of the interaction of spatial velocity fluctuations and diffusion or local-scale dispersion. The velocity fluctuations are induced by spatial medium heterogeneities at the Darcy scale which can enhance mixing but has to be strictly distinguished from it. This work is based on laboratory experiments and theoretical modeling. Pull experiments were performed where a point injection solute is pulled from bottom to top into the porous medium (sand) and visualized with a high resolution camera. Uniform and heterogeneous media are compared. The heterogeneity is obtained by adding finer grains in inclusion regions that upscale to a lower permeability region thus creating heterogneity in the flow on the Darcy scale. The advantage of this novel pull technique is that concentration can be measured outside the porous medium. Making high-resolution concentration sampling possible such that the concentration pdf can be accurately reconstructed. The first observation we make is that homogeneous media always hide heterogeneous signatures of transport behaviors. Heterogeneous media is analyzed thanks to the lamella theory.

Keywords: Mixing, Dispersion, Non-chaotic mixing

Identifying contaminants of emerging concern in urban and rural aquifers: a suspect screening-based approach.

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ABSTRACT

The pressure over the drinking water sources is drastically increasing due to the impact of climate change and water demand. Groundwater has positioned as an important alternative resource to improve the resilience of supply systems, however the presence of contaminants of emerging concern (CECs) threats its potential use. This study applied a suspect screening (SS) workflow to identify CECs in rural (Osona) and urban (Barcelona) aquifers of Catalonia, Spain.

Groundwater samples were cleaned up, pre-concentrated and analyzed by RP-UHPLC–Orbitrap HRMS (ESI±, Full Scan/DDA). Data processing included mass error (±5 ppm), S/N >3, peak area ≥10^6, sample-to-blank ratio >5, and isotopic fit ≥70% in the Compound Discoverer software. Compound annotation relied on mzCloud MS/MS matching (Level 2a) and suspect databases combined with *in-silico* fragmentation and manual verification (Level 3).

In rural groundwater, 139 and 153 annotation records were obtained in two sampling campaigns, including 63 and 50 Level 2a identifications, respectively. Thirteen probable structures were shared, including herbicides and transformation products such as metolachlor ESA and 2-hydroxyatrazine. In urban groundwater, 89 compounds were tentatively annotated across nine sampling locations and six campaigns, with 42 (47%) consistently detected. Industrial compounds like N,N'-Diphenylguanidine and triethyl phosphate showed high frequency detections. Temporal variability was evident, with average detections increasing from 55.1 in C3 to 65.4 in C4. Overall, SS revealed complex mixtures of anthropogenic CECs in groundwater, demonstrating its value for identifying harmful contaminants and prioritizing future research on their sources and environmental fate.

Keywords: Groundwater; Urban/Rural aquifers; Contaminants of emerging concern; Suspected Screening.

Modeling Redox Dynamics in an Urban Aquifer Located in the Besòs River Delta

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ABSTRACT

In the face of increasingly frequent periods of water scarcity, urban groundwater represents an alternative resource to help meet the demand for freshwater. However, urban aquifers are vulnerable to contamination by a wide range of organic substances, including pharmaceutical compounds, personal care products, industrial chemicals, and/or per- and polyfluoroalkyl substances (PFAS). In this context, it is essential to investigate the processes that control the behaviour of these contaminants in aquifers in order to determine when and how urban groundwater can be safely consumed.

A previous study conducted in the shallow aquifer of the Besòs River delta, within the municipality of Sant Adrià del Besòs, identified the influence of the aquifer's redox state on the evolution of certain PFAS. However, the main findings of that study were qualitative. The present work aims to take a step further by quantifying, through numerical modeling, the evolution of PFAS and other organic substances while considering the hydrochemical conditions of the aquifer.

In 2024, a sampling campaign was carried out in the study area, consisting of weekly collection of two river water samples and nine groundwater samples over a period of one and a half months. The hydrochemical data obtained have been used to develop and calibrate a reactive transport model using the PHT3D code, allowing the estimation of kinetic parameters that control the behaviour of selected organic compounds.

Keywords: CECs, degradation rates, reactive transport



SESSION 2

Flash presentations





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A Probabilistic Screening Tool for Pressure-Constrained CO_2 Storage Capacity with Fault Reactivation Risk under Geological Uncertainty

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ABSTRACT

Geological CO_2 storage is a key component of climate mitigation, yet its large-scale deployment is hampered by the risk of rock failure and fault reactivation, which may compromise storage integrity, and scaling it up to the gigatonne level will require multiple injection sites sharing regional aquifers. In this context highly accurate models are often unfeasible, so faster regional screening tools are needed to enable preliminary techno-economic analyses and identify bottlenecks. Here I present CO2BLOCK2, a MATLAB tool that builds on CO2BLOCK and CO2BLOCKSEISM, so that pressure build-up, stress state and fault reactivation risk are solved together and the maximum injection rate and storage capacity come out directly, without the slow trial-and-error that was needed before. Pressure is calculated with an analytical Nordbotten solution for multiple wells, the critical overpressure of each fault follows from Mohr-Coulomb shear and tensile failure criteria, and faults can be either defined by the user or generated stochastically from a size distribution. Uncertainty in permeability and stress is sampled jointly in a Monte Carlo analysis, which means that each realisation is physically consistent and the results are reported as P10, P50 and P90 values instead of a single number. I illustrate the approach with the Troll aquifer in the Horda Platform, North Sea, showing which fault controls the injection and how the stability of faults limits the volume that can be stored safely, which supports early-stage site selection and injection design.

Keywords: CO_2 storage capacity; fault reactivation; pressure build-up; Monte Carlo uncertainty; saline aquifers; regional screening

Machine Learning framework for groundwater quality prediction in the upper Guadiana basin under climate variability

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ABSTRACT

Understanding the interactions between climate variability and groundwater quality remains a major challenge in arid and semi-arid regions, where aquifers are increasingly affected by altered recharge regimes and more frequent droughts. The aims of these study are to: (i) investigate how climate and groundwater quality linkages and, (ii) propose a data-driven machine learning framework to predict hydrochemical parameters in a pilot catchment of the Upper Guadiana Basin (Spain). Daily climatic variables (maximum and minimum temperature and precipitation) from the Spanish Meteorological Agency were compiled together with hydrochemical data collected between 1978 and 2022, including electrical conductivity, pH, and major ions (HCO_3^-, Cl^-, NO_3^-, SO_4^{2-}, Na^+, Mg^{2+}, Ca^{2+}) measured at ten groundwater sampling points from Guadiana River Basin authority. The proposed methodology analyzes the variability, correlations, and long-term behaviour of the hydrochemical dataset in order to identify which parameters respond most clearly to climate conditions. Subsequently, a climate driven predictive component is constructed using multivariate regression models based on ensemble methods, such as Random Forest. The climate predictors obtained from this step allows the estimation of each hydrochemical variable. The resulting data-driven framework will support the prediction of groundwater quality parameters and the assessment of aquifer sensitivity under contrasting climate scenarios. Beyond its local application, the methodology offers a transferable and efficient approach for groundwater management in regions facing increasing climate stress and contributes to the climate change impact assessments and practical decision-support tools.

Keywords: groundwater quality, climate variability, machine learning, upper Guadiana basin.

Synergistic investigation of Organic Pollutants in the urban Atmosphere

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ABSTRACT

Atmospheric organic aerosol (OA) and volatile organic compounds (VOCs) are major components of urban air pollution, contributing to climate forcing and adverse health effects. Their atmospheric behavior is governed by emission sources, chemical composition, atmospheric processing, and meteorological conditions. OA and VOCs are closely linked through atmospheric chemical processes, as the oxidation of VOCs from both anthropogenic and biogenic sources can lead to the formation of secondary organic aerosol (SOA). This study aims to characterize the temporal variability and sources of particulate- and gas-phase organic pollutants in the urban environment of the Western Mediterranean.

Two state-of-the-art instruments, a Q-ACSM and a PTR-TOF-MS, will operate continuously for at least one year at the Palau Reial urban background station in Barcelona, providing simultaneous measurements of aerosol chemical composition and VOCs. OA source apportionment will be performed using Positive Matrix Factorization (PMF), including seasonal and rolling source apportionment approaches. PMF will also be applied to the VOC dataset. A joint source apportionment of OA and VOCs will additionally be explored.

Seasonal and diel variability of raw data and of the outputs of the source apportionment application will be investigated alongside meteorological conditions and emission patterns to identify the processes controlling urban organic pollution. Conclusions will support effective air quality mitigation strategies.

Keywords: organic aerosol, volatile organic compounds, source apportionment, air quality, atmospheric pollution

InSAR data for characterizing the temporal response of aquifers through spectral analysis

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ABSTRACT

Time series analysis of groundwater levels is a useful tool for aquifer characterization, but its applicability is limited by the low density of observation points with sufficiently long records. InSAR products from the European Ground Motion Service (EGMS) provide freely available vertical deformation time series at continental scale and with high spatial density. Given the hydromechanical response of the subsurface to groundwater level changes, part of the observed deformation may be linked to changes in groundwater storage. This work aims to assess whether InSAR vertical deformation data can provide analogous or complementary information on the temporal response of aquifers.

Groundwater level and EGMS Ortho vertical deformation time series (2016–2024) are analyzed in alluvial aquifers from different regions of Europe. The aquifer response is interpreted as a low-pass filter: a characteristic response time is estimated from the cutoff frequency of each series' spectrum and compared between the two signals. The procedure is tested with synthetic series of known characteristic times.

Preliminary results suggest comparable response patterns between piezometric and InSAR records at time scales dominated by regional processes. The frequency-band evaluation identifies ranges of higher coherence as well as informative discrepancies. These results are a first step towards estimating characteristic response times from InSAR where piezometric records are scarce, and towards the regionalization of hydrogeological parameters.

Keywords: InSAR, EGMS, groundwater levels, spectral analysis, aquifer response time, alluvial aquifers



POSTERS





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Air pollution exposure, inhaled doses, and health outcomes in vulnerable populations: A cross-sectional multi-city study

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ABSTRACT

Traditional outdoor monitoring networks overlook indoor microenvironments where urban populations spend 90% of their time, creating misclassification in environmental epidemiology. This PhD research—part of the European HARMONIE project—applies an environmental epidemiology framework to evaluate indoor air quality (IAQ), and immediate health outcomes in vulnerable urban populations. The study implements a cross-sectional design across four European cities (including Barcelona, Barakaldo, Lausanne, and Gävle), assessing 30 households per site divided into healthy individuals and individuals with chronic respiratory conditions (children with asthma and older adults with COPD).

Environmental exposure assessment spans a one-week window combining high-precision indoor and outdoor monitoring. Measured air quality parameters include fine particulate matter ($PM_{2.5}$), ultrafine particles (UFP), black carbon (BC), gaseous pollutants (NO_2, O_3, CO, CO_2), noise, and aerosol Oxidative Potential (OP). Geolocation tracking models microenvironmental movement, while accelerometry estimates minute ventilation to derive the exact Inhaled Dose of Air Pollutants (IDoAP), differentiating indoor-specific contributions from total pollutant intake.

Epidemiological health endpoints evaluate acute pulmonary and systemic physiological responses. Primary outcomes—oxidative potential in exhaled air (OPEA) and lung function (spirometry)—are measured directly in participants' homes at the end of the exposure period. Secondary outcomes include continuous heart rate, perceived stress, and sleep quality.

By linking detailed air pollution metrics, continuous activity-weighted exposure modeling, and non-invasive health biomarkers, this PhD study advances environmental epidemiology. It addresses critical exposure misclassification and provides evidence-based metrics to elucidate how indoor environmental quality drives health risks in susceptible urban demographics.

Keywords: Indoor Environmental Quality; indoor exposure; vulnerable populations;

Distribution of Per- and Polyfluoroalkyl Substances in Human Autopsy

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ABSTRACT

Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants of growing concern due to their widespread occurrence and potential health effects. Although human exposure has been extensively studied in biological fluids, their distribution across internal organs remains poorly understood. This study investigated PFAS in liver, lung, kidney, and bone samples collected during autopsies of 21 individuals from Tarragona (Spain) in 2019. A liquid chromatography–tandem mass spectrometry (LC-MS/MS) method was validated for 29 PFAS, including legacy compounds and short-chain alternatives, to assess tissue-specific accumulation and temporal trends. PFAS were detected in all tissues, with substantial differences in concentrations and chemical profiles. The highest mean total concentrations occurred in lung (21.4 ng/g) and liver (19.9 ng/g), followed by kidney (11.2 ng/g) and bone (4.1 ng/g). PFOS was predominant, particularly in liver (7.8 ng/g, excluding one highly contaminated sample). Lung exhibited the most diverse PFAS profile, while kidney showed a characteristic combination of PFOS, PFHxS, and PFOA. Despite lower concentrations, bone contained several PFAS, including short-chain compounds, highlighting its relevance for exposure assessment. Comparison with liver samples from 2008 suggested declining concentrations of legacy PFAS, particularly PFOS and PFOA, potentially reflecting regulatory restrictions and production changes. However, their continued occurrence alongside short-chain alternatives indicates evolving exposure patterns. These findings demonstrate tissue-dependent PFAS distribution and emphasize the importance of multi-organ analysis for characterizing internal contamination and informing future research on potential human health risks associated with PFAS exposure.

Keywords: PFAS bioaccumulation, Human tissues, Tissue-specific distribution

Synergistic Effects of Extreme Drought and Anthropogenic Pressures on Spring Water Quality in Barcelona Province

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This study examines groundwater quality evolution and nitrate transport across a heterogeneous aquifer system in Barcelona Province (NE Spain), assessing the combined effects of the 2021–2023 drought (the most severe on record) and anthropogenic pressures over 2016–2024. A total of 3,543 samples from 578 natural springs, acting as aquifer discharge points, were analyzed for physicochemical and hydrochemical parameters.

Nitrate contamination showed contrasting trends. Mean concentrations decreased 25% (from 39.82 to 29.84 mg/L), attributable to action programs in vulnerable zones under EU Directive 91/676/EEC. However, the share of springs exceeding the 50 mg/L drinking water threshold remained stable at ~24%, indicating persistent structural contamination unresponsive to conventional management. Elevated nitrates cluster in central and southern sectors, coinciding with intensive agriculture and livestock.

Carbonate aquifers dominate, with 61.2% of springs showing calcium-bicarbonate facies. Facies shifts between 2023 and 2024 reveal diagnostic trajectories: transitions toward sulfate facies indicate contact with evaporitic formations, while shifts toward chloride facies signal increasing anthropogenic pressure in coastal areas and alluvial plains.

Clear climate signals emerge: a 0.5°C temperature increase and rising electrical conductivity consistent with severe drought. Reduced recharge limits natural dilution and increases the contribution of deeper, mineralized flows, so water stress and pre-existing contamination amplify degradation beyond what either stressor would produce alone.

Spring monitoring networks complement official surveillance, offering higher spatial resolution for early detection of localized deterioration. Porous alluvial systems show the highest sensitivity to drought and contamination, with direct implications for prioritizing protection of recharge areas.

Keywords: nitrate contamination; hydrochemical facies; spring monitoring; groundwater vulnerability; carbonate aquifers; climate change

Optimization of sorbents in Ceramic Passive Samplers for marine pollutants from SEATRACE project

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ABSTRACT

The marine environment is facing increasing threats from a myriad of toxic contaminants from both anthropogenic and natural sources, harming marine species and human health. Within the Horizon Europe SEATRACE project, we will deepen our knowledge of marine pollution by characterizing complex cocktails of marine pollutants (MrPs) in the coastal regions of the Atlantic, Arctic, Indian Oceans, and Mediterranean Sea. SEATRACE will strengthen European Union (EU)-India research collaboration on MrPs through joint work by EU and Indian organizations. The MrPs included in the project are contaminants of emerging concern (CECs), such as antibiotics and pharmaceuticals, agrochemicals, tire-derived chemicals and their transformation products, trace metals, marine biotoxins, plastics/micro(nano)plastics, non-intentionally added substances, antibiotic resistance genes, viruses and parasites, PFAS, and persistent organic pollutants (POPs).

Ceramic passive samplers (CPSs) represent a novel and promising alternative to conventional sampling techniques, offering time-integrated measurements while minimizing the influence of short-term concentration fluctuations. To optimize their performance, four adsorbents with different characteristics were tested. The CPSs are filled with the selected optimal adsorbent, which was previously evaluated for the adsorption of 130 CECs.

Furthermore, an LC-MS/MS method was developed to successfully detect all 130 target CECs. Chromatographic and ionization parameters were optimized to ensure low detection limits and high precision.

Acknowledgements

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Keywords: Ceramic passive samplers, contaminants of emerging concern, marine pollutants

Exploring sediment-biota relationships in complex marine environments through chemometric approaches

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ABSTRACT

Marine ecosystems are exposed to conventional and emerging contaminants from natural and anthropogenic sources. Understanding the relationships between contaminant distributions in sediments and biota is particularly challenging in complex environmental systems. This study investigates contamination patterns and potential sediment-biota relationships across six Sicilian coastal areas selected to represent different environmental conditions and anthropogenic pressures, including maritime activities, industrial and urban discharges, agricultural runoff, and bottom trawling. Five demersal and benthic species were selected for their feeding habits, habitat, and ecological relevance. Target analytes include metals and critical metals, polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), pesticides, and per- and polyfluoroalkyl substances (PFAS), reflecting geological contributions and anthropogenic inputs. Elemental analysis used ICP-MS following microwave-assisted digestion. An optimized multiclass QuEChERS method extracted PAHs, PCBs, pesticides and PFAS, followed by GC-MS/MS for organics and UPLC-MS/MS for PFAS. A multi-year dataset was compiled to investigate spatial and temporal contamination patterns in sediments and biota, considering metals and persistent organic pollutants. A targeted subset from a single area includes emerging contaminants, enabling more detailed investigation of spatial variability among bays and bathymetric differences. Chemometric methods are applied to explore multivariate contamination patterns and to identify the main factors driving their variability. PCA results revealed grouping patterns associated with geographical area, sampling season, and year, particularly in sediment samples, while ASCA identified geographical area, season, and year as statistically significant factors. Future work will apply advanced chemometric models to investigate sediment–biota associations and evaluate the relationships between contaminant distributions and environmental and anthropogenic factors.

Keywords: multiclass contaminants; marine contamination; sediment-biota interactions; Principal Component Analysis (PCA); ANOVA Simultaneous Component Analysis (ASCA).

Beyond Growth Inhibition: Uncovering Sub-Lethal CEC Toxicity in Marine Microalgae Through Metabolomics

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ABSTRACT

Chemicals of Emerging Concern (CECs) pose a rising threat to marine ecosystems, yet traditional growth inhibition assays often underestimate sub-lethal toxicological pressures. This study evaluates the integrative ecotoxicological response of the marine microalgae Tetraselmis suecica exposed to both reference toxicants and environmental CEC mixtures collected along the Catalan coast.

Following adapted OECD growth inhibition protocols, cultures were exposed to environmental water extracts and analyzed via liquid chromatography-high-resolution mass spectrometry (LC-HRMS) for targeted and suspect metabolomics. While growth inhibition endpoints alone offered limited insight into complex environmental exposures, multi-platform metabolomic profiling revealed significant sub-lethal alterations.

Key metabolic shifts included reductions in polyunsaturated fatty acids (PUFAs) linked to oxidative stress and photosynthetic impairment, decreases in protective amides, and notable variations in energy-related purine metabolites (such as guanine, xanthine, and hypoxanthine). Furthermore, alterations in choline and acetylcholine pathways suggested potential pesticide-induced enzyme inhibition.

The findings demonstrate that coupling T. suecica bioassays with high-resolution metabolomics provides a sensitive, early-warning diagnostic framework for detecting complex anthropogenic contamination in marine environments, moving beyond conventional toxicity assessments.

Keywords: Microalgae, Bioassay, Metabolomics, CECs, marine waters

Environmental exposure to persistent and non-persistent organic pollutants during pregnancy

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The extensive use of chemicals with endocrine-disrupting potential has posed a threat to both human populations and the environment. Pregnant women constitute a particularly vulnerable group, as prenatal exposure to certain compounds has been associated with adverse effects on child neurodevelopment. This study aims to assess exposure to currently used pesticides (mainly pyrethroids, neonicotinoids and organophosphates), as well as to banned pesticides, such as organochlorine compounds, and other persistent organic pollutants (POPs) in pregnant women from La Garrotxa, Catalonia.

These chemical compounds were analysed in serum and urine samples collected from 60 women participating in the PEHSU La Garrotxa cohort using two complementary methodologies. Urine samples (1 mL) were analysed by solid-phase extraction followed by liquid chromatography–tandem mass spectrometry (LC-MS/MS)[1,2]. Serum samples (0.5 mL) were analysed using a method based on liquid–liquid extraction followed by gas chromatography with electron capture detection (GC-ECD) [3].

In more than 60% of the urine samples, six pesticide metabolites were detected, including acetamiprid, tebuconazole and pirimiphos. In serum, the most frequently detected compounds were vinclozolin, 4,4'-DDE, β-endosulfan and dieldrin, among others, which were found in more than 70% of the samples.

The results confirm widespread exposure in this Catalan population. The combination of both methods provides a robust tool for biomonitoring and highlights the need for public health strategies to reduce prenatal exposure to compounds with endocrine-disrupting potential.

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Assessment of per- and polyfluoroalkyl substances and physiological health in bycaught loggerhead turtles (Caretta caretta) along the Catalan coast

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ABSTRACT

Loggerhead turtles (Caretta caretta) are vulnerable marine species exposed to anthropogenic pollutants, including per- and polyfluoroalkyl substances (PFAS). This study aimed to characterize the pollution burden and physiological status of 53 rescued turtles from the Catalan coast and admitted to the CRAM recovery centre.

An analytical method was optimized to quantify PFAS in plasma. Sample preparation involved acetonitrile-induced protein precipitation followed by solid-phase extraction (SPE) using Oasis WAX cartridges. Analytes were separated using a Hypersil GOLD PFP C18 column via high-performance liquid chromatography (HPLC) coupled to an Orbitrap Exploris 240 high-resolution mass spectrometry (HRMS) system.

Legacy PFAS were widely detected, with PFOS showing the highest detection frequency (96%) and a mean concentration of 0.34 ng/mL. Maximum concentrations of 4.58 and 5.91 ng/mL were observed for PFOA and PFBS, respectively. Trifluoroacetic acid (TFA) reached 645.27 ng/mL in one sample. Emerging PFAS were also detected, with GenX reaching 1489 ng/mL in one individual, alongside frequent detections of ADONA and FOSA.

Clinical assessment established baseline physiological parameters, including mean haematocrit (26.04%) and total protein levels (41.58 g/L). Stable isotope analysis suggested a coastal-pelagic population, with 81.13% of individuals occupying trophic

levels ≤4. Faecal analysis revealed plastic excretion in 49% of turtles, predominantly polypropylene and polyethylene.

Overall, integrating HRMS-based PFAS analysis alongside thorough clinical parameter screening provides a framework for investigating chemical and physical pollution in loggerhead turtles.

Keywords: Per- and polyfluoroalkyl substances (PFAS), loggerhead turtles, high-resolution mass spectrometry (HRMS)

Effects of the short-chain PFAS PFBS on aquatic organisms: a combined *in vivo* and *in vitro* approach

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ABSTRACT

Perfluorobutanesulfonic acid (PFBS) is a short-chain per- and polyfluoroalkyl substance (PFAS) widely used as a replacement for long-chain compounds such as PFOS, whose use has been restricted due to their persistence, bioaccumulation and toxicity. Owing to its high water solubility and mobility, PFBS is increasingly detected in aquatic environments, yet its effects on organisms at different trophic levels remain poorly understood. This study aimed to assess the toxicity of PFBS using two complementary models representing different levels of the aquatic food web: the freshwater cladoceran *Ceriodaphnia dubia*, a primary consumer, and the fish hepatoma cell line PLHC-1, derived from *Poeciliopsis lucida*, as an *in vitro* model of a higher trophic level. Acute toxicity in *C. dubia* was evaluated through a mortality test, which showed that the median lethal concentration (LC50) was higher than 500 mg/L, the highest concentration tested. Genotoxicity in *C. dubia* will be investigated by means of the comet assay, to detect sublethal DNA damage. In PLHC-1 cells, cell viability assays showed no cytotoxic effects at the highest concentrations tested (500µM), while the production of reactive oxygen species (ROS) and the activity of ethoxyresorufin-O-deethylase (EROD), an indicator of CYP1A induction, will be measured to assess oxidative stress and the interaction of PFBS with xenobiotic metabolism. Combining an *in vivo* invertebrate test with an *in vitro* fish cell model provides a broader view of PFBS hazard across biologic scale, and these findings contribute to the environmental risk assessment of short-chain PFAS.

Keywords: PFBS, *Ceriodaphnia dubia,* LC50, PLHC-1, cytotoxicity

Decoding the molecular fingerprints of organophosphate flame retardants with transcriptomics

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Organophosphate flame retardants (OPFRs) are widely used chemicals added to consumer products to reduce flammability. Due to their structural and physicochemical diversity, including differences in polarity, solubility, and persistence, OPFRs can induce a broad range of toxic effects, such as neurotoxicity, hepatotoxicity, metabolic disruption, and alterations in reproductive pathways.

In this study, we evaluated the effects of ten flame retardants in zebrafish embryos: triphenyl phosphate (TPhP), tri(2-butoxyethyl) phosphate (TBOEP), tris(1,3-dichloro-2-propyl) phosphate (TDCIPP), tris(1-chloro-2-propyl) phosphate (TCIPP), tri-n-butyl phosphate (TNBP), tetrabromobisphenol A (TBBPA), 2,4,6-tribromophenol (2,4,6-TBP), hexabromobenzene (HBB), 2,3,4,5,6-pentabromotoluene (PBT), and 2-ethylhexyl diphenyl phosphate (EHDPP). Embryos were exposed from 4 to 5 days post-fertilisation, and developmental effects and survival were assessed. Samples were collected across a concentration range (0, 8.23, 28.27, 100.6, 351, and 1230 µg/L) for dose-response analysis using a high-throughput microfluidic qPCR platform targeting 96 selected genes. In parallel, larval behaviour was evaluated using the DanioVision system, including startle response, non-associative habituation, basal locomotor activity, and visuomotor response. Vibratory and visual stimuli were applied to mimic environmental threats.

Behavioural analyses revealed endpoint- and compound-specific neurotoxicity, demonstrating substantial variability among flame retardants. The startle response emerged as the most sensitive behavioural endpoint, detecting sublethal neurodevelopmental effects at lower concentrations than other assays. TPhP produced the strongest behavioural alterations, primarily affecting mechanosensory and motor circuits involved in startle, habituation, and locomotor responses. Transcriptomic analyses are ongoing. Overall, these findings indicate that OPFR toxicity is driven by compound-specific mechanisms and that chemical diversity plays a key role in determining toxicological outcomes.

Keywords: Organophosphate flame retardants (OPFRs); Zebrafish; Neurotoxicity; Behavioural toxicity.

Machine Learning-Based Gap Filling for PM Long-Term Chemical Speciation

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ABSTRACT

Air pollution is one of the greatest environmental risks worldwide. In this context, atmospheric Particulate Matter (PM) deserves special attention, as its toxicological and health impacts strongly depend on its chemical composition. Therefore, establishing robust, highly resolved observational networks is crucial for supporting effective air quality management and mitigation strategies. However, daily measurements of chemical speciation across PM10, PM2.5, and PM1 fractions are often sampled every few days due to operational. This temporal sparsity poses significant challenges and implications for epidemiological studies and accurate population exposure assessments.

To address this limitation, this study proposes a Machine Learning framework for imputing missing chemical speciation data, leveraging a long-term observational dataset of PM10, PM2.5 and PM1 composition collected at an urban background monitoring station in Barcelona between 2014 and 2025, sampled at irregular intervals ranging from 1 to 6 days. We integrate continuous daily predictors including meteorology, trace gases, black carbon, ultrafine particles, net dust from African intrusion episodes, and temporal context features such past and future observations of the speciated measurements.

We systematically benchmark several tree-based algorithms, including Random Forest and Gradient Boosting (XGBoost and LightGBM), to reconstruct PM chemical species and impute values for unmeasured days, generating a complete long-term chemical time-series over the period. Results demonstrate that the proposed methodology successfully captures variations across multiple PM species. Specifically, incorporating temporal context features, such as lagged and lead observations spanning 1 to 5 days before and after the target date substantially enhances the ML models performance.

Keywords: Atmospheric Chemistry; Air Quality; Machine Learning; Time-Series Gap Filling.

Lithological controls and post-drought flushing: Hydrochemical and isotopic insights from a Mediterranean river basin

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ABSTRACT

Drought-recovery cycles alter solute dynamics in Mediterranean river basins, but the relative roles of lithological controls and recharge-driven solute mobilization remain poorly understood. We investigated the Upper Llobregat River Basin (NE Spain) during drought recovery from the 2021-2024. Major ions, nutrients, and trace elements were analyzed in 88 samples from 23 sites (rivers, tributaries, springs, piezometers and a precipitation collector) across four campaigns (2024-2025). Principal component analysis, inverse geochemical modeling, and flow-normalized comparisons assessed solute dynamics. Separately, stable water isotope data ($\delta^{18}O$ and $\delta^{2}H$) were used to characterize recharge elevations through isotope-altitude relationships.

Groundwater interaction with lithology mainly reflected carbonate dissolution and CO_2 uptake, with additional contributions from evaporite dissolution and cation exchange. River major-ion chemistry reflected springs and tributary mixing, whereas nutrients and trace elements displayed variations not attributable to dilution alone. Flow-normalized patterns indicate flushing of chemical constituents accumulated in soils and sediments during prolonged low-flow conditions. Stable isotopes indicated dominant winter recharge, with substantial contributions from elevations above 1800 m a.s.l., and partial preservation of seasonal signals in groundwater, consistent with short residence times and rapid recharge responses in karst aquifers.

These findings indicate that lithology primarily governs baseline water chemistry, while post-drought hydrological recovery promotes solute mobilization. Stable isotopes constrain recharge dynamics and support groundwater-surface water connectivity. Obtained in a karst-dominated Mediterranean headwater basin subject to recurrent drought, these results are likely transferable to analogous settings across the Mediterranean region, where carbonate geology, seasonal recharge, and increasing drought frequency similarly shape water quality.

Keywords: Hydrogeochemistry; Stable water isotopes; Drought-recovery; Mediterranean river basins.

HRMS Suspect Screening of Pharmaceutical Transformation Products in Simulated Aquifers

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ABSTRACT

Conventional wastewater treatment only partially eliminates pharmaceuticals, allowing these micropollutants to enter surface waters and infiltrate connected alluvial aquifers. In the Besòs River basin (Barcelona), riverbank filtration introduces a wide range of therapeutic classes, most notably beta-blockers, antidepressants, and antihypertensives, into groundwater systems, where their environmental fate is governed by local hydrogeochemistry.

To investigate the attenuation pathways and transformation kinetics of these compounds, parallel batch reactor experiments were conducted under oxic and nitrate-reducing conditions at 25 °C and 35 °C. Over a 21-day period, 11-mL aliquots were collected, concentrated via vacuum-assisted evaporation, and analyzed by liquid chromatography–high-resolution mass spectrometry (LC-HRMS). Suspect screening workflows coupling Compound Discoverer 3.5 with the BioTransformer and FairTPs databases resolved 15 transformation products (TPs) confirmed at Level 2 on the Schymanski scale, including venlafaxine N-oxide, lidocaine N-oxide, O-desmethylvenlafaxine, atenolol acid, and desmethylcitalopram.

These batch experiments reveal how distinct redox regimes and thermal variations dictate pharmaceutical persistence and breakdown mechanisms in groundwater. The resulting metabolic profiles establish mechanistic baselines to guide ongoing field monitoring and pathway validation across the Besòs River catchment.

Keywords: Pharmaceuticals, Transformation products, HRMS

Towards cleaner water: Monitoring micropollutants under the New EU Urban Wastewater Treatment Directive

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ABSTRACT

Organic micropollutants are widely detected in aquatic environments, raising concerns about their potential impacts on human health and ecosystems. The revised Urban Wastewater Treatment Directive (EU) 2024/3019 [1] establishes requirements for their removal and identifies 13 indicator substances to assess quaternary wastewater treatment performance.

This study developed and validated an analytical method for determining these substances in water matrices using online extraction (OLE) coupled with liquid chromatography–high-resolution mass spectrometry (LC-HRMS). The approach simplifies sample preparation and enables retrospective data analysis. Validation was performed according to SANTE 11312/2021 [2] guidelines at 0.1 and 1 µg/L. The method was subsequently applied to influent, effluent, and fortified wastewater samples, including samples analysed in an interlaboratory comparison.

The method demonstrated satisfactory linearity and repeatability for most analytes. Relative recoveries ranged from 43% to 122% at 0.1 µg/L and from 56% to 124% at 1 µg/L, while absolute matrix effects remained below 29% for all compounds. The interlaboratory comparison, assessed using the proficiency assessment standard deviation specified in ISO 13528, yielded satisfactory results for all target compounds and matrices except amisulpride in influent wastewater.

The analysis of real influent and effluent samples revealed different removal behaviors among the target compounds. Some compounds were efficiently removed during wastewater treatment, whereas others showed little or no change in concentration. In contrast, a slight increase in the concentrations of benzotriazoles was observed in the treated effluent, suggesting their possible formation or release during the treatment process.

Keywords: Circular economy, reclaimed water, CECs

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Assessment of the bioaccumulation of mercury and other trace metals in *Anguilla anguilla* in rivers and lagoons of Catalonia and Mallorca

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ABSTRACT

The European eel (*Anguilla anguilla*), currently classified as a critically endangered species, serves as a key bioindicator for assessing the ecological status of aquatic ecosystems. This study evaluates contamination by mercury and other heavy metals in eels from rivers and lagoons in the northwestern Mediterranean (Catalunya and Mallorca) to identify exposure patterns and environmental factors that may compromise the health of these populations. A total of 298 muscle samples, collected during two sampling campaigns (2024 and 2025), were analyzed: total mercury (THg) was measured using a direct mercury analyzer (DMA-80), while eight other metals (As, Cd, Cr, Cu, Ni, Pb, Se, and Zn) were analyzed via inductively coupled plasma mass spectrometry (ICP-MS). THg concentrations ranged from 0.014 to 0.76 µg/g wet weight (ww) and differed significantly across sampling sites ($p < 0.001$), with the highest median value recorded in La Ricarda lagoon (0.25 µg/g ww). Among the other metals, Zn was the most abundant element, peaking in the Ebro Delta (23.9 µg/g ww), while As levels were notably high in the Salses-Leucate and Canet-Sant Nazaire lagoons, as well as in the Ebro Delta, which also exhibited elevated levels of Se and Pb, while the Valencia site showed high concentrations of Cu, Cr, and Se. The remaining sites displayed moderate concentrations, with no consistent enrichment pattern across all elements. These differences suggest an influence from local environmental conditions and anthropogenic pressures and underscore the importance of monitoring for the conservation of this species and Mediterranean ecosystems.

Keywords: *European eel; Mercury; Trace metals; Bioaccumulation; Mediterranean habitats; Ecological risk assessment*

Comprehensive Coverage and Semi-Quantification of Marine Biotoxins in Catalan Coast

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ABSTRACT

Marine biotoxins represent a critical threat to marine ecosystems, seafood safety, and public health. Due to their wide-ranging physicochemical properties, from highly hydrophilic to lipophilic compounds, the simultaneous determination and quantitative evaluation of parent toxins alongside their transformation and degradation products remain a major analytical bottleneck in environmental monitoring.

In this work, we present an integrated high-resolution mass spectrometry platform designed to achieve comprehensive coverage and reliable concentration estimates of marine biotoxins and their related degradation products in seawater, covering azaspiracids, okadaic acid, and saxitoxins. Seawater samples were preconcentrated using an offline tandem solid-phase extraction protocol (HLB and Envi-Carb) prior to analysis by liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS, Exploris240 Orbitrap). Chromatographic separation combined reversed-phase (C18) and hydrophilic interaction liquid chromatography (BEH Amide) to ensure optimal retention and peak resolution across the entire polarity spectrum.

Data were acquired in Full MS/dd-MS² (data-dependent acquisition) mode. A combined targeted and suspect screening workflow—supported by curated in-house databases and *in silico* fragmentation tools—was established to identify candidate biotoxins, transient metabolites, and structural degradation products without requiring prior compound-specific optimization. To address the scarcity of analytical reference standards for degradation derivatives, a semi-quantification approach based on structural analogs and response factor normalization was developed to estimate their environmental concentrations. This workflow demonstrates broad analytical coverage, high identification confidence, and practical semi-quantitative capability, serving as an effective tool for assessing biotoxin occurrence, chemical persistence, and degradation pathways in marine systems.

Keywords: Biotoxins, Suspect screening, Semi-quantification

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