22nd Annual Workshop on Emerging High-Resolution Mass Spectrometry (HRMS) and Lc-Ms/Ms Applications in Environmental Analysis and Food Safety

7th International Conference on Risk Assessment of Pharmaceuticals In The Environment (ICRAPHE)

Barcelona, 9-11 November 2026

ORGANIZED BY

CSIC Consejo Superior de Investigaciones Científicas

Universidad de Almería

Académie nationale de Pharmacie

ABSTRACT BOOK



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*Compared to the ZenoTOF 7600+ system

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CONTENT

COMMITTEES	04
WELCOME	05
PROGRAM	06
KEYNOTE LECTURES	18
ORAL PRESENTATIONS	43
POSTER PRESENTATIONS	76

ORGANIZING AND SCIENTIFIC COMMITTEE

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WELCOME

This edition combines two well-established workshops into a single event.

On one side, we present the 22nd HRMS Workshop, focusing on the practical applications of high-resolution mass spectrometry (HRMS) and tandem mass spectrometric techniques for screening and quantification on of organic contaminants in environmental and food samples.

On the other side, we feature the 7th ICRAPHE Conference, dedicated to exploring the fate, risk, and removal of pharmaceutical residues in the environment.

This joint workshop provides an informal and interactive platform for scientists from academia, governmental agencies, and industry to share the latest research findings, methods, and ideas in a collaborative environment. To further encourage participation, several awards will be presented for outstanding contributions, including prizes for the best oral communication, best poster, and best student presentation, supported by sponsors and scientific partners.

We are offering the possibility to publish your work presented at this workshop at the open access journal of Xenobiotics JoX (IF 4.4, JCR Q1) as part of the Special Issue entitled: «Emerging Contaminants as Vectors of Global Change: Ecotoxicology, Bioaccumulation and Risk».

In a similar way as in previous years, the workshop is jointly organized by IDAEA- CSIC (Barcelona, Spain), University of Almería, Académie nationale de Pharmacie and Royal Academy of Pharmacy of Catalonia.

Wishing to all of you a safe trip to Barcelona next November.

Prof. Dr. Damià Barcelo
University of Almería and Académie nationale de Pharmacie

MONDAY,9th November 2026

08:15 **Registration**

08:45 **Opening ceremony**

HRMS 2026

Topic: Advances in HRMS instrumentation and their applicability in environmental analysis of PFAS

09:00 **Opening lecture.** Isomers Matter: Revealing the distributions of branched and linear PFAS in environmental samples using cyclic ion mobility spectrometry

Diana S. Aga, *Department of Chemistry and RENEW Institute, University of Buffalo, NY, US*

09:45 **Keynote lecture.** Studying the ionization of neutral PFAS with flexible microtube plasma source and LC-MS

Juan Francisco Garcia Reyes, *Department of Analytical Chemistry, University of Jaen, Spain*

10:15 **Keynote lecture.** PFAS in AFFF contaminated sites – What can we learn from LC-HRMS analysis

Christian Zwiener, *Environmental Analytical Chemistry, University of Tübingen, Germany*

10:45 **David Solomon Jalajel, Prince Sultan Bin Abdulaziz International Water Prize**

11:00 **Coffee break & poster session 1**

CHAIR: Diana S. Aga

11:30 **Keynote lecture.** Expanding the PFAS Atmospheric Inventory: From Legacy Ionic Compounds to Volatile Precursors

Natalia Soares Quinete, *Institute of Environment, Department of Chemistry and Biochemistry, Florida International University, US*

12:00 **Contributed lecture.** Application of HRMS-based suspect screening for the investigation of the fate of mobile organic contaminants in urban blue-green infrastructures

Sandra Pérez, *IDAEA-CSIC, Spain*

12:20 **Contributed lecture.** PFAS analysis and removal in aquatic systems: the role of advanced mass spectrometry in supporting treatment strategies

Maryam Mallek, *Faculty of Sciences, University of Sfax, Sfax, Tunisia*

12:40 **Oral communication.** Analytical strategies and removal treatments of a broad spectrum of PFAS in Drinking Water Treatment Plants: A LC-MS/MS study

Anna Barrera Duque, *Institut Químic de Sarrià*

12:50 **Oral communication.** Overcoming chromatographic and extraction challenges for the determination of PMT/vPvM substances in water

Natalia Sáez Rosique, *Catalan Institute for Water Research (ICRA)*

13:00 **Lunch break & poster session 1**

CHAIR: Torsten C. Schmidt

Topic: Non-Target Analysis (NTA) and Bioinformatics applied to environmental and food samples

14:00 **Keynote lecture.** Comprehensive Chemometric Analysis of Ion Mobility coupled with Liquid Chromatography High Resolution Mass Spectrometry Data

Roma Tauler Ferre, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Spain*

14:30 **Keynote lecture.** Advancing Environmental Monitoring Through LC-HRMS-Based Non-Targeted Approaches: From Contamination Profiling to Contaminant Prioritization

Miren López de Alda, *IDAEA-CSIC, Spain*

15:00 **Oral communication.** From arid to Arctic: Non-target screening of CECs across climatic extremes

Monika Adanyi, *Università del Piemonte Orientale*

15:10 **Oral communication.** Non-target LC–HRMS/MS screening of ceramic passive sampler extracts from groundwater and river sites

Giacomo Moro, *IDAEA – CSIC*

15:20 **Oral communication.** Estimating Concentration of Emerging Contaminants from their MS/MS Spectra in Environmental Samples

Carlos Pérez López, *National and Kapodistrian University of Athens*

15:30 **Oral communication.** Expanding the Scope of NTS in High-Throughput EDA: Uncovering Transthyretin-binding Compounds in Stormwater Ponds via Orthogonal Separation Modes and Ion Mobility HRMS

Lyen Castro, *Institute of Environmental Assessment and Water Research, Barcelona, Spain*

15:40 **Oral communication.** Integrated Analysis of IM-MS Imaging and LC–IMS–MS Using Trilinear MCR for Non-Target Lipid Identification

Chenxi Peng, *Universitat de Barcelona*

15:50 **Oral communication.** Multimodal high-resolution mass spectrometric screening of leachates from recycled plastics: what is new and what is already known?

Carsten Jaeger, *Federal Institute for Materials Research and Testing (BAM)*

16:00 **Oral communication.** Integrating targeted LC–MS/MS and high-resolution mass spectrometry suspect screening for comprehensive characterization of emerging contaminants in a legacy landfill-impacted river

Sara Abdelli, *Institute for Energy Technology (IFE), University of Turin (UNITO), Polytechnic University of Valencia (UPV)*

CHAIR: Kevin Tucker

Topic: Advanced Wastewater Based Epidemiology (WBE) and Human Exposome

16:10 **Keynote lecture.** Water-based epidemiology for community health early warning: advances in analytics and data triangulation approaches

Barbara Kasprzyk-Hordern, *Department of Chemistry, University of Bath, UK*

16:40 **Keynote lecture.** Beyond Single Samples: Mapping Chemical Transport Across the Human Exposome

Pablo Gago Ferrero, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Spain*

17:10 **Sponsored lecture.** Insight Profiler streamlines non-targeted analysis of river water contaminants of environmental concern in a single software solution

Emily G. Armitage, *Shimadzu Corporation, Manchester, UK*

17:40 **Break**

18:00 **Keynote lecture.** Wastewater Omics for Population Health and Lifestyle

Montserrat Carrascal, *Department of Experimental Pathology, Institute of Biomedical Research of Barcelona, Spain*

18:30 **Contributed lecture.** Metabolic profiling reveals structure-based common metabolites for liquid crystal monomers

Japhet Cheuk-Fung Law, *Hong Kong Baptist University*

18:50 **Oral communication.** The application of wastewater-based epidemiology for the nationwide assessment of drug consumption patterns

Magdolna Petrics, *National Center for Public Health and Pharmacy (NNGYK) and Environmental Doctoral School, Eötvös Loránd University (ELTE)*

19:00 **Oral communication.** Wastewater-based assessment of lifestyle and dietary patterns in Croatian regions

Ivan Senta, *Rudjer Boskovic Institute*

19:10 **Oral communication.** Integrating wastewater-based epidemiology with socioeconomic and health indicators to characterize patterns of psychoactive substance consumption across Catalonia

Rocío Inés Bonansea-García, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Spanish National Research Council (CSIC)*

19:20 **End of day 1**

TUESDAY, 10th November 2026

CHAIR: Christian Zwiener

Topic: HRMS and LC/M S-MS applied to environmental and food authenticity

09:00 **Keynote lecture.** From source to tap: Perspectives of water monitoring using liquid chromatography high-resolution mass spectrometry

Torsten C. Schmidt, *Instrumental Analytical Chemistry and Centre for Water and Environmental Research (ZWU), University of Duisburg-Essen, Germany*

09:30 **Keynote lecture.** Mass Spectrometry and Ion Mobility for the Characterization and Determination of Arsenosugars in Algae

Encarnación Moyano, *Deptartment Section of Analytical Chemistry, University of Barcelona, Spain*

10:00 **Keynote lecture.** High-Resolution Mass Spectrometric Monitoring of Dissolved Organic Matter and Pollutants in Basilicata Region Reservoirs

Giuliana Bianco,*Coordinator, Degree Course in Chemistry, Department of Basic and Applied Sciences, University of Basilicata, Italy*

Angela Di Capua, *Department of Basic and Applied Sciences, University of Basilicata, Italy*

10:30 **Keynote lecture.** Two Decades of HRMS in Pesticide Residue Analysis: From Milestones to Future Directions

Amadeo R. Fernández-Alba, *Department of Chemistry and Physics, University of Almeria, Spain*

11:00 **Coffee break & poster session 2**

11:30 **Sponsored lecture.** Ultra sensitive quantitation and targeted/ non targeted analysis of water and food contaminants using the SCIEX ZenoTOF 8600 system

Jianru Stahl-Zeng, *SCIEX, Germany*

12:00 **Contributed lecture.** Beyond Antibiotic Exposure: Salinity Modulates Oxytetracycline Toxicity in Mytilus galloprovincialis

Rosa Freitas, *University of Aveiro*

12:20 **Contributed lecture.** Advanced materials for the selective extraction of pharmaceuticals from environmental water samples

Rosa Maria Marcé, *Universitat Rovira i Virgili*

12:40 **Oral communication.** From in-vitro to in-vivo: liquid chromatography-mass spectrometry elucidation of mammalian metabolism of tire-related chemicals

Belén Ameijeiras Lois, *Aquatic One Health Research Center (ARCUS) & Department of Analytical Chemistry, Nutrition and Food Chemistry, Universidade de Santiago de Compostela*

12:50 **Oral communication.** Occurrence of Tire-Derived Chemicals in Environmental Waters of the Barcelona Metropolitan

Aurelio Foscari, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC)*

13:00 **Oral communication.** Methodologies based on high-performance liquid chromatography coupled with mass spectrometry for the determination of emerging contaminants in water: application to hospital effluents

Laura Diaz Espla, *LABAQUA*

ICRAPHE 2026

CHAIR: Giuliana Bianco

Topic: Remediation Technologies including adsorption, advanced oxidation processes, bioremediation and NBS for Pharmaceutical residues and other Pollutants

13:10 **Keynote lecture.** Biomass-Derived Carbons as a Sustainable Strategy for Mitigating Pharmaceutical Pollution: Challenges and Opportunities

Vânia Calisto, *Department of Chemistry and CESAM, University of Aveiro, Portugal*

13:40 **Keynote lecture.** Closing the Loop: Solar Hydrogen Production from Wastewater-Derived Organics

Laura Clarizia, *Department of Chemical, Materials and Industrial Production Engineering, University of Naples «Federico II», Italy*

14:10 **Lunch break & poster session 2**

15:00 **Keynote lecture.** Assessment of the health status of the Ebro River after remediation of the dumped waste from a chlor-alkali plant

Joan O. Grimalt, *Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research (IDAEA), Spanish Council for Scientific Research (CSIC), Spain*

15:30 **Keynote lecture.** Passive samplers for the monitoring of contaminants in surface waters

Núria Fontanals Torroja, *Analytical Chemistry and Organic Chemistry, Rovira i Virgili University, Tarragona, Spain*

16:00 **Contributed lecture.** Release of a quaternary effluent on a water body – Assessment of its environmental impact mitigation by natural attenuation processes

Paola Verlicchi, *University of Ferrara, Italy*

16:20 **Contributed lecture.** Removal of pharmaceuticals from synthetic human urine using ozone-based advanced oxidation processes

Henry Zúñiga-Benítez, *University of Antioquia, Colombia*

16:40 **Oral communication.** Selection and Preliminary Evaluation of Biomass and Sludge-Derived Biochars for Pharmaceutical Removal from Wastewater

Ana Rita Alves, *REQUIMTE/LAQV, Instituto Superior de Engenharia do Porto, Instituto Politécnico do Porto, Portugal*

CHAIR: Antoni Ginebreda

Topic: Risk Assessment and Sustainable Management of Pharmaceuticals and other Emerging Contaminants-first session

16:50 **Keynote lecture.** Integrating environmental data with dynamic modelling for urban water risk assessment

Demetris F. Lekkas, *Waste Management Laboratory, Department of Environment, University of the Aegean, Greece*

17:20 **Break**

17:40 **Contributed lecture.** COST Action ENVIRANT: Anthelmintics, from its farming use to the environment

María Martínez Valladares, *CSIC – Consejo Superior de Investigaciones Científicas, Instituto de Ganadería de Montaña*

18:00 **Contributed lecture.** Assessing organic pollutant benchmarks in a Mediterranean catchment facing climate-driven flood risks

Julian Campo, *Environmental and Food Safety Research Group, Desertification Research Centre, Valencia, Spain*

18:20 **Contributed lecture.** From Water to Eel Tissues: LC–HRMS/MS Characterization of Emerging Contaminant Exposure across Mediterranean Aquatic Systems

Nicola Montemurro, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Barcelona, Catalonia, Spain*

18:40 **Oral communication.** Pharmaceutical-containing pollutant mixtures in freshwater: independent action predicts acute lethality while sub-lethal endpoints reveal masking in Daphnia magna

Leonid Antonov, *Dublin City University*

18:50 **Oral communication.** Beyond the aquatic compartment: persistent, mobile and toxic pharmaceuticals in wastewater-impacted agroecosystems — field evidence for integrated health risk assessment

Lesly Ayala Cabana, *IMDEA Water Institute*

19:00 **Oral communication.** Will warmer summers increase the impact of UV filters on marine bivalves?

Diana Bordalo, *Universidade de Aveiro*

19:10 **End of day 2**

20:00 **Dinner at Restaurant la Poma (la Rambla 117)**

WEDNESDAY, 11th November

CHAIR: Natalia Soares Quinete

Topic: Risk Assessment and Sustainable Management of Pharmaceuticals and other Emerging Contaminants-second session

09:00 **Keynote lecture.** Toxicological Impacts of Environmentally Relevant Pharmaceuticals: Bioconcentration, Tissue-Specific Distribution, and Ecological Implications Revealed by Advanced Mass Spectrometry

Kevin Tucker, *Department of Chemistry, Southern Illinois University Edwardsville, US*

09:30 **Keynote lecture.** Contrasting Mediterranean coastal wetlands: emerging contaminants environmental interactions

Vicente Andreu Pérez, *Universitat de València – CSIC (CIDE), Spain*

10:00 **Keynote lecture.** New chemometric approaches on the occurrence and risk assessement modelling of pharmaceuticals in the freshwater environment

Antoni Ginebreda, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Spain*

10:30 **Keynote lecture.** Fair, efficient, and sustainable management of urban wastewater without compromising access to medicinal products

Emili Esteve, *Technical Department, Farmaindustria, Spain*

11:00 **Coffee break**

CHAIR: Damià Barceló

11:30 **Topic Panel discussion on Risk and Sustainable Management of Pharmaceuticals under the new Urban WasteWater Directive from November 2024**

Antoni Ginebreda, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Spain*

Demetris F. Lekkas, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Spain*

Emili Esteve, *Technical Department, Farmaindustria, Spain*

Miquel Salgot, *Royal Academy of Pharmacy of Catalonia, Spain*

Paola Verlicchi, *University of Ferrara, Italy*

Marc Moliner, *Catalan Water Agency, Spain*

12:45 **Awards and closing ceremony**

13:00 **End of the workshop**

LIST OF POSTERS

POSTER SESSION 1 – HRMS 2026 (MONDAY, 9th November)

S1-1 **Monika Adanyi** (Università del Piemonte Orientale)
Beyond grab sampling: Monitoring CECs in wastewater effluent using Affinisep AttractSPE membranes

S1-2 **Ruben Ballesteros** (Aigües de Barcelona)
Glyphosate and AMPA in source water and drinking water: occurrence, fate, and treatment implications in Barcelona (Spain)

S1-3 **Mohamed El-sheikh** (Botany & Microbiology Department, College of Science, King Saud University, Saudi Arabia)
Assessing the Presence of Pesticides, Pharmaceuticals, and Personal Care Residuals in Water, Soil, and Plants in Riyadh Urban Ecosystem, Saudi Arabia

S1-4 **Júlia Marsol Clop** (Aigües de Barcelona)
Comparative distribution of linear and branched PFAS isomers in water treatment

S1-5 **Maria Mendoza Manzano** (Florida International University)
Occurrence and depth-related distribution of PFAS in the deep-sea shrimp Eurythenes atacamensis from the Atacama Trench

S1-6 **Dana Orlando-Véliz** (IDAEA-CSIC)
Comprehensive profiling of contaminants of emerging concern in northern Antarctic Peninsula waters through liquid chromatography–ion mobility–high-resolution mass spectrometry

S1-7 **Dana Orlando-Véliz** (IDAEA-CSIC)
Development of an LC-HRMS analytical method for organic micropollutants indicators established in the recently adopted urban wastewater Directive

S1-8 **Junwu Xiong** (Catalan Institute for Water Research (ICRA))
Diffusive Gradients in Thin-films (DGT) as a Time-Integrated Tool for Monitoring Emerging Contaminants in Groundwater

S1-9 **Tin Županović** (Rudjer Boskovic Institute)
Wastewater-based assessment of pharmaceutical use in Croatia: regional differences and the importance of conjugates

S1-10 **Jianru Stahl-Zeng** (SCIEX)
Ultra-Sensitive Quantitation and Targeted/Non-Targeted Analysis of Pharmaceuticals, Pesticides and Personal Care Products (PPCPs) in Water Using the SCIEX ZenoTOF 8600 System

S1-11 **Josep Lliberia** *(SCIEX)*
Ultra-sensitive quantitation of top 20 PFAS in drinking, surface and wastewater samples by direct injection using the SCIEX ZenoTOF 8600 system

S1-12 **Marc Roca** (IDAEA-CSIC)
Tissue-Specific Distribution of Emerging Contaminants in European Eel by LC–HRMS

S1-13 **Sara Abdelli** (IFE, UNITO, UPV)
Spatial and temporal patterns of pesticides in Nordic surface waters revealed by targeted analysis supported by HRMS

S1-14 **Santiago Gómez-Herrera** (IDAEA-CSIC)
Complex chemical mixtures occur in Pyrenean high-mountain rivers: impacts on ecosystem health

POSTER SESSION 2 – ICRAPHE 2026 (TUESDAY, 10th November)

S2-1 **Ana Rita Alves** (REQUIMTE/LAQV, Instituto Superior de Engenharia do Porto, Instituto Politécnico do Porto, Portugal)
Influence of Biomass Feedstock on the Biochar Physicochemical Properties and Adsorption Performance of Pharmaceuticals

S2-2 **Leire Besga-Oyanarte** (IMDEA Water)
Antimicrobial resistance genes and potential co-selective pressures under unplanned water reuse across the water–soil–plant continuum

S2-3 **Benouareth Djamel Eddine** (Laboratory of Molecular and Cellular Biology (LBMC), Biology Department, Faculty of Natural and Life Sciences, Earth and Universe Sciences. University 8 Mai 1945 Guelma, BP 401 Guelma 24000, Algeria)
Bioremediation of Municipal Sewage Sludge: The Role of Bacteria in Organic Degradation and Heavy Metal Immobilization

S2-4 **Filomena Lelario** (University of Basilicata)
Comparative removal of erectile dysfunction pharmaceuticals from water using microwave-activated carbon and organically modified montmorillonite

S2-5 **Petra Matoušková** (Charles University, Faculty of Pharmacy)
The metabolic adaptation of Haemonchus contortus to fenbendazole

S2-6 **Erik Mestanza-Castelltort** (IDAEA CSIC)
Identification of Pharmaceutical Transformation Products in Reactors Simulating Natural Aquifer Conditions Using HRMS Suspect Screening

S2-7 **Maria Fernanda Nogueira** (Grupo de Reação e Análises Químicas (GRAQ))
Influence of Matrix Effects on the QuEChERS Extraction of Pharmaceuticals from Wastewater Sludge

S2-8 **Goreti Pereira** (Department of Chemistry & CESAM, University of Aveiro)
Silver Telluride Nanocrystals as Amplifiers for Pharmaceuticals Monitoring by SEIRA

S2-9 **Lucie Raisová Stuchlíková** (Department of Biochemical Sciences, Faculty of Pharmacy, Charles University)
Environmental residues of albendazole drug induce adaptive changes in Caenorhabditis elegans

S2-10 **Laura Moreno** (Laboratorio de Farmacología, Centro de Investigación Veterinaria de Tandil (CIVETAN), UNCPBA-CICPBA-CONICET, Facultad de Ciencias Veterinarias, Tandil, Argentina)
Persistence and fecal elimination of fluralaner in cattle following pour-on administration over 31 days using LC-MS/MS

S2-11 **Isabel Díez-Palet** (Institute of Environmental Assessment and Water Research (IDAEA-CSIC))
Optimization of analytical procedures for marine pollutants in seawater from SEATRACE project

S2-12 **Rosa Freitas** (University of Aveiro)
Silent exposure, delayed damage: GenX and enrofloxacin effects in marine mussels

S2-13 **Melissa Di Rocco** (Teagasc Food Research Centre)
Development of a multi-residue method for macrocyclic lactones in animal waste by UHPLC-MS/MS

S2-14 **Emily G. Armitage** (Shimadzu Corporation, Manchester, UK)
LC-MS/MS QTOF analysis of river water identifies contaminants of environmental concern by non-targeted analysis

KEYNOTE LECTURES

Isomers matter: Revealing the distributions of branched and linear PFAS in environmental samples using cyclic ion mobility spectrometry

Diana S. Aga[a,*]

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Per- and polyfluoroalkyl substances (PFAS) produced by electrochemical fluorination are complex mixtures of linear and branched isomers that differ in physicochemical properties, environmental fate, bioaccumulation potential, and biological activity. Increasing evidence shows that not only linear but also branched PFAS isomers are prevalent in the environment. Yet, current monitoring frameworks and regulatory approaches largely rely on total PFAS isomer metrics, masking the distinct behaviors and toxicities of individual isomers and introducing uncertainty into exposure and risk assessments. For instance, perfluorooctane sulfonic acid (PFOS) exists in the environment as a mixture of linear (L-PFOS) and branched (Br-PFOS) isomers. Although it is one of the most frequently detected per- and polyfluorinated alkyl substances (PFAS), it is often analyzed and reported as total PFOS with limited attention to the distribution of individual isomers. Here, we used cyclic ion mobility spectrometry (cIMS) with a tunable drift length as an added dimension of separation combined with ultra-performance liquid chromatography-quadrupole-time-of-flight mass spectrometry (UPLC-cIMS-qToF-MS) to separate six PFOS isomers. By applying six passes in the cIMS, the differences in drift times (DT) allowed us to distinguish L-PFOS from four Br-PFOS isomers. The disubstituted PFOS isomers were not separated from each other because they have the same DTs. Calibration curves prepared with individual isomers revealed that all Br-PFOS had higher ionization efficiencies (more than 2 to 5 times higher) in electrospray MS than L-PFOS, emphasizing the need for isomer-specific analysis for accurate PFOS quantification. The optimized UPLC-cIMS-qToF-MS method was then used to determine PFOS isomer patterns in influent and effluent wastewater samples as well as in bird egg yolk samples. The results showed that Br-PFOS isomers dominate in wastewater (more than 50% of total PFOS), while L-PFOS is significantly enriched in egg yolk samples (over 88%). This study highlights the effectiveness of UPLC-cIMS-qToF-MS for separating and quantifying PFOS isomers in complex matrices and underscores the importance of evaluating the isomer distribution of other PFAS compounds in environmental and biological samples. Reliance on the sum of PFAS isomers rather than individual isomers may bias PFAS quantification, weaken exposure-response assessments, and limit the development of scientifically robust, isomer-informed risk assessment and regulation. Advancing PFAS risk evaluation will require a shift from aggregate measurements to isomer-resolved science and policy.

Contrasting Mediterranean coastal wetlands: Emerging contaminants environmental interactions

Vicente Andreu, Julian Campo

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Mediterranean Wetlands support a high number of important species, including birds, mammals, reptiles, amphibians, fish and invertebrates, many of which are endemic to the region. However, these wetlands are the world's most threatened ecosystem and they are in danger of collapse without policies of restoration.

In this work two important wetlands of the Mediterranean Spain has been comparatively studied, the Oliva-Pego marsh and the Albufera of Valencia, both are Natural Parks under protection. The presence of emerging contaminants, heavy metals and 17 pharmaceuticals, in waters and the interrelationships between and with the intrinsic characteristics of waters and environmental parameters were also studied in both marshes.

Total concentrations of 17 pharmaceuticals, covering the most frequently used classes (anti-inflammatories, antibiotics, etc) were measured. The simultaneous determination of pharmaceuticals was performed by solid phase extraction (SPE). Extracts were analyzed by liquid chromatography–tandem mass spectrometry (UHPLC-MS/MS), using both, positive and negative ionization with an ESI interface. Concentrations of Al, As, B, Cd, Co, Cr, Cu, Fe, Li, Ni, Pb, Sr, Tl, and Zn were determined using microwave-assisted acid digestion. Total of concentration were measured using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES), except As and Cd that were quantified by an Inductively coupled plasma mass spectrometry spectrometer (ICP-MS). Two pollution indexes were applied, Heavy Metal Evaluation Index (HEI) and Water Pollution Index (WPI), to assess the water quality state in the area. Two pollution indexes were applied, Heavy Metal Evaluation Index (HEI) and Water Pollution Index (WPI), to assess the water quality state in these areas.

In the Albufera, for B, Sr, and Tl, all samples exceeded WHO limits, EU legislation, or EPA benchmarks, with 61.76 % and 85.71 % of samples surpassing standards for Al and Li, respectively. Regarding Oliva-Pego marsh, the values of the studied elments are very low in all cases. Only Li, Ni, and Sr show one value higher than the UE or WHO limits.

All water samples appeared contaminated with at least two pharmaceuticals, being ibuprofen and codeine those more frequently detected. Tetracycline and oxytetracycline were not detected in any sample, and fenofibrate and norfloxacin were not present in in La Albufera. However, both zones showed significant differences and pollution sources inherent to their own characteristics and circumstances. Salinity is one of the environmental parameters that affects in an important way the dynamics of inorganic and organic compounds.

Analysis using both indexes (HEI and WPI) revealed poor water quality in both areas, but mainly in the Albufera Natural Park.

Acknowledgements

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High-Resolution Mass Spectrometry- based monitoring of dissolved organic matter and pollutants in Basilicata region reservoirs

Giuliana Bianco[a,b]*, Angela Di Capua[a], Maria Assunta Acquavia[c] , Filomena Lelario[a], Rosanna Ciriello[a], Antonio Guerrieri[a], Giuseppe Martelli[a], Antonio Vassallo[a]

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The Pertusillo reservoir (Basilicata, Southern Italy) is a strategic freshwater resource for drinking water supply and irrigation. Owing to agricultural activities, urban settlements, and oil and gas exploitation within its watershed, comprehensive monitoring is essential to assess both natural biogeochemical processes and potential anthropogenic impacts.

Within the LUCAS (Lucania Ambiente e Salute) project, an integrated high-resolution mass spectrometry-based workflow was developed to investigate dissolved organic matter (DOM) and organic pollutants in reservoir waters. Water samples were collected during two monitoring campaigns at five representative stations and two sampling depths.

Targeted analyses of volatile organic compounds, organohalogenated compounds and petroleum hydrocarbons were performed using validated EPA and ISO methods. In parallel, DOM was extracted by solid-phase extraction (Bond Elut PPL) and characterized by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS). Molecular formula assignment, van Krevelen diagrams, Kendrick Mass Defect analysis and molecular networking were applied to characterize DOM composition and transformation processes.

Targeted analyses showed an overall good chemical status of the reservoir, with contaminants detected at concentrations below regulatory limits. These findings provide a reliable baseline for interpreting ultrahigh-resolution molecular fingerprints and discriminating natural organic matter from possible anthropogenic inputs. The integration of targeted contaminant determination with FT-ICR MS-based molecular characterization provides a powerful framework for environmental monitoring and supports the identification of molecular indicators for freshwater ecosystem assessment.

Acknowledgements

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Biomass-Derived Carbons as a Sustainable Strategy for Mitigating Pharmaceutical Pollution: Challenges and Opportunities

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Micro and mesoporous carbons and, in particular, biochar and activated carbon (AC), are massively applied in a large number of well-established and emergent environmental problems, with a global market that has been continuously growing. Currently available commercial options strongly rely on non-renewable fossil sources as AC precursors or on the pyrolytic conversion of biomass under harsh conditions, which raises concerns due to possible mid/long-term shortage of raw materials and the sustainability of these carbons. In this context, finding valid and reliable alternative precursors and sustainable production routes would trigger a significant increase in the greenness scale of these widely applied materials.

This communication presents recent advances in the use of carbon-rich residual biomass from industrial activities (namely, paper and brewing industries) for the development of micro and mesoporous carbons, with subsequent application in advanced water treatment, either as adsorbents or as photocatalysts. Along with the advantages of replacing non-renewable sources for AC production, the use of residual biomass contributes to the valorization and sustainable management of such residues, often significantly underutilized before disposal. Residual biomass from the referred industries were subjected to thermal and chemical treatments of different complexity, with strong focus on the precursors adequacy to repeatedly achieve materials with stable characteristics and on the evaluation of their potential to obtain microporous carbons with distinct key features. In this sense, this research was focused on the development of biochar and AC and further functionalization considering different strategies: grafting functionalization, incorporation of magnetic iron oxides, modification with molecular imprinting polymers and modification with oxidoreductase enzymes. Along with conventional heating for the conversion of the biomass into a microporous carbon net, microwave-assisted pyrolysis was applied in view of investing in more sustainable production routes, by optimizing low-energy processes, minimizing the use of reagents, and promoting after-use regeneration strategies. The developed materials were fully characterized, addressing their chemical, physical and textural properties, and their correlation with production conditions. Then, the efficiency of these materials in the removal of pharmaceuticals from water, foreseeing their application in the advanced treatment of wastewater, was evaluated either in single or competitive conditions, batch, or continuous modes. This research made a significant contribution to encourage the introduction of wastes in the productive chain, deconstructing the idea that secondary raw materials necessarily result in carbons with inferior properties.

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Wastewater Omics for Population Health and Lifestyle

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Wastewater is a complex but information-rich reflection of the society that generates it, integrating signals from human metabolism, diet, consumption patterns, health status, domestic activities, industry, and the surrounding urban ecosystem. Wastewater-based epidemiology (WBE) has traditionally focused on predefined chemical biomarkers and pathogen nucleic acids. However, advances in high-resolution mass spectrometry now allow us to study a wider range of small molecules and proteins without focusing on specific targets, providing much more information from wastewater.

We present complementary metabolomic and proteomic approaches to explore wastewater as a multidimensional fingerprint of population, lifestyle, and health. Untargeted metabolomics was applied to influent samples from five wastewater treatment plants differing in population size and industrial influence, collected over three seasonal campaigns. The combination of GC-MS, RPLC-MS, and HILIC-MS provided highly complementary coverage, yielding 828 unique annotated compounds with minimal overlap between platforms. Reproducible site-associated chemical fingerprints emerged after accounting for seasonal variability. Lipids, organic acids, organic oxygen compounds, organoheterocyclic compounds, and benzenoids were major contributors to these differences. The detected chemical space also included signatures related to tobacco and caffeine consumption, pharmaceuticals, endogenous metabolism, and food-related inputs, showing that untargeted metabolomics can reveal different aspects of community lifestyle.

Proteomics adds an orthogonal biological dimension. Wastewater profiling across municipalities with contrasting demographic and industrial characteristics revealed proteins originating from humans, livestock, rodents, plants, and microorganisms. Human pancreatic α-amylases emerge as promising population and normalization markers, while species-specific amylases, immunoglobulins, and albumins provide information on rodent populations and livestock-related activities. Moreover, hundreds of human proteins, including immune- and disease-related candidates, open the possibility of monitoring population health. Immunoproteomic strategies further extend this concept towards surveillance of host immune responses and pathogen antigens.

Together, metabolomics and proteomics transform wastewater into a population-scale observatory. Rather than relying on individual biomarkers, integrating complementary omic fingerprints may allow us to read how communities live, consume, interact with their environment, and respond to disease.

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Closing the Loop: Solar Hydrogen Production from Wastewater-Derived Organics

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The transition toward circular and resource-efficient water treatment requires technologies that not only remove contaminants, but also exploit their residual chemical value. Photocatalytic reforming offers this dual opportunity by using oxidizable organic species in aqueous streams as electron donors while simultaneously driving hydrogen evolution. Compared with conventional photocatalytic water splitting, the oxidation of organics can promote charge separation by scavenging photogenerated holes, thereby limiting electron-hole recombination and enhancing H2 production.

This concept is particularly attractive for industrial and municipal wastewaters containing readily oxidizable compounds, including alcohols and carboxylic acids. Rather than being treated exclusively as pollutants, these species can become reactive substrates in a solar-driven conversion process. Their transformation can therefore contribute to wastewater purification while recovering part of their chemical energy as a clean fuel, shifting advanced treatment from contaminant abatement toward integrated pollutant valorization and resource recovery.

Material design remains central to the feasibility of this approach. Photocatalysts intended for application in complex water matrices should combine efficient visible-light absorption and effective charge separation with high surface reactivity, chemical and photochemical stability, low toxicity, reusability, and economically sustainable preparation. Nanoscale metal-based semiconductors are particularly promising in this respect and have been widely investigated for photocatalytic and photoelectrocatalytic solar hydrogen production and environmental remediation (1).

This contribution discusses photocatalytic organic reforming from the perspective of advanced wastewater treatment and pollutant valorization, with emphasis on visible-light-active metal-based semiconductor nanomaterials (2). Particular attention is devoted to the relationships between crystallinity, particle size, band-gap characteristics, surface properties, and photoactivity, as well as to the role of the nature and concentration of organic substrates in controlling hydrogen evolution. Reaction pathways linking organic oxidation to proton reduction are considered together with kinetic aspects of photocatalytic H2 production (3). These elements are critically examined to identify the main opportunities and limitations for developing solar-driven processes capable of coupling water decontamination with renewable hydrogen recovery.

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Fair, efficient, and sustainable management of urban wastewater without compromising access to medicinal products

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Directive (EU) 2024/3019 of the European Parliament and of the Council of 27 November 2024 on urban wastewater treatment requires quaternary treatment of urban wastewater. In practice, the new extended producer responsibility (EPR) regime will apply only to the pharmaceutical and cosmetics sectors, which must cover at least 80% of the related treatment costs.

This approach marks a substantial departure from the traditional model of urban wastewater treatment, whose costs in Spain have historically been borne by public administrations. In Spain alone, the ministry responsible for environmental affairs estimates that implementing quaternary treatment will cost approximately €5 billion over the next 20 years.

According to the Directive, pharmaceutical and cosmetic residues are currently the main sources of micropollutants in urban wastewater that require quaternary treatment. On that basis, the EPR regime is applied to those two sectors.

However, imposing EPR exclusively on pharmaceutical and cosmetics producers raises questions about compliance with the polluter-pays principle and the principle of equal treatment.

Pharmaceuticals and cosmetics undoubtedly contribute to wastewater contamination, but they are not the only sources of micropollutants. Other product groups appear to have been underestimated during the legislative process, possibly because pharmaceuticals and cosmetics were selected for EPR without a scientific comparison with other producer categories. Consequently, other relevant sources—including pesticides, plastics, food products and chemicals—are initially excluded from the obligations.

The EPR regime created by the Directive is both novel and exceptional: it transfers a mechanism from waste regulation into the field of water treatment, creating several distortions and weaknesses.

Unlike traditional EPR schemes, in which producers can organise the management of waste generated by their products, this regime imposes mainly financial obligations linked to public infrastructure and pre-existing treatment systems. Producers therefore have limited ability to influence decisions that determine costs, including the choice of treatment technologies, the selection of facilities and the design of operating models.

When producers must bear the costs of removing contamination, they are generally encouraged to consider more environmentally friendly substitute materials. For most medicinal products, however, reformulation or material substitution is not feasible.

Where substitution is neither possible nor desirable, producers might ordinarily incorporate the additional costs into product prices and pass them on to customers and consumers, who could then consider alternatives. This option is also constrained in many countries, including Spain, because the prices of reimbursed medicinal products are regulated and marketing authorisation holders cannot increase them unilaterally.

If “no reformulation” of the product and “no increasing” of prices, the product itself would be in compromised situation related to its continuity in the market, mainly in the case of critical medicinal products. But if these products are exempted to pay the costs of quaternary treatment, it will be producers of the products not exempted that will have to pay for what they have not contaminated.

In short, we are in a very complex situation (and now judicialized) to determine who should finance this, who is exempt and how the application of this important directive will be carried out in the coming years.

Passive samplers for the monitoring of contaminants in surface waters

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In recent years, the analytical chemistry community has increasingly focused on developing methods that align with the principles of Green Analytical Chemistry. In addition, when designing methods for monitoring contaminants in environmental water samples, the sampling procedure must be efficient, reliable, and representative of the water body, while also remaining simple and easy to implement. In this context, passive sampling has attracted considerable attention as a suitable approach for water quality assessment, as it has been proposed as a feasible alternative to conventional monitoring techniques. Its advantages over active sampling include the elimination of complex pumping systems, improved representativeness, the ability to obtain time-weighted average concentrations, and the avoidance of solvent use when thermal desorption is applied (1).

Passive samplers (PS) as sampling devices for the determination of a group of polar emerging contaminants in environmental water samples, followed by liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) is overviewed. Two types of PS were evaluated: macroporous ceramic samplers (Fig. 1A), consisting of a porous ceramic tube that enables compound diffusion (2), and a PS developed through 3D printing using polylactic acid (Fig. 1B), in line with the use of sustainable materials. In both cases, the samplers were filled with different sorbent materials to provide a range of retention capabilities for the target compounds. Key parameters, including analyte stability, diffusivity, and sampling rates, were assessed to enable proper calibration of the PS. Once calibrated, the samplers were deployed for monitoring contaminants in surface waters.

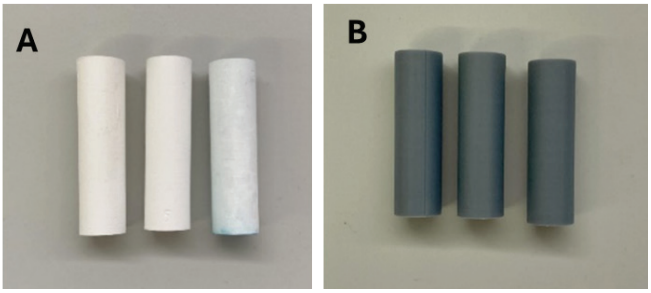


Figure 1. Ceramic (A) and 3D printing polylactic acid (B) passive samplers.

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Multi-Matrix exposomics: Mapping chemicals across the human body

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Understanding how environmental chemicals distribute and persist across human tissues is essential to interpret exposure and biological response. This question becomes especially critical in certain situations, such as during fetal development, when multiple biological barriers regulate the exchange of chemicals between the mother and the developing child. Yet, characterizing this complex chemical landscape remains analytically challenging due to the diversity of matrices, concentrations, and compound classes involved.

In this talk, I will discuss how advanced LC–high-resolution mass spectrometry (LC-HRMS) can be applied to map chemical distribution across interconnected biological compartments, including urine, serum, placenta, and cord blood, providing an integrated view of internal exposure. HRMS workflows enable the detection of hundreds of environmental chemicals and transformation products spanning a broad polarity and volatility range. Combining targeted and untargeted analyses allows us to resolve tissue-specific partitioning patterns and identify physicochemical and biological determinants of transport across interfaces such as the placenta.

In this context, I will also address one important analytical bottleneck in multi-matrix exposomics: the high intraindividual variability observed in chemical concentrations. Such variability can arise from short-term exposure fluctuations, sampling conditions, and analytical uncertainty, complicating the interpretation of exposure levels and highlighting the need for strategies to obtain more reliable and adjusted estimates. These approaches are essential to draw meaningful conclusions and enhance biological interpretability.

Together, these efforts illustrate how multi-matrix exposomics provides a scalable analytical framework to understand chemical transport within the human body, ultimately linking exposure to molecular and health outcomes.

Studying the ionization of neutral PFAS with flexible microtube plasma ionization and LC-MS

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Dielectric barrier discharge ionization (DBD) is a versatile ionization technique adaptable to different analytical platforms, including liquid and gas chromatography interfaces or ambient mass spectrometry formats. The relatively mild DBD conditions generate positive or negative ions via multiple processes such as Penning ionization, electron capture, proton transfer, among others. Most research has predominantly focused on positive ion mode, though. In this presentation, flexible microtube plasma (FμTP) source was evaluated for negative ionization using liquid chromatography-high resolution mass spectrometry (LC-HRMS). A set of 18 per- and polyfluoroalkyl substances (PFAS), including nine compounds covered by the Spanish drinking-water Σ20 PFAS parameter (Real Decreto 3/2023), was selected as model analytes due to their environmental relevance as persistent contaminants. The set included perfluoroalkyl carboxylic acids (PFCAs), perfluoroalkyl sulfonic acids (PFSAs), the perfluoroether carboxylic acid HFPO-DA (GenX), and fluorotelomer compounds, namely fluorotelomer alcohols (FTOHs), and fluorotelomer olefins (FTOs). These comprised both compounds readily analyzed by electrospray ionization (ESI), such as PFCAs or PFSAs, and less ESI-amenable neutral fluorotelomer compounds. The ionization performance of FμTP was compared with conventional LC ionization sources (ESI and atmospheric pressure chemical ionization (APCI), with ion assignment confirmed by Orbitrap-HRMS. Distinct ionization and fragmentation patterns were observed across sources, reflecting differences in ionization mechanisms. For carboxylic and sulfonated PFAS, FμTP showed gas-phase-like behaviour with enhanced in-source fragmentation compared to ESI and APCI. For neutral PFAS, not efficiently detected by ESI, FμTP enabled ionization via -H_nF_m loss and subsequent fragmentation, generating diagnostic fragment ions. Overall, FμTP represents a promising alternative ionization source for PFAS analysis, providing characteristic ionization fingerprints and enhanced suitability for full-scan screening approaches, with reduced reliance on tandem mass spectrometry (MS/MS) experiments for compound identification.

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New chemometric approaches on the occurrence, risk assessment and modelling of chemical mixtures in the freshwater environment

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Pollutants in freshwater environments occur as complex and highly variable mixtures rather than as individual compounds. This complexity challenges current regulatory frameworks, including the Water Framework Directive (WFD) and its daughter legislation, where prioritisation and Environmental Quality Standards (EQSs) are largely based on single-compound risk assessment (e.g., priority substances, river-basin-specific pollutants, Watch List substances). Over the past decade, several EU-funded projects (e.g., SOLUTIONS and GLOBAQUA) have highlighted these limitations and called for mixture-oriented assessment approaches (1).

Recent advances in chemical analysis, particularly LC-HRMS, together with chemometric methods, have generated extensive monitoring datasets that offer new opportunities for mixture characterization. Among these, Multivariate Curve Resolution–Alternating Least Squares (MCR-ALS) enables the resolution of environmentally occurring mixtures into their compositional, spatial, and temporal profiles (2), typically regarded as "pollution sources". The approach presented thus integrates environmental risk assessment into the MCR-ALS framework. First, the concentration of each compound is transformed into a risk quotient (RQ) by dividing the measured concentration by its predicted no-effect concentration (PNEC), following current environmental risk assessment practice (3). The resulting RQ matrix is subsequently analysed by MCR-ALS using a multilinear model (i.e., bilinear or trilinear) (2), allowing the identification of characteristic risk-based composition profiles and their spatial and temporal distributions. Finally, the obtained spatiotemporal and compositional risk profiles are modelled within a scalar field matrix.

The proposed methodology is demonstrated using monitoring data from the Llobregat River basin (NE Spain) (4). The dataset comprises 71 contaminants of emerging concern—including pharmaceuticals, pesticides, perfluoroalkyl substances, endocrine-disrupting compounds, and drugs of abuse—monitored at 14 sampling sites (seven along the main river and seven in two tributaries) during two monitoring campaigns. The risk matrix was successfully factorized using a bilinear MCR-ALS model, resolving five major risk sources. The resulting compositional profiles revealed pharmaceuticals as the dominant contributors to environmental risk in three of the five resolved sources. Overall, the proposed methodology provides an integrated chemometric framework for identifying, characterising, and modelling environmentally relevant contaminant mixtures (sources) from a risk perspective, offering a valuable complement to conventional single-substance assessment approaches.

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Assessment of the health status of the Ebro River after remediation of the dumped waste from a chlor-alkali plant

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One hundred km upstream from the Ebro estuary, there was a chlor-alkali plant that was the one who manufactured PCBs in Spain and the major producer of DDT in this country when these activities were legal. It was also a main manufacturer of dicalcium phosphate using phosphorite. As a result of these activities, 500,000-700,000 tons of waste containing large amounts of PCBs, DDTs, Hg and radionuclides, originating from the phosphorite, were dumped in the water reservoir located in front of the factory. Between 2010 and 2023, actions were carried out to remove this waste, treat it, and dispose of it in a landfill.

After remediation, in 2025, the concentrations of Ni, Hg, Cr, As, Se, PCBs, pentachlorobenzene, hexachlorobenzene, hexachlorocyclohexane and DDTs in the sediments of the reservoir were lower than those present before the waste removal.

However, these sediments were still polluted at levels harmful for the organisms by As, Cd, Hg, Cr, Pb, PCBs, hexachlorobutadiene, DDTs and dioxins (polychorodibenzodioxins, polychlorodibenzofurans, dioxin-like PCBs). A unique aspect of these sediments was the dominance of 4,4'-DDT over the other species in this group, including 4,4'-DDE. Concerning fluoranthene, benz[a]anthracene, chrysene, benzo[a]pyrene and dibenz[a]anthracene the concentrations nearby the old discharge sites of waste were also harmful for the organisms.

The sedimentary concentrations of Ni, Cd, Pb, hexachlorobutadiene, pentachlorobenzene, hexachlorobenzene and hexachlorocyclohexanes in the reservoir were higher than those found in the Flix meander. Those of Zn and As were similar both in the reservoir and the meander. In contrast, the concentrations of PCBs, dioxins, DDTs, anthracene, fluoranthene, benz[a] anthracene, chrysene, benzo[a]pyrene, indeno[1,2,3-cd]pyrene and dibenz[a] anthracene were lower than those found in the meander.

In the meander, the concentrations of Hg, PCBs, DDTs, dioxins and polycyclic aromatic hydrocarbons exceeded concentrations known to cause harmful effects to organisms.

One especial case concerned the DDT concentrations, 9.0-150,000 µg/kg, that were even higher in the meander than in the reservoir before waste removal. This feature was consistent with dumping sites in the meander that were not remediated. The concentrations of hexachlorobutadiene, pentachlorobenzene and hexachlorobenzene were also consistent with local dumping sites in the meander.

In fish (carps) from the meander, the high concentrations of chlorinated compounds, especially the coplanar ones, and polycyclic aromatic hydrocarbons correlated with higher EROD and BFCOD enzymatic activities in microsomes from hepatic tissue and, together with metals, caused increased oxidative stress. This impact was also observed in transplanted Asian clams after two week exposure in the meander, that also showed increased accumulation of Hg...

The results obtained showed that there was a very significant contamination in the sediment samples from the Flix reservoir and meander. This contamination was transferred downstream during floods, primarily in the cases of Cd, Pb, Hg, DDTs, and benzo[a]pyrene. The observed concentrations of these compounds in the particles collected during the high-flow events were higher than those reported for deleterious effects in organism and resulted in increased toxicity of the Ebro River waters. Under non-flooding conditions, , reduced but detectable inputs of DDTs (predominantly 4,4'-DDT), polycyclic aromatic hydrocarbons, dioxins, dicofol, As, Cd, Cu, Cr, Ni, Pb, and Zn were still observed. However, regarding the metals, their concentrations in 2025 were lower during flooding than those observed in 2006, a difference that is consistent with the waste extraction work carried out at the Flix reservoir.

Water-based epidemiology for community health early warning: advances in analytics and data triangulation approaches

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This talk will present recent advances in water-based epidemiology (WBE) as a transformative approach for community health surveillance and early warning. By analysing chemical and biological markers in wastewater and environmental waters, WBE provides anonymised, near real-time insights into population health, exposure, behaviour, and infectious disease dynamics at the community scale.

This presentation will showcase our recent advances in WBE analytics, particularly high-resolution mass spectrometry, which are expanding the scope of WBE beyond its established applications in drug monitoring and infectious disease surveillance to include the assessment of dietary patterns, nutritional status, environmental exposures to hazardous chemicals, and broader determinants of health within populations.

A particular focus will be placed on data triangulation approaches that integrate community-level wastewater measurements with socioeconomic, demographic, environmental, and spatial datasets, highlighting both their advantages and limitations. Such integration enables more robust interpretation of wastewater signals, supports the identification of vulnerable populations and emerging health threats, and facilitates the development of fit-for-purpose public health surveillance systems.

Integrating environmental data with dynamic modelling for urban water risk assessment

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Climate change, urbanisation and ageing infrastructure are pushing cities to move from fragmented, centralised water management towards integrated, decentralised schemes. These schemes reuse wastewater and stormwater, which also carry pharmaceuticals, other contaminants of emerging concern (CECs), microplastics and pathogens. Reliable risk assessment therefore needs to link the quantity of water moving through the urban water cycle with its quality. This presentation discusses how monitoring data, sensors and dynamic models can be integrated into decision support for Integrated Urban Water Management. It also examines the data, structural and parameter errors that can make a model or Digital Twin perform well for the wrong reasons.

A daily urban water balance model of the Greater Athens Area (about 3.8 million inhabitants) was compared against measured imported water and wastewater discharge. It was then used to evaluate decentralised water saving strategies under climate change scenarios: a 20% decrease in precipitation and a 1°C temperature increase. On-site wastewater treatment and reuse reduced imported water by 17.7% and wastewater discharge by 20.7%. Rainwater harvesting reduced stormwater runoff by 27.2%. These results show that reuse can substantially reduce freshwater demand.

To address this quality dimension, the work is being extended within the EU-funded UrbaQuantum project. UrbaQuantum combines novel in situ sensors for pathogens, chemical CECs and microplastics with new models of sewer overflows and stormwater pollutant pathways, and feeds both into an Urban Water Platform for risk-based decision support. In the Attica case study, effluents from two wastewater treatment plants and urban runoff are characterised in the laboratory and monitored with sensors. Coupling these concentration data with modelled flows allows contaminant loads and exposure pathways to be estimated. This supports risk-informed water reuse and the EU Zero Pollution ambition.

Keywords: urban water cycle; Digital Twin; water reuse; contaminants of emerging concern; sensors; risk-based decision support

Advancing Environmental Monitoring Through LC-HRMS-Based Non-Targeted Approaches: From Contamination Profiling to Contaminant Prioritization

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Environmental monitoring is increasingly challenged by the diversity of organic contaminants occurring in complex matrices. Targeted approaches provide robust quantitative information for predefined substances, but can overlook unknown or unexpected contaminants. Suspect screening and non-target analysis (NTA) using liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS) can broaden the chemical space investigated. This keynote will discuss how sample preparation, identification confidence, occurrence assessment and contaminant prioritization influence the information obtained from HRMS-based screening.

Recent applications will illustrate this approach across contrasting scenarios. In wastewater effluents, comparison of lyophilization, direct injection and online solid-phase extraction showed that sample preparation strongly affects the chemical fingerprint: 119 CECs were identified with high confidence, but detection differed markedly among approaches (1). In a reclaimed-water irrigation system, wide-scope LC-HRMS screening using lyophilization for sample preparation identified 158 contaminants of emerging concern (CECs), whose occurrence and ecotoxicity were combined to prioritize site-specific pollutants relevant to water reuse (2). In Antarctic Peninsula waters, LC coupled to trapped ion mobility and HRMS detected 88 CECs in 19 samples, including 54 confirmed with reference standards. Ion mobility provided additional structural information and improved discrimination of isobaric and conformational isomers, supporting risk assessment and prioritization.

Finally, LC-HRMS NTA of urban PM2.5 from eight monitoring stations in Barcelona enabled the confident annotation of 40 CECs, including 21 compounds reported for the first time in urban air (3). Together, these studies demonstrate how HRMS-based non-targeted strategies can move environmental monitoring beyond the detection of individual contaminants towards comprehensive contamination profiling, improved identification confidence, semi-quantitative assessment and evidence-based prioritization across diverse environmental matrices.

Acknowledgements

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Mass Spectrometry and Ion Mobility for the Characterization and Determination of Arsenosugars in Algae

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Arsenic is an environmental and food contaminant whose toxicity depends strongly on its chemical form. In edible seaweeds, arsenosugars (As-sugars) are the predominant arsenic species, but uncertainties regarding their long-term health effects require reliable analytical approaches for their characterization.

This study presents an LC-HRMS workflow for arsenosugar profiling in edible macroalgae, combining hydrophilic interaction liquid chromatography (HILIC), Orbitrap HRMS, and ion mobility quadrupole time-of-flight mass spectrometry (IMS-QTOF-MS). A zwitterionic HILIC column enabled the simultaneous separation of the four major arsenosugars commonly found in seaweeds: glycerol (Gy-Sug), phosphate (PO_4-Sug), sulfonate (SO_3-Sug), and sulfate (SO_4-Sug) arsenosugars.

Accurate-mass measurements and high-resolution tandem MS data acquired in positive and negative ionization modes provided detailed structural characterization of all target compounds. Diagnostic fragments and neutral-loss pathways were established, while ion mobility separation improved spectral selectivity by reducing matrix interferences.

A key outcome of this work is the first experimental determination of collision cross-section (CCS) values for the four principal arsenosugars. CCS measurements showed excellent repeatability (RSD < 0.3%) and offered an additional identification parameter independent of retention time and less affected by matrix effects.

The methodology was applied to twelve edible seaweed samples from brown, red, and green algae. Arsenosugars were the dominant arsenic species, with distinct distribution patterns among algal groups. The results demonstrate the value of integrating LC-HRMS and ion mobility spectrometry for arsenic speciation in food and environmental samples, supporting exposure assessment, food safety monitoring, and future studies on organoarsenic compounds.

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Two Decades of HRMS in Pesticide Residue Analysis: From Milestones to Future Directions

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High-resolution mass spectrometry (HRMS) has undergone a remarkable evolution over the last two decades, moving from a highly specialized research tool to an increasingly important platform for small-molecule analysis, particularly in the field of pesticide residues and environmental contaminants. Improvements in resolving power, mass accuracy, acquisition speed, sensitivity and full-scan capabilities have expanded its role from targeted confirmation to wide-scope screening, suspect and non-target analysis, and retrospective data reprocessing.

HRMS offers clear advantages for reliable identification, helping to reduce the risk of false positives and false negatives while providing additional information on metabolites, degradation products, transformation products and unexpected residues. Its relevance is particularly evident in complex food and environmental matrices, where analytical selectivity, regulatory requirements, monitoring scopes and decision-making criteria may vary across regions and applications.

This presentation reviews key milestones in the application of HRMS to pesticide residue and environmental contaminant analysis, including the development of LC-HRMS and GC-HRMS workflows, accurate-mass screening, spectral libraries, data-independent acquisition and improved confirmation strategies. Particular attention is given to the practical challenges that still limit broader implementation in routine laboratories, especially sensitivity, robustness, cost, data processing and harmonized identification criteria.

Finally, future directions are discussed, including microflow LC, enhanced dynamic range approaches, adaptive acquisition strategies, artificial intelligence-assisted data evaluation and integrated workflows combining targeted quantification with suspect and retrospective screening. These developments may help bring HRMS closer to routine control needs while preserving its unique strength: the generation of reliable, information-rich data beyond classical targeted analysis.

From source to tap: Perspectives of water monitoring using liquid chromatography high-resolution mass spectrometry

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High-resolution mass spectrometry (HR-MS) has been increasingly used over the past years in water analysis, mostly for suspect screening or non-target analysis. At the same time the focus has shifted towards inclusion of polar compounds by more suitable separation techniques than classical reversed-phase chromatography. Finally, spot sampling can nowadays be complemented by time-averaged approaches. All these developments contribute to a much more comprehensive coverage of the chemical space in water ranging from sources such as municipal and industrial wastewater to receiving aquatic ecosystems and eventually drinking water. To maximise the benefits of these approaches reliable data processing and advanced chemometric data analysis are prerequisites (1). The presentation will highlight current trends and will give examples from recent case studies in my group in all these areas.

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Expanding the PFAS Atmospheric Inventory: From Legacy Ionic Compounds to Volatile Precursors

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Per- and polyfluoroalkyl substances (PFAS) in the atmosphere remain mostly understudied despite growing evidence that both legacy ionic PFAS and volatile precursor compounds contribute to long-range environmental transport and human exposure. In this work, we integrated two complementary approaches to broaden the PFAS atmospheric inventory across gaseous and particle-bound phases. First, we developed and conducted a year-long assessment of particle-bound PFAS in outdoor air at a coastal urban site in South Florida using a six-stage Tisch cascade impactor, which mimics the human respiratory system (1). The air sampler was equipped with glass fiber filters in each stage. PFAS were extracted from the filters by sonication with methanol and analyzed by LC-MS/MS. Secondly, to explore PFAS occurrence and distribution in the gas phase, we developed a method for measuring gaseous fluorotelomer alcohols (FTOHs) and perfluoroalkane sulfonamides (FASAs) using solid-phase microextraction (SPME) coupled with GC-MS/MS, which enabled the sensitive detection of six FTOHs (4:2–10:2), Me/Et- FOSA and Me/Et-FOSE with minimal use of solvent and without the need of traditional pre-concentration systems (Figure 1). Air samples were collected by a cascade impactor sampler equipped with glass fiber filters at each stage and a polyurethane foam (PUF) after the last stage, which allowed the capture of gas-phase compounds and evaluation of their phase distribution. The estimated method detection limits ranged from 0.08 pg/m^3 to 1.19 pg/m^3 for the non-volatile and semi-volatile PFAS in the atmospheric particulate matter (APM). PFBA was the most frequently detected compound in APM, while PFOS exhibited a bimodal size distribution with enrichment in fine particles relevant to tracheobronchial and alveolar deposition. Meteorological factors, including temperature, humidity, and rainfall, were found to influence PFAS occurrence and persistence in airborne particles. The SPME-GC-MS method was optimized (by varying extraction time, temperature and desorption time) and validated using headspace, achieving the lowest instrument detection limit (LOD) of 0.1 µg/L for most of the targeted compounds. Longer extraction time and higher temperatures generally improved the detection for major compounds, including 8:2 FTOH and 10:2 FTOH, and heavier compounds (N-MeFOSA, N-EtFOSA), but affected the more volatile PFAS, such as 5:2 FTOH. Together, these studies demonstrate that both volatile precursors and particulate PFAS can have important contributions to atmospheric PFAS burdens. By integrating optimized and complementary analytical workflows (LC-MS/MS and GC-MS) with long-term air ambient monitoring, this work advances our understanding of PFAS behavior in air and supports the development of more comprehensive human exposure assessments and guide future regulatory frameworks.

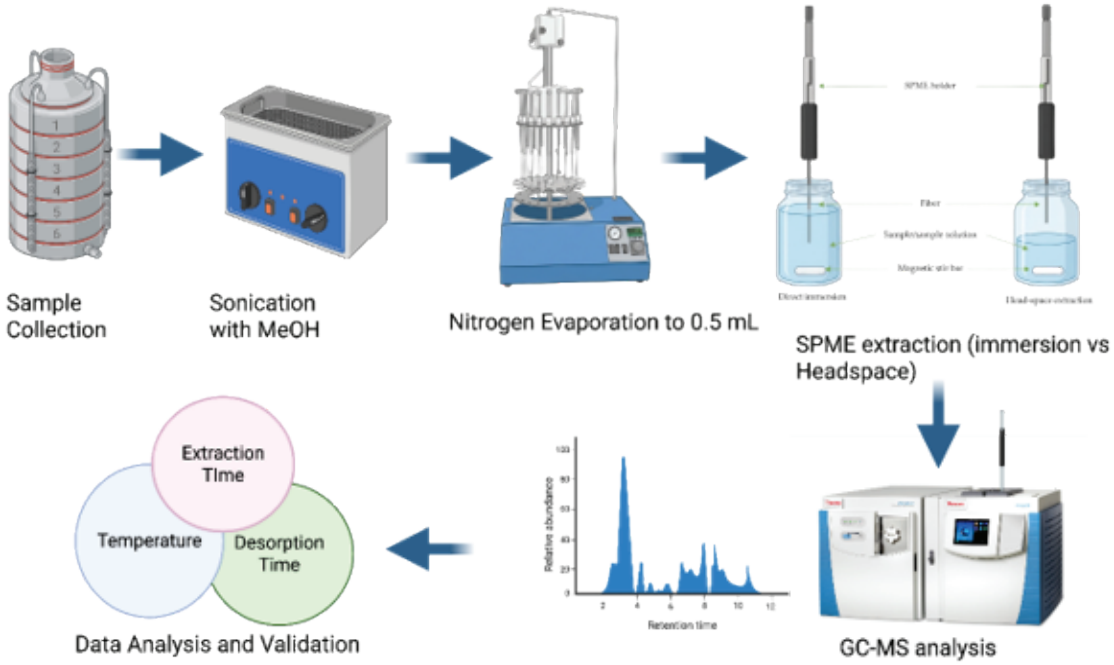


Figure 1. Sample collection and processing for air samples analysis by SPME GC-MS/MS. Created with Biorender.

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Comprehensive Chemometric Analysis of Ion Mobility coupled with Liquid Chromatography High Resolution Mass Spectrometry Data

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Ion mobility mass spectrometry coupled with liquid chromatography (LC-IMS-MS/MS) is a powerful analytical technique for the in-depth characterization of complex environmental and biological samples. However, the large, multidimensional datasets generated by LC-IMS-MS/MS present significant challenges for data interpretation. To address this issue, we have introduced the Regions-of-Interest-Multivariate Curve Resolution (ROIMCR) strategy[1,2]. Unlike conventional approaches that reduce ion mobility information to a single collision cross-section (CCS) value, ROIMCR preserves the complete ion mobility profile, enabling a more comprehensive and accurate analysis.

The core of the proposed approach is a three-way data formulation implemented through either bilinear or trilinear multivariate curve resolution models. This framework simultaneously resolves the three principal dimensions (ways or modes) of the dataset: chromatographic elution profiles, ion mobility profiles, and mass spectra, including both MS1 and MS2 data. By enforcing chemically consistent solutions across these three dimensions, the model generates interpretable component profiles with high analytical performance.

Compound annotation is achieved by directly comparing the resolved drift-time and tandem mass spectral profiles with reference library data. The effectiveness of the three-way ROIMCR approach proposed in this work is validated using two distinct datasets: a synthetic mixture of four analytes, and an experimental lipid-mixture dataset[3]. Overall, the proposed three-way MCR framework provides an accurate, powerful and chemically meaningful solution for the analysis of high-dimensional LC-IMS-MS/MS data, particularly in lipidomics analysis.

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Toxicological Impacts of Environmentally Relevant Pharmaceuticals: Bioconcentration, Tissue-Specific Distribution, and Ecological Implications Revealed by Advanced Mass Spectrometry

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Pharmaceuticals and related contaminants of emerging concern are continuously introduced into aquatic and terrestrial environments, creating the potential for chronic exposure in non-target organisms. Assessing their ecological significance requires understanding not only whether exposure occurs, but whether contaminants accumulate, where they localize within an organism, and how that internal distribution relates to toxicological response.

The development of mass spectrometry imaging as an emerging technique over the past decade in environmental science when applied as a complementary mass spectrometry approach to investigate localization in addition to accumulation and toxicity. While targeted liquid chromatography–mass spectrometry provides quantitative measurements of contaminant uptake and bioconcentration, MSI preserves spatial information that is lost during conventional tissue homogenization. The use of MSI to visualize the distribution of contaminants directly within biological tissues provides spatially resolved analysis that can identify regions of localized accumulation, distinguish compound-specific distribution patterns, and provide insight into potential uptake and transport pathways. The approach has been applied across aquatic and terrestrial model organisms, with additional method development required in the future aimed at expanding the accessibility of MSI for environmental applications.

PFAS in AFFF contaminated sites - What can we learn from LC-HRMS analysis

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The analysis of PFAS in environmental samples is very challenging because of their diverse physical/chemical properties and the high number of individual PFAS compounds. Therefore, nontarget screening (NTS) approaches are highly attractive and provide promising results. For assessment of risks and long-term behaviour of PFAS in contaminated sites, semi-quantification and identification of transformation products and their formation kinetics is furthermore required.

In this work we present data from an AFFF contaminated soil site from a large fire event in 2008 in southwest Germany. Based on NTS and data prioritization and evaluation using our software tool PFAScreen we identified a much larger extent of PFAS contaminants than previously known: 124 PFAS and their transformation products from 42 subclasses at confidence levels for identification between 1 and 3. These included anionic, cationic, and zwitterionic substances with 3 to 14 perfluorinated carbon atoms. Only 28 PFAS could be quantified based on standard calibration functions. We therefore developed and applied a semi-quantification method based on matrix-matched average calibration curves of suitable authentic standards taking four different functional and/or ionization groups into consideration: carboxylic acids, sulfonic acids, sulfonamides, and cationic PFAS. We achieved a median prediction error of 2.2x, at a range between 1.3x and 5x. This showed that in the topsoil of the contamination cationic and zwitterionic PFAS dominate, that semi-quantified PFAS more than doubled the sum concentration of quantified PFAS in soil (7.3 µg/g) and that the total sum finally explains completely the extractable organic fluorine (EOF) of the contamination. To predict the long-term behaviour of the contamination we performed photocatalytic oxidation processes (PhotoTOP) and identified potential intermediates and final oxidation products by target and NTS and investigated their transformation kinetics. The results provide insight into the occurrence, behaviour and persistence of PFAS in contaminated soil and their potential fate in the environment.

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ORAL PRESENTATIONS

Integrating targeted LC–MS/MS and high-resolution mass spectrometry suspect screening for comprehensive characterization of emerging contaminants in a legacy landfill-impacted river

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Legacy landfills are long-term sources of complex mixtures of contaminants of emerging concern (CECs), yet environmental monitoring is often limited to a relatively small number of regulated compounds. Integrating targeted and suspect screening approaches can substantially improve the characterization of these complex contaminant mixtures and provide a more comprehensive understanding of their environmental impact. To evaluate contaminant dispersion from a legacy landfill into a receiving water body, surface water samples were collected from the Nitelva River and the adjacent landfill tributary upstream and downstream of the Brånåsen landfill (Norway). Samples were analyzed using a complementary analytical workflow that combined targeted liquid chromatography–tandem mass spectrometry (LC–MS/MS) for the quantification of selected per- and polyfluoroalkyl substances (PFAS), gas chromatography–tandem mass spectrometry (GC–MS/MS), and ultra-high-performance liquid chromatography coupled to Orbitrap high-resolution mass spectrometry (UHPLC–HRMS) for suspect screening. Compound identification was supported by accurate mass measurements, isotopic pattern evaluation, data-dependent MS^2 fragmentation, spectral library matching, and confidence assignment according to the Schymanski framework. Targeted analysis revealed a distinct contamination gradient along the Nitelva River, confirming the landfill as a continuing source of PFAS. Perfluorooctanesulfonic acid (PFOS) was the predominant compound, reaching 780 ng L^1 in the landfill tributary before decreasing to 110 ng L^1 approximately 3 km downstream in the river. Other perfluorinated compounds (PFOA, PFHxS, PFHxA, PFPeA, and PFBS) were also detected, indicating a diverse PFAS profile. HRMS suspect screening considerably expanded the investigated chemical space by identifying polymer-derived contaminants, including diethylene glycol dimethacrylate (DEGDMA) and triethylene glycol dimethacrylate (TEGDMA), together with additional dimethacrylate-related compounds assigned to Schymanski confidence Levels 2 and 3. Several of these compounds followed spatial trends consistent with landfill-derived inputs. The combined analytical workflow significantly expanded the chemical information that could be obtained with targeted analysis alone, demonstrating the value of integrating quantitative LC–MS/MS with HRMS suspect screening for comprehensive environmental monitoring, source characterization, and environmental risk assessment of legacy pollution sources.

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From arid to Arctic: Non-target screening of CECs across climatic extremes

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Extreme environments are increasingly recognized as important areas for investigating the occurrence and behaviour of emerging organic contaminants. Non-target screening provides a powerful approach for exploring complex chemical profiles without restricting the analysis to a predefined list of compounds. This study presents a non-target screening workflow applied to environmental samples collected across contrasting climatic regions, including Mediterranean and arid areas in northern and southern Tunisia and Arctic environments in the Tromsø region of northern Norway.

In Tunisia, 20 sites were sampled once, including nine sites in the north around Tunis and Bizerte and eleven sites in the south around Gafsa and Tozeur. The northern campaign focused mainly on surface waters, whereas the southern campaign covered a broader range of water types, including groundwater, river, cascade and thermal waters. In the Tromsø region, eight sites were sampled over three consecutive days, including background sites in the fjord and locations potentially influenced by urban, wastewater-related, airport and industrial activities.

The samples were filtered through glass-fiber filters and extracted by solid-phase extraction using hydrophilic–lipophilic balanced sorbent cartridges to enrich a broad range of organic micropollutants. System blanks were included to assess potential contamination introduced during sample preparation, while internal standards were used to evaluate extraction performance. The extracts were analyzed by high-resolution mass spectrometry using a SCIEX X500R QTOF in non-target screening mode. Data-independent SWATH acquisition provided precursor and fragment ion information, supporting broad compound detection and identification.

Data processing combines non-target screening in SCIEX OS with suspect screening based on internal spectral libraries. The resulting chemical fingerprints give a comparison across sites, water types and climatic regions to investigate spatial differences, short-term variability and potential anthropogenic influences. This comparative approach aims to reveal region-specific chemical patterns and broaden current knowledge of emerging organic contaminants across highly contrasting environments.

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Selection and Preliminary Evaluation of Biomass and Sludge-Derived Biochars for Pharmaceutical Removal from Wastewater

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The management of increasing quantities of sewage sludge and the continuous release of pharmaceutical contaminants into aquatic environments represent two major environmental challenges requiring sustainable and integrated solutions [1,2]. Converting sewage sludge into biochar through co-pyrolysis with lignocellulosic residues offers a promising approach to simultaneously valorise waste streams and develop low-cost adsorbents for advanced wastewater treatment [3].

This work aimed to develop and optimise biochar-based adsorbents for the removal of pharmaceuticals included in the Urban Wastewater Treatment Directive (EU) 2024/3019, namely carbamazepine, citalopram, diclofenac and venlafaxine [4]. Initially, biochars produced from acacia, eucalyptus, and vine pruning were prepared by pyrolysis (700 °C, 4 h), ground (<75 µm), and physiochemically characterised, including determination of the pH at the point of zero charge. In parallel, an HPLC method was developed and validated for the simultaneous quantification of the selected pharmaceuticals. Batch adsorption experiments were subsequently performed to optimise key parameters, including adsorbent dosage, particle size and contact time. Among the biomass-derived biochars tested, eucalyptus-derived biochar showed the best overall adsorption performance, achieving removal efficiencies above 70% for most of the target pharmaceuticals. Based on these results, eucalyptus biomass was selected for co-pyrolysis with sewage sludge (50:50, w/w; 461 °C, 4 h). The resulting biochar was subsequently evaluated under batch and continuous-flow conditions using experimental conditions established during optimisation studies. This work contributes to the development of cost-effective adsorbents for quaternary wastewater treatment while promoting the valorisation of sewage sludge and agroforestry residues in line with the Directive (EU) 2024/3019 and circular economy principles.

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From *in-vitro* to *in-vivo*: liquid chromatography-mass spectrometry elucidation of mammalian metabolism of tire-related chemicals

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Tire anti-degradant N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD) and the cross-linking agent hexamethoxymethylmelamine (HMMM) are widely used in rubber products, despite their potential to leach from polymeric materials and accumulate in the environment (1). Furthermore, 6PPD transformation product 6PPD quinone (6PPDQ) is known to be toxic to some aquatic species (2), and 6PPD in aqueous media usually suffers an oxidative deamination to generate 4-hydroxyphenylamine (4-HDPA). However, information on the mammalian metabolism and toxicokinetic behavior of these compounds remains scarce. Firstly, we investigated the *in-vitro* Phase I and II metabolites of the above compounds using human liver microsomes and cytosolic fractions through a suspect screening workflow by liquid chromatography-high resolution mass spectrometry (LC-HRMS), where up to 13 metabolites were tentatively identified. Subsequently, an *in-vivo* toxicokinetic study was conducted with Wistar rats for validating *in-vitro* findings. Animals were orally administered with 1 mg/kg of each compound individually, and urine and plasma samples were collected at multiple time points. A target LC-triple quadrupole-tandem mass spectrometry (LC-MS/MS) method was developed for parent compounds and their metabolites in the biological samples, and their concentration-time profiles were evaluated through a semi-quantitative approach to characterize their toxicokinetic behavior and relative bioavailability. All parent compounds were detected in both urine and plasma of the corresponding treated rats and most *in-vitro* metabolites could be confirmed *in-vivo*. In animals exposed to 6PPD, a mono-hydroxylated metabolite was detected in plasma, along with the mono-hydroxylated metabolite of 6PPDQ. Following 6PPDQ administration, mono-, di- and tri-hydroxylated metabolites, along with two sulfate conjugates, were detected in both rat urine and plasma. Administration of 4-HDPA derived in the detection of glucuronidated and sulfated metabolites in both matrices. Finally, a hydroxylated metabolite of HMMM was also detected in urine.

Acknowledgments

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Pharmaceutical-containing pollutant mixtures in freshwater: independent action predicts acute lethality while sub-lethal endpoints reveal masking in *Daphnia magna*

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Pharmaceuticals occur in freshwater ecosystems alongside other pollutants, including metals and pesticides, yet environmental risk assessment remains largely based on a chemical-by-chemical approach and may overlook mixture effects[1]. To determine whether standard models reliably predict toxicity across various biological endpoints, *Daphnia magna* were exposed to a six-component pharmaceutical-containing mixture comprising propranolol, diltiazem, metformin, nickel, lithium, and the herbicide glyphosate. The chemicals were tested at a mechanistically informative high concentration range selected to magnify mixture interactions. In 24 h acute immobilisation tests, the mixture exhibited higher toxicity than any individual component, with LC_{50} of 8.573 mg/L. Independent Action model closely predicted the observed mixture response (LC_{50} = 8.997 mg/L), whereas Concentration Addition predicted substantially greater toxicity (LC_{50} = 4.550 mg/L). Acute lethality was consistent with an Independent Action-type additive response. However, at the tested sub-lethal concentrations, 1 and 3 mg/L, comparisons with individual compounds revealed endpoint-specific antagonism or masking. Inhibition of lipase, alkaline and acid phosphatases, aminopeptidase and β-galactosidase by individual chemicals was not consistently intensified in the mixture. Similar masking was observed at the physiological level: single-chemical effects on feeding rate[3] after 24 h and growth at 7, 14 and 21 days did not translate into greater inhibition by the mixture. The mixture itself caused concentration-dependent sub-lethal effects. Feeding[3] declined significantly from 2 mg/L, reaching 17% below the control at 7 mg/L, while growth was inhibited from 3 mg/L at days 7, 14 and 21. Chronic survival showed a threshold-like dose-dependent decline above 7.5 mg/L. Although Independent Action adequately described acute mortality due to a complex pollutant cocktail, at other, more informative endpoints, the additivity needed for the single chemical predictions was lost. A multi-endpoint *D. magna* framework complements mixture testing and supports the development of effect-based approaches aligned with New Approach Methodology principles for pharmaceutical-mixture risk assessment[2]. Ongoing work aims to extend the covered endpoints through LC-MS untargeted metabolomics and river-water exposures to strengthen mechanistic interpretation and environmental transferability.

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Insight Profiler streamlines non-targeted analysis of river water contaminants of environmental concern in a single software solution

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Advances in non-targeted analysis (NTA) increasingly rely on integrated workflows which can handle complex spectral deconvolution, feature alignment, multivariate interpretation and compound identification. Several software applications provide complementary capabilities for ion feature extraction, statistical interrogation and spectral annotation; however, transitioning data across discrete platforms increases workflow fragmentation. This presentation will introduce Insight Profiler, a single software application developed to automate feature detection and alignment, statistical analysis, compound screening and identification, delivering an integrated solution using a single processing method. To highlight an end-to-end workflow for environmental toxicology screening, the data processing application was applied to NTA of river water contaminants of environmental concern.

NTA using high-resolution mass spectrometry enables detection of emerging contaminants associated with wastewater discharges and environmental inputs. River water samples collected from 22 sites across two urban rivers were analysed to determine whether NTA could differentiate locations based on chemical composition. Samples were filtered and analysed by LC-DIA-MS/MS using a Shimadzu LCMS-9050 QTOF. Data were processed using Insight Profiler software for feature detection, alignment, filtering, and compound identification. NTA successfully distinguished samples according to sampling location and revealed significant impacts of wastewater treatment facility (WWTF) discharge on downstream water chemistry.

Samples collected downstream of a WWTF contained substantially greater numbers and concentrations of pharmaceutical compounds and metabolites than upstream sites. Detected compounds included venlafaxine, desmethylvenlafaxine, tramadol, O-desmethyltramadol, gabapentin, ketamine, clarithromycin, metronidazole, carbamazepine, and lidocaine. In contrast, upstream samples showed markedly lower pharmaceutical abundance, providing clear evidence of WWTF influence on river contaminant profiles. Recognised tracers of wastewater inputs were detected at all sampling locations at relatively low and consistent concentrations.

The observed differences between upstream and downstream sites demonstrate the utility of Insight Profiler for identifying spatial variations in complex environmental datasets. These findings highlight the value of NTA workflows for monitoring wastewater-derived contaminants and support the need for systematic surveillance of rivers located near WWTF discharge points.

Beyond the aquatic compartment: persistent, mobile and toxic pharmaceuticals in wastewater-impacted agroecosystems — field evidence for integrated health risk assessment

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Persistent, mobile and toxic (PMT) substances are receiving increasing scientific and regulatory attention because they resist degradation, spread through connected aquatic ecosystems, and contribute to long-term exposure of ecosystems and humans. Many human and veterinary pharmaceuticals meet PMT criteria, yet their assessment has so far been confined to aquatic compartments. Whether and under which conditions PMT pharmaceuticals cross into agricultural soils and edible crops remains largely unresolved, particularly under unplanned water reuses, where effluent-dominated waters are used for crop irrigation.

We conducted a field-scale, integrated assessment of the occurrence, attenuation, fate and transfer pathways of 30 prioritized PMT pharmaceuticals across the water–soil–plant continuum in an intensively irrigated area south-eastern of Madrid (Spain). Data from aquatic compartments, agricultural soils, and edible tissues of lettuce and maize were integrated with ecological and human health risk assessments.

Despite natural attenuation, several PMT pharmaceuticals persisted in surface water downstream of WWTP effluents and in groundwater throughout the hydrological year. This persistence was ecotoxicologically relevant, as 60% of the investigated PMTs occurred at concentrations associated with moderate-to-high ecological risk for aquatic organisms. Following irrigation, several PMTs detected in irrigation water were also found in agricultural soils, demonstrating that even highly mobile substances can be retained. Retention was governed by substance-specific properties (particularly ionization state), soil characteristics, and local agricultural inputs, indicating that soils act simultaneously as sinks and secondary sources. Transfer to crop was selective and significantly correlated with soil concentrations, with 43% of the investigated PMTs detected in edible tissues of lettuce and/or maize.

Estimated non- and carcinogenic risks from crop consumption was negligible. However, imidacloprid, a neonicotinoid used both in veterinary medicinal products and in local greenhouse, exceeded the EU maximum residue level in lettuce. Risk-based thresholds also identified lorazepam, diazepam, sitagliptin, and fluconazole as having narrow margins of safety. These findings show that PMT contamination extends beyond aquatic compartments: irrigation links environmental persistence to soil retention and crop exposure. Assessing PMT substances across the water–soil–plant continuum is therefore essential for realistic exposure and risk characterization.

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Analytical strategies and removal treatments of a broad spectrum of PFAS in Drinking Water Treatment Plants: A LC-MS/MS study

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Per- and polyfluorinated compounds (PFAS) are highly persistent and toxic substances with strong carbon-fluorine bonds that make them difficult to eliminate from the environment, despite their widespread use in consumer products and industrial applications. Human exposure to PFAS can cause adverse effects on the immune system and other health outcomes. In response to this concern, the European Union has implemented regulatory measures to progressively restrict PFAS production and use. [1,2]

The most widely employed removal methods are reverse osmosis and activated carbon filtration, both demonstrating considerable effectiveness in reducing PFAS concentrations.

To address the complexity of PFAS contamination, an advanced analytical method has been developed capable of simultaneously detecting and quantifying 63 different PFAS compounds, along with 18 internal standards (ISTD) using liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS), with a SCIEX 7500 mass spectrometer. This comprehensive methodology specifically includes PFAS regulated under current European Union directives, ensuring compliance with community water quality standards and providing unprecedented insight into the full spectrum of PFAS contamination.

This study focused on drinking water treatment plants (DWTP) operated by Aigües de Barcelona: Sant Joan Despí (Besòs river basin) and La Llagosta (Llobregat river basin), comparing reverse osmosis and activated carbon filtration for removing emerging PFAS compounds. The study successfully determined PFAS concentration levels and provided valuable data on the effectiveness of both treatment methods in removing these persistent contaminants from drinking water supplies.

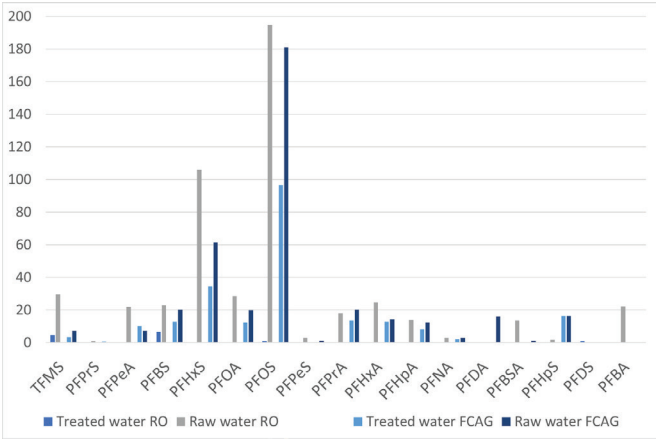


Figure 1. Comparison of treatment methods

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Integrating wastewater-based epidemiology with socioeconomic and health indicators to characterize patterns of psychoactive substance consumption across Catalonia

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Harmful alcohol and drug use remains a major public health challenge worldwide. Wastewater-based epidemiology (WBE) has emerged as an objective tool for monitoring population-level consumption of psychoactive substances and supporting evidence-based public health policies. This study combined WBE with socioeconomic and health indicators to characterize spatial and temporal patterns of alcohol, illicit drug, and psychopharmaceutical consumption across Catalonia.

Wastewater samples were collected from ten wastewater treatment plants (WWTPs), representing approximately 45.5% of the Catalan population, during two seven-day campaigns in spring and autumn 2025. Alcohol biomarkers were quantified by high-performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS), whereas illicit drugs and psychopharmaceuticals were determined using online solid-phase extraction followed by ultra-high-performance liquid chromatography coupled with quadrupole time-of-flight high-resolution mass spectrometry (online SPE-UHPLC-QTOF-HRMS). Population consumption was estimated through back-calculation, and chemical data were integrated with socioeconomic and health indicators using correlation analysis, principal component analysis (PCA), and hierarchical clustering.

Results revealed spatial, weekly, and seasonal consumption patterns across Catalonia. Recreational substances, including cocaine biomarkers, MDMA, and ethyl sulfate, showed significant weekend increases, while seasonal differences reflected changes in recreational activities and psychopharmaceutical use. Clustering and correlation analyses identified groups of compounds with similar consumption patterns and clusters of WWTPs according to population density, suggesting higher and more diverse consumption profiles in more urbanized areas. Integration with socioeconomic and health indicators revealed positive associations between socioeconomic status and stimulant consumption, inverse relationships between cannabis use and educational level, while diazepam emerged as a key biomarker associated with regional suicide mortality.

These findings demonstrate that integrating WBE with socioeconomic and health data extends its application beyond estimating substance consumption towards a public health surveillance framework, supporting the identification of territorial hotspots and evidence-based public health interventions.

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Will warmer summers increase the impact of UV filters on marine bivalves?

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Increasing pressures on coastal organisms are enhanced by emerging contaminants and multiple stressors, including personal care products (PCPs) and climate change-derived factors. The ultraviolet (UV) avobenzone (AVO) is widely used in PCPs, being often detected in environmental samples from aquatic systems, its toxicological effects combined with warming remain poorly understood. Therefore, this research focused on studying the responses of the Mediterranean mussel, *Mytilus galloprovincialis*, to environmentally relevant concentrations of AVO (0.5 µg/L), alone and in combination with warming (21 °C). Moreover, to assess life-stage-level effects, the exposures were tested in sperm cells and adults. For that, acute 30-min *in vitro* exposures of sperm cells were performed to evaluate oxidative status, viability, DNA integrity, motility, and kinetic parameters. In adults, chronic 28-day *in vivo* exposures were performed to assess energy reserves, metabolism, antioxidant and biotransformation defences, cellular damage, and neurotransmission. Exposure to AVO alone led to a loss of DNA integrity and increased respiration rate in sperm cells, whereas biotransformation enzymes' activity was induced in mussels. Warming enhanced respiration rate, reactive oxygen species production, cellular damage, and decreased sperm cells' viability, whilst adults' metabolic capacity increased. The multiple-stressor exposure to AVO and warming intensified oxidative stress, led to greater cellular damage, higher DNA integrity loss, and impaired sperm cell motility, whereas antioxidant enzyme activity increased in adults. More pronounced responses were observed with combined exposure to AVO and warming, emphasising the importance of studying multiple stressors to predict responses in future scenarios. Sperm cells appeared more sensitive than adults, demonstrating that early life stages are valuable as an early proxy for assessing ecological risks posed by emerging contaminants under future climate change scenarios.

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Assessing organic pollutant benchmarks in a Mediterranean catchment facing climate-driven flood risks

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Climate change can alter ecosystems and human health by intensifying extreme phenomena associated to altered precipitation regimes or increased temperatures. In October 2024, Valencia region (E Spain) experienced very intense rainstorms, which resulted in catastrophic floods in the final part of the Jucar River basin. In this study, river water, sediment and nine fish species from this catchment were analysed for the determination of numerous persistent organic pollutants (POPs) and microplastics (MPs), in samples taken four months before the floods. Extractions were based on microwave-assisted extraction and solid- phase extraction, optimised for each different matrix and analyte type. Analyses were performed by High Pressure Liquid Chromatography Tandem High-resolution mass spectrometry, micro-FTIR, Pyrolysis coupled with Gas Chromatography-Mass Spectrometry (Py-GC–MS) and GC–MS/MS. Ecological and human health risks were also estimated by different indices. The results reveal a multi-matrix pollution pattern dominated by pharmaceuticals, pesticides, perfluoroalkyl substances (PFAS), polycyclic aromatic hydrocarbons (PAHs), flame retardants (PFRs), and MPs, with the highest levels detected in urban-influenced sites (Magro River, Jucar River near the mouth). Water samples were particularly enriched in tebuconazole (mean: 519.2±33.4 ng L^{-1}), tramadol (104.2±2.9 ng L^{-1}) and ibuprofen (94.1±6.2 ng L^{-1}). Sediments, acting as pollutant sinks, contained elevated levels of PFAS, triazole pesticides, salicylic acid and methylparaben, which average concentration reached up 2538.4±43.5 ng g^{-1} dw. Fish from the Jucar River showed substantial bioaccumulation of PFAS, tris(2-butoxyethyl) phosphate (TBEP) and lipophilic pharmaceuticals. One fish sample (*A. alburnus*) presented a high concentration of polypropylene (PP) and was contaminated by 11 PAHs, including benzo[*a*]pyrene. The ecological risk assessment flagged perfluorooctanesulfonic acid (PFOS), perfluorooctanoic acid (PFOA), ibuprofen and TBEP as high-risk compounds, particularly in sediments and fish. Incremental life cancer risk values for MPs and PAHs in water samples, and for the highly polluted fish sample indicated potential risk. Principal component analysis suggested positive correlation between PP, benzo[*a*]pyrene and potential cancer risk. These findings, recorded just four months before the October 2024 floods, underscore the vulnerability of Mediterranean river systems to pollutant mobilisation during extreme hydrological events, a scenario expected to intensify with ongoing climate change. This work highlights the urgent need to integrate spatiotemporal risk-based monitoring and climate-adapted management strategies in ecotoxicologically sensitive watersheds.

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Expanding the Scope of NTS in High-Throughput EDA: Uncovering Transthyretin-binding Compounds in Stormwater Ponds via Orthogonal Separation Modes and Ion Mobility HRMS

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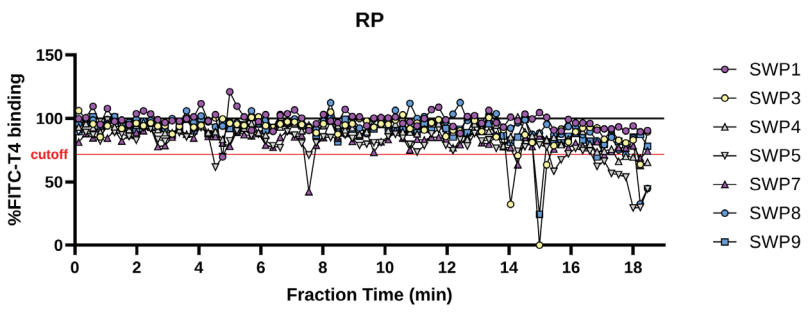
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High-throughput effect-directed analysis (HT-EDA) has been a powerful tool for prioritizing and identifying unmonitored endocrine-disrupting compounds in complex environmental mixtures. Its effectiveness can be greatly enhanced when coupled with multidimensional chromatography and ion mobility separation - high-resolution mass spectrometry (IMS-HRMS). This approach allows to expand chemical coverage, improve separation of coeluting and isomeric compounds, and increase confidence in compound annotation. The present study applies this expanded HT-EDA strategy to identify endocrine-active transthyretin (TTR)-binding chemicals in outdoor stormwater ponds, which are hotspots for urban-derived micropollutants. Water from outdoor stormwater ponds around Uppsala (Sweden) was collected and concentrated through solid-phase extraction (SPE). The stormwater extracts were screened on their ability to compete with thyroid hormone (TH) for binding to TTR, the TH distributor protein in plasma and cerebrospinal fluids. The extracts with higher binding affinity to TTR were selected for parallel fractionation into 96-well plates using two orthogonal separation modes: hydrophilic interaction chromatography (HILIC) and reversed-phase liquid chromatography (RP). The fractions were screened on a fluorescent competitive TTR-binding assay, and the chemical analysis of the same extracts was performed using trapped ion mobility-quadrupole time-of-flight MS. Suspect and nontarget screening was performed, and features within the fractions exhibiting high TTR-binding activity (Figure 1A and 1B) were prioritized for compound annotation. This prioritization workflow uncovered over 200 unique compounds with potential TTR-binding activity at confidence level 2 or 3, and at least 3 compounds of which have confirmed TTR-binding potencies reported in literature. Combining orthogonal separation modes proved essential for broadening the chemical space coverage. While RPLC was still able to capture majority of the active features, the integration of HILIC enabled the identification of unique features not retained by RPLC. In addition, several shared features were detected in both HILIC and RP active fractions, further validating their potential as TTR binders. The incorporation of ion mobility as a dimension helped to distinguish analytes from coeluting matrix interferences, while acting as an additional line of evidence that increases the confidence level of the annotated features.



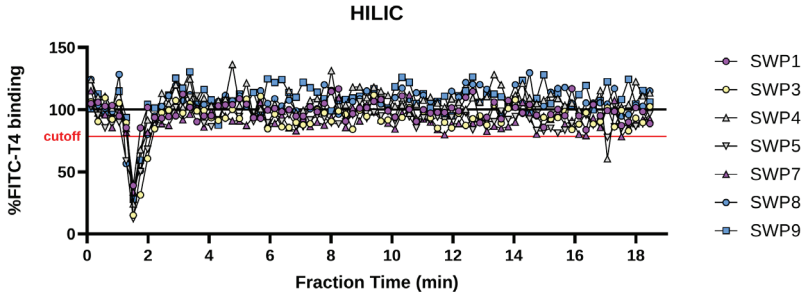


Figure 1. Transthyretin (TTR)-binding activity of the fractions obtained via (A) reversed-phase liquid chromatography and (B) hydrophilic interaction liquid chromatography for 7 outdoor stormwater pond extracts. Each plotted point represents an individual chromatographic fraction, and the y-axis represents the bioactivity, expressed as the signal of bound fluorescently-labelled thyroxine relative to negative controls. Fractions below the cutoff threshold (red line) indicate strong TTR-binding competition and were prioritized for compound annotation.

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Methodologies based on high-performance liquid chromatography coupled with mass spectrometry for the determination of emerging contaminants in water: application to hospital effluents

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Emerging pollutants are substances whose presence in the environment is generating growing concern due to their potential effects on human health and ecosystems. Their appearance in wastewater from healthcare facilities, such as hospitals, is common. However, there is currently no specific, detailed legislation regulating these discharges, despite their potential environmental impact. Given this situation, it is essential not only to begin regulating their presence in water, but also to design effective strategies for their elimination. These strategies must include studies to identify the actual sources of contamination, as well as the application of advanced technologies to control and eliminate these compounds.

A key element in this process is having reliable information on the concentrations of these contaminants. This requires robust and versatile analytical methodologies. In this context, liquid chromatography-coupled mass spectrometry techniques, such as LC/MS-QQQ and LC/MS-QTOF, are essential due to their ability to detect and quantify contaminants at trace levels. Advances in these techniques have allowed for the identification of a greater number of emerging compounds.

This study focuses on the evaluation of discharges from hospitals in the Community of Madrid, analyzing four main groups of contaminants: hormones, perfluorinated compounds, pharmaceuticals, and drugs of abuse. The aforementioned analytical techniques were used. The results obtained to date confirm the presence of these compounds at all sampling points, with the detection of pharmaceuticals and drugs being particularly notable. This study constitutes a crucial starting point for understanding the behaviour of these contaminants in the environment, as well as for assessing their potential risk at the concentrations observed in real samples.

Table 1. List of investigated hospitals in the present study

ID	Facility type	Number of beds	Level of care	Wastewater volume (m^3/day)
A	General university hospital	650–700	III	196
B	Specialized public hospital	450–500	III	100
C	General university hospital	350–370	II	55
D	General private hospital	200–230	II	21
E	Private hospital	200–250	II	25
F	Private hospital-clinic	150–170	I	12
G	Private hospital	90–120	I	6
H	Private clinic	70–90	I	3
I	Private hospital-clinic	80–100	I	4
J	Laboratory	–	–	16

Occurrence of Tire-Derived Chemicals in Environmental Waters of the Barcelona Metropolitan

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Tire and road-wear particles (TRWPs) are a major source of tire-related chemicals (TRCs) and potentially toxic transformation products (TPs) in aquatic environments[1], yet their occurrence remains poorly characterized, particularly in coastal waters. This study investigates TRCs and their TPs in Barcelona's aquatic systems under dry and rainy conditions, addressing knowledge gaps on their occurrence and behavior in urban coastal regions.

A total of 20 water samples were collected from channels, streams, and ponds in the Llobregat Delta surrounding Barcelona–El Prat Airport. After filtration (0.2 µm), samples were analyzed by LC–MS/MS and HRMS using target and suspect screening approaches. Transformation products were identified after blank correction and peak filtering.

TRC concentrations were highest in waters adjacent to densely urbanized areas and the perimeter of Barcelona–El Prat Airport, reaching cumulative levels above 3 µg/L and increasing after rainfall events. Nevertheless, elevated concentrations were also detected in natural and protected areas, indicating widespread contamination. Benzothiazole-2-sulfonic acid (BTSA), hexamethoxymethylmelamine (HMMM), and 1,3-diphenylguanidine (DPG) were the predominant compounds (Table 1), showing a 100% detection frequency across all sampling campaigns. In addition, 23 suspect transformation products, mainly derived from DPG and HMMM, were identified, highlighting the importance of including these compounds in future monitoring of traffic-derived contaminants.

		1st Sampling (Dry Period)	2nd Sampling (First rain)	3rd Sampling (Rainy period)	Nº of Associated TPs
Compound	Abbr.	Conc. (ng/L)	Conc. (ng/L)	Conc. (ng/L)	
Benzothiazole-2-sulfonic acid	BTSA	21 - 755	21 - 1633	14 - 3751	-
Hexamethoxymethyl melamine	HMMM	1.0 – 1446	1.0 - 1304	2.0 - 3198	9
Diphenylguanidine	DPG	0.3 – 167	0.3 – 229	2.8 – 241	14

Table 1. Concentrations of the most abundant detected compounds

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Beyond Antibiotic Exposure: Salinity Modulates Oxytetracycline Toxicity in *Mytilus galloprovincialis*

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Pharmaceuticals used in aquaculture can reach transitional coastal systems where their effects may be modulated by climate-driven changes in abiotic conditions. Oxytetracycline (OTC), a broad-spectrum antibiotic widely used in aquaculture, is frequently detected in aquatic environments, yet its sublethal effects during salinity shifts associated with marine heatwaves remain poorly understood. This study evaluated the combined effects of OTC and increased salinity on *Mytilus galloprovincialis*, using biochemical biomarkers as early-warning indicators of physiological disturbance. Mussels collected from the Ria de Aveiro (Portugal) were acclimated for 10 days and exposed for 14 days to six treatments in triplicate aquaria: salinities of 30 and 40, each combined with 0, 1, or 10 µg L-1 OTC. Whole soft tissues were analysed for antioxidant defences, detoxification capacity, cellular damage, neurotoxicity, osmotic regulation, and energy metabolism. Overall, the biochemical profile of *Mytilus galloprovincialis* revealed that salinity modulated oxytetracycline toxicity. At salinity 30, OTC exposure mainly affected neurotoxicity-related and physiological adjustment pathways, with 1 µg/L OTC associated with neurotoxicity, and 10 µg/L OTC associated with alterations in antioxidant defence, metabolic capacity, protein content, and osmotic regulation. Under salinity 40, the response shifted towards detoxification and antioxidant mechanisms. In particular, 1 µg/L OTC was associated with increased involvement of detoxification enzymes, while 10 µg/L OTC elicited a marked antioxidant response involving antioxidant enzymes. These findings indicate that higher salinity not only intensifies OTC toxicity but also alters the biochemical pathways underlying the response, highlighting the importance of accounting for climate-driven salinity changes when assessing antibiotic toxicity in marine bivalves.

Keywords: Oxytetracycline; bivalves; Climate Change; Biochemical biomarkers; Aquaculture pharmaceuticals

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Multimodal high-resolution mass spectrometric screening of leachates from recycled plastics: what is new and what is already known?

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Plastics contain thousands of chemical compounds that can enter the environment through the leaching of plastic waste, potentially posing risks to both human health and ecosystems. Recycled plastics, which are expected to play a key role in the transition toward a circular economy, may further exacerbate this issue because, in addition to known and catalogued additives, they can contain numerous contaminants originating from previous use cycles. However, the identity and leaching behaviour of many of these substances remain poorly characterized.

In the present study, GC-HRMS and LC-HRMS were employed for suspect and non-target screening to detect and identify substances released from recycled and conventional high-density polyethylene (HDPE) as comprehensively as possible. Rather than investigating plastic pellets, the study focused on finished HDPE products (containers), reflecting items that frequently enter the environment where they are exposed to weathering. To simulate different exposure conditions, the containers were subjected to five HDPE-compatible aqueous and organic solvents.

GC-HRMS analysis revealed 788 distinct chromatographic components, of which 257 were identified through comparison with multiple spectral libraries. In contrast, LC-HRMS analysis yielded 2,560 components after combining RPLC and HILIC datasets acquired in both ESI(+) and ESI(-) modes, of which 213 could be identified. Additional putative annotations were obtained through de novo molecular formula prediction using SIRIUS, followed by suspect screening against PlastChem and other chemical inventories. The major classes of annotated compounds included aromatics, phthalates, fatty acid esters, terpenoids and alkanes, among them well-known plasticizers such as dibutyl phthalate and dibutyl hexanedioate.

A central aspect of the study was determining which leached substances are already known to be associated with plastics and which are not. For this purpose, an extensive comparison with PubChem metadata based on “short” InChIKeys was conducted. This approach indicated that fragrance compounds such as tonalide and galaxolide, along with numerous other substances, were most likely introduced through previous use cycles as no plastic-associated use is known. The study also demonstrated that such classifications are often challenging because many compounds are used across multiple industrial sectors and because of data gaps in available chemical databases.

The presentation will introduce the analytical and bioinformatic workflows applied in the study and discuss both the major methodological challenges and the broader question of how the growing number of “new” leachables from recyclates can be adequately addressed in routine analysis and regulatory frameworks.

Metabolic profiling reveals structure-based common metabolites for liquid crystal monomers

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Liquid crystal monomers (LCMs) are emerging contaminants with persistent, bioaccumulative and toxic properties that are widely detected in various environmental and human matrices. However, their metabolism in humans and the toxicity of them and their metabolites are still poorly understood. In this talk, we will present our study on the biotransformation of LCMs. The phase I metabolism of six representative LCMs were investigated using human liver microsomes, revealing convergence towards common metabolites among structurally related LCMs. Targeted analysis further confirmed the presence of these metabolites in meconium from newborns, indicating potential prenatal exposure. *In silico* toxicity predictions indicated that, while parent LCMs were generally more bioaccumulative, several metabolites strongly suggested mutagenicity, developmental toxicity, skin sensitization, and endocrine disruption properties. Together, these findings demonstrate that the potential toxicity of LCM biotransformation should not be underestimated, and that using common metabolites from structurally related LCMs warrants exploration for future human biomonitoring and risk assessment of LCMs.

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PFAS analysis and removal in aquatic systems: the role of advanced mass spectrometry in supporting treatment strategies

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Per- and polyfluoroalkyl substances (PFAS) are persistent and mobile contaminants widely detected in surface water, groundwater, wastewater, sludge, and landfill leachates. Their environmental assessment remains challenging because conventional targeted methods do not fully capture the diversity of legacy, emerging, and ultrashort-chain PFAS, while precursor transformation and matrix effects can complicate interpretation. This presentation highlights recent progress in PFAS analysis and removal in aquatic systems, with emphasis on the role of advanced mass spectrometric tools in supporting remediation strategies.

Targeted LC-MS/MS remains essential for the sensitive quantification of regulated PFAS, whereas high-resolution mass spectrometry enables broader characterization through suspect screening and non-target analysis of emerging PFAS, isomers, precursors, and transformation products. These approaches have considerably expanded PFAS detection in complex environmental matrices and improved understanding of contamination profiles beyond conventional target lists. From a treatment perspective, conventional wastewater processes are often insufficient and may even promote precursor conversion into terminal PFAS. More effective options include adsorption onto activated carbon and ion-exchange resins, membrane separation by nanofiltration and reverse osmosis, and destructive treatments such as electrochemical, plasma, oxidative-reductive, and thermal processes. However, important limitations remain, including selectivity, matrix effects, cost, energy demand, and management of PFAS-concentrated residual streams. Overall, integrated workflows combining advanced analytical detection with selective separation and destructive polishing are needed for more effective PFAS management in aquatic systems.

ADVANCED MATERIALS FOR THE SELECTIVE EXTRACTION OF PHARMACEUTICALS FROM ENVIRONMENTAL WATER SAMPLES

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The determination of pharmaceuticals in environmental samples represents a challenging analytical task owing to the high complexity of environmental matrices and the very low concentrations at which these contaminants are typically present in the samples. Due to their chemical properties, their determination is mainly performed using liquid chromatography coupled to mass spectrometry-based detection.

Despite the advanced capabilities of these detection systems, sample preparation remains essential to both concentrate analytes and reduce matrix interferences. In this context, sorptive extraction techniques are widely employed for liquid samples thanks to the large variety of available sorbents, including both commercial and in-house-developed materials [1]. A great group of pharmaceuticals are ionic or ionizable compounds, which typically exhibit low retention on standard sorbents. To address this, several strategies have been developed, with mixed-mode ion-exchange sorbents emerging as an excellent option due to their improved retention capabilities and the high selectivity they can provide, especially when a clean-up step is included [2]. However, the selective and simultaneous extraction of both acidic and basic compounds remains an analytical challenge. Among the various strategies that have been explored, the use of amphoteric materials has proven to be an effective approach [3-5].

Different strategies for the preparation of amphoteric mixed-mode ionic-exchange materials will be presented, and their application to the determination of pharmaceuticals in environmental water samples using sorptive extraction techniques will be demonstrated.

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COST Action ENVIRANT: Anthelmintics, from its farming use to the environment

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Pasture-based animal production systems play a vital role in sustainable European farming, relying on grass grazing as a cost-effective feed source. However, grazing livestock are highly susceptible to helminth parasite infections, which impose a substantial economic burden on food production. Anthelmintic drugs remain the most widely used control method, yet these compounds are increasingly recognised as emerging environmental contaminants whose presence in terrestrial and aquatic ecosystems poses significant ecological risks.

ENVIRANT (CA23154) is a European COST Action network that aims to advance, consolidate and disseminate research on the environmental occurrence and ecological impact of anthelmintics administered to livestock, and to promote more sustainable helminth control practices. The Action investigates factors governing anthelmintic persistence in the environment, assesses their impact on non-target ecosystems, develops sustainable alternatives to reduce drug use across diverse European settings, and models the benefit-risk balance between animal health and ecosystem protection.

As part of this work, a Stakeholder Advisory Board process has revealed a number of critical gaps at the intersection of science and policy. Anthelmintics remain largely absent from EU environmental monitoring programmes, and no substance-specific Environmental Quality Standards have been established for this drug class. The current Environmental Risk Assessment framework for veterinary medicinal products falls short of capturing the full range of ecological effects, particularly on non-target organisms. At the regulatory level, pharmaceutical authorisation and EU water quality policy continue to operate in separate silos, with little coordination between them. Finally, the possible role of environmental residues in driving anthelmintic resistance selection remains an open and largely unexplored question.

These gaps highlight an urgent need for coordinated research and policy action at the European level.

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From Water to Eel Tissues: LC–HRMS/MS Characterization of Emerging Contaminant Exposure across Mediterranean Aquatic Systems

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The European eel (*Anguilla anguilla*) is critically endangered and is exposed throughout its continental life stage to complex mixtures of anthropogenic chemicals. High-resolution mass spectrometry (HRMS) offers the selectivity, mass accuracy and broad chemical coverage required to characterise this exposure across environmental and biological matrices. This study applies complementary liquid chromatography–HRMS workflows to surface water and European eel muscle and brain collected from rivers, lagoons and wetlands in the Pyrénées-Orientales and Catalonia.

Matrix-adapted extraction and cleanup procedures were used prior to reversed-phase LC analysis with electrospray ionisation in positive and negative modes on a Thermo Orbitrap Eclipse Tribrid HRMS system. For water analysis, solid phase extraction (SPE) using Oasis HLB 200 mg cartridges was performed (1). Muscle tissue were homogenized using an IKA A11 Basic blade grinder and 0.5 g of tissue was taken for analysis. For brain tissue, only 20–200 mg was available per specimen. Samples were extracted by bead beating with 0.5 mL of cold acidified acetonitrile/methanol, followed by ultrasonication and centrifugation adapting a previous methodology (2). Cleanup was performed with HybridSPE dispersive pipette extraction tips and automated on a Hamilton robotic platform, reducing manual handling and solvent consumption while increasing sample throughput. Compound identification and quantification were performed through a wide-scope target-screening workflow supported by accurate mass, retention time, isotopic pattern and HRMS/MS fragmentation.

Brain analyses revealed widespread occurrence of pharmaceuticals and personal care products, pesticides and industrial additives. Salicylic acid and 4-hydroxybenzoic acid showed the highest mean concentrations across sites, followed by valproic acid and 2-acrylamido-2-methylpropane sulfonic acid. Valproic acid, 2,6-di-tert-butyl-4-(hydroxymethyl)phenol, acetaminophen, trimethoprim and propranolol were frequently quantified at multiple locations. The Fluvià site samples presented the highest overall contaminant burden, whereas samples collected from La Massona, la Ricarda, and El Remolar ponds also displayed relevant and distinct chemical profiles, indicating both recurrent exposure and site-specific contamination signatures.

The multi-matrix HRMS strategy provides a comprehensive framework for tracing emerging contaminants from aquatic habitats to sensitive eel tissues. The combination of broad-scope Orbitrap analysis with miniaturised and automated sample preparation is particularly valuable for biomonitoring threatened species when sample mass is limited.

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Non-target LC–HRMS/MS screening of ceramic passive sampler extracts from groundwater and river sites

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Grab sampling provides only a snapshot of water contamination and may overlook temporally variable or low-level chemical exposure. Passive samplers integrate exposure over extended periods while accumulating contaminants on a receiving phase, producing enriched extracts suitable for high-resolution mass spectrometry. Combined with suspect and non-target screening, they can reveal compounds outside predefined target lists [1–2]. This study evaluated ceramic passive samplers (CPSs) as time-integrative enrichment tools for non-target LC–HRMS/MS screening in a connected river–groundwater system.

Duplicate CPSs containing 300 mg Oasis HLB and 100 mg Porapak Rxn were deployed for 14 days in 14 groundwater wells and at two river sites in the Besòs catchment, Barcelona, Spain. After retrieval, the sorbents were extracted with methanol. The extracts were analysed in separate positive- and negative-ionisation runs using a Thermo Scientific Orbitrap Eclipse Tribrid mass spectrometer. Data were processed in Compound Discoverer through feature detection, molecular-formula assignment, MS/MS spectral processing and comparison against procedural blanks. Candidate structures were searched concurrently against mzCloud and ChemSpider; mzCloud spectral matches were used when available, whereas candidates retrieved only from ChemSpider were evaluated by in-silico fragmentation [3,4].

The workflow detected 52,423 LC–HRMS features, of which 45,514 received proposed molecular formulas and 15,513 had associated MS/MS spectra. Features producing an mzCloud best-match confidence score above 90 were prioritised for further evaluation. High-scoring library matches included pharmaceuticals and transformation products not covered by the targeted LC–MS/MS method, including vildagliptin, citalopram, bisoprolol and venlafaxine N-oxide, as well as diethyl phthalate and 2,4-dinitrophenol. Several candidate compounds showed contrasting occurrence patterns between river and groundwater sites, with some predominantly detected at the river sites and others distributed across both river and groundwater samples.

CPS-based enrichment produced information-rich extracts suitable for broad LC–HRMS/MS screening, expanding the observable chemical space beyond the predefined target list. This approach supports the prioritisation of emerging contaminants and transformation products for further investigation and quantitative monitoring.

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Integrated Analysis of IM-MS Imaging and LC–IMS–MS Using Trilinear MCR for Non-Target Lipid Identification

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Ion mobility–mass spectrometry imaging (IM-MS imaging) and liquid chromatography–ion mobility–mass spectrometry (LC–IMS–MS) both generate multidimensional datasets containing chemical and structural information [1]. These techniques have shown considerable potential for non-target lipid identification. However, their integrated analysis remains challenging because of differences in data structure and acquisition modes. In this study, we propose a joint analytical framework that combines IM-MS imaging and LC–IMS–MS using multivariate curve resolution (MCR) to simultaneously resolve spatial distributions, chromatographic elution profiles, ion mobility profiles, and mass spectra.

Skin tissue samples contaminated through air exposure were selected as the study subjects. IM-MS imaging and LC–IMS–MS datasets were acquired from the same tissue samples. Regions of interest (ROIs) were first applied to reduce the m/z dimension, yielding compact data cubes for both techniques [2]. The mobility and m/z dimensions of the two datasets were subsequently aligned through interpolation. The aligned imaging and LC-IM-MS data matrices were column-wise augmented and analyzed by MCR-ALS [3], while trilinearity constraints were imposed separately within each data block. This approach enabled the simultaneous extraction of spatial images, retention time profiles, drift time profiles, and mass spectral profiles for individual chemical components. Collision cross section (CCS) values were further calculated from the resolved drift times. Finally, the resolved retention times, CCS values, and m/z information were matched against lipid databases to achieve non-target lipid identification, and the identified lipid species were visualized according to their spatial distributions.

Overall, this study demonstrates that trilinear MCR enables the integrated analysis of IM-MS imaging and LC–IMS–MS datasets, providing simultaneous resolution of imaging, chromatographic, mobility, and mass spectral information within a unified framework. Combined with database matching based on retention time, CCS, and m/z, the proposed workflow facilitates non-target lipid identification and visualization, offering a promising strategy for multimodal mass spectrometry data integration.

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Application of HRMS-based suspect screening for the investigation of the fate of mobile organic contaminants in urban blue-green infrastructures

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Rapid urbanization and climate change are driving cities to adopt sustainable urban water management strategies. Stormwater runoff transports anthropogenic contaminants from sources such as traffic and construction, threatening surface water and groundwater quality [1]. Nature-based solutions, including Blue-Green Infrastructure (BGI) and Sustainable Urban Drainage Systems (SUDS), use soil, vegetation, and microbial processes to reduce runoff and remove pollutants. While effective for conventional pollutants such as metals, their ability to retain mobile organic contaminants remains poorly understood [2]. Moreover, biological processes within SUDS can generate transformation products (TPs) that may be more persistent or toxic than their parent compounds and often escape conventional monitoring. High-resolution mass spectrometry (HR-MS)-based suspect screening combined with in silico approaches provides a powerful means to identify these compounds and their TPs [1]. Since contaminant fate depends on both physicochemical properties and environmental conditions, field studies are essential [3]. However, limited field data hinder the assessment of groundwater risks and the optimization of BGI and SUDS for organic contaminant removal.

The objectives of this work were to: i) to prioritize mobile contaminants in stormwater and SUDS effluents, across Barcelona; and ii) identify with in-silico methods transformation products of the most frequent prioritized analytes via HRMS suspect screening with LC-Orbitrap Eclipse tribrid. 52 contaminants were prioritized for water samples The prevalence of TRCs, industrial chemicals, and artificial sweeteners indicates a diverse mixture of anthropogenic contaminants. SUDS effluents revealed a partial reduction of total load concentrations, which reports Log Removal Values (LRV) in comparison to rainwater and street runoff. While the biofilter significantly reduces the contaminant load of influent stormwater, specific compounds are able to bypass the biofilter and elute into the effluent. Particular attention should be paid to persistent and toxic compounds such as TCPP and melamine, which appear enriched or poorly retained in SUDS effluents.

Major contaminants identified in runoff were used to create a list of transformation products for suspect screening. The suspect list was compiled from i) known TPs of original targets and ii) TPs generated through open-source prediction softwares targeting both biotransformation and abiotic degradation products. Acquired NTA data across the two compartments (Runoff and SUDS effluent) are currently being processed to unveil transformation and degradation processes occurring during infiltration.

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Estimating Concentration of Emerging Contaminants from their MS/MS Spectra in Environmental Samples

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Recent advancements in liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS) have facilitated the identification of diverse compound classes within environmental matrices. Certain chemicals, including pharmaceuticals, personal care products, and illicit substances, fall within the broader category known as emerging contaminants (ECs). Continuous exposure of wildlife or humans to ECs has been linked to endocrine disruption, carcinogenesis and other adverse health outcomes [1]. Within this framework, advanced computational tools are important for identifying and structurally characterizing detected compounds using non-targeted analysis (NTA) workflows. In NTA studies, the quantitative or semiquantitative determination of ECs is essential for assessing their toxicity and potential environmental risks. However, the chemical structures of many of these detected peaks remain unidentified. This ambiguity regarding structural elucidation as well as the prevalence of thousands of potential false positives in most cases, presents a significant challenge to predicting chemical properties or estimating concentrations via ionization efficiency. Currently, most reliable semi-quantitative analysis tools require accurate chemical structure of analytes analyzed via LC-HRMS [2]. This study presents a robust method for predicting the logarithm of ionization efficiency (logIE) and response factors (logRF) based on MS/MS data, thereby facilitating the estimation of analyte concentrations without prior knowledge of their chemical structures. This novel framework employs deep learning-based transformer models to generate structure representations from MS/MS data. These arrays comprise (i) molecular fingerprints and SMILES codes predicted from MS/MS spectra using the IDSL_MINT program [3] and (ii) an embedding array with structural information also predicted from MS/MS spectra using DreaMS [4]. The models underwent fine-tuning via machine learning algorithms to predict logIE and logRF for over 700 ECs. The proposed framework was evaluated using sewage sludge samples from wastewater treatment plant of Athens and compared with methods constructed with known chemical structures. The results indicate overall acceptable accuracy (median Fold error of 7-12, for low (20 μg/L) and high (300 μg/L) spiked concentration, respectively). User-friendly software with quantified uncertainty is provided to implement the entire procedure. Notably, it is necessary to transfer and calibrate the models for each new instrumental configuration and matrix using a calibration curve generated from a series of reference compounds spiked into the environmental samples.

Acknowledgements

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The application of wastewater-based epidemiology for the nationwide assessment of drug consumption patterns

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Wastewater-based epidemiology (WBE) represents a modern and innovative tool that enables monitoring of population health status as well as lifestyle-related behaviours. By determining the concentrations of biomarkers in untreated influent wastewater, it is possible to estimate pathogen circulation and other health risks in the community, as well as the associated consumption of pharmaceutical products and illicit drugs. Data obtained through WBE complement information derived from traditional public health surveillance systems. As a public health tool, WBE offers distinct advantages: it provides anonymous, population-wide data while being relatively cost-effective and capable of delivering rapid results.

The analysis of illicit drugs and their metabolites in wastewater have become a major area of research in recent years. In Europe, the first large-scale investigation of illicit drug residues in wastewater was conducted in 2011 within the Sewage Analysis CORe Group Europe (SCORE) project, which included 19 European cities. The study revealed significant regional differences in illicit drug consumption across Europe. Following the success of this initial survey, annual monitoring campaigns have been conducted, and by 2024 the network had expanded to 128 cities across 26 countries, including Hungary. Building on this initiative, Hungary has introduced a national monthly surveillance of illicit drug concentrations in wastewater since May 2025. Concentrations of benzoylecgonine (cocaine metabolite), ketamine and amphetamine were the highest in the capital, Budapest. Spatial distribution of THC was the most even. Year-round variability was also significant.

The next step of the research involves optimizing the methodologies for sample preparation and measurement of other pharmaceuticals in wastewater matrices. Selected pharmaceutical residues (including Nonsteroidal Anti-Inflammatory Drugs (NSAIDs), antibiotics, etc.) will also be analysed on a monthly basis in samples collected from untreated influent wastewater. Results will be compared with pharmaceutical retail data. A secondary objective is to characterize the removal efficiency of specific treatment technologies by comparing data obtained from treated effluent and untreated influent wastewater samples collected at a wastewater treatment facility. These investigations will also support the implementation of the revised EU Urban Wastewater Treatment Directive (2024/3019).

Overcoming chromatographic and extraction challenges for the determination of PMT/vPvM substances in water

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The occurrence of persistent, mobile, and toxic (PMT) and very persistent and very mobile (vPvM) substances in the aquatic environment has gained growing attention within the scientific community due to their potencial impact on environmental and human health. Their high polarity and strong ionisation mean that many of these substances are poorly retained in most natural attenuation processes. At the same time, routine monitoring programmes still rely largely on analytical methods that are not well suited to the most mobile compounds, and show limited retention for the "gap compounds". There is therefore a clear need to develop and apply dedicated analytical approaches that can reliably capture these highly polar PMT and vPvM substances in real environmental samples.

This study addresses this challenge by developing and optimising a robust ultra-high-performance liquid chromatography–tandem mass spectrometry (UHPLC–MS/MS) method for the identification and quantification of representative PMT and vPvM substances in water, and by applying it to groundwater monitoring in Catalonia (north-eastern Spain). A set of 55 substances was selected to represent a broad range of physicochemical and ionic properties. Compounds with logD < 0 and no robust methods available, such as cyanoguanidine, acesulfame, melamine or trifluoroacetic acid, were deliberately included to challenge method performance. Different chromatographic columns were evaluated and optimised exploring the effects of pH, buffer concentration and aqueous content. In parallel, three water preconcentration strategies were assessed: mixed-mode solid-phase extraction, hydrophilic–lipophilic balanced solid-phase extraction and lyophilisation.

The optimised workflow, with a mixed-mode chromatography, significantly improved retention and peak shape for the most mobile analytes and enabled the determination of previously problematic PMT substances with method detection limits between 0.06 – 9.83 ng/L. Application to groundwater samples from the Baix Fluvià alluvial aquifer and the Llobregat River Basin aquifer confirmed the presence of several PMT substances in different hydrogeological sectors, highlighting their relevance in regional water resources. Overall, the study demonstrates that dedicated chromatographic and extraction strategies are essential to close current analytical gaps in groundwater monitoring and to provide more reliable occurrence data for the identification and prioritisation of PMT and vPvM substances in environmental protection and water-management frameworks.

Acknowledgements

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Ultra sensitive quantitation and targeted/non targeted analysis of water and food contaminants using the SCIEX ZenoTOF 8600 system

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SCIEX

Emerging contaminants in food and water require analytical solutions capable of delivering both highly sensitive quantitation and confident compound identification. The SCIEX ZenoTOF 8600 system combines high-resolution accurate-mass detection with Zeno trap-enhanced MS/MS sensitivity to enable targeted, suspect, and non-targeted analysis within a single workflow. The platform supports multiple acquisition strategies, including TOF-MS, MRMHR, data-dependent acquisition (DDA), and data-independent acquisition (DIA), providing flexibility for quantitative and qualitative applications.

Application examples covering pharmaceuticals and personal care products (PPCPs), pesticides, PFAS, hormones, and veterinary drugs demonstrate the system's ability to achieve ultra-trace detection in complex environmental matrices while maintaining accurate mass measurements and high-quality MS/MS spectra. Quantitative performance was evaluated in drinking water, surface water, groundwater, and treated wastewater samples, with results demonstrating the capability to meet SANTE identification and quantitation requirements.

Beyond targeted quantitation, the workflow supports suspect screening and non-targeted analysis through accurate-mass feature detection, isotopic pattern evaluation, MS/MS spectral matching, and library searching. This enables the identification of known contaminants, emerging pollutants, and previously unrecognized compounds with increased confidence. Integration with advanced data processing tools further enhances annotation and chemical characterization capabilities.

The SCIEX ZenoTOF 8600 system provides a comprehensive analytical solution for laboratories seeking to combine high-sensitivity quantitation with broad contaminant screening, supporting regulatory compliance, environmental monitoring, and food safety investigations.

Keywords: ZenoTOF 8600, high-resolution mass spectrometry, MRMHR, suspect screening, non-target

Wastewater-based assessment of lifestyle and dietary patterns in Croatian regions

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Wastewater-based epidemiology (WBE) is now a well-established approach that complements traditional epidemiological methods for assessing illicit drug use. In recent years, it has been increasingly used to estimate the consumption of other lifestyle chemicals, such as alcohol, nicotine, and caffeine, while its potential for assessing dietary patterns has been less explored [1].

In this study, WBE was used to assess spatial and temporal differences in lifestyle and dietary patterns across six Croatian regions during two seasons (November/December and June/July). Twenty-four-hour composite wastewater samples were collected over one week from 12 cities throughout Croatia. Samples were analysed by liquid chromatography coupled with tandem mass spectrometry, following a previously developed analytical method that included more than 40 biomarkers from several categories: alcohol, tobacco/nicotine, caffeine, artificial sweeteners, vitamins, the antidiabetic drug metformin, and various components of plant-based and animal-based foods [2]. Biomarker concentrations were converted to population-normalized mass loads (PNMLs) to enable intercity comparisons. The capital urban area was generally characterized by higher PNMLs for most lifestyle–related and plant food–related biomarkers. PNMLs of biomarkers associated with Mediterranean dietary patterns, such as higher citrus and fish consumption, were generally greatest in the Southern Adriatic region, followed by the capital urban area.

Although WBE can provide useful insights into regional and seasonal differences in lifestyle and dietary patterns, these data should be combined with dietary surveys, food purchase records, and other conventional methods to provide a more accurate, comprehensive, and reliable assessment of dietary patterns at the population level.

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Release of a quaternary effluent on a water body - Assessment of its environmental impact mitigation by natural attenuation processes

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The revised Urban Wastewater Treatment Directive (UWWTD) (1) requires the implementation of a quaternary treatment (QT) for large wastewater treatment plants (WWTPs) (≥ 150,000 person equivalent, PE) and medium ones (≥ 10,000 PE) located in areas where there is a risk. Its goal is to achieve an average removal efficiency of ≥80% for the load of ≥ 6 out of the 12 indicator micropollutants (MPs) set out in the directive. Although QT may significantly reduce concentrations of MPs, their released amounts can persist in the receiving water bodies. Hydraulic dilution and natural degradation processes (e.g. photodegradation) can further reduce their occurrence, consequently decreasing their impacts on aquatic species.

This study aims to assess the mitigation of the environmental impacts of a selection of 25 MPs (including 8 out of the 12 MPs set by the directive) present in a QT effluent as a result of natural attenuation processes. QT consists of a full scale hybrid membrane bioreactor (MBR), that is a MBR where powdered activated carbon (PAC, 0.1–0.2 g/L) is added to the bioreactor (2). The plant treats a mixture of hospital effluent (75%) and domestic wastewater (25%), has a treatment capacity of 700 m^3/day, and discharges its effluent into a small channel that is part of the local irrigation surface water network. The environmental risk assessment is based on the risk quotient (RQ), that is the ratio between the measured MP concentration and its predicted no-effect concentration, and assumes the three risk levels (3): low (RQ<0.1), medium (0.1≤RQ<1) and high (RQ≥1) risk. RQ was evaluated for the 25 compounds in the QT effluent, after its mixing with the receiving water, assuming the default value of 10 [4] and the real value (ranging from 2 to 3). To account for photodegradation contribution, the study evaluates the distance from the release point required to guarantee RQ< 0.1. Limiting here the attention to the MPs of the UWWTD, the results showed that only two compounds (diclofenac and venlafaxine) in the QT pose a high risk, being RQ for the other MPs< 0.1. Assuming the default dilution factor of 10, RQ after the complete mixing is reduced by 90%, dropping from high to medium risk for both diclofenac and venlafaxine. Continuous sunlight exposure can reduce RQ below 0.1 for diclofenac at a distance from the release point within 0.020 km (with 0.2 g PAC/L) and 0.052 km (with 0.1 g PAC/L) by direct photodegradation, and 0.19 km to 0.48 km (with 0.1 and 0.2 g PAC/L respectively) by indirect one. In contrast, venlafaxine exhibits much greater persistence, requiring substantially longer distances to reduce its concentration at low risk through photodegradation (>600 km for direct photodegradation and 39–65 km for indirect photodegradation).

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Removal of pharmaceuticals from synthetic human urine using ozone-based advanced oxidation processes

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This study examines the application of ozone-based treatment technologies for removing pharmaceuticals from human urine, a significant source of nutrients and organic contaminants. Although urine accounts for a relatively small portion of domestic wastewater volume, it contributes significantly to the overall load of pharmaceuticals and nutrients. Consequently, source-separated urine treatment represents a promising strategy to reduce environmental pollution, limit the spread of antimicrobial resistance, and promote nutrient recovery within a circular economy perspective (1, 2).

The study focused on the removal of carbamazepine (CBZ), sildenafil (SDF), and amoxicillin (AMX) in synthetic fresh and hydrolyzed urine using ozonation (O_3) and ozone-based advanced oxidation processes, including O_3/H_2O_2 and O_3/UV. Experiments evaluated the influence of several operational factors, such as urine composition, oxidant configuration, ozone dosage, and reaction time.

Pharmaceutical concentrations were quantified by chromatographic methods, while key physicochemical parameters were monitored to track changes in the urine matrix throughout the treatment. The findings revealed removal efficiencies above 90.0% for all target pharmaceuticals in both fresh and hydrolyzed urine. Moreover, degradation occurred more rapidly in hydrolyzed urine, which can be attributed to its alkaline pH and altered chemical composition. These conditions enhance ozone decomposition and stimulate the formation of hydroxyl radicals (HO•), thereby promoting indirect, non-selective oxidation reactions.

The integration of hydrogen peroxide (H_2O_2) and ultraviolet radiation (UV) further enhanced pharmaceutical elimination compared with ozonation alone. Both O_3/H_2O_2 and O_3/UV processes increased HO• generation and minimized matrix interferences from organic and inorganic components in urine.

In addition to contaminant removal, ozone-based treatments support circular sanitation approaches by enabling the recovery and reuse of valuable nutrients, including nitrogen and phosphorus, for agricultural applications. By lowering pharmaceutical concentrations while maintaining nutrient content, these technologies may facilitate the safe reuse of urine-derived streams within sustainable resource management strategies.

Overall, the study demonstrates the strong potential of ozone-based advanced oxidation processes for removing antibiotics from urine and highlights their relevance for integrated sanitation strategies that combine contaminant control with nutrient recovery.

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POSTERS

S1-1 Beyond grab sampling: Monitoring CECs in wastewater effluent using Affinisep AttractSPE membranes

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Wastewater treatment plant effluents are a significant route for the release of contaminants of emerging concern (CECs) into aquatic environments. Conventional grab sampling provides information limited to the time of collection and may not adequately capture temporal variability. Passive sampling offers a complementary approach by providing time-integrated information throughout the deployment period.

This study evaluates Affinisep AttractSPE passive sampling membranes containing a mixed sorbent composition of 50% HLB, 25% MCX and 25% WCX, designed to retain compounds with diverse physicochemical properties. Before field deployment, laboratory kinetic experiments were conducted in a recirculation system using tap water spiked with eleven selected contaminants. Eight membranes were retrieved over a 96 h exposure period, together with corresponding water samples, to investigate contaminant uptake kinetics.

Following the laboratory experiments, the samplers were deployed during two field campaigns in the effluent of a wastewater treatment plant in Saint-Point Maxence, France. During each deployment, six membranes were exposed, with three retrieved after one week and three after two weeks. Grab water samples were collected in parallel to enable comparison between passive and conventional grab sampling.

After retrieval, the sampler extracts were prepared for non-target analysis. In addition, residues collected from the membrane surface were extracted separately to determine whether they could provide complementary information on the overall chemical profile.

By combining laboratory calibration, field deployment, grab-sample comparison and separate analysis of residues collected from the membrane surface, this study aims to evaluate the performance and complementary information provided by mixed-sorbent passive sampling for the monitoring of CECs in complex wastewater matrices.

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S1-2 Glyphosate and AMPA in source water and drinking water: occurrence, fate, and treatment implications in Barcelona (Spain)

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The pesticide Glyphosate, one of the world's most widely used herbicides and its metabolite AMPA are widespread aquatic contaminants, yet their sources and fate in drinking water remain poorly understood. This study analyzed 345 water samples from two Barcelona river basins (Llobregat and Besòs) that supply drinking water to the city. AMPA consistently exceeded glyphosate levels at 95% of sampling sites, and remarkably, AMPA was detected without glyphosate in 60% of samples, indicating that AMPA originates from multiple independent sources beyond glyphosate degradation. In the Llobregat basin, peak concentrations reached ~20 µg/L for both compounds, exceeding EU drinking water standards (0.1 µg/L), with agricultural activities and urban wastewater discharges identified as major contamination sources. During the 2024 drought, water reuse significantly increased AMPA levels. In the Besòs basin, downstream concentrations were even higher, with AMPA showing seasonal variation and peaking in autumn, while groundwater contamination remained minimal. Surprisingly, at drinking water treatment plants, reverse osmosis antiscalants containing phosphonates introduced AMPA into treated water (up to 14 µg/L), which only resolved after switching to non-phosphonate alternatives. These findings reveal that AMPA originates from multiple sources and that treatment chemicals themselves can contaminate drinking water, necessitating integrated monitoring and process-level management strategies.

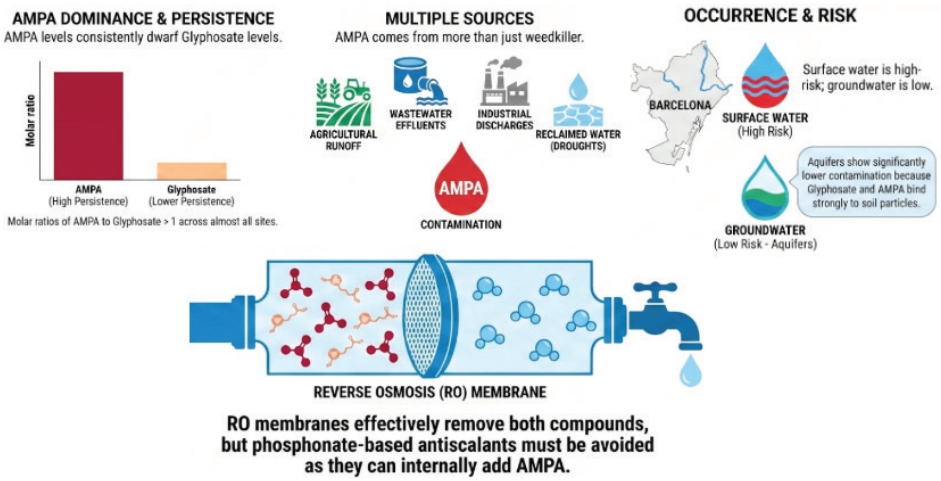


Figure 1. Occurrence and treatment of Glyphosate and AMPA in source water and drinking water

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S1-3 Assessing the Presence of Pesticides, Pharmaceuticals, and Personal Care Residuals in Water, Soil, and Plants in Riyadh Urban Ecosystem, Saudi Arabia

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Purpose: This study assessed the presence of pesticides, pharmaceuticals, and personal Care Residuals in Water, Soil and Plants in Riyadh's urban ecosystem. The study aimed to evaluate the potential of the presence of these commonly emergent pollutants (Pesticides, Pharmaceuticals and Personal Beauty Care Residuals) in the urban ecosystem of Riyadh region.

Methods: Samples of wastewater, soil, and plants were selected from the polluted sites such as sewage-draining canals and hospitals in the urban ecosystem of different locations in the Riyadh region. Solid phase extraction was used to extract these organic pollutions from water, soil, and plant samples. Ultra-High-Performance Liquid Chromatography (UHPLC) instrument was used to measure concentrations of these pesticides, pharmaceuticals, and personal care residuals. Additionally, Compound Discoverer™ software was used to achieve quantification, data interpretation, and structure.

Results: 16 pesticides in water, soil, and plants with high and low concentrations such as Terbuthylazine-2-hydroxy (388.8ng/ml) and Chlorpyrifos (0.3ng/ml). However, the results showed 16 pharmaceuticals such as Ibuprofen with high concentration (3645.3ng/ml) and Clofibric acid (0.033ng/ml) in water, soil and plant samples. Eight personal care products were detected and accumulated in water, soil, and plants, with high and low concentrations such as PFOS (30.7 ng/ml) and PFBA (0.78 ng/ml).

Conclusions: Results of the study showed that pesticides, pharmaceuticals, and personal care items were more prevalent in water samples than in soil and plant samples. All of these pesticides, pharmaceuticals, and personal care usage and disposal must be given attention to prevent their occurrences in the environment. Furthermore, treated wastewater must be given attention, as it is an important source of water in Saudi, which suffers from water shortages.

Keywords:
Emergent pollutants; Pharmaceuticals Urban Ecosystem; Wastewater; Riyadh; UHPLC

S1-4 Comparative distribution of lineal and branched PFAS isomers in water treatment

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PFAS (perfluoroalkylated and polyfluoroalkylated substances) are characterized by highly polar structures and very strong carbon-fluorine bonds. This bond gives strong thermal and chemical stability to these compounds in both linear and branched isomers. The toxicity of linear versus branched PFAS isomers differs significantly (1). Therefore, identifying and understanding the fate of individual isomers during water treatment is critical.

This study investigates the fate of PFAS in a drinking water treatment scenario involving water reuse (2). A total of 31 PFAS were analyzed across four sampling points during 2 years in reclaimed water (RW), river water 0.2 km upstream of a RW discharge point (UP), drinking water intake after RW discharge (CP), and final treated water (TW). The distribution and isomeric composition of PFAS were characterized at each stage.

Among the 31 PFAS analyzed, the main compounds identified were PFOS, PFOA, 6:2 FTS, PFBS, PFHxA, PFPeA, PFHpA. PFOS and PFOA presented both branched and linear isomers and therefore the ratio between species was quantified throughout the treatment and water reuse process.

Statistically significant differences (Kruskal-Wallis: $\chi^2 = 38.056$, $p < 0.001$)were observed in the lineal/branched isomeric ratios of PFOS across sampling points.The highest ratio was observed at the upstream point (UP: 1.79 ± 0.29), while the lowest was at the treated water point (TW: 1.35 ± 0.34), representing a 24% reduction. Post-hoc comparisons revealed significant differences between UP and TW ($p < 0.001$), and between CP and TW ($p < 0.001$), indicating that water treatment effectively reduces the linear PFOS fraction, considered more toxic due to its higher bioaccumulation potential, relative to branched isomers (3).

In contrast, the linear/branched ratio of PFOA remained relatively constant (Kruskal-Wallis: $\chi^2 = 7.789$, $p = 0.051$) across all sampling stages, indicating differential isomeric behaviour between these two compounds.

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S1-5 Occurrence and depth-related distribution of PFAS in the deep-sea shrimp *Eurythenes atacamensis* from the Atacama Trench

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Per- and polyfluoroalkyl substances (PFAS) are a diverse class of synthetic chemicals widely used in consumer and industrial products due to their chemical stability. The strong carbon–fluorine bonds make them persistent environmental contaminants capable of long-range transport through aquatic systems, sediments, organic matter, and the atmosphere, resulting in their widespread global distribution, including in remote marine environments. Despite increasing evidence of PFAS global contamination in marine organisms, information on their occurrence in deep-sea ecosystems remains limited. This study investigated the presence and distribution of PFAS in a novel deep-sea species *Eurythenes atacamensis* inhabiting the Atacama Trench, and evaluated whether collection depth influences PFAS accumulation. Eleven shrimp samples collected from 4,000 m to 8,000 m were freeze-dried, extracted using ultrasonic-assisted extraction, and analyzed by liquid chromatography–tandem mass spectrometry (LC–MS/MS) targeting 40 PFAS compounds representing multiple chemical classes, including perfluoroalkyl carboxylic acids, perfluoroalkane sulfonates, fluorotelomer sulfonates, and emerging PFAS. Quantification was performed based on analyte responses relative to isotope-labeled internal standards. Twenty-three PFAS were detected across the samples, with PFAS classes and concentrations varying among individual samples. Although no clear depth-related trend was visually observed, the heterogeneous distribution of PFAS suggests complex transport pathways and accumulation processes within the deep-sea environment. Statistical analyses were conducted to determine whether total PFAS concentrations differ significantly between the two collection depths. These findings provide the first evidence of PFAS occurrence in *Eurythenes atacamensis* and establish important baseline data on PFAS contamination in the Atacama Trench. The research contributes to a better understanding of contaminant transport through the marine water column and supports continued monitoring of PFAS in deep-sea ecosystems and potential marine food resources.

S1-6 Comprehensive profiling of contaminants of emerging concern in northern Antarctic Peninsula waters through liquid chromatography–ion mobility–high-resolution mass spectrometry

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The Antarctic Peninsula region is among the most remote and least populated regions on Earth. Despite its geographic isolation and the protective measures to safeguard its fragile ecosystem, anthropogenic pressures are increasing. Early research provided evidence on the presence of persistent organic pollutants, capable of long-range environmental transport in such a remote area. In recent years, the occurrence of contaminants of emerging concern (CECs) has also been flagged and linked to human activity taking place in the region. These findings are based on targeted studies examining a limited range of compounds, leaving a significant gap in the comprehensive characterization of water chemistry pollution. To address this issue, advanced analytical techniques based on wide-scope target screening and non-target analysis (NTA) by means of liquid chromatography coupled with hybrid ion mobility spectrometry - high resolution mass spectrometry were applied to the analysis of 19 water samples collected from ice-free areas of Deception, King George, and Livingston Islands (South Shetlands archipelago). These methods support retrospective analysis, providing a broad-spectrum detection of compounds not previously identified or anticipated. Incorporating ion mobility adds a complementary dimension to compound identification, enhancing confidence in NTA results. A semi-quantitative approach has also been employed to assess environmental risk.

In total, 88 compounds were detected in at least one sample with different identification confidence levels: 53 of them were confirmed with reference standards (Level 1), 28 matched with spectral libraries (Level 2A), and 7 were annotated with Level 3, following the Celma et al. (2020) criteria [1]. Ion mobility data enabled the identification of conformational isomers, such as adenosine, and differentiation of isobaric compounds like paraxanthine and theobromine. Most compounds presented concentrations in the ng/L range (91.8%), although a few of them reached the µg/L level. 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. Regarding aquatic environmental risk, only 15 of the identified compounds showed some occasional (usually in only 1 or 2 samples) high risk (RQ > 1).

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S1-7 Development of an LC-HRMS analytical method for organic micropollutants indicators established in the recently adopted urban wastewater Directive

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Concern about organic micropollutants has increased considerably in recent years due to their widespread occurrence in different environmental compartments and their potential impact on human health through environmental exposure. These compounds include pharmaceuticals, personal care products, and pesticides, among others, and are commonly detected throughout the water cycle owing to their physicochemical properties and incomplete removal by conventional treatment processes. Wastewater treatment plants (WWTPs) play a crucial role in mitigating their release into the environment. The recently adopted Urban Wastewater Treatment Directive (EU) 2024/3019 [1] reinforces this approach by establishing strict requirements for micropollutant removal and the progressive implementation of advanced quaternary treatment technologies in WWTPs. The Directive identifies 13 indicator substances to assess the performance of quaternary treatment processes, classifying them into Category 1 (substances that can be very easily treated) and Category 2 (substances that can be easily disposed of).

In this study, an analytical method was developed for the determination of these analytes in different water matrices. The method is based on the use of an Elute Online Extraction (OLE) system coupled with liquid chromatography-high resolution mass spectrometry (LC-HRMS). This approach provides simple and efficient sample preparation while enabling retrospective analysis using HRMS data. The method was validated following the SANTE 11312/2021 [2] guidelines at two concentration levels, 0.1 and 1 µg/L. The validated method was then applied to influent, effluent, and fortified samples as part of an interlaboratory comparison exercise.

The method showed good analytical performance in terms of linearity, repeatability, matrix effects (%ME), and relative recoveries (%RE) for most of the compounds. %RE values ranged from 43% to 122% at 0.1 µg/L and from 56% to 124% at 1 µg/L. Absolute %ME values were below 29% for all compounds. According to the interlaboratory comparison, evaluated using the standard deviation for proficiency assessment defined in ISO 13528, satisfactory results were obtained for all compounds and water matrices, except for amisulpride in influent wastewater.

The analysis of real influent and effluent samples revealed different removal behaviours 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.

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S1-8 Diffusive Gradients in Thin-films (DGT) as a Time-Integrated Tool for Monitoring Emerging Contaminants in Groundwater

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Neonicotinoid insecticides (NNIs) are among the most widely used insecticides worldwide, and their potential threat to non-target organisms has drawn increasing attention. To overcome the limited temporal representativeness of conventional grab sampling, a diffusive gradients in thin films (DGT) passive sampling technique using HLB as the binding gel (HLB-DGT) was developed for in situ monitoring of time-weighted average (TWA) concentrations of NNIs in groundwater. HLB-DGT enabled quantitative sampling over a wide range of conditions (pH 5–9.5, ionic strength 0.001–0.5 M, dissolved organic matter 0–10 mg L^{-1}) and was independent of typical groundwater ionic environments. The in situ diffusive boundary layer thicknesses were 0.35 mm in groundwater. Uptake remained linear over 14–18 days of deployment, and concentrations and occurrence patterns agreed well with grab samples, confirming its reliability and stability.

The technique was subsequently applied to investigate NNIs in surface water and groundwater of the Honghu region. All 15 target NNIs were detected, but concentrations and composition differed clearly between media: the mean Σ_{15}NNIs concentration in groundwater (21.9 ng L^{-1}) was significantly lower than in surface water (104 ng L^{-1}; $p < 0.05$). Groundwater was strongly dominated by the first-generation compound imidacloprid, whereas surface water carried larger contributions from currently used second- and third-generation NNIs. The predominance of imidacloprid in groundwater indicated the influence of historical residues, delayed infiltration and subsurface storage, illustrating how time-integrated sampling captures persistent and lagged contamination signals that may be underrepresented by individual grab samples.

Groundwater NNI concentrations exhibited clear seasonal variation, peaking in spring and summer in association with agricultural application, rainfall-driven leaching and seasonal groundwater recharge. This indicates that groundwater contamination was governed by both rapid vertical transport of highly soluble NNIs through agricultural soils and slower, longer-term infiltration of seed-treatment residues. Redundancy analysis further highlighted wetlands as the most influential factor for groundwater, indicating that low-lying wetlands and input from the Sihu Main Canal act as recharge sources that enhance NNI loading to the aquifer.

Overall, HLB-DGT provides a robust, time-integrated tool for monitoring emerging contaminants in groundwater, improving the characterization of average exposure, seasonal dynamics and delayed contaminant inputs, and thereby supporting a more comprehensive understanding of the sources, transport and persistence of NNIs in groundwater systems.

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S1-9 Wastewater-based assessment of pharmaceutical use in Croatia: regional differences and the importance of conjugates

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Beyond tracking illicit drugs and lifestyle chemicals such as alcohol, nicotine, and caffeine, wastewater-based epidemiology (WBE) is increasingly used to estimate pharmaceutical consumption [1]. WBE is particularly well suited to assessing the use of drugs with misuse potential, including anxiolytics, hypnotics, sedatives, and erectile dysfunction medications.

In this study, the consumption of benzodiazepines, zolpidem, methylphenidate, and phosphodiesterase type V inhibitors in six Croatian regions was assessed using a WBE approach. Raw wastewater samples were collected from several cities during a one-week sampling campaign, and additional samples were collected in the city of Zagreb in different seasons to assess the contribution of benzodiazepine conjugates (glucuronides), which are usually neglected in WBE studies, although recent work has highlighted their importance [2]. In total, more than 30 biomarkers, including parent compounds, metabolites, and glucuronides, were analysed by ultra-high-performance liquid chromatography coupled with tandem mass spectrometry after enrichment by solid-phase extraction.

In addition to identifying regional differences in the use of several pharmaceuticals, this study confirmed the importance of glucuronides in the overall mass balance of benzodiazepines, particularly during colder periods, when the activity of β-glucuronidase enzymes in faecal bacteria is reduced. However, further sampling campaigns spanning different seasons, together with triangulation with traditional epidemiological data, are needed for a comprehensive assessment and for the detection of potential pharmaceutical misuse.

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S1-10 Ultra-Sensitive Quantitation and Targeted/Non-Targeted Analysis of Pharmaceuticals, Pesticides and Personal Care Products (PPCPs) in Water Using the SCIEX ZenoTOF 8600 System

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Introduction

Pharmaceuticals, pesticides and personal care products (PPCPs) are increasingly detected in aquatic environments due to continuous release from wastewater, agricultural runoff, industrial discharge and other anthropogenic sources. Regulatory initiatives, including the EU Water Framework Directive and Drinking Water Directive, require sensitive and reliable analytical methods capable of detecting contaminants at trace and ultra-trace levels. High-resolution mass spectrometry (HRMS) provides a powerful solution for both targeted quantitation and comprehensive screening of known and emerging contaminants.

Methods

A multi-residue method comprising 176 PPCPs was developed using an ExionLC™ system coupled to the SCIEX ZenoTOF 8600 system. Water matrices included drinking water, surface water, groundwater and treated wastewater. Calibration standards were prepared from 0.1–1000 ng/L with isotopically labelled internal standards. Samples were analyzed using three HRMS acquisition strategies: information-dependent acquisition (DDA), SWATH® data-independent acquisition (DIA), and Zeno MRMHR. Quantitative performance was evaluated according to SANTE criteria, including accuracy, linearity, signal-to-noise ratio and ion-ratio confirmation.

Results

The SCIEX ZenoTOF 8600 system demonstrated excellent sensitivity and quantitative performance across a broad range of PPCPs. Limits of quantitation reached sub-ng/L levels, with many analytes meeting SANTE requirements at 0.5 ng/L and below. Representative compounds, including atenolol, bezafibrate, gabapentin, isoproturon, metribuzin, propamocarb and thiamethoxam, exhibited robust calibration performance and accurate recoveries in diverse water matrices. Trimethoprim recovery experiments showed quantitative accuracy between 90% and 103%. The system also maintained excellent mass accuracy without significant mass shifts, even at high analyte concentrations. Comparison with triple quadrupole MRM workflows demonstrated comparable or improved sensitivity while simultaneously providing accurate-mass confirmation

Beyond quantitation, the workflow enabled high-confidence suspect and non-target screening through accurate-mass TOF-MS and MS/MS data. Wastewater and surface water samples were successfully profiled using suspect screening lists and comparative screening approaches, enabling identification of known contaminants as well as previously unmonitored compounds and transformation products.

Conclusions

The SCIEX ZenoTOF 8600 system provides a unified high-resolution workflow for ultra-sensitive quantitation, suspect screening and non-target analysis of PPCPs in water. The platform delivers quantitative performance consistent with SANTE guidelines while enabling comprehensive contaminant characterization through accurate-mass MS/MS. This approach supports current and future.

S1-11 Ultra-sensitive quantitation of top 20 PFAS in drinking, surface and wastewater samples by direct injection using the SCIEX ZenoTOF 8600 system

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Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants of increasing regulatory concern because of their widespread occurrence, bioaccumulation potential, and possible adverse health effects. As drinking water regulations increasingly require detection at low ng/L (ppt) levels, laboratories need workflows that combine highly sensitive targeted quantitation with confident confirmation and the ability to investigate emerging PFAS compounds.

This study evaluated the SCIEX ZenoTOF® 8600 system for direct-injection, high-resolution accurate-mass analysis of 20 regulated and emerging PFAS in drinking, surface, and wastewater samples, using Zeno MRMHR, DDA, and SWATH DIA workflows to support quantitation, confirmation, and retrospective screening.

Samples were analyzed on an ExionLC™ system coupled to the SCIEX ZenoTOF 8600 system in negative electrospray ionization mode. Calibration standards from 0.1–100 ng/L were prepared with isotopically labeled internal standards, and performance was assessed for linearity, sensitivity, mass accuracy, precision, recovery, and matrix effects.

The workflow achieved excellent sensitivity for all 20 PFAS analytes, with limits of quantitation at or below current drinking water monitoring requirements and calibration linearity of $R^2 > 0.99$ across the investigated range. MRM-HR MAX acquisition with a broad set of product ions improved sensitivity and enabled MS/MS spectral library matching.

Accurate-mass precursor and fragment ion measurements supported high-confidence identification, with typical mass errors below 2 ppm and ion-ratio confirmation improving specificity in complex matrices.

Spike recovery experiments produced recoveries between 80% and 120% with excellent repeatability, while the Zeno trap enhanced low-level MS/MS detection without compromising high-resolution accurate-mass performance.

Beyond targeted quantitation, the HRMS data enabled retrospective investigation of emerging PFAS and transformation products without re-analysis, providing a future-ready advantage over targeted-only workflows.

Conclusions

Overall, the SCIEX ZenoTOF 8600 system provides an ultra-sensitive HRMS workflow for PFAS analysis in drinking, surface, and wastewater samples, combining low-ppt quantitation, accurate-mass confirmation, high-confidence MS/MS identification, suspect screening, and retrospective data mining.

The workflow enables laboratories to meet current drinking water monitoring requirements while establishing a future-ready platform for expanding PFAS surveillance programs.

Keywords: PFAS, Drinking Water, ZenoTOF 8600, High-Resolution Mass Spectrometry, MRMHR, Zeno DDA, SWATH, SWATH DIA, Environmental Analysis, Regulatory Monitoring.

S1-12 Tissue-Specific Distribution of Emerging Contaminants in European Eel by LC–HRMS

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The European eel (*Anguilla anguilla*) is a critically endangered species whose population has declined dramatically since the second half of the twentieth century. This decline has been associated with multiple interacting stressors, including overexploitation, habitat alteration and fragmentation, infectious diseases, barriers to migration, and chemical pollution. During their long continental growth phase, eels may be continuously exposed to complex mixtures of environmental contaminants, including metals, pharmaceuticals, pesticides and other contaminants of emerging concern (CECs). Some of these compounds may bioaccumulate in tissues and interfere with physiological processes relevant to eel health, reproduction and migration.

This study investigates the tissue-specific distribution of CECs in European eels by analysing muscle and liver samples collected from different aquatic environments in Catalonia (Spain) and the Pyrénées-Orientales (France). Sampling sites in Catalonia included Congost (Besòs), Massona (Fluvià), Ricarda and Remolar (Llobregat Delta), Fluvià, Ter, Llançà and Basses d'en Coll (Daró), whereas French sites included Salses-Leucate, Canet-Saint-Nazaire, Tech, Têt and Verdouble. The inclusion of several tissues with different physiological functions provides an opportunity to investigate contaminant partitioning and potential differences in tissue-specific accumulation.

For contaminant extraction, muscle and liver samples (500 mg) were homogenised using a TissueLyser II system with cold acidified acetonitrile/methanol (50:50, v/v). Samples were subsequently sonicated for 10 min and centrifuged for 12 min. Matrix interferences were reduced using a cleanup procedure based on HybridSPE dispersive pipette extraction (DPX) technology. Sample preparation was automated using a Hamilton robotic platform, improving reproducibility while reducing manual handling and solvent consumption.

Target compounds were analysed by liquid chromatography coupled to a Thermo Orbitrap Eclipse Tribrid high-resolution mass spectrometer (LC–HRMS), using electrospray ionisation in both positive and negative modes. The HRMS workflow enables the simultaneous determination of a broad range of contaminants belonging to different chemical classes and supports their reliable identification through accurate mass measurements and MS/MS fragmentation. The resulting multi-tissue dataset will provide new information on the occurrence and distribution of emerging contaminants in European eel and will contribute to a better understanding of internal contaminant exposure in this threatened species.

Acknowledgements

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S1-13 Spatial and temporal patterns of pesticides in Nordic surface waters revealed by targeted analysis supported by HRMS

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Current pesticide monitoring does not adequately capture short-term exposure variability, transformation products or overlapping contamination sources in Nordic surface waters. Integrated high-resolution spatial and temporal sampling, combining targeted quantification with HRMS screening and hydrological information, is therefore needed to distinguish sources, elucidate transformation pathways and assess mixture-related ecological risks under rainfall, snowmelt and freeze-thaw conditions. Combining quantitative targeted analysis with high-resolution mass spectrometry (HRMS) screening can broaden chemical coverage and provide complementary information on contaminant occurrence and distribution. Here, an integrated mass spectrometric workflow was applied to investigate pesticide contamination in the Nitelva River, Norway, within a catchment affected by multiple anthropogenic pressures, including the Brånåsen legacy landfill. Surface water samples were collected at seven locations during five sampling days in October 2024. The sites included a landfill-associated collector receiving drainage from Brånåsen, an upstream river reference, and five downstream locations representing urban, road-influenced, recreational and lower-river environments. Targeted quantification was performed by LC–ESI–MS/MS using an AB Sciex Exion LC coupled to a 6500+ triple-quadrupole mass spectrometer in multiple reaction monitoring mode. Separate methods covered glyphosate, AMPA and glufosinate and a broader multiresidue pesticide panel, with method quantification limits predominantly of 0.01 μg L^{-1}. Complementary UHPLC–Orbitrap HRMS screening used accurate mass, isotopic information and data-dependent MS^2 fragmentation to support tentative compound annotation. Targeted analysis revealed a complex pesticide fingerprint with pronounced spatial and day-to-day variability. Herbicides, fungicides, insecticides and transformation products were detected, including atrazine-related compounds, terbuthylazine/desethyl-terbuthylazine, chlorpyrifos-methyl, boscalid, diuron, imidacloprid, MCPA and 2,4-D. Polar analysis showed substantial spatial variability in glyphosate and AMPA, with elevated responses at selected downstream locations rather than a simple gradient originating from the landfill-associated site. HRMS screening complemented targeted quantification by providing tentative annotations of additional pesticide-related compounds outside the predefined quantitative target list. Overall, pesticide occurrence was characterized by heterogeneous spatial and short-term temporal patterns, suggesting contributions from multiple sources within the catchment rather than a single contamination source. Integrating quantitative LC–MS/MS with HRMS screening and repeated spatial sampling provided complementary information on pesticide occurrence and transformation products, demonstrating the value of combined targeted and HRMS approaches for characterizing complex contaminant mixtures and supporting source-oriented freshwater monitoring.

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S1-14 Complex chemical mixtures occur in Pyrenean high-mountain rivers: impacts on ecosystem health

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High-mountain rivers sustain biodiversity and provide key ecosystem services, including freshwater supply and downstream ecological integrity. Although often considered pristine, these environments are increasingly exposed to environmental pressures. In regions characterised by intense seasonal tourism, such as ski areas, additional inputs from wastewater, infrastructure, and recreational activities may further contribute to their occurrence. However, the presence and potential biological relevance of these contaminants in remote waters remain insufficiently characterised.

We investigated chemical contaminants in Pyrenean rivers across three Naut Aran locations to assess ecosystem health impacts. Sampling along a gradient from pristine headwaters to tourism-influenced areas was conducted in April and July 2025 to compare varying anthropogenic pressures. Chemical characterisation was performed by LC-MS/MS and GC-MS/MS for target analysis (including plastic additives, personal care products, bisphenols, flame retardants, PFASs); and LC-HRMS/MS for suspect screening of unknown chemicals. Toxicity assays were performed to assess in vivo acute to subchronical effects on feeding, behavioural and cardiological functions in *Daphnia magna* juveniles and zebrafish larvae.

Target analyses determined the presence of 54 contaminants. Phtalates were the most ubiquitous compounds, which is explained by their frequency of use as plastic additives in many products including packaging, cosmetics, or textiles. The solar filter UV-328 was detected at levels up to 865 ng/L in April, during peak tourism and ski season, which confirmed the relevance of anthropogenic pressure in the area studied. Suspect screening revealed the presence of therapeutics and prescription drugs, and industrial chemicals related to tire wear runoff from rubber and polymer manufacturing, textile chemicals such as some surfactants or caprolactam, related to the production of nylon fibbers and plastics, as well as sports doping drugs/drugs of abuse and their main metabolites.

Toxicity results highlighted sublethal alterations in feeding activity, locomotor behaviour, and cardiac responses, in both, invertebrate and vertebrate models. These findings indicate that contaminant mixtures present even in apparently low-impact mountain environments may still exert biologically relevant effects with potential ecological consequences.

Overall, this study shows that remoteness does not preclude chemical exposure in mountain areas and underlines the importance of combining chemical analysis with effect-based assessment to improve the understanding of the impact of complex chemical mixtures on ecosystems health.

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S2-1 Influence of Biomass Feedstock on the Biochar Physicochemical Properties and Adsorption Performance of Pharmaceuticals

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The increasing occurrence of pharmaceutical compounds in aquatic environments has intensified the search for sustainable adsorbents for advanced wastewater treatment. Biochar has emerged as a promising alternative due to its low production cost and tuneable physicochemical properties, which are strongly influenced by the nature of the feedstock and pyrolysis conditions. Understanding how these factors affect adsorption behaviour is essential for the rational design of high-performance biochars [1,2].

In this work, biochars produced from abundant biowaste resources, namely acacia, eucalyptus, vine pruning residues, and a 50:50 (w/w) mixture of eucalyptus biomass and wastewater treatment plant sewage sludge, were investigated as adsorbents for the removal of carbamazepine, citalopram, diclofenac and venlafaxine. These pharmaceuticals were selected because they are included among the indicator micropollutants defined in the Urban Wastewater Treatment Directive (EU) 2024/3019 [3] for assessing micropollutant removal performance. The materials were produced by pyrolysis and characterised in terms of surface chemistry, thermal stability, textural properties and surface charge using Fourier Transform Infrared Spectroscopy (FTIR), Differential Scanning Calorimetry (DSC), specific surface area analysis (BET) and pore volume determination (Mercury Intrusion Porosimetry) [4]. The relationship between feedstock composition, biochar physicochemical properties and adsorption performance was assessed to identify the key characteristics governing pharmaceutical removal. The outcomes of this work are expected to provide insights into the selection of suitable biomass resources to produce efficient and sustainable biochar adsorbents while promoting the valorisation of agroforestry residues and sewage sludge within a circular economy framework.

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S2-2 Antimicrobial resistance genes and potential co-selective pressures under unplanned water reuse across the water–soil–plant continuum

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Crop irrigation with surface waters impacted by wastewater discharges, a form of unplanned water reuse, may introduce pharmaceutical residues, antimicrobial resistance genes (ARGs), and other selective agents into agroecosystems. Metals and soil physico-chemical properties may further influence the persistence and distribution of resistance determinants, potentially contributing to co-selection processes. From a One Health perspective, agricultural environments represent important interfaces connecting water, soil, crops, and potential human exposure. This study provides a preliminary assessment of these factors across the water–soil–plant continuum in six agricultural plots with a gradient of agricultural management practices and irrigated with surface water under unplanned water reuse conditions.

Water, soil, root and leaf samples were collected from the plots to characterize pharmaceutical residues, ARG profiles, total metal concentrations and soil physico-chemical properties. ARGs were screened across the different environmental compartments using metagenomic analysis, while antibiotics and antifungals were screened to identify priority compounds for subsequent quantitative analysis. Total metal concentrations and key edaphic parameters were also determined to explore their potential association with resistance occurrence and distribution patterns.

Initial screening showed differences among environmental compartments. Water samples exhibited a more differentiated resistome profile, whereas soil and plant compartments displayed greater similarity in their ARG composition. Overall, genes associated with efflux pumps predominated. Pharmaceutical screening indicated a higher occurrence of antibiotics in water, while antifungal compounds were more frequently detected in soil as expected. Differences among plots were also observed in total metal concentrations and soil characteristics, suggesting that local environmental conditions and agricultural management may modulate ARG occurrence and distribution. The integrated analysis of pharmaceutical occurrence, ARG profiles, metal concentrations and edaphic variables is currently underway to identify co-occurrence patterns and potential drivers of antimicrobial resistance.

These findings highlight the importance of a comprehensive assessment of antimicrobial resistance in agricultural environments, considering not only antibiotic residues but also antifungals, metals, soil properties and agricultural management. The ongoing prioritization and quantification of selected pharmaceutical compounds will enable a more detailed evaluation of the chemical pressures associated with ARG occurrence and help identify potential co-selection processes under unplanned water reuse scenarios.

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S2-3 Bioremediation of Municipal Sewage Sludge: The Role of Bacteria in Organic Degradation and Heavy Metal Immobilization

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Sewage sludge disposal is a major environmental problem, because of its large organic load and presence of harmful heavy metals. The present study examines the efficiency of microbial anaerobic digestion as a bioremediation technique for the stabilization of municipal wastewater sludge and reduction in heavy metal toxicity. Samples of sludge were collected from wastewater treatment plants of Guelma and Annaba in Northeast of Algeria. The study investigated the metabolic activity of the indigenous microbial community and its function in organic matter breakdown and heavy metal dynamics.

Microbiological investigation after 30 days of anaerobic digestion process showed the active role of different bacterial populations including *Pseudomonas spp., Bacillus spp.* and *Staphylococcus spp*. These bacteria carried out a sophisticated biotransformation of the sludge matrix, which resulted in a highly efficient digesting stage with a decrease of 43.79% of the organic matter and 49.95% of the dry matter.

Some enzymes can be inactivated by heavy metals, inhibiting the metabolism of the bacteria, nevertheless, the detected microflora showed a high degree of tolerance and could stabilize the sludge. Despite high reduction of total solid mass, physically concentrating the residual inorganic elements, the microbial digestion process guaranteed that the heavy metal concentrations were safely within permissible limits for agricultural application.

Indigenous bacterial communities during anaerobic digestion have bioremediation potential that provides a useful means of detoxifying sewage sludge. In addition to degrading organic waste, this biological process stabilizes heavy metals and produces a safe, nutrient-rich digestate for sustainable agronomic valorization.

Keywords: wastewater treatment, sludge, anaerobic digestion, heavy metals.

S2-4 Comparative removal of erectile dysfunction pharmaceuticals from water using microwaveactivatedcarbon and organically modified montmorillonite

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The widespread occurrence of emerging contaminants (ECs) in aquatic environments has raised growing concern due to their persistence and potential ecological and human health risks [1]. Among these, phosphodiesterase type 5 (PDE-5) inhibitors, such as sildenafil (SILD) and tadalafil (TAD), are receiving growing attention because of their increasing detection in water bodies and the limited effectiveness of conventional wastewater treatment processes in removing them [2]. Adsorption represents a promising and sustainable strategy for the removal of these pharmaceuticals, particularly through the use of low-cost and environmentally friendly adsorbents [3-5]. In this study, the adsorption performance of biomass-derived activated carbons (ACs) was compared with that of montmorillonite (MMT). Spent brewery grains (SBG) were used as a renewable precursor to produce AC via conventional and microwave-assisted pyrolysis, while raw MMT and didodecyldimethylammonium bromide (DDAB)-modified MMT were investigated as alternative clay-based adsorbents. Batch adsorption experiments showed that AC produced via microwave-assisted pyrolysis exhibited superior adsorption performance compared with AC produced via conventional pyrolysis. Microwave-derived AC reached equilibrium within 2 h, achieving removal efficiencies of 90.3 ± 0.1% for SILD and 95 ± 2% for TAD at an adsorbent dosage of 50 mg L^{-1}. The maximum Langmuir adsorption capacities were 207 ± 10 mg g^{-1} and 119 ± 6 mg g^{-1} for SILD and TAD, respectively. The DDAB-modified MMT markedly outperformed raw MMT, reaching equilibrium within 1 h, with removal efficiencies of 84.9 ± 0.1% for SILD and 91 ± 3% for TAD at an adsorbent dosage of 250 mg L^{-1}. The corresponding maximum Langmuir adsorption capacities were 39 ± 3 and 38 ± 1 mg g^{-1}, respectively. These results demonstrate that microwave-derived AC and DDAB-modified MMT represent complementary adsorption platforms and provide valuable guidelines for the rational design of sustainable adsorbents for removing pharmaceutical contaminants from water.

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S2-5 The metabolic adaptation of *Haemonchus contortus* to fenbendazole

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Anthelmintic resistance in parasitic nematodes poses a critical threat to global livestock health and agricultural sustainability. Unravelling the molecular mechanisms of nematodes adaptation to anthelmintics is essential for identifying novel targets and biomarkers. We have previously shown that environmental circulation of the anthelmintic drug albendazole affects the expression and activity of drug-metabolizing enzymes contributing anthelmintic resistance in the parasitic nematode *Haemonchus contortus* (1) and that such alterations are stable across generations (2). Our preliminary study comparing metabolism of fenbendazole (FBZ) in adults of *H. contortus* among three different strains, a benzimidazole-susceptible strain (ISE), a benzimidazole-resistant strain (IRE), and a multidrug-resistant strain (WR), revealed that the susceptible ISE strain exhibited a significantly lower rate of FBZ metabolization (with a portion of metabolites being completely undetected) compared to the resistant IRE and WR strains (Figure 1). In this project, we study the complex changes in *H. contortus* metabolism under FBZ selection pressure. Using an integrative multi-omics framework, we combine *in vitro* larval selection and *in vivo* sheep infection models to trace phenotypic and molecular shifts across life stages. Here, we present preliminary bioinformatics analyses of high-throughput RNA-sequencing (RNA-seq) data derived from adult *H. contortus* subjected to FBZ exposure. These initial findings lay the bioinformatics foundation for ongoing genomic and metabolomic integration, enhancing our understanding of anthelmintic resistance acquisition due to environmental contamination in veterinary parasite populations.

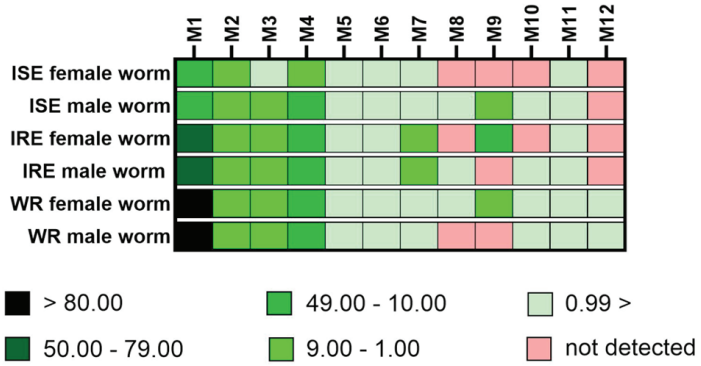


Figure 1. Comparison of FBZ metabolization rates among individual *H. contortus* strains (ratio of peak areas of individual metabolites to the internal standard normalized to mg of protein).

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S2-6 Identification of Pharmaceutical Transformation Products in Reactors Simulating Natural Aquifer Conditions Using HRMS Suspect Screening

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Pharmaceutical products are widely detected in the environment due to anthropogenic pollution, as their removal in wastewater treatment plants is only partial. Consequently, these compounds reach surface rivers and infiltrate into adjacent aquifers, leading to groundwater contamination. Once in the subsurface, their environmental fate depends heavily on hydrochemical processes and ambient aquifer conditions. Previous studies in Barcelona have reported a high frequency of pharmaceuticals, including atenolol, benzotriazole, citalopram, climbazole, gabapentin, iopromide, irbesartan, lamotrigine, lidocaine, losartan, metoprolol, oxazepam, sertraline, sitagliptin, sulfamethoxazole, trimethoprim, valsartan, and venlafaxine, in groundwater due to infiltration from the Besós River. Once in the aquifer, these contaminants may undergo degradation, making it essential to identify their resulting transformation products.

Therefore, this study aims to evaluate the attenuation pathways and potential transformation processes of these pharmaceuticals within the subsurface, specifically investigating how distinct redox conditions and temperatures influence their natural attenuation. To achieve this, parallel batch reactor experiments were conducted under oxic and suboxic (nitrate-reducing) conditions at two temperatures (25 °C and 35 °C). Over a 21-day period, 11-mL samples were collected, concentrated via vacuum-assisted evaporation, and analyzed using Liquid Chromatography-High Resolution Mass Spectrometry (LC-HRMS). A comprehensive suspect screening of parent compounds and their transformation products (TPs) was performed using Compound Discoverer 3.5 alongside specialized databases such as BioTransformer and FairTPs. To date, 15 TPs from various pharmaceuticals have been detected and confirmed at Level 2 of the Schymanski scale, including venlafaxine N-oxide, lidocaine N-oxide, and O-desmethylvenlafaxine, atenolol acid and desmethylcitalopram.

The parallel reactor systems successfully enabled the controlled investigation of the mechanisms governing the fate and attenuation of these compounds. These findings provide valuable insights into the pathways regulating pharmaceutical degradation in groundwater, and future work will involve monitoring and validating these specific TPs in real-world samples collected throughout the Besós River basin.

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S2-7 Influence of Matrix Effects on the QuEChERS Extraction of Pharmaceuticals from Wastewater Sludge

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The agricultural reuse of sewage sludge supports circular economy strategies by recycling nutrients and organic matter [1]. However, the presence of pharmaceutical residues in this matrix raises environmental concerns and demands analytical methods for their determination. Due to the complexity of sewage sludge, matrix effects remain one of the main challenges affecting the accuracy and precision of chromatographic analyses of pharmaceutical residues [2].

This study evaluated the influence of matrix effects on the determination of nine pharmaceuticals in dewatered sludge collected from a Wastewater Treatment Plant (WWTP) serving approximately 300,000 p.e.. Target analytes were extracted using the AOAC QuEChERS (Quick, Easy, Cheap, Effective, Rugged and Safe) method followed by a dispersive solid-phase extraction (d-SPE) clean-up step [3,4]. Quantification was performed by High-Performance Liquid Chromatography (HPLC) with fluorescence (FLD) or photodiode array (PDA) detection. Method performance was evaluated in terms of recovery, precision and matrix effects using sludge samples spiked at three concentration levels (2250, 3000 and 4000 ng g^{-1} dry weight, n = 3) with a mixture of atenolol (ATN), carbamazepine (CBZ), diclofenac (DCF), fluoxetine (FLX), ibuprofen (IBU), ofloxacin (OFL), propranolol (PRP), sulfapyridine (SP) and sulfamethoxazole (SMX).

Matrix effects varied among the target pharmaceuticals, with both signal suppression and enhancement depending on the analyte. Across the three spiking levels, ATN and SP exhibited minimal matrix effects, ranging from −8.9% to 7.4% and −10.7% to 15.6%, respectively. In contrast, OFL showed the greatest matrix interference, with matrix enhancement reaching up to 169% (4000 ng g^{-1}), indicating a strong influence of the sludge matrix. Overall, the most favorable results were obtained at the 3000 ng g^{-1} fortification level, where all analytes except OFL remained within the ± 20% acceptance criteria [5].

Recovery was compound-dependent, reflecting the heterogeneous interactions between pharmaceuticals and the sludge matrix. Recovery values generally improved with increasing fortification level, with the best overall performance obtained at 4000 ng g^{-1}, as seven of out the nine pharmaceuticals showed recoveries inside the acceptance criteria of 70 - 120% established by the SANTE guidelines [5]. Exceptions were PRP with a poor recovery efficiency of 33% and CBZ which surpassed the limit with 141%.

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S2-8 Silver Telluride Nanocrystals as Amplifiers for Pharmaceuticals Monitoring by SEIRA

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Rapid demographic and industrial growth have led to increasing levels of anthropogenic contaminants in water resources and ecosystems. Among them, organic microcontaminants, such as pharmaceuticals and pesticides, are of particular concern because they can affect non-target organisms even at trace concentrations (ng to µg/L). In this context, the new Urban Wastewater Treatment Directive (EU) 2024/3019 (EU-UWWTD) introduces requirements for monitoring and removing organic microcontaminants from urban wastewater. Thus, to improve wastewater treatment and reduce organic pollutant loads, practical, fast, and reliable monitoring tools are essential to support environmental compliance and water-quality control.

Conventional water analysis techniques, such as liquid chromatography coupled with mass spectrometry (MS), are costly, time-consuming, and require specialized personnel. By contrast, surface-enhanced infrared absorption (SEIRA) spectroscopy has emerged as a promising approach for sensitive and portable detection of microcontaminants. As a Green Analytical Chemistry (GAC) technique, SEIRA minimizes sample handling, enables in situ measurements, and generates minimal waste.

Infrared spectroscopy can be used for molecular identification through vibrational fingerprints, but its sensitivity decreases for weakly absorbing compounds or low analyte concentrations. To overcome this limitation, in this work, silver telluride (Ag_2Te) quantum dots (QDs) were evaluated as SEIRA amplifiers for the detection of the pharmaceutical venlafaxine (VEN). The Ag_2Te QDs were prepared in water using different stabilizing molecules, namely mercaptosuccinic acid (MSA), cysteine (Cys), or glutathione (GSH). All Ag_2Te QDs exhibited SEIRA activity, with enhancement factors (EF) varying according to the stabilizer, with Cys and GSH showing the best performance. Preliminary results showed an EF of up to 17× at the 1611 cm^{-1} band of VEN, demonstrating substantial signal amplification.

Overall, these results show that the stabilizing agent strongly influences analyte–substrate interactions and support the use of Ag_2Te QDs as promising and sustainable SEIRA-active materials for sensitive pharmaceutical monitoring in water.

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S2-9 Environmental residues of albendazole drug induce adaptive changes in *Caenorhabditis elegans*

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Environmental contamination by veterinary anthelmintics is increasingly recognized as an important factor influencing biological interactions within ecosystems. Although residues of these pharmaceuticals have been detected in soils and plants, their long-term effects on target and non-target nematodes remain poorly understood. The extensive use of anthelmintic drugs in agriculture and veterinary medicine has raised concerns regarding their environmental persistence and the potential consequences of chronic exposure to environmentally relevant concentrations. Even trace levels of these compounds may induce adaptive responses that contribute to the development of anthelmintic resistance and have broader ecological implications. Previous studies have confirmed the environmental circulation of anthelmintics and demonstrated alterations in the expression of detoxification enzymes in the parasitic nematode *Haemonchus contortus* following exposure to these compounds [1, 2].

The study used the free-living nematode *Caenorhabditis elegans* as a model organism to investigate the effects of long-term exposure to environmentally relevant concentrations of albendazole (veterinary anthelmintics). Chronic exposure resulted in altered susceptibility to albendazole, as demonstrated by changes in IC_{50} values across generations. In addition, biotransformation analysis (using HRMS) revealed differences in albendazole metabolism following prolonged low-dose exposure, indicating adaptive modifications of metabolic pathways. These findings provide new insights into the responses of non-target nematodes to environmental anthelmintic residues and suggest that chronic exposure to trace concentrations of albendazole may contribute to the development of reduced drug susceptibility.

Acknowledgements

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S2-10 Persistence and fecal elimination of fluralaner in cattle following pour-on administration over 31 days using LC-MS/MS

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Fluralaner is an isoxazoline widely used in veterinary medicine due to its high efficacy against ectoparasites. While its systemic disposition is well documented in companion animals, data regarding its excretion pathways in livestock remain limited. Evaluating fecal elimination in cattle following topical (*pour-on*) application is particularly critical, as excreted residues can reach surrounding soil and pastures, raising potential environmental safety and ecotoxicological concerns for non-target terrestrial organisms. Objective: This study aimed to monitor the excretion levels and persistence of fluralaner in bovine feces across a 31-day post-treatment window (days 5, 16, and 31) following topical administration, using LC-MS/MS to evaluate preliminary environmental exposure potential. Methods: Fifteen steers were treated with a single pour-on dose of fluralaner (2.5 mg/kg). Paired plasma and fecal samples were collected on days 5, 16, and 31 post-treatment. Quantification in plasma and feces was carried out by LC-MS/MS adapting the method previously established for plasma (Berkovic *et al*., 2026) with specific modifications optimized for the fecal matrix. Results: Fluralaner was quantifiable in plasma and fecal matrixes throughout the 31-day evaluation period, exhibiting substantial inter-individual variability. Plasma concentrations remained low and stable across sampling points, with medians of 11.4 ng/mL (range: 0.0–42.1 ng/mL) on day 5, 12.1 ng/mL (range: 0.0–73.2 ng/mL) on day 16, and 9.1 ng/mL (range: 0.0–28.8 ng/mL) on day 31. In contrast, fecal elimination displayed higher overall levels, peaking at day 16 with a median concentration of 445.2 ng/g (range: 68.7–1879.7 ng/g) compared to 142.1 ng/g (range: 21.6–2257.2 ng/g) on day 5 and 146.2 ng/g (range: 23.4–385.2 ng/g) on day 31. Fecal concentrations of fluralaner were markedly higher than those observed in plasma throughout the study, remaining substantial at 31 days post-administration. These findings demonstrate that fecal excretion constitutes a major route of elimination for fluralaner in cattle. Given the persistence and magnitude of residues excreted in manure, potential environmental repercussions must be carefully evaluated, forming the basis for ongoing and future research.

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S2-11 Optimization of analytical procedures for marine pollutants in seawater from SEATRACE project

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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).

In the present study, a solid-phase extraction (SPE) procedure coupled to liquid chromatography–high-resolution tandem mass spectrometry (LC-HRMS/MS) was optimized for the determination of CECs in seawater (Figure 1). Different SPE conditions were evaluated using hydrophilic–lipophilic balanced (HLB) sorbents, with particular attention to sample dilution, cartridge washing and elution. Dilution of seawater 1:1 with ultrapure water substantially reduced the salt load retained by the cartridge and transferred to the final extract. The best overall performance was obtained using a single rinse with 0.01 N HCl followed by elution with 2 × 3 mL MeOH, which provided improved recoveries and broadened the range of compounds efficiently extracted. Extracts were evaporated to dryness, reconstituted in H_2O (90:10, v/v) and analysed by LC-HRMS/MS.

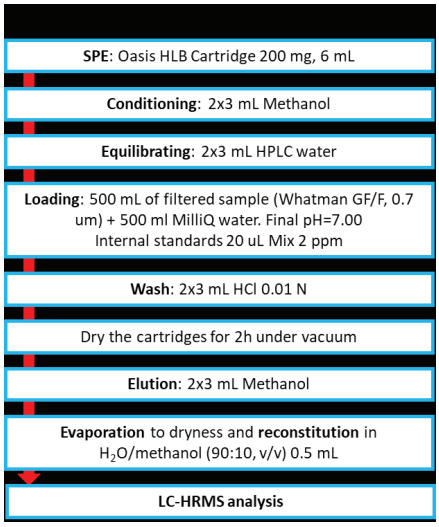


Figure 1. Procedure for sea water extraction of CECs.

To complement organic micropollutant characterization with information on seawater chemistry, a method for the determination of inorganic nutrients and major ions was developed using a Thermo Scientific Dionex INTEGRION Reagent-Free

Ion Chromatography (IC) system. IonPac AS18 and CS12A columns, electrolytically generated hydroxide and methanesulfonic acid eluents, respectively, and suppressed conductivity detection enabled the analysis of common anions and cations in seawater with minimal sample pretreatment.

The optimized procedures were subsequently applied during a preliminary sampling campaign in the Mar Menor coastal lagoon (Spain) to evaluate their performance under real environmental conditions (Figure 2). Surface seawater samples covering contrasting areas of the lagoon were used to assess SPE robustness, residual salt interference and matrix effects during HRMS analysis, together with the applicability of the IC method to nutrient-rich marine waters. This pilot campaign represents the first field validation of the SEATRACE analytical workflow and provides the basis for its application to the geographically diverse marine sampling campaigns planned within the project.

The combination of optimized sample preparation, broad-scope HRMS analysis and complementary nutrient characterization provides a robust analytical strategy for the comprehensive assessment of pollutant prevalence in complex marine environments.



Figure 2. Study area and sampling locations in the Mar Menor hotspot during the pre-sampling campaign carried out in October 2026.

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S2-12 Silent exposure, delayed damage: GenX and enrofloxacin effects in marine mussels

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Per- and polyfluoroalkyl substances (PFAS) and fluorinated pharmaceuticals are increasingly detected in coastal waters, where filter-feeding bivalves may experience episodic exposure followed by partial depuration. This study assessed the individual and combined sublethal effects of hexafluoropropylene oxide dimer acid (HFPO-DA; GenX) and enrofloxacin (ENR) in *Mytilus galloprovincialis*. Mussels collected from Ria de Aveiro were acclimated and exposed for 14 days to 50 ng/L GenX, 50 ng/L ENR or their mixture, followed by 14 days of recovery in clean seawater. A battery of biomarkers was evaluated in whole soft tissues, including energy metabolism, energy reserves (carbohydrates and proteins), antioxidant defences, biotransformation, oxidative damage (lipid peroxidation and protein carbonylation) and neurotoxicity. During exposure, ENR did not trigger obvious oxidative stress or neurotoxicity. However, GenX and the mixture increased carbohydrate reserves, suggesting energy reallocation in response to low-dose chemical stress. Furthermore, mixture-exposed mussels displayed a more distinct position, primarily associated with carboxylesterases and acetylcholinesterase, suggesting early modulation of biotransformation- and neurotoxicity-related responses under combined exposure. After depuration, contaminant-exposed mussels exhibited higher antioxidant-related responses, along with increased lipid peroxidation and protein carbonylation, indicating delayed oxidative damage. The mixture also reduced carboxylesterase activity during recovery, pointing to potential interactive effects on biotransformation capacity. Multivariate analysis separated exposure-phase treatments from contaminant-exposed recovery groups, confirming that the 14-day recovery period was insufficient to restore control-like biochemical profiles. Overall, environmentally relevant levels of GenX and ENR induced mainly sublethal and delayed effects in *M. galloprovincialis*, highlighting the need to include mixture scenarios and post-exposure phases in the risk assessment of emerging contaminants in marine environments.

Keywords: PFAS, pharmaceuticals; bivalves; biomarkers; recovery; emerging contaminants.

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S2-13 Development of a multi-residue method for macrocyclic lactones in animal waste by UHPLC-MS/MS

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Macrocyclic lactones (MLs) are broad-spectrum endectocides widely used in livestock production. Due to limited metabolism, a substantial fraction of the administered drug is eliminated as parent compound via faeces, resulting in direct inputs to terrestrial systems through dung deposition and land application of manure and slurry. Existing analytical methods, mainly based on HPLC-FLD detection, target the single compounds or a limited number of them. In this work, a multi-residue method for the simultaneous quantification of six MLs, including abamectin, doramectin, emamectin, eprinomectin, ivermectin and moxidectin in bovine manure, bovine slurry and ovine manure, was developed using UHPLC-MS/MS. Samples were extracted with acetonitrile and subsequently cleaned-up using solid-phase extraction (SPE). The total run time to achieve the separation of all six analytes was 12 minutes. Quantification was performed using isotope-labelled internal standards (moxidectin-D_3, $^{13}C_6$-eprinomectin, emamectin-D_3) and a structural analogue (3,4-dihydrodoramectin). The method is currently undergoing validation according to the SANTE/11813/2017 guidelines, before being applied to the analysis of field manure and slurry samples. Preliminary method performance results showed recoveries in the range 75-120% and precision ≤20% across the three different matrices. To the best of our knowledge, this is the first UHPLC-MS/MS method covering all six MLs in both cattle and sheep waste matrices and can be efficiently employed in the assessment of ML environmental exposure within agricultural systems.

S2-14 LC-MS/MS QTOF analysis of river water identifies contaminants of environmental concern by non-targeted analysis

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Water-based epidemiological studies have yielded valuable insights into wastewater treatment processes and have enabled the identification of contaminants of environmental concern (CEC) in recent years. Both targeted and non-targeted analysis have been applied to detect emerging contaminants that may originate from treated or untreated wastewater as a result of storm overflows. In this study, river water samples were measured from both tidal and freshwater locations. Novel non-targeted analysis (NTA) profiling software was applied to identify key differences between samples.

River water samples were taken from twelve sites on the River Thames and ten sites on the River Hogsmill. Samples were measured using a reversed-phase forensic toxicology LC-DIA MS/MS method (LCMS-9050, Shimadzu Corporation). Insight Profiler software was used to process data with a method configured to detect trace level components in all samples, align features, filter features based on data quality criteria and identify components with high confidence using multiple MS/MS data repositories.

The results highlighted the need for systematic monitoring of river samples close to wastewater treatment facilities (WWTFs) as samples taken downstream of the Hogsmill River facility contained a high number of pharmaceutical compounds and metabolites, including venlafaxine, desmethylvenlafaxine, tramadol, O-desmethyltramadol, gabapentin, ketamine, clarithromycin, metronidazole, carbamazepine, and lidocaine, whilst upstream samples showed a markedly lower distribution and concentration of pharmaceuticals evidencing of the impact of the WWTF on downstream profiles. It was also notable that acetaminophen (paracetamol), recognized as a well-established tracer of wastewater influent, was detected at all sampling sites at relatively consistent but low levels.

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