20TH ANNUAL WORKSHOP ON EMERGING HIGH-RESOLUTION MASS SPECTROMETRY (HRMS) AND LC-MS/MS APPLICATIONS IN ENVIRONMENTAL ANALYSIS AND FOOD SAFETY

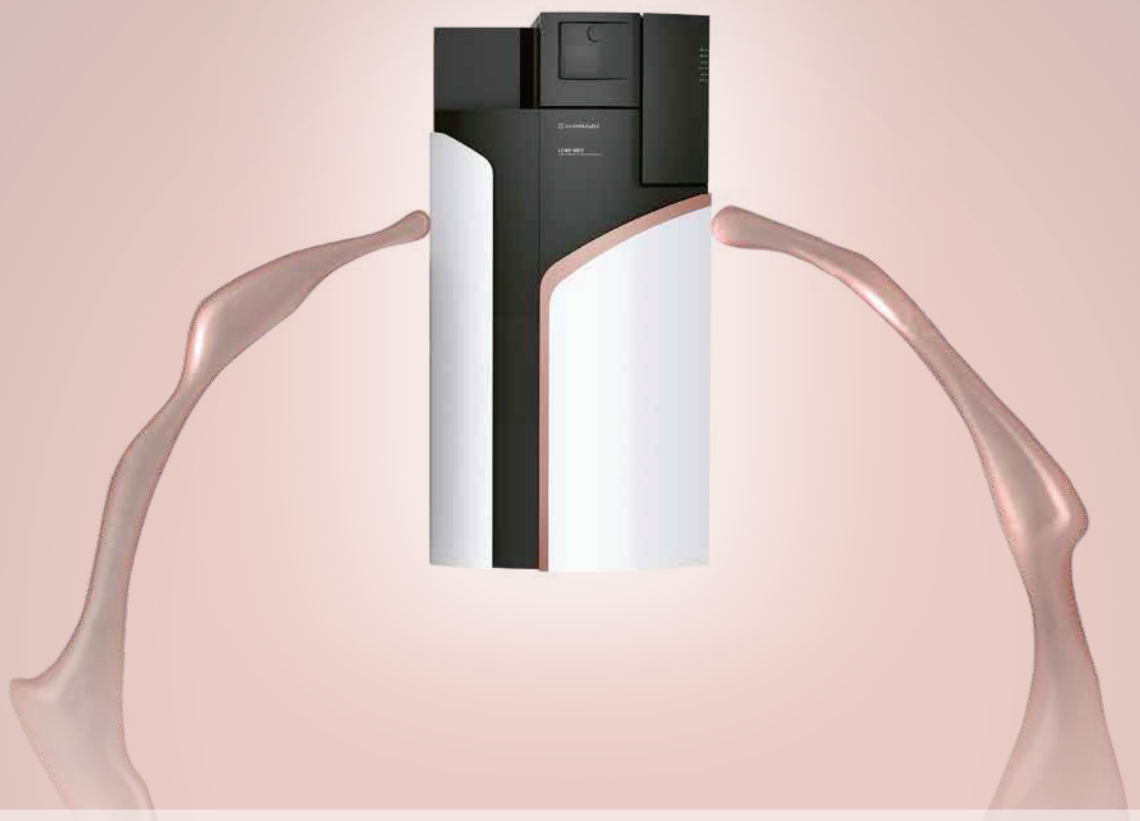
BARCELONA, 7-8 OCTOBER 2024

ORGANIZED BY

CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

UNIVERSIDAD DE ALMERÍA

ABSTRACT BOOK



CONTENT

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WELCOME

Following the success of previous 19th International workshops on LC-MS/MS in environmental analysis and food safety (Barcelona 2005, Barcelona 2006, Guelph, Ontario 2007, Barcelona 2008,Toronto2009, Barcelona 2010, Buffalo 2011,Barcelona 2012, Toronto 2013, Barcelona2014, Burlington, 2015, Barcelona 2014,Buffalo 2017, Barcelona 2018, Miami Beach2019, Barcelona 2020-virtual and Ottawa-2021 virtual),Barcelona 2022 and Buffalo 2023) we are presenting here the 20th International workshop on emerging high-resolution mass spectrometry (HRMS), as well as on LC-MS/MS applications in environmental analysis and food safety. The conference is planned to be IN PERSON.

The main objectives of the workshop is to evaluate practical aspects of the usefulness of high resolution mass spectrometry and tandem mass spectrometric techniques for screening and quantitation of organic contaminants in the environmental and food samples. The following practical aspects and state of the art applications will be discussed:

- Advances in HRMS instrumentation and their applicability in environmental analysis and food authenticity
- Non Target Analysis (NTA) and Bioinformatics applied to environmental and food samples
- Advanced Wastewater Based Epidemiology (WBE) for public health
- Large number of applications in environmental analysis and food authenticity such as water and soil/ sediment, biota and food, like fruits and vegetables, juices and meat including green methods

This workshop is intended to be an informal venue that encourages an exchange of the latest information and ideas among scientists from academia, governmental agencies and industry. In a similar way as last years the workshop is jointly organized by IDAEA- CSIC (Barcelona, Spain), in collaboration with CTA-RSEQ, PSIPW and the University of Almeria.

A virtual special issue (VSI) in Methods Elsevier) is planned. Authors interested to submit a contribution to this VSI please contact the conference chair. Deadline for submission of papers is December 1, 2024.

Welcome to Barcelona!

Damià Barcelo
Emeritus Professor at the University of Almeria, Spain
Chair of the Scientific Committee

MONDAY, 7th October 2024

09:00 **Registration**

CHAIR: Damià Barceló

Topic: Advanced Wastewater Based Epidemiology (WBE) for public health

9:00 **Opening lecture**. Chlorination of Emerging Contaminants for Application in Potable Wastewater Reuse: Disinfection By-Product Formation, Estrogen Activity, and Cytotoxicity
Susan Richardson, *University of South Carolina*

9:45 **Keynote lecture.** Mass spectrometry enabled water-based early warning systems for environmental and public health protection: an importance of chemical profiling in longitudinal studies
Barbara Kasprzyk-Hordern, *University of Bath*

10:15 **Contributed lecture.** SPE and HPLC-HRMS/MS protocol for multi-residue analysis of chemicals from degraded polyester fibres
Julian Campo, *Environmental & Food Safety Research group of the University of Valencia (SAMA-UV), Desertification Research Centre CIDE (CSIC-UV-GV)*

10:35 **Contributed lecture.** The potential of wastewater-based epidemiology for the assessment of lifestyle and dietary habits
Ivan Senta, *Rudjer Boskovic Institute*

10:55 David Solomon Jalajel, Prince Sultan Bin Abdulaziz International Water Prize

11:10 **COFFEE BREAK & POSTER SESSION 1**

CHAIR: Barbara Kasprzyk-Hordern

11:45 **Keynote lecture.** High-Resolution Mass Spectrometry and Proteomics Unveils The Capsule Of Time All Vertebrates Share
José Luis Capelo Martínez, *NOVA University Lisbon*

12:15 **Contributed lecture.** Application of a metabolomic approach based on the use of high-resolution mass spectrometry for the discrimination of agricultural practices
M.J. Martinez Bueno, *University of Almeria*

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

12:35 **ORAL COMMUNICATIONS**

Detecting PFAS beyond the Current Regulative Request: a Comprehensive Overview of the Contamination in Water by UPHLC-ion mobility-HRMS

Carsten Baessmann, *Bruker Daltonik GmbH & Co KG*

Non-targeted analysis of a biodegradable bio-based food packaging material by LC-ESI-Q-Orbitrap

Antía Lestido Cardama, *Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Pharmacy, University of Santiago de Compostela / Instituto de Materiales (iMATUS), University of Santiago de Compostela*

How Wastewater Reflects Human Metabolism – Suspect Screening of Pharmaceutical Metabolites in Wastewater Influent

Corina Meyer, *Eawag (Swiss Federal Institute of Aquatic Science and Technology)*

Discovery of new contaminants and their metabolites in fertilizing residue materials (FRMs) and amended agricultural soils using NTA: A case study of deinking residues-amended soils

Jingyun Zheng, *Department of Food Science and Agricultural Chemistry, McGill University*

Discovering pharmaceutical transformation products in intermittent rivers using open cheminformatics approaches

Olga Gómez-Navarro, *Institute of Environmental Assessment and Water Research (IDAEA), Spanish National Research Council (CSIC)*

13:25 **LUNCH BREAK & POSTER SESSION 1**

CHAIR: Susan Richardson

14:30 **Keynote lecture.** Combining Target and Non-Targeted Approaches for PFAS characterization in recreational fisheries

Natalia Soares Quinete, *Florida International University*

15:00 **Contributed lecture.** Efficient Data Prioritization for dentification and Semi-Quantification in Nontarget Screening of PFAS

Christian Zwiener, *Environmental Analytical Chemistry, Department of Geosciences, Universität Tübingen*

15:20 **Keynote lecture.** Non-Target HRMS analysis using the ROIMCR chemometrics method

Romà Tauler, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC)*

15:50 **Sponsored lecture.** Applying a novel component detection algorithm to untargeted screening

Neil Loftus, *Shimadzu Corporation*

16:20 **Keynote lecture.** Chemical Exposome, Ultrafine Particles, and Glioblastoma: A New Perspective

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

16:50 **COFFEE BREAK**

CHAIR: Natalia Soares Quinete

17:20 **Contributed lecture.** Source apportioning of wastewater intrusions: merging Non-target Analysis and traditional water quality parameter datasets. A South Florida case study

Piero R. Gardinali, *Florida International University*

17:40 **Contributed lecture.** Tracking organic pollutants occurrence and sources in urban groundwaters using LC-HRMS

Sandra Pérez, *IDAEA-CSIC, ONHEALTH, Department of Environmental Chemistry Institute of Environmental Assessment & Water Research (IDAEA), CSIC*

Topic: Green Analytical Chemistry using HRMS and/or LC/MS-MS applied to environmental and food analysis

18:00 **ORAL COMMUNICATIONS**

Quantification of quaternary ammonium compounds in meat and seafood products by LC-MS/MS

Kahina Slimani, *Anses*

Hyphenation of Electrochemistry and Mass Spectrometry to Elucidate Environmental Transformation Processes of Organic Pollutants

Valentin Göldner, *University of Vienna*

Assessment of potentially hazardous chemicals during pregnancy

Esteban Restrepo-Montes, *Institute of Environmental Assessment and Water Research, IDAEA-CSIC*

Comprehensive Assessment of Endocrine Disruptors: Evaluating Hair, Blood, and Urine Matrices

Ana González-Ruiz, *Institut d'Investigació Sanitària Pere Virgili (IISPV)*

18:40 End of the day

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

TUESDAY, 8th October 2024

Topic: Green Analytical Chemistry using HRMS and/or LC/MS-MS applied to environmental and food analysis

CHAIR: Stephane Bayen

9:00 **Keynote lecture.** Strategies to facilitate high throughput determinations by Solid Phase Microextraction

Janusz Pawliszyn, *University of Waterloo*

9:30 **Keynote lecture.** Sample treatment prior chromatography-MS based detection techniques to determine High Production Volume Chemicals in environmental samples

Rosa Maria Marcé, *Universitat Rovira i Virgili*

10:00 **Keynote lecture.** Use of advanced analytical techniques coupled to mass spectrometry to greening analytical methods for food safety

Luigi Mondello, *Università degli Studi di Messina*

10:30 **Sponsored lecture.** Hydrogen – green renewable source in analytical chemistry applications

Filippo Bonadonna, *LNI SWISSGAS*

11:00 **COFFEE BREAK & POSTER SESSION 2**

CHAIR: Luigi Mondello

Topic: Advances in HRMS instrumentation and their applicability in environmental analysis and food authenticity

11:30 **Keynote lecture.** Liquid Chromatography – Ion Mobility – High Resolution Mass Spectrometry, a new tool in the study of palytoxin-like compounds produced by Ostreopsis cf. Ovata

Encarna Moyano, *University of Barcelona*

12:00 **Keynote lecture.** Flexible micro-tube miniaturized plasma ionization source for the effective ionization of non-easily ionizable pesticides in food with liquid chromatography/mass spectrometry

Juan Francisco García Reyes, *Universidad de Jaén*

12:30 **Keynote lecture.** Latest advances in HRMS to address critical challenges in environmental monitoring and food authenticity issues

Nikolaos S. Thomaidis, *University of Athens*

13:00 **LUNCH BREAK & POSTER SESSION 2**

Topic: Large number of applications in environmental analysis and food authenticity such as water and soil/ sediment, biota and food, like fruits and vegetables, juices and meat

CHAIR: Nikolaos S. Thomaidis

14:00 **Keynote lecture.** Analysis of plastic-related chemical contaminants in food and environmental matrices using targeted and non-targeted screening

Stephane Bayen, *McGill University*

14:30 **Keynote lecture.** Importance of correct chromatography and its common oversights

Amadeo R. Fernández-Alba, *University of Almeria*

15:00 **FLASH POSTER PRESENTATIONS**

CHAIR: Antoni Ginebreda and Damià Barceló

15:30 **Closing lecture.**

How contaminates can affect soil ecosystem services?

Paulo Pereira, *Research Institute for Analytical Instrumentation, INCDO INOE, Cluj-Napoca, Romania*

16:00 Awards and closing ceremony

16:15 End of the workshop

POSTER SESSION 1 (Monday, October 7)

1. Highly Improved Compound Identification in the Non-target Analysis of Wastewater using a Novel HRMS with Simultaneous EI and CI
   Carsten Baessmann, *Bruker Daltonics GmbH & Co KG, Germany*
2. Pesticide residues in the Palancia River Basin: Groundwater vs Surface water bodies
   Jhesibel Chavez Ortiz, *Desertification Research Centre (CIDE) CSIC-GV-UV*
3. Dithiothreitol-Based Protein Equalization in the Context of Multiple Myeloma: Enhancing Proteomic Analysis and Therapeutic Insights
   Inês F. Domingos, *BIOSCOPE Research Group, LAQV-REQUIMTE, Department of Chemistry, NOVA School of Science and Technology, Universidade NOVA de Lisboa; PROTEOMASS Scientific Society*
4. Enhancing Feature Detection and Biomarker Validation through Optimized Proteomics MS-data Normalization Using the Protein Deglycase DJ-7 (PARK-7)
   André Figueiredo, *BIOSCOPE Research Group, LAQV-REQUIMTE, Department of Chemistry, NOVA School of Science and Technology, Universidade NOVA de Lisboa; PROTEOMASS Scientific Society*
5. Improved efficiency of ion trapping time-of-flight mass spectrometry for the analysis of pesticide residues and mycotoxins at trace levels in baby food
   Lorena Manzano Sánchez, *University of Almeria*
6. Migration of additives and other chemicals present conventional plastics and bioplastics used in agriculture using HRMS analyses
   M.J. Martinez Bueno, *University of Almeria*
7. Tracking emerging pollutants from effluents of wastewater treatment plants to supply water using high-resolution mass spectrometry and non-target analysis
   Erik Mestanza-Castelltort, *IDAEA CSIC*
8. Wide screening of urban pollutants and transformation products in runoff water samples using quadrupole-ion trap-Orbitrap high resolution mass spectrometer
   Sergio Santana-Viera, *ONHEALTH, Department of Environmental Chemistry Institute of Environmental Assessment & Water Research (IDAEA), CSIC*
9. Assessment of Environmental Contaminant Exposure in Children Through Urine Analysis Using High-Resolution and Low-Resolution Mass Spectrometry
   Julen Segura Abarrategi, *IDAEA-CSIC*
10. Comprehensive air quality assessment including non-target approaches in primary schools from Spain
    Clara Coscolla, *FISABIO*
11. Intelligent data acquisition metabolomic workflow for biomarker hunting in serum of cattle for early prediction of defective meat: A pilot study of usefulness of liquid biopsy in meat quality assessment
    Pablo Dualde, *Food Safety Research Area. Foundation for the Promotion of Health and Biomedical Research in the Valencian Region, FISABIO-Public Health*
12. Exploring the Organic Composition of Polar and Semi-Polar Compounds in Ultrafine Particles (UFPs) in Barcelona, Spain: Validation and Application of an LC-HRMS Method
    Daniel Gutiérrez-Martín, *Institute of Environmental Assessment and Water Research (IDAEA), CSIC*
13. Machine learning for predicting environmental mobility based on retention behaviour
    Tobias Hulleman, *Queensland Alliance for Environmental Health* Sciences
14. Air Quality of Health Facilities in Spain
    Antonio López, *Foundation for the Promotion of Health and Biomedical Research in the Valencia Region, FISABIO-Public Health*

15. Non-targeted analysis of household dust by UHPLC-HRMS and feature-based molecular networking: Pilot study
    Pablo Miralles, *Foundation for the Promotion of Health and Biomedical Research of the Valencian Region (FISABIO)*
16. New methodological insights on non-target HRMS analytical profiling, spatiotemporal characterization, and modeling of pollution sources affecting an urban aquifer
    Carlos Pérez-López, *Institute of Environmental Assessment and Water Research (IDAEA-CSIC)*
17. Impact of Wastewater Treatment Plants on Surface Water Quality and Organic Contaminant Mixtures
    Cristina Postigo, *Dept. Civil Engineering and Institute of Water Research, Universidad de Granada*
18. Target and non-target analytical methodology to ensure the water quality in reclaimed, river and drinking waters
    Aniol Roca Rodriguez, *Aigües de Barcelona*
19. Application of NH2-UiO-66 MOF for the Dispersive Solid Phase Extraction of Nine PFAS from Environmental Water Samples Followed by High-Resolution Mass Spectrometry Analysis
    Vasileios Alampanos, *Aristotle University of Thessaloniki*
20. Broad screening of food and feed supplements for marine and cyanobacterial toxins
    Elena de Vries, *Wageningen Food Safety Research (WFSR)*
21. SICRIT® analysis of pesticides and environmental pollutants in complex matrices using a standard ESI workflow on Shimadzu LCMS- 9030 QTOF
    Stephane Moreau, *Shimadzu Europa GmbH*
22. Targeted quantitative screening pesticides in food matrices using high resolution DIA spectral library matching
    Neil Loftus, *Shimadzu Corporation*

POSTER SESSION 2 (Tuesday, October 8)

1. Characterization of the non-volatile fraction focusing on the identification of oligomers in a PHA biopolymer packaging using LC-MS/MS
   Carlos Vivanco, *Universidad de Santiago de Compostela (USC)*
2. Development of analytical methods for the determination of lifestyle and dietary biomarkers in municipal wastewater
   Karlo Jambrosic, *Rudjer Boskovic Institute*
3. Simultaneous analysis of pesticides and mycotoxins in primary processed foods: the case of bee pollen
   Maria Antonietta Carrera, *Estación Experimental de Zonas Aridas (EEZA- CSIC)*
4. Pesticide water dynamics and prioritization: The first steps to improve water management strategies in irrigation hydro-agricultural areas
   Adriana Catarino, *Escola Superior Agrária, Instituto Politécnico de Beja; Instituto de Ciências da Terra (ICT), Universidade de Évora; Center for Sci-Tech Research in Earth system and Energy (CREATE), Universidade de Évora; Marine and Environmental Sciences Centre (MARE), Universidade de Évora*
5. Static and dynamic flow biochar systems for the remediation of per- and polyfluoroalkyl substances in contaminated stormwater
   Alberto Celma, *Department of Aquatic Sciences and Assessment, Swedish University of Agricultural Sciences (SLU)*
6. Urban Stormwater Contamination: LC-QTOF-MS Analysis of PMTs in Barcelona
   Filippo Chierchini, *IDAEA-CSIC*
7. Assessing the Presence of Pesticides, Pharmaceuticals and Personal Care Residuals in Water, Soil and Plants in Riyadh Urban Ecosystem, Saudi Arabia
   Mohamed El-Sheikh, *Botany & Microbiology Department, Faculty of Science, Damanhour University, Egypt*
8. Polybrominated diphenyl ethers in household dust of breastfeeding mothers: Exposure levels and health risk assessment
   Esther Fuentes-Ferragud, *Foundation for the Promotion of Health and Biomedical Research in the Valencian Region*
9. Presence and Quantification of Per- and Polyfluoroalkyl Substances (PFAS) in Surface Water of the Miccosukee Reservation and Coastal Environment of Miami, FL, US
   Courtney Heath, *Florida International University*
10. Determination of highly polar anionic pesticides in foods using ion chromatography coupled to tandem mass spectrometry
    Florencia Jesús, *Chemistry and Physics Department. University of Almeria, Agrifood Campus of International Excellence (ceiA3)*
11. Levels and risk assessment of dl-PCBs and dioxins in soils surrounded by cement plants from industrial areas of Colombia and Spain
    Iñaki Lacomba, *Foundation for the Promotion of Health and Biomedical Research in the Valencian Region, FISABIO Public Health*
12. Pesticide Pathways Revealed: Combining Complementary Analytical Methods for Comprehensive Multi-compound Monitoring in Urban and Agricultural Catchments
    Kim Ngoc Tram Luong, *Eawag (Swiss Federal Institute of Aquatic Science and Technology)*
13. First study on the impact of plastic greenhouses on airborne microplastics presence
    Maria Jesús Martinez Bueno, *University of Almeria*

14. Metabolomic profiling for European eel exposed to contaminants of emerging concern
    Alicia Medina Peris, *Food and Environmental Safety Research Group of the University of Valencia (SAMA-UV), Desertification Research Centre (CIDE) CSIC-GV-UV*

15. Use of ceramic passive samplers and HR-MS for the analysis of pharmaceuticals in groundwater samples
    Giacomo Moro, *Department of Environmental Chemistry, IDAEA-CSIC*

16. Identification of bisphenol A diglycidyl ether derivatives after in vitro digestion process by LC-MS/MS
    Lara Pazos-Soto, *FoodChemPack Research Group, Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Pharmacy, University of Santiago de Compostela; Instituto de Materiales (iMATUS), University of Santiago de Compostela*

17. Risk assessment of the exposure to bisphenols, parabens, benzophenone-3 and triclosan in the Spanish adult population by urinary human biomonitoring
    Borja Peris-Camarasa, *Foundation for the Promotion of Health and Biomedical Research in the Valencian Region, FISABIO – Public Health; Department of Analytical Chemistry, University of Valencia*

18. Inexpensive and low-tech sampler to collect time-integrated samples for multi-residue LC-MS analysis of organic contaminants in water
    Cristina Postigo, *Dept Civil Engineering and Institute of Water Research, Universidad de Granada*

19. Suspected and non-targeted analysis of environmental contaminants in water and sediments of L'Albufera Natural Park using liquid chromatography-high resolution mass spectrometry
    Yolanda Soriano, *University of Valencia*

20. Surveillance of commercial frauds in honey sold in the Italian market by isotope ratio mass spectrometry
    Giovanna Esposito, *Istituto Zooprofilattico Sperimentale del Piemonte*

21. Removal and accumulation of pharmaceutical compounds in sediments and biota of a full-scale constructed wetland
    María Eugenia Valdés, *Catalan Institute for Water Research (ICRA-CERCA)*

22. NG(A) CASTORE XL iQ: Advanced On-Site Nitrogen Generation for LC-MS Applications
    Filippo Bonadonna, *LNI Swissgas Srl*

PROGRAM
LECTURES

Analysis of plastic-related chemical contaminants in food and environmental matrices using targeted and non-targeted screening

STEPHANE BAYEN, *McGill University;* **JINGYUN ZHENG,** *McGill University;* **ZHI HAO CHI,** *McGill University;* **ZIYUN XU,** *McGill University;* **LEI TIAN,** *McGill University*

As a result of the widespread use of plastic materials in our societies, a range of chemicals defined as plastic-related chemicals (PRCs) may be disseminated into the environment, contaminate food or accumulate in human and animal tissues. PRCs may correspond to the initial components of the plastics (e.g., monomers, additives and non-intentionally added substances) or their degradation products. PRCs are commonly reported in a variety of foods as a result of the interaction between the food and the packaging material, but they may occur in food as the result of other processes such as environmental and food processing contamination. In many cases, and notably for NIAS, the identity of the compounds leaching from plastics is unknown.

Suspect and non-targeted analyses (NTA), using high resolution mass spectrometry and advanced data processing tools, allow for the rapid characterization of thousands of never-before-studied chemicals in complex matrices. In this talk, key applications of targeted, suspect and non-targeted analyses for PRCs in agri-food systems or as FCMs will be presented. First, methods using LC-QTOF-MS will be introduced for water, agricultural soil and food, and we will show how their application has revealed the contamination of agri-food systems by many previously unreported manmade chemicals, all with plastics as a common origin. In the second part, we will show how we detected unreported bisphenols recently in food in Canada and South Africa, identified thermal labels on packaging and fertilizers as sources of food contamination, and eventually demonstrated their accumulation in human milk from hundreds of mothers in Canada and South Africa. Using NTA, large chemical fingerprints can be recorded for each sample, offering novel perspectives on the exposure to plastic-derived chemical contaminant mixtures.

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Hydrogen - green renewable source in analytical chemistry applications

Filippo Bonadonna, *LNI SWISSGAS*

The constant reduction of helium worldwide, mainly due to its depletion as a natural gas on Earth and the growing demand from both military and nuclear industries, poses a significant issue for analytical chemistry laboratories, which face continuous increases in price and delivery times for this noble gas.

In gas chromatography, replacing the carrier gas from helium to hydrogen represents a sustainable strategy both economically and environmentally. For this purpose, instrument and method adjust-ments are required.

Materials that are in contact with hydrogen must be appropriately selected or inertized due to the reactivity of hydrogen, and the pressure gauges must be correctly calibrated. The optimization of gas chromatographic methods must consider the specific characteristics of hydrogen as a carrier gas, including the verification of the fragmentation process of each analyte in spectrometric terms.

As the required gas flow rate depends on the number of gas chromatographs, the number of FIDs or similar detectors, and the sample injection methods, an adequate generator dimension is required. Furthermore, being an explosive gas, hydrogen generators should not be accumulated.

In this scenario, hydrogen generators using water electrolysis represent a promising strategy to al-low “on-demand” production. Safety criteria for using hydrogen generators make it inappropriate to have a backup with pressurized hydrogen cylinders.

Crucially, the residual moisture in the hydrogen gas must be reduced below 1 ppm, and the resi-dual oxygen below 0.1 ppm. To achieve this, a gas purification system has been developed using high-pressure molecular exclusion (up to 16 bar), coupled with thermal desorption of purification columns.

The electronic development of a centralized control system for multiple units (up to 30) allows for an automatic backup of gas production even during routine or extraordinary maintenance. Pressure in line is reduced to the desired value while maintaining the maximum hydrogen generation pres-sure.

In conclusion, the use of hydrogen generators improves chromatographic resolution, opening a new era based on the development of spectrometric equipment and international standards adjustments in the agro-food, environmental, pharmaceutical, and industrial fields.

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SPE and HPLC-HRMS/MS protocol for multi-residue analysis of chemicals from degraded polyester fibres

Julian Campo, *Environmental & Food Safety Research group of the University of Valencia (SAMA-UV), Desertification Research Centre CIDE (CSIC-UV-GV), Road CV-315 Km 10.7, 46113, Moncada, Valencia, Spain;* **Vasiliki Soursou**, *Environmental & Food Safety Research group of the University of Valencia (SAMA-UV), Desertification Research Centre CIDE (CSIC-UV-GV), Road CV-315 Km 10.7, 46113, Moncada, Valencia, Spain;* **Francesca De Falco**, *School of Biological and Marine Sciences, University of Plymouth, Drake Circus, PL4 8AA Plymouth, Devon, UK;* **Yolanda Picó**, *Environmental & Food Safety Research group of the University of Valencia (SAMA-UV), Desertification Research Centre CIDE (CSIC-UV-GV), Road CV-315 Km 10.7, 46113, Moncada, Valencia, Spain;* **Julián Campo**, *Environmental & Food Safety Research group of the University of Valencia (SAMA-UV), Desertification Research Centre CIDE (CSIC-UV-GV), Road CV-315 Km 10.7, 46113, Moncada, Valencia, Spain;*

Microfibers released from textiles are common in the environment. Synthetic or natural, they undergo degradation that depends on the textile fibre property and on environmental conditions. This process can cause the release of a great variety of chemicals, mainly textile dyes and additives of high toxicity that need to be regulated. A novel approach is proposed to identify and quantify monomers, dyes, and additives in alkaline degradation solution (neutralized), seawater, and similar laboratory-simulated solutions. Thirteen compounds, that belong to common textile fibre released products, were determined by target analysis. Extraction was performed using a solid-phase extraction protocol, followed by UHPLC-HRMS/MS (Orbitrap Exploris 120). Intra-day precision (% RSD, n = 3) ranged from 0.08 to 8.85%, while linearity (R2) values were higher than 0.9980. Good recoveries were obtained for all compounds (%), while matrix effects ranged from -6 to 30%, depending on the analyte. Eleven compounds were detected and quantified in the degradation solution of the two different polyester (PES) fibres, with three of them (benzothiazole, 4-nitrophenol, 2,6-dichloro-4-nitroaniline) being PES type-dependent. The others were found in both PES types. Non-target analysis was, also, applied to detect a wider range of possible leachates, allowing the identification of 55 compounds in positive ionization mode and 24 in negative one.

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High-Resolution Mass Spectrometry and Proteomics Unveils The Capsule Of Time All Vertebrates Share

Jose-Luis Capelo-Martínez, *NOVA Univeristy of Lisbon*

Teeth are highly resistant to environmental degradation, making them invaluable in forensic and archaeological analyses, especially when traditional DNA-based methods fail due to degradation. This study explores the use of mass spectrometry (MS) to analyze dental proteins, allowing for accurate determination of sex and estimation of age. The protein amelogenin, present in tooth enamel, is encoded by both the X (AMELX) and Y (AMELY) chromosomes. Through MS analysis, the presence of AMELY indicates male sex, while its absence signifies female sex. Additionally, the desamidation of proteins such as collagen and amelogenin provides a reliable method for age estimation. Desamidation, the removal of amide groups from asparagine and glutamine, occurs in a predictable manner over time. By measuring these post-translational modifications through MS, it is possible to estimate the age of individuals, particularly when other methods, such as skeletal analysis, are limited. This approach offers a complementary solution in cases where DNA is unavailable or degraded, enhancing forensic and bioarchaeological investigations.

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Importance of correct chromatography and its common oversights

Amadeo R. Fernandez-Alba, *European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables, Ctra. Sacramento S/N, La Cañada de San Urbano, 04120, Almeria, Spain*; **Francisco Garrido**, *Centro de Innovacion Tecnologica CO-EXPHAL, La Mojonera, Almeria, Spain*

The significant expansion in the range of compounds analyzed in modern techniques has led to a common misconception that high-end mass spectrometers can solve all challenges. This has often resulted in the misuse of analytical methodologies, leading to poor performance of the applied methods. In many instances, the importance of proper chromatography is overlooked.

In this presentation, we will emphasize the importance of chromatography in the analysis of highly polar compounds, such as pesticides like glyphosate, and showcase efficient, eco-friendly approaches utilizing microflow chromatography.

Highly polar pesticides, such as glyphosate and its related compounds, are among the most extensively used agrochemicals globally. Despite their widespread application, the monitoring of these residues in food remains challenging, mainly due to the need for specialized analytical methods. These pesticides require highly selective and sensitive techniques for accurate quantitation to ensure regulatory compliance and food safety. Ion chromatography, coupled with tandem mass spectrometry (IC-MS/MS), has become a powerful technique for the direct analysis of highly polar pesticides. This combination enhances the detection capabilities, providing low quantitation limits critical for the accurate monitoring of residues. In this study, a method for the direct determination of 13 target highly polar anionic pesticides using IC-MS/MS is presented.

The development of green analytical methods is essential, especially considering the millions of pesticide analyses performed annually in the EU, which generate tons of organic waste, negatively impacting the environment and increasing analytical costs. In this context, the introduction of microflow techniques is of great interest, as they can reduce organic waste by up to sixfold without compromising the quality of the results. This represents a clear objective for the future of routine laboratories.

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Chemical Exposome, Ultrafine Particles, and Glioblastoma: A New Perspective

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Glioblastomas (GBM) are the most common primary brain tumors in adults, but their causes remain largely unknown. Environmental exposures are suspected to play a role; however, the data is limited due to analytical challenges and the difficulty of obtaining brain samples for cohort studies. This study investigates the chemical exposome in GBM, with a focus on an underexplored source: Ultrafine particles (UFPs), the smallest component of air particulate matter. UFPs are known to penetrate the brain and transport hazardous substances, and previous epidemiological studies suggest a potential link between ambient air UFPs and disease incidence.

This study leveraged the Bellvitge Glioma Cohort (BGC) from HUB-IDIBELL, a unique retrospective cohort of 400 patients with high-quality histopathology brain tumor samples collected from 2005 to present. Additionally, non-tumor brain samples from autopsies were analyzed. In this proof-of-concept study, 33 GBM samples and 20 non-tumoral brain samples were examined using a comprehensive HRMS-based wide-scope target and nontarget analysis. We also analyzed 20 UFP samples from the metropolitan area of Barcelona, where cohort patients lived.

A total of 49 exogenous chemicals, including various industrial compounds, were identified. While chemical profiles in GBM differed significantly from those in healthy brain tissue, no direct link to disease onset could be established. However, the results underscore the need for thorough assessments of potential chemical contributions to GBM. Notably, several air pollutants linked to road traffic, such as tire additives, were detected, supporting the hypothesis that hazardous chemicals may access the brain via the olfactory pathway. Our UFP analysis from the Barcelona area revealed over 20,000 features, including chemicals previously identified in the brain (e.g., tire additives), further substantiating this hypothesis.

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Flexible micro-tube miniaturized plasma ionization source for the effective ionization of non-easily ionizable pesticides in food with liquid chromatography/mass spectrometry

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Dielectric barrier discharge ionization (DBDI) has gained attraction in recent years as a versatile ionization method available in different formats (ambient ionization probes, GC-MS and LC-MS) intended for many applications including ambient mass spectrometry imaging, environmental analysis, biological and pharmaceutical and food safety. In this work, we have studied the potential of flexible microtube plasma (FuTP) as ionization source for the liquid chromatography high-resolution mass spectrometry detection of non-easily ionizable pesticides (viz. nonpolar and non-ionizable by acid/basic moieties). Phthalimide-related compounds such as dicofol, dinocap, o-phenylphenol, captan, captafol, folpet and their metabolites were studied. Dielectric barrier discharge ionization (DBDI) was examined using two electrode configurations, including the miniaturized one based on a single high-voltage (HV) electrode and a virtual ground electrode configuration (FuTP), and also the two-ring electrode DBDI configuration. Different ionization pathways were observed to ionize these challenging, non-easily ionizable nonpolar compounds, involving nucleophilic substitutions and proton abstraction, with subtle differences in the spectra obtained compared with APCI. An average sensitivity increase of 5-fold was attained compared with the standard APCI source. In addition, more tolerance with matrix effects was observed in both DBDI sources. The importance of the data reported is not just limited to the sensitivity enhancement compared to APCI, but, more notably, to the ability to effectively ionize nonpolar, late-eluting (in reverse-phase chromatography) non-ionizable compounds. Besides o-phenylphenol ([M-H]-), all the parent species were efficiently ionized through different mechanisms involving bond cleavages through the effect of plasma reagent species or its combination with thermal degradation and subsequent ionization. This tool can be used to figure out overlooked nonpolar compounds in different environmental samples of societal interest through non-target screening (NTS) strategies.

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Source apportioning of wastewater intrusions: merging Non-target Analysis and traditional water quality parameter datasets. A South Florida case study

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Introduction of novel analytical chemistry technologies such as Non-Target Analysis (NTA) have moved the needle outside of the chemist comfort zone. Sample preparation and chromatography separations have become secondary to computerized tools like peak deconvolution and the benefits of FTMS. Features, chemical formulae, in-silico fragmentation and other discriminating tools are now available at the click of a mouse button. Nevertheless, the wealth of information produced by these new workflows are not exempt of challenges in both the computer and human domain. In this presentation we explore the fusion of NTA results with other quite valuable environmental data often gathered in large monitoring efforts including nutrients, inorganic tracers, metals and other basic water quality parameters. Biscayne Bay, the economic driver of South Florida tourism, is becoming impaired due to decades of chronic eutrophication from urban sources. Benthic habitat losses, recurring fish kills, and algal blooms have prompted the implementation of a myriad of projects targeted to reduce Phosphorous loadings, the limiting nutrient for the Bay. In this work we use a combination of NTA workflows, specific target analysis of organic and inorganic tracers, nutrients and other basic water quality parameters to provide a clearer identification of wastewater sources contributing the significant loadings of “P” to the main bay tributaries. The NTA workflow is used to segregate water sources, relationships between specific tentatively identified compounds (herbicides, surfactants), organic tracers (Splenda and caffeine) and inorganic tracers (zinc and copper) are used to isolate specific parts of the watershed where projects need to be implemented. Wagner Creek in the Miami River and the North Spur Canal in the Little River are good examples where efforts in reducing wastewater intrusions will result in significant reduction of “P” loadings.

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Mass spectrometry enabled water-based early warning systems for environmental and public health protection: an importance of biochemical profiling in longitudinal studies

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WBE is now established as a complimentary tool in public health surveillance (pathogen and illicit drug tracking). WBE aims to quantify community exposure, discover exposure-outcome associations, and trigger policy, technological or societal intervention strategies with the overarching aim of exposure prevention and public health promotion. As discussed in our recent paper (Kasprzyk-Hordern et al. 2023), to achieve WBE's full potential, the following key aspects require further action: (1) Integration of WBE-HBM (human biomonitoring) initiatives that provide comprehensive community-individual multichemical exposure assessment. (2) Global WBE monitoring campaigns to provide much needed data on exposure in low- and middle-income countries (LMICs) and fill in the gaps in knowledge especially in the underrepresented highly urbanised as well as rural settings in LMICs. (3) Combining WBE with One Health actions to enable effective interventions. (4) Advancements in new analytical tools and methodologies for WBE progression to enable biomarker selection for exposure studies, and to provide sensitive and selective multiresidue analysis for trace multi-biomarker quantification in a complex wastewater matrix. This talk will focus on utilisation of mass spectrometry in water mining for wide-ranging biochemical markers with particular focus on the need for comprehensive spatiotemporal profiling over large geographical areas and longitudinal studies capturing seasonal impacts to provide a truly transformative tool for One Health interventions.

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Applying a novel component detection algorithm to untargeted screening

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Introduction: To accelerate small molecule component detection in complex mixtures a novel algorithm has been developed for high resolution accurate mass Q-TOF data sets. As with other techniques, the algorithm locates ions that behave as a recognised chromatographic feature (ion intensities rise and fall in abundance in a covariant manner). This algorithm was evaluated using a series of HRAM Q-TOF data sets including food safety screening.

Methods: Unknown samples and calibration samples were prepared using a standard QuEChERS sample preparation method. Reverse phase liquid chromatography was used (Shim-pack Velox Biphenyl) 17 min analysis time per sample. LC-MS/MS Q-TOF measurement (LCMS-9050, Shimadzu Corporation, Japan) was performed by full scan MS (m/z 140-925, 100 msec scan time) with DIA MS/MS scans resulting in a 1 second cycle time.

The component detection algorithm used default processing parameters with a spectral intensity threshold set to low.

Results: The high resolution LC-MS/MS acquisition method was designed to quantitate a primary target list of 317 pesticides and to report detected pesticides with high reporting confidence using precursor mass accuracy, isotope pattern matching and retention time together with DIA-MS/MS library verification. The MS and DIA-MS/MS method was also capable of retrospective analysis and to explore the potential of this approach a secondary target list of pesticides was included in the post-acquisition processing method resulting in a total of 486 pesticides. For example, in a nectarine extract, the secondary screening list detected high levels of pyrimethanil which is not routinely quantified, and in grape extracts the fungicides boscalid, fluopyram, penconazole and pyrimethanil were detected with high reporting confidence.

This method highlights the need for nonbiased scope testing using full scan untargeted acquisition, allowing retrospective analysis of pesticides not included a priori but then revised in a post-targeted manner enabling expanded search lists even to other potential food-borne hazards.

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Sample treatment prior chromatography-MS based detection techniques to determine High Production Volume Chemicals in environmental samples

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Among organic contaminants, high production volume chemicals (HPVC) are a group of increasing concern. These compounds are widely used across the world. According to the Organisation for Economic Co-operation and Development, HPVC include chemicals that are produced or imported at levels greater than 1,000 tons per year in at least one member country. Due to their extensive use, HPVC can be found in different environmental compartments and their presence has been confirmed in several samples. The occurrence of some of these compounds poses potential risks to human health through exposure via ingestion, inhalation or dermic contact. Therefore, it is essential to evaluate their presence in the environmental samples.

The large number of chemicals classified as HPVC involves the use of powerful chromatographic techniques and mass spectrometry-based detection for their determination. Both gas chromatography (GC) and liquid chromatography (LC) are used depending on the characteristics of the HPVC. For example, phthalates or benzothiazoles can be determined using either LC or GC, while musk fragrances have to be determined by GC. Due to the complexity of environment samples, a sample treatment technique is required, and a wide range of techniques can be used to this purpose.

In this presentation, different analytical methods will be discussed for the determination of a broad group of HPVC, including organophosphate esters, phthalate esters, benzotriazoles, benzothiazoles, benzosulfonamides, synthetic musk fragrances, UV-stabilizers and phenolic antioxidants in different environmental samples such as air, dust, water, and biota. Given the diversity of the environmental samples, different extraction techniques will be described, highlighting the use of solid-phase extraction, pressurised liquid extraction and QuEChERS. The developed methods will be applied to assess of the occurrence of these HPVC in the different types of environmental samples.

Acknowledgements

The author would like to thank the Ministerio de Ciencia e Innovación, the Agencia Estatal de Investigación, MCIN/AEI/10.13039/501100011033 and the European Regional Development Fund (ERDF) under project PID2020-114587GB-I00

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Application of a metabolomic approach based on the use of high-resolution mass spectrometry for the discrimination of agricultural practices

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The lack of chemical markers capable of distinguishing between different agricultural practices makes the organic market susceptible to food fraud. To address this issue, this study employs a metabolomics approach using ultra-high-performance liquid chromatography coupled with high-resolution mass spectrometry (UHPLC-HRMS) and multivariate statistical analysis to identify differences among crops produced through conventional, organic, and simulated fraudulent organic practices. Specifically, the impact of small applications of synthetic fertilizers and phytosanitary products on the metabolism of tomato (Solanum lycopersicum) crops was examined. Potential marker compounds were identified using Compound DiscovererTM 3.2 software (Thermo Scientific), by evaluating their MS and MS2 spectra, and utilizing libraries, spectral databases, and in silico fragmentation tools. Finally, the classification of confidence levels described by Schymanski et al. [1] was utilized to identify the compounds, owing to its high number of citations and significant impact within the scientific community.

The approach allowed for the discrimination of different agricultural practices evaluated and the differentiation of genuinely organic crops (T1) from those fraudulently managed as organic (T2 and T3), which had been treated with synthetic fertilizers. A total of 14 bioactive compounds were identified as potential markers of the production method, with levels strongly correlated to the type of fertilization applied. These compounds included six carotenoids, three sterols, two vitamins, two phospholipids, and one carboxylic acid. The bioactive compounds identified in this study are of particular interest due to their higher concentrations in organic tomatoes. This significance is twofold. Firstly, it highlights the impact of small applications of synthetic fertilizers on organic crops. Secondly, some of these compounds, such as vitamins, carotenoids, and sterols, offer notable nutritional benefits for human health.

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Use of advanced analytical techniques coupled to mass spectrometry to greening analytical methods for food safety

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In the evolving field of "Green Chemistry," current trends emphasize the simplification and acceleration of analytical methods, alongside a significant reduction in the use of organic solvents. The integration of advanced analytical techniques with tandem mass spectrometry (MS) has streamlined sample preparation, minimizing the need for solvents and adsorbent materials, thereby enhancing operator safety. Additionally, the combination of liquid and gas chromatography techniques enables the development of fully automated analytical methods. This lecture will showcase how these advanced analytical approaches couple to MS detectors facilitate the development of rapid, accurate, and robust methods for detecting various food contaminants—such as pesticides, phthalates, and polycyclic aromatic hydrocarbons—complying with the legal limits established by the European Community.

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Liquid Chromatography–Ion Mobility–High Resolution Mass Spectrometry, a new tool in the study of palytoxin-like compounds produced by Ostreopsis cf. Ovata

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Palytoxin (PLTX) and its analogues produced by Ostreopsis cf. ovata represent a concerning health issue. These compounds are marine toxins that act as powerful vasoconstrictors and are often responsible for seafood poisoning. PLTX analogues contain many chiral centres leading to numerous isomers, making their separation and analysis difficult by both mass spectrometry and liquid chromatography. In this work, the ion mobility spectrometry (IMS) behaviour of this family of compounds is explored for the first time to overcome these analytical challenges. Drift tube (DTIMS) and traveling wave (TWIMS) ion mobility spectrometry were used and the results were compared. Moreover, to justify some unexpected results, trapped ion mobility spectrometry (TIMS) and computational studies of molecular dynamics simulation were performed as complementary techniques. The higher resolution provided by TIMS allowed us to distinguish isomeric ions generated in the electrospray source by losing n-units of water molecules from different sites in the toxin structure. Computational studies provided a theoretical basis for understanding the ion mobility behaviour of triply charged calcium and sodium adduct ions and indicated a possible folded conformation of these molecules. DT-CCS-N2 values were obtained for PLTXstd, as well as for ovatoxin-a and ovatoxin-b present in the extracts of microalgae samples collected in Sant Andreu de Llavaneres (Barcelona, Spain). These results were comparable (ΔCCSs < 2%) to those measured on the TWIMS instrument when calibrated using PLTXstd. In this work, a list of 102 CCS values calculated from DTIMS and TWIMS data were obtained for adducts and fragment ions observed in the mass spectra of PLTX analogues (PLTX standard, ovatoxin-a and ovatoxin-b). These values can serve as reference values and be included in databases to aid in the detection of these toxins in complex samples.

Acknowledgments: The authors thank the different financing agencies that supported the study. FI-SDUR2020-00254 and 2021 SGR 00281 (AGAUR, Government of Catalonia); PID2021-122743NB-I00 (Ministry of Science and Innovation, Spain); Water Research Institute (IdRA, University of Barcelona); CoCliME (ERA4CS, ERA-NET); ERC-2019-CoG-863934-GlycoSpec (European Research Council).

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Strategies to facilitate high throughput determinations by Solid Phase Microextraction

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Recent world-wide efforts towards implementation of sustainable technologies will have impact on future practice of analytical chemistry including sampling and sample preparation steps. The current sample preparation techniques used in extraction of compound of interests from complex samples, such as animal tissue, food and environmental matrices involve time-consuming procedures that are not always effective at minimizing matrix interferences. These methods often involve the use of large amounts of organic solvents which lead to hazardous waste. Moreover, they lack automation and high-throughput capabilities.

Development of devices to facilitate chemical determination of organic compounds in complex matrices involves two main directions. One is to design sensors, which are simple portable on-site devices performing well for real samples, even in-vivo. However they are typically limited to single component determination with selectivity determined by membrane and/or readout characteristics. The other approach is to use hyphenated separation with mass spectrometry technologies such as GC/MS and LC/MS which allow multicomponent determination including comprehensive characterization of the composition of the complex samples facilitated by recent rapid development in mass spectrometry as well as multidimensional approaches. The main limitation of this direction is demand placed on sample preparation for complex samples to deliver good analytical performance. Miniaturized, on-site versions of the instruments are already available or being constructed, so the size and portability are addressed. What missing are effective sampling/ sample preparation tools.

To address the above challenges we have been proposing to combine sensor design strategy offering good isolation selectivity with the chromatography/ spectrometry technologies facilitating multicomponent characterization with high accuracy, reproductivity and precision. For this approach to be effective the "sensor" would need to accumulate enough analyte during sampling to facilitate sensitive determinations. To accomplish this task we have been designing matrix compatible high analyte capacity probes with flexible shapes and morphologies to facilitate GC/MS, LC/MS or direct mass spectrometry readout. The probes consist of thin matrix compatible coating of extraction phase containing sorbent particles and the binder forming the protection layer preventing direct contact of the particles with the matrix while also facilitating adhesion of the particles to the support. The designed probes perform non-exhaustive sampling in similar way as sensor does, but for much longer times to allow accumulation of sufficient amount of analytes required for sensitive detection. Such chemical biopsy probes selectively enrich smaller molecules which are able to diffuse though the protection layer formed by the binder, while leaving investigated system intact and therefore eliminating effect of macromolecules present in the sample on the measurement quality. After completion of the sampling/sample preparation step the probes are introduced to analytical instrument where the isolated components via thermal or solvent desorption.

Such flexible Solid Phase Microextraction (SPME) approach has been applied to wide range of the applications demonstrating superior performance compared to traditional approaches developed in the past for complex sample determinations. In addition to better analytical performance it has much better sustainability characteristics by replacing or minimizing use of organic solvents making it suitable tool for future generations of chemists. The main challenge in adoption of SPME approach is that the sampling process as in case of sensors in non-exhaustive, while standard technologies utilize exhaustive approaches evaluating their performance based on recovery of spikes. This situation creates some resistance in adoption of the SPME technologies by many regulatory agencies. However despite this challenge the technology is being used in many areas where there no good solutions exist. Many applications for different scientific disciplines are also fueled by its “green” features. During the talk several examples of SPME designs will be given addressing important world challenges, so the audience can appreciate impact of this chemical sensing approach.

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How contaminates can affect soil ecosystem services?

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Ecosystem services (ES) are understood as the goods the ecosystems supply to the people. Soils supply a vast number of regulating (e.g., water purification, flood and erosion regulation) and provisioning (e.g., food, raw material) ES. Human activities, such as agriculture and urbanization harm soil functions and ES. It is well known that high amounts of contaminants (e.g., minor and microelements, organic pollutants, pharmaceuticals) negatively impact soil microbiology, such as reduced microbial biomass, species diversity, enzyme activity or respiration. On the other hand, it is also known that microbes can bio-degrade contaminants. Contaminants can also indirectly affect soil physical properties and increase degradation. For instance, soils heavily polluted are less suitable to be colonized by vegetation. This has implications for soil cover and the vulnerability to erosion, increased flood impacts or reduced soil capacity to filter water. Although this is well known, more studies need to be developed on the effects of soil contaminants on ES. This presentation will assess the direct and indirect links between pollutants and ES.

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Tracking organic pollutants occurrence and sources in urban groundwaters using LC-HRMS

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Groundwater (GW) is an essential water resource for meeting the world's water needs for industrial, agricultural, and drinking uses. However, GW may be polluted by their recharge sources, such as stormwater, surface water, and leaking from the sewer system. A myriad of contaminants such as pharmaceuticals, personal care products, as well as artificial sweeteners, and industrial chemicals may end up in urban GW. The Directive 2006/118/EC amendment on GW quality and protection was published in October 2022. Although it includes persistent organic substances such as carbamazepine, sulfamethoxazole and 24 PFAS other persistent and polar compounds are not included yet. In our study, urban water from Barcelona was analyzed to determine 127 organic compounds including very polar and very mobile analytes (vPvM) used in various applications such as pharmaceuticals, industrial chemicals, and tire wear substances, using an evaporative enrichment methodology combined with two LC columns and their detection with Orbitrap-HRMS. Special attention was paid to 31 vPvM, whose analysis is particularly challenging. Although the modified C18 column Acquity HSST3 is designed to improve the retention of polar analytes; vPvM still suffer from weak retention and poor peak shape. Switching to the HILIC column Acquity BEH Amide allows for drastic improvement in both retention and peak shape. The analytical protocol was successfully applied to real samples from the four matrices determining the presence of 127 analytes and their distribution across several urban waters such as sewer, stormwater and river waters. A general trend was observed in the results: as polarity (log D) decreases, and mobility increases, the higher detection frequencies and concentrations were found. Considering the number of variables involved and the large amount of data generated, a multivariate analytical method, principal component analysis, was employed. Multivariate statistical analysis (PCAs and Mixing Ratios Calculations) allowed to capture differences between sources. PCA conducted using only vPvM compounds was able to capture the differences between stormwater, sewer, surface and groundwater clusters. Several vPvM correlated with stormwater points. The study highlighted a clear need for updating existing monitoring schemes to include vPvM in all matrices.

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Chlorination of Emerging Contaminants for Application in Potable Wastewater Reuse: Disinfection By-Product Formation, Estrogen Activity, and Cytotoxicity

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With increasing water scarcity worldwide, many drinking water utilities are considering potable reuse of wastewater as a source of drinking water. However, not all chemicals are removed in conventional wastewater treatment, and disinfection byproducts (DBPs) can form from these contaminants when disinfectants are applied during or after reuse treatment, especially if applied upstream of advanced treatment processes to control biofouling. We investigated the chlorination of seven priority emerging contaminants (17β-estradiol, estrone, 17α-ethinylestradiol, bisphenol A (BPA), diclofenac, p-nonylphenol, and triclosan) in ultrapure water, and we also investigated the impact of chlorination on real samples from different treatment stages of an advanced reuse plant to evaluate the role of chlorination on the associated cytotoxicity and estrogenicity. Many DBPs were tentatively identified via liquid chromatography (LC)- and gas chromatography (GC)-high resolution mass spectrometry, including 28 not previously reported. These encompassed chlorinated, brominated, and oxidized analogs of the parent compounds, as well as smaller halogenated molecules. Chlorinated BPA was the least cytotoxic of the DBPs formed, but was highly estrogenic, whereas chlorinated hormones were highly cytotoxic. Estrogenicity decreased by ~4-6 orders of magnitude for 17β-estradiol and estrone following chlorination, but increased 2 orders of magnitude for diclofenac. Estrogenicity of chlorinated BPA and p-nonylphenol were ~50% of the natural/synthetic hormones.

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The potential of wastewater-based epidemiology for the assessment of lifestyle and dietary habits

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Wastewater-based epidemiology is a very useful complementary approach for estimating illicit drug use at the population level. In recent years, it has also been used to assess other lifestyle habits, such as alcohol, nicotine and legal drug use [1]. On the other hand, its potential in the assessment of dietary habits has only been investigated in a few studies [2,3].

The present work aims to fill this gap by developing analytical methods for the determination of several classes of lifestyle and dietary biomarkers in raw municipal wastewater. In addition to biomarkers of alcohol, nicotine/tobacco and caffeine, the suitability of a broader range of dietary biomarkers will be investigated, focusing on specific compounds from plant foods that may be good indicators of healthy dietary habits and health outcomes, such as lignans, phenylethanoids and various classes of flavonoids. The study will also include major representatives of artificial sweeteners, as well as some vitamins and biomarkers from animal foods.

The target compounds will be analyzed by ultra-high performance liquid chromatography – tandem mass spectrometry (UHPLC-MS/MS). Some compounds, such as ethyl sulfate, the biomarker of alcohol (ethanol), will be injected directly, but in most cases solid-phase extraction will be used. The suitability of the biomarkers will be assessed by stability tests in real wastewater and in a model sewer system, and the developed methods will be used to assess spatial and temporal differences in lifestyle and dietary habits in six Croatian regions. The preliminary results, including the selection of potential biomarkers, the development of the LC-MS/MS methods, the optimization of the solid-phase extraction procedures and the analysis of real wastewater samples from the city of Zagreb, will be presented together with the future work.

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Acknowledgments: This work was supported by the Croatian Science Foundation under the project number HRZZ-IP-2022-10-5332.

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Combining Target and Non-Targeted Approaches for PFAS characterization in recreational fisheries

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Per-and polyfluoroalkyl substances (PFAS) are a group of synthetic, highly fluorinated, and emerging contaminants that are reportedly used for both industrial applications and consumer products. Florida is the "Fishing Capital of the World" with Biscayne Bay supporting a high degree of biodiversity and habitat for a variety of sport fishes and other marine life, and also counting with great weather, therefore allowing for year-round fishing activities. Several PFAS are shown to be persistent and bioaccumulative in marine organisms, posing human and ecological health concerns. Although some PFAS (such as PFOA and PFOS) have been regulated and banned from use, new fluorinated compounds have been produced to serve as replacements for legacy PFAS. Furthermore, there is limited information on new chemicals, their precursors, as well as metabolites, and degradants in the environment. Although targeted analysis is highly sensitivity and has been used for the identification and quantification of legacy and some emerging PFAS contaminants, there are > 10,000 PFAS listed in the U.S EPA Master List in global circulation, for which authentic reference standards are not commercially available. Hence application of high-resolution mass spectrometry (HRMS) becomes crucial for the comprehensive characterization and identification of novel and/or not routinely monitored PFAS compounds in the environment.

In this research, our primary aim was to characterize PFAS in recreational fisheries by targeted and non-targeted analysis (NTA), improving food safety by proving better understanding of how PFAS get into human diet and identifying PFAS that should be considered in risks assessments. Based on PFAS surface water concentrations, we were able to estimate PFAS bioaccumulation potentials in blackfin tuna (Thunnus atlanticus) and lobsters (Homarus americanus), that are commonly consumed among South Florida's residents. An alkaline based extraction followed by dispersive solid phase extraction (dSPE) was implemented for extraction and clean-up step, respectively. An NTA workflow was developed for the holistic screening of PFAS in the tissue samples using a liquid chromatography (LC)- Q-Exactive Orbitrap system followed by data processing and identification using Compound Discoverer v 3.3. As a complementary approach, LC-TIMS-qTOF was applied for assessment of unknown PFAS, in which molecular trendlines were generated for PFAS based on mass and structural relationships. Targeted 30 PFAS were detected in at least one sample except for N-EtFOSAA in lobster which was below the method detection limit. ΣPFAS body burden ranged from 0.15 - 3.40 ng/g ww in blackfin tuna samples and 0.37- 5.15 ng/g ww in lobster samples, respectively. Wilcoxon rank paired test ($\alpha = 0.05$) shows that there was statistical significance ($\rho < 0.05$) of ΣPFAS between species. Bioaccumulation factors (BAF) suggest an increasing trend in PFAS classes (PFCAs <PFSAs < FTSs), with higher BAF observed in tuna species compared to lobster. Long chain PFESAs and FASAA were reported higher in lobster in comparison to tuna species due to their bioavailability through sediment-sorption interactions. Hazard risk (HR) based on available toxicological data of few PFAS suggests low risk to human health based on the consumption of the species studied, however, the risk to contaminant exposure might be underestimated. Multidimensional data such as high mass accuracy, CCS ion mobility values and Kendrick mass analysis processed on MetaboScape data analysis tool increased confidence for tentatively identified untargeted PFAS in tissue samples.

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Non-Target HRMS analysis using the ROIMCR chemometrics method

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Non-target analysis of LC-HRMS environmental omic datasets demands highly extensive processing of a vast amount of (big) data. Different LC-MS data analysis packages have been developed in the last few years to facilitate this analysis. However, most of these strategies involve the chromatographic alignment of every analytical “feature” (i.e., chromatographic peak) defined by a single unique m/z measurement. Alternative data analysis strategies applicable to HRMS chromatographic data, addressing properly these issues, are still a challenge in different environmental and omics fields.

Here, we present the ROIMCR approach [1] as an alternative methodology to: i) filter and compress massive LC-HRMS non-target analytical datasets while transforming their original uneven data structure into a regular data matrix of selected MS signals, without losing their relevant chemical information through the search of the Regions Of Interest (ROIs) in the m/z domain, ii)component resolution (componentization) of the contributing chemical constituents, defined by their elution and mass spectra profiles without previous peak alignment nor peak shaping using the Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS), chemometrics method [2,3] iii) filtering, identification and annotation of these chemical constituents, using the recently developed Sygsel [4] and MSident [5] spectral data treatments methods.

In this presentation, these different chemometrics methods will be applied to the analysis of: a) PFAs mixtures in bird egg samples by LC-HRMS/MS [2], b) mixtures of aminoacids and other metabolites in biological samples by LC-HRMS/MS in positive and negative ionization acquisition modes [3], and c) changes in the rhizosphere metabolome profile of wastewater-irrigated lettuces using non-target LC-HR-MS/MS [6]

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Latest advances in HRMS to address critical challenges in environmental monitoring and food authenticity issues

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In recent decades, environmental pollution and food fraud have emerged as major threats to human health and ecosystems. Environmental monitoring is increasingly challenged by the presence of chemicals of emerging concern (CECs), often with unknown toxicological properties, necessitating comprehensive analysis beyond traditional targets. The European Commission's "Chemicals Strategy for Sustainability" and resolutions from the UN Environment Assembly highlight the global urgency of these issues. In-depth characterization of environmental samples is essential, not only for pollution prevention and sustainable water resource management, but also for ensuring the safety and authenticity of our food supply chain. Economically motivated food fraud, frequently involving the substitution of ingredients with cheaper alternatives, demands robust analytical methods for detection and mitigation. Compounding these concerns, food safety is further compromised by factors, such as environmental contamination, climate change, and intensive animal farming practices. Establishing stringent quality standards, effective mitigation measures, and comprehensive monitoring systems for both environmental and food contaminants is paramount to safeguarding public health.

High-Resolution Mass Spectrometry (HRMS) has emerged as a transformative tool in addressing the complexities of environmental and food analysis. Leveraging the unique ability of HRMS instruments to record a theoretically unlimited number of compounds in full-scan mode, holistic screening strategies have been developed, utilizing MS/MS databases and advanced software for confident identification of known, unexpected, and even unknown compounds, with the added benefit of retrospective data mining. Recent advancements have led to integrated HRMS-based screening workflows (target, suspect, and non-target), emphasizing high analytical performance and comprehensive compound identification across diverse domains. These approaches have significantly improved compound detection and identification, enabling thorough sample characterization, the discovery of characteristic markers, and the detection of food adulteration. Notably, several sophisticated software tools have been developed to support non-target screening (NTS), including Quantitative Structure-Retention Relationship (QSRR) models for retention time prediction [1], Retention Time Indices (RTI) for inter-laboratory harmonization [2], and pH-dependent elution patterns for unknown identification [3]. Additionally, machine learning models aid in selecting the most appropriate instrumental method (LC-HRMS, GC-HRMS, or both) [4], while novel semi-quantification methods estimate concentrations without reference standards [5,6]. Innovative trend analysis tools have unveiled crucial patterns in chemical occurrence and fate [7,8,9], and a harmonized identification scoring system for LC-HRMS-based NTS has been proposed [10]. Furthermore, the integration of Trapped Ion Mobility Spectrometry (TIMS) into LC-HRMS platforms has shown promise in tackling complex challenges, such as differentiating isomers in olive oil for authenticity assessment [11] and identifying emerging PFAS contaminants in environmental matrices, leveraging improved separation and collision cross section values for enhanced confidence. Additionally, recent advances in fast-screening techniques, such as Matrix-Assisted Laser Desorption Ionization-Time of Flight Mass Spectrometry (MALDI-TOFMS) and Direct Analysis in Real Time - High Resolution Mass Spectrometry (DART-HRMS) have spurred the development of novel omics-based methods for comprehensive sample characterization, including holistic proteomics- and lipidomics-based workflows for the rapid detection of adulteration and contamination in protected designation of origin (PDO) food products, as PDO feta cheese [12].

Overall, the ongoing evolution of HRMS-based technologies, encompassing comprehensive analytical workflows, sophisticated chemometric tools, and cutting-edge instrumentation, represents a paradigm shift in our ability to address the complex challenges facing food safety and environmental monitoring. These advancements offer unprecedented potential for protecting the food chain, safeguarding the environment, and ultimately, promoting human health.

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Efficient Data Prioritization for Identification and Semi-Quantification in Nontarget Screening of PFAS

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Per- and polyfluoroalkyl substances (PFAS) are ubiquitous contaminants posing adverse effects to humans and the environment. 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. Target analysis is not feasible for a comprehensive characterization as only a few PFAS can be quantified and hence the total PFAS burden is often drastically underestimated. Thus, current analytical trends emphasize non-target screening (NTS) and organofluorine sum parameters for a higher PFAS coverage.

In this work a focus will be on promising workflows for data prioritization, identification and semi-quantification of PFAS and potential transformation products in environmental samples by LC-HRMS. In the first part, PFAS prioritization of LC-HRMS data of soil and sediment samples is demonstrated. For example, data reduction by 90 to 95% was achieved for more than 12,000 features by the carbon-normalized mass defect vs. mass plot (MD/C-m/C). This step resulted in much less false positives in a preceding Kendrick mass analysis with 26 homologue series with CF2-repeating units rather than 74 series without suitable prioritization. The most promising steps of the whole NTS workflow are accessible from the newly developed open-source code PFAScreen, which further includes mass defect filtering, the use of mass fragment differences, diagnostic fragments, and matches with suspect lists for further data identification. In the second part we used prioritized NTS features from soils, sediments, and ashes from different locations in Europe and correlated them with the sum parameter extractable organic fluorine (EOF). The results show a high correlation between quantitative EOF data with the prioritized number of feature number as well as with the total peak area of prioritized features, while commonly applied mass defect ranges for filtering showed much weaker correlation with EOF. The possibilities and limitations of the presented approaches are discussed in light of the wide range of PFAS occurring in environmental samples and products.

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Prince Sultan Bin Abdulaziz International Prize for Water

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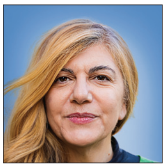
Creativity Prize

Creativity Prize

[1] The team of Maria Cristina Rulli (Polytechnic of Milan, Italy) and Paolo D'Odorico (University of California, Berkeley, USA)

for spearheading novel analyses of the water-energy-food nexus that describe how numerous complex factors interact, providing for better freshwater stewardship in a changing, globalised world.


Maria Cristina Rulli


Paolo D'Odorico

[2] The team of Zhiguo He (Zhejiang University, China)

for developing working, versatile soft robots with unprecedented manoeuvrability that have the capacity for numerous underwater research and monitoring applications. Team members include: Pengcheng Jiao and Yang Yang.


Zhiguo He

Surface Water Prize

Surface Water Prize

Qiuhua Liang (Loughborough University, UK) and his team

for developing innovative, open-source, multi-GPU hydrodynamic models to support real-time flood forecasting at high temporal-spatial resolutions. Team members include: Huili Chen, Xiaodong Ming, Xilin Xia, Yan Xiong and Jiaheng Zhao.


Qiuhua Liang

Groundwater Prize

Groundwater Prize

Chunmiao Zheng (EIT, Ningbo, China) and his team

for powerful modelling tools to understand groundwater processes and manage groundwater resources under diverse eco-hydrological and climatic conditions, considering environmental and socioeconomic factors at local and national scales.

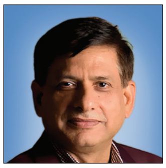

Chunmiao Zheng

Alternative Water Resources Prize

Alternative Water Resources Prize

Virender K. Sharma (Texas A&M University, USA) and his team

for the effective removal of antibiotics and pharmaceuticals from wastewater through advanced oxidative processes by activated ferrate, which work at high, even enhanced, efficiency in water containing commonly occurring natural organic matter. Team members include: Ching-Hua Huang, Chetan Jinadatha and Radek Zbořil.


Virender K. Sharma

Water Management & Protection Prize

Water Management & Protection Prize

Joseph Hun-wei Lee (Macau University of Science & Technology, China)

for developing unique and highly effective hydro-environmental modelling systems for the sustainable water management of smart cities.


Joseph Hun-wei Lee

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ORAL COMMUNICATIONS

Detecting PFAS beyond the Current Regulative Request: a Comprehensive Overview of the Contamination in Water by UPHLC-Ion mobility-HRMS

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PFAS are known as "forever chemicals" due to their persistent, bio-accumulative, toxic (PBT) properties and ubiquitous presence in the environment and organisms. Ca. 5000 PFAS are marketed worldwide, making their systematic environmental monitoring an extremely challenging task. On top, there is a lack of reference standards or spectral libraries, and there are plenty of isomers. Adding trapped ion mobility spectrometry (TIMS) to UHPLC-HRMS allows for comprehensive monitoring of organic micropollutants in environmental matrices such as water and soil. Presented here is a complete solution for PFAS characterization in environmental samples, combining ion mobility supported target analysis with wide scope non-target screening against the complete set of 5000 compounds.

Water was sampled at 10 sites in the Netherlands and pre-concentrated by SPE. Data acquisition was performed on a timsTOF Pro (Bruker)equipped with ion mobility. Kendrick mass defect (KMD) analysis filtered potential PFAS from the matrix background, based on the fluorine content (repeating CF2 units). Spectra were compared with the Norman network and NIST suspect lists of 5000 entries for non-targeted analysis. These contain information about the PFAS elemental composition and the InChI structure which were matched with the four criteria of exact mass, isotope pattern, MS/MS fragmentation and CCS value of the experimental data for an automated and untargeted identification of all PFAS present in the sample.

The ion mobility feature of the system was utilized for several purposes. First, it could separate coeluting isobars and isomers. Second, the TIMS filter resulted in higher sensitivity and lower detection limits of the targeted PFAS as well as significantly higher quality of full-scan MS and bbCID MS/MS spectra. Finally, collisional cross sections (CCS) as additional identification criteria enhanced the identification confidence with was based on retention time, exact mass, diagnostic fragmentation ions and the isotope pattern fit. Starting from a total of 15,700 detected features, 1181 potential PFAS have been filtered by KMD (92% data reduction). In total, 98 PFAS were found in the water samples, including genuine and degradation products with distinct differences for the various sampling sites which point to individual environmental circumstances and origins for PFAS.

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Hyphenation of Electrochemistry and Mass Spectrometry to Elucidate Environmental Transformation Processes of Organic Pollutants

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It has been demonstrated that electrochemical transformation products are comparable to products formed by enzyme-catalyzed redox reactions for a multitude of small organic molecules. This approach has been particularly useful for predicting metabolites formed by human xenobiotic metabolism. In the context of environmental transformation processes, enzyme-catalyzed and abiotic redox reactions also play a central role. Thus, hyphenation of electrochemistry and mass spectrometry has been investigated as method for predicting environmentally relevant transformation products. This work demonstrates the added value of such hyphenation through the structural elucidation of a soil degradation product of the sulfonylurea-herbicide tritosulfuron using an online coupling of electrochemistry and high-resolution mass spectrometry. The annotation is verified by scaled-up electrosynthesis and isolation of 1 mg of the transformation product followed by nuclear magnetic resonance spectroscopy. Moreover, the antihypertensive drug valsartan is investigated by electrochemistry coupled to high-resolution mass spectrometry, and the presence of a predicted transformation product in wastewater treatment plant effluent is verified. By generating a standard of the predicted compound in situ, the annotation confidence is increased and a targeted detection method using liquid chromatography-tandem mass spectrometry is set up. These examples highlight the capability of electrochemistry to predict environmentally relevant transformation products. The purely instrumental setup and simple and fast implementation allow for high-throughput screening applications that can be used to study the transformation behavior of multiple environmental pollutants in the future and increase annotation confidence of their transformation products in non-target and suspect screening.

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Discovering pharmaceutical transformation products in intermittent rivers using open cheminformatics approaches

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Due to the widespread use of pharmaceuticals, and their partial elimination in conventional wastewater treatment plants (WWTP), they are frequently detected in the aquatic environment. An essential factor in assessing their potential hazards is understanding their fate once they enter the environment thus, it is also important to study their transformation products (TPs). Previous research has demonstrated that certain TPs can be as toxic, or even more toxic than their parent compounds. Hence their study and identification are essential to assess the health of a watercourse. However, the identities of many TPs are still unknown, resulting in a limited understanding of their environmental fate and ecotoxicity. The aim of this study was to tentatively identify pharmaceutical TPs present in Spanish intermittent rivers and to evaluate possible temporal variations. Samples were collected from various intermittent rivers, impacted by WWTP discharges, and several points along the river were collected in order to study possible in-stream attenuation of pharmaceuticals and to identify the corresponding TPs formed. Samples were analyzed by means of liquid chromatography coupled to a high resolution mass spectrometer Q-Exactive Orbitrap using both positive and negative ionization modes. The ShinyTPs app (https://gitlab.com/uniluxembourg/lcsb/eci/shinytps) was used to create a suspect list of TPs related to 80 parent pharmaceuticals. While many TPs were already documented in open TP libraries, 107 newly curated reactions related to 11 pharmaceuticals were added into the HSDBTPS dataset (https://zenodo.org/records/12752099) and thus the PubChem Transformations library (e.g. https://pubchem.ncbi.nlm.nih.gov/compound/2826#section=Transformations). This suspect list, including over 400 entries, will be used to perform suspect and non-target analysis using the open source R-package patRoon, with MetFrag and additional database information from PubChemLite for compound identification, coupled with the patRoon TP functionality to complement the ShinyTPs suspect list. Compound identification, semi-quantification and if possible, confirmation quantification will be performed to determine which TPs are relevant in intermittent rivers. These results will be compared with similar screening exercises in Luxembourgish surface water samples from small water bodies. The findings in this study will complement existing knowledge and will help to better understand pharmaceuticals and their TPs fate in the environment.

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Comprehensive Assessment of Endocrine Disruptors: Evaluating Hair, Blood, and Urine Matrices

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Endocrine disruptors (EDs) are chemicals commonly found in consumer products that have the potential to interfere with the endocrine system, leading to adverse health effects. Traditional methods of assessing exposure typically rely on blood and urine samples. While these matrices offer valuable insights into recent exposure, they may not accurately reflect long-term exposure due to the relatively short half-lives of EDs in the body. In contrast, hair samples can integrate exposure over more extended periods, potentially offering a more comprehensive and complementary approach for biomonitoring studies.

This study aims to evaluate and compare the presence of EDs in hair, blood, and urine samples from patients with frontal fibrosing alopecia and age-matched controls at Hospital del Mar in Barcelona. The extraction process followed previously developed in-house methods. Briefly, hair samples were cleaned of surface contaminants with DCM and MeOH, ground with bead beating and extracted with MeOH. Urine samples underwent centrifugation to remove solids, and endogenous chemicals were filtered using Captiva cartridges. Serum samples were deproteinized with ACN.

Using a liquid chromatography-high resolution mass spectrometry (LC-HRMS) approach, we analyzed 48 EDs, detecting 35 of them. The highest number of chemicals was found in hair samples (63%), followed by urine (42%) and serum (27%). Notably, parabens and flame retardants were consistently present across all matrices, with hair samples showing a significantly higher concentration range (<LOQ-3134 µg/kg) compared to serum (<LOQ-88.12 µg/L) and urine (<LOQ-26.47 µg/L).

The findings suggest that hair samples are particularly valuable in detecting a broader range of EDs and in higher concentrations, underscoring their potential as a reliable biomonitoring matrix for assessing long-term exposure to organic chemicals. This study highlights the importance of incorporating hair analysis into biomonitoring protocols to achieve a more comprehensive understanding of ED exposure and its implications for human health.

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Non-targeted analysis of a biodegradable bio-based food packaging material by LC-ESI-Q-Orbitrap

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Polymers derived from renewable biological resources and biodegradable polymers designed to decompose easily in the environment are being developed and promoted as alternatives to conventional petroleum-based non-biodegradable plastics for food packaging. However, these materials typically do not perform as well as traditional plastics and often require additional chemicals, such as plasticizers, antioxidants, etc., to improve their properties. It is important to study the chemical safety of these sustainable materials since, like other materials in contact with food, they can release low molecular weight components into food, which may represent a risk to consumers´ health.

In this study, a non-target analysis using liquid chromatography coupled with high-resolution mass spectrometry equipped with an electrospray source (UHPLC Q Exactive) was employed in positive and negative ion mode, using a C18-like column (100 mm × 2.1 mm, 1.9 µm). Both MS1 and MS2 experiments were performed to carry out the elucidation of the molecules.

A sample consisted of industry-provided polyhydroxybutyrate (PHB) pellets, the most common polyhydroxyalkanoate. Several PHB derivatives below 1000

Da, both linear and cyclized, were tentatively identified by comparing their characteristic m/z as well as the fragmentation pattern with a homemade database developed, taking into account possible starting substances. As toxicological data are not yet available for these compounds, their toxicity was estimated using Cramer's decision tree based on the molecular structures, and it was found that many of them belong to the high toxicity class (Cramer class III).

This study highlights the potential of high-resolution mass spectrometry as a powerful tool for in-depth chemical characterization of complex matrices, facilitating the identification of unknown compounds through accurate mass measurements and fragmentation patterns. The findings of this study contribute to the understanding of the chemical safety of bio-based biodegradable packaging materials, emphasizing the need for comprehensive risk assessments before their application in food packaging.

Acknowledgement: The study was financially supported by the Ministerio de Ciencia e Innovación, Agencia Estatal de Investigación and by Fondo Europeo de Desarrollo Regional (FEDER). Ref.No. PID2021-124729NB-I00 "MIGRABIOQUANT" (MCIN/AEI/ 10.13039/501100011033/FEDER, UE).

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How Wastewater Reflects Human Metabolism - Suspect Screening of Pharmaceutical Metabolites in Wastewater Influent

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Pharmaceuticals and their human metabolites are contaminants of emerging concern in the aquatic environment. Most monitoring studies focus on a limited set of parent compounds and even fewer metabolites. However, more than 50% of the most consumed pharmaceuticals are excreted in higher amounts as metabolites than as parents, as confirmed by a literature analysis within this study. Hence, we applied a wide-scope suspect screening approach to identify human pharmaceutical metabolites in wastewater influent from three Swiss treatment plants. Based on consumption amounts and human metabolism data, a suspect list comprising 268 parent compounds and over 1500 metabolites was compiled. Online solid phase extraction combined with liquid chromatography coupled to high-resolution tandem mass spectrometry was used to analyze the samples. Different data pre-processing workflows were compared in advance, whereby final pre-processing was conducted with Compound Discoverer. Further data processing, annotation and structure elucidation was achieved with various tools, including molecular networking as well as SIRIUS/CSI:FingerID and MetFrag for MS2 spectra rationalization. We confirmed 37 metabolites with reference standards and 16 by human liver S9 incubation experiments. More than 25 metabolites were detected for the first time in influent wastewater. Semiquantification with MS2Quant showed that metabolite to parent concentration ratios were generally lower compared to literature expectations, probably due to further metabolite transformation in the sewer system or limitations in the metabolite detection. Nonetheless, metabolites pose a large fraction to the total pharmaceutical contribution in wastewater, highlighting the need for metabolite inclusion in chemical risk assessment.

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Assessment of potentially hazardous chemicals during pregnancy

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Chemical exposures are a major risk factor in the onset of a wide range of chronic diseases, and this risk increases during early stages of gestation, with potential adverse effects throughout the life course. This study aimed to comprehensive evaluate the occurrence of organic contaminants in pregnant women, and their potential transfer to the foetus.To achieve this, we focused on two biological matrices (serum and placenta). The chemical expsome was measured with a validated methodology based on liquid chromatography coupled to high-resolution mass spectrometry that allowed to assess >700 potentially hazardous chemicals in 294 maternal serum (First trimester of pregnancy) and 253 placenta samples (114 nested with serum) from the Barcelona Life Study Cohort (BiSC).

For serum and placenta different a wide amount of chemicals were found (149 and 147, respectlively), with 33 and 60 chemicals having a detection rate >50% and at least 28 and 52 >80%. These chemicals included plasticizers, tire additives, UV-filters, PFAS, personal care products, among others. The concentrations found varied, ranging from low ng/L to low mg/L. Sixty-three of the chemicals detected were present in both placenta and serum, for index, tris(2-chloroisopropyl) phosphate, N,N'-Diphenylguanidine and Di-n-octyl phthalate. The concentration ratios between these matrices were studied, revealing significant variability depending on the physicochemical properties of the chemicals, with some showing higher retention in one matrix than the other. Further studies will be conducted, including the analysis of paired cord blood samples, to better understand how the placental barrier affects the mobility of chemicals from maternal to cord blood.

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Quantification of quaternary ammonium compounds in meat and seafood products by LC-MS/MS

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Biocides substances are widely used as disinfectants, preservatives and pest control products, as well as antifouling and taxidermy products. Among them, Quaternary Ammonium Compounds (QACs) are the active substances which can be present in the composition of disinfection products for professional and domestic use (e.g. Benzalkonium chlorides (BACs), dialkyldimethylammonium chlorides (DDACs), alkyldimethyl(ethylbenzyl) ammonium chlorides (ADEBACs)), but also in products used as wood preservatives (alkyltrimethylammonium chlorides (TMAC)). Due to their wide use, particularly in the agri-food industry, these biocidal substances can unintentionally end up in foodstuffs, following their use during the disinfection of surfaces but also in food storage areas. Therefore, to ensure consumer safety, European Commission has set maximum residue levels (MRL) at 100 µg/kg, for BACs and DDACs only, and to be applied for products of animal origin.

A reliable method was developed for the quantification of 18 QACs in meat and seafood products by isotope-dilution liquid chromatography-tandem mass spectrometry (LC-MS/MS). QACs were extracted from sample with a mixture of acetonitrile and ethyl acetate, followed by dispersive purification with primary and secondary amines (PSA). Finally, the residue was reconstituted in methanol for analysis on Thermo® TSQ Vantage triple quadrupole operating in positive electrospray mode.

The method has been validated according to standard NF V03-110 and document No. SANTE/11312/2021, guidelines relating to the validation of quantitative analysis methods in food products. Method performance criteria (e.g. limit of quantification (LOQ), repeatability and reproducibility, trueness) were evaluated using the total error approach with e.noval® 4.1 software. Results obtained will be presented and discussed. Finally, the method is intended to be used for quantifying QACs within the framework of the 3rd French total diet study.

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Discovery of new contaminants and their metabolites in fertilizing residue materials (FRMs) and amended agricultural soils using NTA: A case study of deinking residues-amended soils

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Deinking residues, composite waste materials generated from paper deinking processes, are considered as fertilizing residual materials (FRMs) that are utilized to enhance soil properties and promote plant growth. However, the presence of organic contaminants (e.g. bisphenols, plasticizers, etc.) in deinking residues may pose potential health risks to humans and the environment. Some contaminants may even undergo degradation or metabolism in soils and form compounds with unknown toxic effects. This study aims to investigate the accumulation behavior and fate of plastic-related contaminants in soils amended with deinking residues using simultaneous targeted and non-targeted analysis. This is the first study on the application of NTA to contaminants in soils amended with deinking residues.

Soils amended with deinking residues were collected at four time points (prior to the application, and then 7 and 56 days post-application, and at harvest) from a two-year controlled field experiment conducted in Quebec, Canada. Soil samples were freeze-dried, homogenized, and extracted using an ultrasound-assisted method. Extracts were analyzed by LC-QToF-MS. The analytical method was validated (recoveries, matrix effects, method detection limits, and precision using a certified reference material - SRM 2781). The extraction method showed overall satisfactory performance (with a median recovery above 85%) and was applied to samples. In NTA, features were extracted, prioritized, and searched against an in-house library of contaminants metabolites predicted by BioTransformer (https://biotransformer.ca/). The annotated features were further confirmed through SIRIUS (https://bio.informatik.uni-jena.de/software/sirius/) based on MS/MS.

DEHP, DEP, D-8, TGSA, and BPS were the dominant targeted contaminants detected in deinking residues, with levels up to 36 μg g-1. These chemicals were all quantifiable in agricultural soils 7 days after the amendment, at levels up to 20 ng g-1. Many previously unreported contaminants were identified in fertilizers using NTA, including 2,4-Bis(phenylsulfonyl)phenol (DBSP), N-(2-((Phenylcarbamoyl)amino)phenyl)benzenesulfonamide (NKK-1304), etc. The non-targeted workflow was also able to highlight some novel degradation products/metabolites of those emerging contaminants. For example, two hydroxylated metabolites of Cyanox 2246 (an antioxidant), predicted by BioTransformer, were tentatively identified and shown to increase in amended soils. These results confirmed that NTA based on LC-QToF-MS can provide essential information for the surveillance of chemical mixtures in agri-food systems.

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POSTERS

S1-P01 Highly Improved Compound Identification in the Non-target Analysis of Wastewater using a Novel HRMS with Simultaneous EI and CI

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Wastewater plants can release aqueous effluents containing harmful pollutants, posing risks to ecosystems and human health. Given the dynamic nature of wastewater composition, regular target and non-target analyses are frequently conducted. Due to its complimentary polarity range, GC-MS is often employed alongside LC-MS to evaluate potential hazard profiles, to identify compounds and to gain a more complete overview of the present hazards. Non-target analyses in GC-MS suffer from ambiguous scores of EI (electron ionization) data in NIST searches and are prone to false positives. Therefore, often additional GC runs are performed with a CI (chemical ionization) source to add the molecular ion information for filtering the NIST search results or when appropriate reference standards are not available. However, that requires mechanical source switching, separate GC runs and generates issues with peak alignments. Presented here is a novel GC-HRMS with simultaneous operation of EI and CI. Structural as well as accurate molecular ion information is generated in single GC runs which highly improves the confidence for identifying unknown compounds in wastewater.

24h effluent samples were collected from an industrial plant over two months. Analytes were enriched by headspace SPME using a hydrophilic-lipophilic balanced (HLB) fiber coating (CTC, CH). A 7890A GC (Agilent, USA) and was coupled to a novel dual ionization source TOF-MS (ecTOF, Tofwerk, CH)). Here, a standard 70 eV EI source and a medium pressure CI source are operated simultaneously on a single mass analyzer. Additionally, the CI source allows for a selection of different reagent ions (e.g., [NH4]+, [N2H]+, [H3O]+) enabling the adjustment of reactant selectivity and the degree of fragmentation.

Several examples for non-target wastewater analysis will be shown to illustrate the benefit of adding CI information to NIST-searchable EI data. The number of hits is largely reduced, the confidence of identification increased, and the rate of false positives minimized. Results show that this approach as well increases the number of compounds detected and identified leading to a more complete overview of contamination in wastewater and improving measures for treatment. The novel GC-EI/CI-HRMS can efficiently complement commonly employed methods such as LC-ESI-HRMS used in industrial wastewater analysis.

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S1-P02 Pesticide residues in the Palancia River Basin: Groundwater vs Surface water bodies

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The sustainable management of freshwater resources is a major challenge in the European Union as well as in the Mediterranean region. Groundwater stands out as the largest body of fresh water in the European Union, but it is also the most vulnerable, so the deterioration of the quality of this resource is a significant problem in many aquifers. In the specific case of Spain, pollution related to agricultural activities represents the main problem that affects groundwater because these activities are extensive in the Valencian Community and soil intrinsic characteristics favor lixiviation and runoff. Pesticide residues due to their continuous use and low elimination are widely dispersed in the environment. However, they are not fully regulated yet, and gaps remain regarding their environmental levels and potential adverse effects on ecosystems and human health. This study aims to establish the occurrence and spatial distribution of pesticides in surface and groundwater at the Palancia River Basin to identify possible pesticide sources. Six sampling points were established in the main course of the Palancia River, 16 in underground aquifers, and 8 points in the Almenara and Los Moros wetlands at the mouth of the River, which have made it possible to cover the upper, middle, and lower parts of the basin comprehensively. As a starting point, the presence of pesticides was evaluated considering that agricultural activity is practiced in a large part of the basin and the basis of the traditional irrigation system are springs, which are largely nourished by groundwater. For the chemical identification of pesticides, Target (T) and non-target (NT) analytical detection methods based on high-performance liquid chromatography (HPLC) coupled with high-resolution mass spectrometry (HRMS) have been developed. We will use the reversed-phase liquid chromatography (RPLC) mode, using a C18 chromatography column coupled to a quadrupole-Orbitrap mass spectrometry (MS) (Q Exactive Plus, Thermo Scientific) with an electrospray ionization (ESI) source. The results obtained provide important information for the management of water resources on the fate and behavior of these pollutants.

Acknowledgments: This work has been supported by Grant PID2022-138556OB-C22 funded by MCIN/AEI/10.13039/501100011033 and by “ERDF A way of making Europe”. Jhesibel Chavez acknowledges her pre-doctoral contract by the grant PRE2022-000791 funded by MCIN/AEI/ 10.13039/501100011033 and by “ESF Investing in your future”.

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S1-P03 Dithiothreitol-Based Protein Equalization in the Context of Multiple Myeloma: Enhancing Proteomic Analysis and Therapeutic Insights

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Multiple myeloma (MM) is a slowly growing and complex haematological malignancy characterized by abnormal proliferation of plasma cells in the bone marrow, leading to bone destruction, monoclonal gammopathy (i.e. increased immunoglobulin synthesis), and potential complications such as renal failure and anaemia. Despite treatment advancements, MM remains associated with significant morbidity and mortality, with approximately 160,000 new cases and 106,000 deaths annually worldwide.

In the field of analytical proteomics, significant advances have been made in understanding, detecting, and monitoring MM. Despite these advancements, proteomics applied to serum samples faces challenges, notably the dynamic range of protein concentrations, where abundant proteins overshadow disease-specific ones. To better understand myeloma diseases, we employed the dithiothreitol (DTT)-based protein equalisation technique and analytical proteomics by comparing the proteomes of pellets and supernatants formed upon application of DTT on serum samples. The number of unique proteins found in pellets was 252 for healthy individuals and 223 for multiple myeloma patients, with the comparison of these proteomes showing 97 dysregulated proteins. The unique proteins found in supernatants were 264 for healthy individuals and 235 for multiple myeloma patients, with the comparison of these proteomes revealing 87 dysregulated proteins.

The analytical proteomic comparison of both groups of dysregulated proteins was translated into parallel dysregulated pathways, including chaperonemediated autophagy and protein folding, addressing potential therapeutic interventions. Future research endeavors in personalized medicine should prioritize refining analytical proteomic methodologies using serum DTT-based protein equalization to explore innovative therapeutic strategies. We highlight the advanced insights gained from this analytical strategy in studying multiple myeloma, emphasising its complex nature and the critical role of personalized, targeted analytical techniques in enhancing therapeutic efficacy in personalized medicine.

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S1-P04 Enhancing Feature Detection and Biomarker Validation through Optimized Proteomics MS-data Normalization Using the Protein Deglycase DJ-7 (PARK-7)

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Renal cell carcinoma (RCC), the third most prevalent genitourinary cancer after prostate and bladder cancer, presents significant diagnostic challenges due to its heterogeneity and the lack of specific biomarkers [1]. In this study, we employed a proteomics approach to investigate the impact of mass spectrometry (MS) data normalization on detecting and selecting significant features for biomarker validation in RCC. Utilizing high-resolution MS, we analyzed protein expression profiles from RCC tissue samples and adjacent normal tissues. The normalization of MS data was critical in minimizing variability and enhancing the accuracy of protein quantification.

Proteomic techniques based on mass spectrometry now enable the estimation of relative or absolute amounts for thousands of proteins across a wide range of biological systems. This advanced technology is particularly useful for identifying stably expressed proteins that can serve as superior loading controls compared to traditional ones. Typically, ubiquitously expressed proteins such as β-actin, β-tubulin, and glyceraldehyde phosphate dehydrogenase are commonly used for normalization in proteomic studies. However, these proteins exhibit considerable variability across different samples, potentially leading to inconsistent data. Large-scale proteomic analyses of cultured cells and tissues have revealed deglycase DJ-1 (PARK-7) as the protein with the lowest variability in abundance among different human cell types. Consequently, we used DJ-1 to normalize our data, ensuring more reliable and accurate quantification. This protein typically constitutes 0.069% ± 0.017% of the total cellular protein and is present at a specific concentration of 34.6 ± 8.7 pmol/mg of total protein.

This research underscores the transformative role of optimized MS data normalization in enabling the detection and validation of biomarkers, providing new insights into RCC pathology as well as opening avenues for improved diagnosis and treatment options. The integration of advanced proteomic approaches in clinical environments is expected to greatly improve the precision and effectiveness of RCC diagnosis and treatment.

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S1-P05 Improved efficiency of ion trapping time-of-flight mass spectrometry for the analysis of pesticide residues and mycotoxins at trace levels in baby food

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The analysis of pesticide residues and mycotoxins in baby food requires exceptionally low limits of quantitation, necessitating highly sensitive instruments for trace analyses. Traditional high-resolution instruments often fail to detect such low levels. However, recent advancements in liquid time-of-flight (TOF) technology, coupled with ion trapping, enable ion enrichment, significantly improving detection levels. This allows for the analysis of these substances at low concentration levels with enhanced mass accuracy, eliminating matrix interferences and enabling high-confidence identification.

In this study, a multi-residue method was developed to analyze 219 pesticide residues and 9 mycotoxin residues in baby food matrices. Utilizing a QuEChERS-based extraction method, the samples were then analyzed using an LC-ZenoTOF 7600 system with mass window screening acquisition. For pesticides, the limits of quantitation were 0.001 - 0.003 mg/kg for 81% of the evaluated compounds, 0.005 mg/kg for 13%, 0.010 mg/kg for 4%, and 0.020 – 0.030 mg/kg for 2%. Good linearity was obtained at these levels. Apparent recoveries were evaluated at 0.003, 0.005, and 0.010 mg/kg, with 93% of compounds at the lowest recovery level showing recoveries between 70-120%, and the rest in the range of 63-129%, with relative standard deviation values below 20%.

For mycotoxins, the limits of quantitation ranged from 0.0001 to 0.100 mg/kg, with matrix-matched concentrations assessed within this range. Recoveries were evaluated at low concentration ranges (0.001-0.003 mg/kg) and high ranges (0.020-0.050 mg/kg), with apparent recovery values between 92-140%. Finally, 31 commercial baby food samples were analyzed using this method, revealing 16 samples with pesticide residues and two with mycotoxins.

The presence of pesticide residues and mycotoxins in commercial samples underscores the importance of analysis at low concentration levels. The combined use of SWATH® acquisition mode, enhanced by activated ion trap (Zeno pulsing), has proven effective in detecting trace-level results in routine analysis. This approach also allows for retrospective analysis and the potential identification of unknown substances using mass accurate commercial libraries. Furthermore, complementing the initial analysis with a second using MRMHR mode can produce mass spectra of higher cleanliness and accuracy, particularly beneficial in cases of uncertain identification.

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S1-P06 Migration of additives and other chemicals present conventional plastics and bioplastics used in agriculture using HRMS analyses

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Plastics and bioplastics, which are frequently used in agricultural applications (e.g., PE and PP), often contain additives that are essential to improve their performance. These include flame retardants, antioxidants, optical brighteners, and UV protectants, among others, which have the potential to migrate into the medium in contact with them. There is a substantial body of scientific literature on the migration of these chemicals from plastic packaging materials into food. However, there is a paucity of studies on the migration of substances from agricultural plastics into soil and the environment.

In this work, migration experiments from the different types of plastic materials were carried out using an aqueous solution as water/soil simulant. Square of 10 x 10 cm of the plastic materials were introduced in glass recipients and cover with the simulant. Three replicates were conducted plus one control sample (only stimulant). Samples were placed in an incubator for fifteen days at a fixed temperature, UV light and humidity. Experiments were carried out at 40 °C, which is the temperature that is reached during the summer months in the greenhouses of this area, therefore, conditions equivalent to the worst foreseeable use. After the incubation time, aliquots of each of the samples were injected in the analytical instrument for the analysis of plastic additives, monomers, oligomers, and other chemicals migrating from the materials. Analysis was made by liquid chromatography (LC) coupled to high resolution mass spectrometry (HRMS) for the nontarget analysis of chemicals with a wide variety of chemical-physical properties. Non-targeted analysis and processing of samples were carried out using different strategies, such as library search, filtering workflows using case-control samples.

Acknowledgments: The authors are grateful to the MICINN for the financial support given to the project PLEC2021-007693 and TED2021-131609B-C31

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S1-P07 Tracking emerging pollutants from effluents of wastewater treatment plants to supply water using high-resolution mass spectrometry and non-target analysis

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Ensuring the safety of drinking water resources from undesired and toxic chemicals is a primary goal of human health protection and it is one of the Sustainable Development Goals of the United Nations. The European Union has established much stricter quality criteria for surface and groundwater, so that it can continue to be used safely in the future. Since surface water and groundwater are both important sources for drinking water, their quality has to be evaluated. Groundwater is threatened by emerging contaminants such as products used in agriculture that infiltrate after use, pharmaceuticals and personal care products, industrial and pesticides that are not completely eliminated in wastewater treatment plants (WWTPs) and are discharged into rivers that infiltrate the groundwater, and industrial products carried by runoff water after storm events in cities.

From all above, in this work, water samples were collected in the effluents of several WWTPs, in the rivers that receive the treated wastewater, in wells near the rivers and in springs in the area where supply water is obtained. We developed a target method based on LC-HRMS for the analysis of 35 in water samples. For obtaining complementary information about the organic pollutants' occurrence, a suspect screening method was applied. Using on-line and homemade libraries, hundreds of contaminants were determined at different confidence levels of the Schymanski scale, and were tracked through the samples taken.

This research is funded thanks to the CLIMADAPT project of the SINERGIA call of the IDAEA-CSIC, Severo-Ochoa center of excellence.

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S1-P08 Wide screening of urban pollutants and transformation products in runoff water samples using quadrupole-ion trap-Orbitrap high resolution mass spectrometer

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Urban stormwater runoff contains many urban pollutants (UPs) from different sources vehicles and traffic areas, commercial or industrial areas, buildings, etc. Therefore, this type of pollution is variable depending on the area and time, and more studies are needed to understand its distribution for an efficient management of this resource. However, the large number of UPs present in the runoff makes its analysis by traditional liquid chromatography tandem mass spectrometry approaches very complicated, so high-resolution mass spectrometry would be a better option. To date, more than 600 UPs have been measured in runoff samples, highlighting pesticides, pharmaceuticals and personal care products, and chemical or industrial products (Zhang et al., 2024). This task is even more complicated if the standards are not available for confirmation purposes for instance for the detection of transformation products which come from the transformation processes that UPs may undergo in surfaces and runoff waters. These compounds can be even more toxic and dangerous substances. The alarm generated due to the discovery of the transformation product (TP) N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine-quinone (6PPD-quinone) indicates that it is crucial to pay attention to TPs (Ankley et al., 2024). More TPs of urban organic pollutants have been detected in water, such as hexamethoxymethylmelamine (HMMM), which is also polymer crosslinking agent used in tires (Johannessen & Parnis, 2021) or biocidal substances that cover building facades and can be released during wind-driven rain, as well as their TPs created by solar irradiation (Junginger et al., 2023). However, the identification of new TPs is complicated and long, and requires very sensitive and high-resolution state-of-the-art techniques to be able to identify them. In this work, with the aim of increasing the knowledge of TPs in urban runoff water, 25 runoff samples were analyzed by high-resolution mass spectrometry, specifically Orbitrap Eclipse Tribrid Mass Spectrometer. The high performance of this cutting-edge equipment has allowed us to detect dozens of contaminants and transformation products.

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S1-P09 Assessment of Environmental Contaminant Exposure in Children Through Urine Analysis Using High-Resolution and Low-Resolution Mass Spectrometry

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Chemical exposure in humans has been a topic of public health concern for decades. Several toxic chemical compounds to which the population is exposed has been detected, however a large number of them are still not yet identified. These facts highlight the need for biomonitoring to assess and mitigate the impact of these contaminants on human health, especially in vulnerable populations such as children. Urine is a convenient and non-invasive biological sample for assessing such exposure in children.

In this study, a suspected screening list of several endocrine-active substances, including herbicides, plasticizers, fungicides, lubricants, and plasticizers commonly present in the environment, was developed. Urine samples from a cohort of 8-year-old children from the same geographical area were analyzed to determine the most prevalent contaminants from a list of approximately 350,000 suspected compounds. High-resolution liquid chromatography coupled with tandem mass spectrometry was employed using a Thermo Fisher Q-Exactive Orbitrap MS system to perform the tentative determination.

From the established suspected list, benzophenone-3 and daidzein were found in all analyzed samples. Additionally, other compounds, mainly plasticizers and pesticides, were tentatively detected in more than 20% of the samples.

Subsequently, the samples were analyzed using low-resolution mass spectrometry coupled with tandem mass spectrometry, employing an Agilent 6475 LC/TQ system, to quantify the previously detected compounds.

Among the quantified compounds, bisphenol A was found in 70% of the samples at a median concentration of 1.6 µg/L, benzophenone-3 in 80% of the samples at a median concentration of 10.2 µg/L, and methyl paraben in 67% of the samples at a median concentration of 8.0 µg/L.

In conclusion, this study reveals that 8-year-old children are exposed to various environmental contaminants that can influence their health and quality of life. Furthermore, it demonstrates the powerful of combining high-resolution and low-resolution mass spectrometry for human biomonitoring and the detection and quantification of chemical contaminants.

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S1-P10 Comprehensive air quality assessment including non-target approaches in primary schools from Spain

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Children spend most of their time in indoor environments, especially in schools. Thus, indoor air quality (IAQ) in schools has an important impact on child health and is related to discomfort, reduced academic performance and productivity, allergies and some respiratory diseases. Moreover, the pandemic situation produced by COVID-19 disease has caused a pressing concern related to this issue.

This work aims to comprehensively assess the IAQ in four primary schools in Spain. Common indoor pollutants, like CO2, NO2, O3, CO, particulate matter (PM10, PM2.5), ultrafine particles (UFP), total volatile organic compounds (TVOCs), and formaldehyde (HCHO), have been assessed in terms of maximum recommended levels, daily variations, also, seasonality and school location influences. Additionally, fungi and bacteria have been assessed indoors and were always found at adequate levels. The most commonly identified fungi genera were Aspergillus, Penicillium, and Cladosporium. Seventeen respiratory viruses were measured in the air of the assessed classrooms and none were detected. Volatile and semivolatile organic compounds have been identified indoors and outdoors of schools using non-targeted approaches based on GC-HRMS and UHPLC-HRMS analytical methodologies. High-confidence identified compounds were classified according to their chemical and toxicological characteristics, revealing that 44% and 26% of the identified compounds presented a high toxicological risk in outdoor and indoor environments, respectively.

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S1-P011 Intelligent data acquisition metabolomic workflow for biomarker hunting in serum of cattle for early prediction of defective meat: A pilot study of usefulness of liquid biopsy in meat quality assessment

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Rejection of dark, firm, and dry (DFD) meat by consumers causes significant economic loses in cattle sector. This defective meat is characterized by its dark colour, atypical consistency and high pH finding diverse pre-slaughter stressing conditions such as transportation, fasting periods or fatigue of animals as main contributors. Early detection of defective meat and identification of stressed animals before slaughter can improve trading profits and minimize food waste. Intelligent data acquisition through iterative high resolution mass spectrometry (LC-HRMS, Orbitrap ID-X Tribrid) metabolomic analysis successfully addressed the unveiling of biomarkers characterizing DFD meats. Furthermore, current study represents a step forward since there was proposed a metabolomic approach based on the same LC-HRMS workflow but this time aiming at the elucidation of unambiguous meat quality biomarkers in serum from cattle before slaughter. In brief, a pool of five serum samples from Normal meat cattle (pH24 <5.7) and a pool of five serum samples from DFD meat cattle (pH24 >5.9) were analysed. Preparation of samples included an initial deproteinization step, evaporation, redisolution in 0.1% formic acid and addition of a mix of internal standards. Sample pools were injected following an intelligent MS3 AcquireXTM workflow. In order to obtain discriminatory signals during the acquisition step, DFD sample was considered as a blank during the Normal serum analysis and the Normal pool was used as a blank during the DFD sample approach. Compound Discoverer 3.3 data processing proposed 266 features (135 in negative and 131 in positive ionization modes) with high quality MS2 and MS3 spectra, appearing over or underexpressed in DFD sample compared to its normal counterpart. After manual filtering, 170 features were kept for tentative identification using the Chemspider and MzCloud databases. Among them, 80 were annotated with a proposed structure, finding how 6 of these potential descriptors showed a MS2 spectra match higher than 80% in mzCloud database and they were finally proposed as DFD biomarkers.

This pilot study demonstrated advantages of using a straightforward intelligent iterative acquisition workflow to obtain discriminant features for early detection of DFD bovine meat through liquid biopsy before slaughter avoiding the use of complex chemometric strategies.

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S1-P12 Exploring the Organic Composition of Polar and Semi-Polar Compounds in Ultrafine Particles (UFPs) in Barcelona, Spain: Validation and Application of an LC-HRMS Method

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The worsening of air pollution is a global concern due to its severe impact on human health. Particulate matter (PM), a critical pollutant, is linked to respiratory and cardiovascular diseases, cancer, and other health issues. The chemical composition of PM, particularly ultrafine particles (UFPs) that can deeply penetrate the human body, remains poorly understood. To better assess exposure to airborne PM pollution, a comprehensive analytical methodology is needed. This study optimized and validated a robust analytical protocol for UFPs analysis using liquid chromatography-high resolution mass spectrometry (LC-HRMS) for both targeted and non-targeted approaches. A curated set of over 150 chemicals was chosen to ensure coverage of a wide range of physicochemical properties, considering both logP values and retention times. This list included pharmaceuticals, biocides, flame retardants, corrosion inhibitors, tire additives, UV filters, personal care products (PCPs), plasticizers, PFASs, drugs of abuse, food/tobacco-related compounds and transformation products. The protocol was successfully validated for extraction recoveries, linearity, matrix effect, sensitivity, and reproducibility. It was then applied to 32 samples from the metropolitan area of Barcelona, Spain, revealing the presence of a wide variety of chemicals, including plastic additives, flame retardants, corrosion inhibitors, drugs of abuse, UV filters, and tire additives. This underscores the need for thorough analytical protocols to assess exposure to these airborne chemicals. Notably, the presence of tire additives is significant, as air pollution is a major exposure pathway. Additionally, non-targeted approaches identified over 25,000 features in the UFPs samples, highlighting the necessity of non-targeted strategies to fully characterize this matrix.

Acknowledgement: We thank support from AEI-MICI (RYC2019–027913-I, P. Gago-Ferrero) as well as the Spanish Ministry of Science and Innovation through the support received as “Centro de Excelencia Severo Ochoa 2019–2023". The project that gave rise to these results received the support of a fellowship from “la Caixa” Foundation (ID 100010434). The fellowship code is LCF/BQ/DR23/12000031 awarded to D. Gutiérrez Martín (INPhINIT Retaining Fellow). We also acknowledge the support received from the European Union through the Marie Skłodowska-Curie Postdoctoral Fellowship awarded to M.C. Nika

(HORIZON-MSCA-2022-PF-01, ID 101105240). Finally, we acknowledge nPETS, a project funded by the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 954377.

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S1-13 Machine learning for predicting environmental mobility based on retention behaviour

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Persistent and mobile organic contaminants (PMOC) have garnered significant attention in policy implementations and academic research due to their challenging removal from aquatic environments. The European Commission has identified very persistent and very mobile substances as categories of very high concern. Mobility of chemicals in the environment is typically assessed using the log Koc, the partition equilibrium between organic carbon and water. Chemicals with lower log Koc values are more mobile, but experimental log Koc values are often unavailable, necessitating the use of quantitative structure-activity relationships (QSAR) and other metrics like log Dow for ionizable compounds.

To enhance the classification of chemical mobility, our study utilizes the extensive RepoRT database, which includes 139,064 separations via reverse-phase liquid chromatography (RPLC). We developed a random forest classifier model to categorize chemicals into three mobility classes: very mobile, mobile, and non-mobile, based on the fraction of organic modifier at elution. Molecular fingerprints, which encode structural information of molecules, were used as features for classification. Unlike traditional molecular descriptors, fingerprints provide a comprehensive and computationally efficient representation of molecular structures.

This approach addresses the limitations of log Koc-based classification by providing a more direct and experimentally grounded method for assessing chemical mobility. The random forest model, trained on a large dataset of experimental RPLC data, offers improved robustness in classifying chemical mobility compared to current methods. We also applied the model to the EU REACH database and classified each of the 65000 chemicals according to their mobility

This study demonstrates the potential of advanced chemometric and machine learning tools in environmental chemistry, providing a valuable tool for regulatory agencies and researchers in managing PMOC.

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S1-P14 Air Quality of Health Facilities in Spain

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The present study is the first one to examine indoor and outdoor air pollution in the surroundings of health facilities in Spanish health facilities using liquid chromatography (LC) and gas chromatography (GC) coupled to high-resolution mass spectrometry (HRMS). This work has focused on compounds from various sources, such as industrial products, healthcare activities and building materials. Different places like two public hospitals, two public healthcare centres, and one public health laboratory were studied in two different areas (industrial and agricultural area) in the Valencian Region (Spain).

The results showed that around 400 substances (61 in indoor environments and 355 substances in outdoor air) were tentatively identified at a high confidence level, with over 50 % of compounds classified as of high toxicological risk taking into account Cramer rules. For the first time, three indoor and 26 outdoor compounds were fully confirmed with standards. These confirmed substances were linked to medical, industrial and agricultural activities.

Examining and comparing the results obtained in indoor and outdoor air, only three substances were tentatively identified in both environments. On the other hand, despite the fact that two areas were studied (industrial and agricultural areas), no significant differences were observed between areas, taking into account that more than 50 % of the confirmed substances were detected in both environments. This study will contribute by providing new data to inform policy frameworks, for harmonising available data, and improving the carbon footprint linked to health facility emissions.

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S1-P15 Non-targeted analysis of household dust by UHPLC-HRMS and feature-based molecular networking: Pilot study

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Household dust is a complex mixture of particulate matter that includes pollen, dead skin cells, natural and synthetic fibers, soil particles, and materials from furnishings and buildings. As people spend significant time indoors, exposure to household dust poses potential health risks, influencing respiratory and cardiovascular diseases according to the World Health Organization. Despite its significance, the chemical composition of household dust remains under-characterized, presenting a challenge for non-targeted analysis (NTA).

In this study, we developed and applied a non-targeted UHPLC-HRMS approach to analyze 19 household dust samples from urban and rural regions in Spain. Dust samples underwent microwave-assisted extraction (MAE), followed by concentration and dilution with deuterium-labeled pesticide standards before injection into an Orbitrap ID-X Tribrid mass spectrometer (Thermo Scientific). Samples were randomized, and pooled quality controls (QC) and blanks were included throughout the sequence.

During LC-MS analysis, both MS1 and MS2 data were acquired using two data-dependent acquisition (DDA) strategies with AcquireX MS2 (Thermo Scientific). MS2 data from all samples were collected using a background exclusion list based on blanks (Background Exclusion mode), while MS2 data from QC samples were acquired through successive injections with inclusion/exclusion lists (Deep Scan mode).

Data processing was performed using mzmine v4.1.0 to generate feature tables through a series of steps, including peak picking, feature deconvolution, retention time alignment, gap filling, and MS2 annotation against MassBank, MoNA, and GNPS libraries. The integrated areas of the extracted features were then subjected to exploratory data analysis using PCA and classification models using PLSDA, with the latter employing the sampling location as the classification criterion based on population and town density. These analyses were conducted using MATLAB (MathWorks) and PLS Toolbox (Eigenvector Research).

Preliminary results indicated interesting regional patterns in the PCA, although significant PLSDA models were not achieved as confirmed by permutation tests. Additionally, compound dereplication highlighted the potential of molecular networking in identifying and characterizing indoor pollutants.

This pilot study demonstrates the feasibility of combining DDA with AcquireX, feature-based molecular networking, and chemometrics for the NTA of household dust, offering a valuable tool for screening indoor pollutants in complex matrices.

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S1-P16 New methodological insights on non-target HRMS analytical profiling, spatiotemporal characterization, and modeling of pollution sources affecting an urban aquifer

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Urban aquifers are recognized as essential water sources for human supply and other industrial and general services like urban cleaning, irrigation, etc. Their preservation is crucial to cope with increasingly occurring water scarcity and global warming scenarios. Therefore, monitoring of physical, chemical, and biological parameters is necessary to characterize the quality of aquifers. Monitoring is generally based on water sampling carried out on certain sites and time frequencies. In this work, eleven groundwater samples were collected from February 2021 to January 2022 in seven points of an urban shallow alluvial aquifer of Besòs River, located in Barcelona. The samples were analyzed following a non-target approach by LC-HRMS in 2 steps to obtain the comprehensive information: i) a first analysis using Full MS acquisition to obtain the compound MS signals and ii) a second analysis using DDA mode to obtain the fragmentation pattern (MS2 signals) of those MS signals of interest obtained in the Full MS acquisition. Data treatment of full-scan datasets (first analysis) was performed using the Regions of Interest – Multivariate Curve Resolution (ROIMCR) algorithm, thereby filtering and compressing the MS signals and resolving chemical compounds. The results of ROIMCR were used to elaborate a list of the MS signals of interest to obtain their fragmentation pattern in a DDA analysis (second analysis). A total of 82 chemical compounds were annotated using the MSident application, most of them related to industrial activities, personal care products, or pharmaceutical products among others. The peak areas of these identified compounds were used for source apportionment in a second MCR (using the trilinear constraint to study separately the sampling time and the collection site). From this analysis, 5 main sources were selected (each one with a value of total explained variance > 10%). Finally, the areas from source apportionment analysis were used to elaborate advection-reaction models. Our approach allows obtaining relevant quantitative information relative to the dynamics of the pollution sources (expressed as composite mixtures of the resolved contaminants) such as the relative importance of the two main processes involved, i.e., the conservative transport across the aquifer vs. the local dynamics.

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S1-P17 Impact of Wastewater Treatment Plants on Surface Water Quality and Organic Contaminant Mixtures

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This study aims to investigate the impact of the construction and operation of a wastewater treatment plant on the water quality of Genil River as it flows through the municipalities of Huetor Tajar and Villanueva de Mesía (Granada, Spain). For this, grab water samples were collected before and after the plant operation upstream and downstream the treated wastewater effluent was discharged. Upstream locations include non-treated wastewater-impacted areas. The samples collected were analyzed for general water quality parameters like chemical oxygen demand and E. coli counts, and emerging organic contaminants. For the latter, samples were freezed-dried to achieve a 200x concentration factor, and obtained sample extracts were analyzed with liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS) using a quadrupole-orbitrap analyzer and a non-targeted approach. HRMS-data are being treated using chemometrics to identify differences among the organic contaminant mixtures in the different locations and sampling events. Expected results will reveal the organic contaminants that survive the water treatment to further explore their environmental risks and removal with currently-used advanced treatments.

Acknowledgments: CP acknowledges grant RYC2020-028901-I funded by MCIN/AEI/10.13039/501100011033 and “ESF investing in your future”. This work has been partially funded by the University of Granada Plan (Programme 1, #24) and grant PID2022-138229NB-I00 funded by MICIU/AEI/10.13039/501100011033 and ERDF/EU

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S1-P18 Target and non-target analytical methodology to ensure the water quality in reclaimed, river and drinking waters

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The main source of organic micropollutant contamination in rivers is the release of effluents from wastewater treatment plants (WWTPs). The Llobregat River, with more than 60 WWTPs in its basin, many industrial estates and significant flow rate fluctuations, has high pollution levels, which are likely to worsen due to climate change. In 2019, a special trial discharged reclaimed water from the largest WWTP into the lower Llobregat River to enhance water availability [1].

Currently, in drought conditions, reclaimed water is becoming one of the key resources to ensure the supply of drinking water to the metropolitan area of Barcelona. The reclaimed water is discharged into the Llobregat River a few kilometers upstream from the drinking water treatment plant (DWTP) intake. River water before discharged, reclaimed water, water intake DWTP and treated water, are analyzed using all analytical methodologies that are systematically analyzed according to RD 3/2023 [2] for drinking water.

Moreover, a target and non-target method has been developed in order to assess organic micropollutant presence in these waters. 28 compounds were selected for the analysis based on prior trials and recent scientific literature. Quantitative target analysis revealed 14 contaminants in reclaimed and raw water, with only iomeprol detected in all treated water samples between 280 to 910 ng/L. The non-target suspect screening methodology was applied to analyze water and assess that there was no significant presence of any contaminant. A large list of contaminants was confirmed at level 2a in reclaimed and river water [3], but only amantadine was suspected in treated water samples. After purchasing the analytical standard, amantadine was unequivocally confirmed at level 1 [3], quantified (around 170 ng/L in the treated water samples) and subsequently added to the target list. After that, the concentration levels found are compared with the predicted no-effect concentration (PNEC) found in the literature to determine if they are levels of significant presence in the environment.

[1] Munné A, et. al. Sci Total Environ. 866 (2023), 161339.

[2] Real Decreto 3/2023. BOE num. 9, Sec. I. Pág. 4253.

[3] Schymanski EL et. al. Environ Sci Technol 48 (2014), 2097–2098.

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S1-P19 Application of NH2-UiO-66 MOF for the Dispersive Solid Phase Extraction of Nine PFAS from Environmental Water Samples Followed by High-Resolution Mass Spectrometry Analysis

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Metal-organic frameworks (MOFs) have been widely integrated with various pretreatment techniques because of their exceptional properties, such as high porosity, significantly increased specific surface area, and chemical stability. NH2-UiO-66 MOF was synthesized with respect to green chemistry principles. Subsequently, a rapid and efficient method for extracting nine per- and polyfluoroalkyl substances (PFAS) from environmental water samples was developed using MOF-assisted dispersive solid phase extraction (d-SPE). This analytical method was enhanced by liquid chromatography tandem high-resolution mass spectrometry. Key parameters affecting extraction efficiency were systematically evaluated and optimized using one-variable-at-a-time (OVAT) approach and a central composite design (CCD). The OVAT approach revealed that 10 mL sample volume, 15 minutes extraction time, and 5 minutes elution time were ideal. Based on these optimized parameters, the design of experiments (DoE) included assessing eluent volume, sorbent amount, and sample pH. ANOVA confirmed the model's suitability with a p-value less than 0.05, and multiple diagnostic tests supported the findings. Optimal conditions identified were pH 7, 10 mg sorbent, and 750 µL eluent volume. The method's accuracy, repeatability, and detection limits were validated, showing recoveries above 70%, relative standard deviations below 20%, and detection limits ranging from 4 to 95 ng/L. Before application to real samples, the method's environmental friendliness was evaluated using the ComplexGAPI index, demonstrating high "green" attributes. The method's efficacy was tested on various environmental water matrices with different complexities, including runoff, river water, seawater, and wastewater effluent, confirming its capability for PFAS detection in diverse samples.

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S1-P20 Broad screening of food and feed supplements for marine and cyanobacterial toxins

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Products of aquatic origin are broadly and increasingly used as dietary supplements for humans and as feed supplements for pets and cattle. The origin of these supplements is diverse, ranging from phytoplankton to seaweed, mussels, fish and krill. This diversity implies that these supplements could be contaminated with a wide range of phycotoxins, both originating from freshwater and marine systems. The aim of our study was to determine the presence of phycotoxins in food and feed supplements of aquatic origin. To this end, we performed a quick literature survey and found that some combinations of supplements and toxins are more intensively studied than others. Next, we optimized and validated our high resolution mass spectrometry (LC-hrMS) method in order to reliably detect both marine and cyanobacterial toxins in a wide range of supplements. Finally we screened over 80 food and feed supplements by LC-hrMS, using a database containing more than 1200 toxins for data processing. When needed and if possible, the LC-hrMS results were confirmed by tandem mass spectrometry (LC-MS/MS).

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S1-P21 SICRIT® analysis of pesticides and environmental pollutants in complex matrices using a standard ESI workflow on Shimadzu LCMS- 9030 QTOF

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This study explores the use of SICRIT® ionization technology integrated into a standard LC-ESI workflow for the detection and analysis of 78 pesticides and across complex biological matrices. The primary goal was to evaluate the performance of SICRIT as a viable alternative to ESI, the industry-standard ionization technique, by comparing the ionization, detection, and identification of various pesticide classes. Complex matrices such as plasma, milk, urine, and saliva were spiked with pesticide standards at different concentrations to assess the effectiveness of SICRIT. Results demonstrated that SICRIT provided comparable results to ESI in terms of signal intensity, signal-to-noise ratios, and matrix effects for the majority of pesticides, showing its adaptability even in methods specifically optimized for ESI. Importantly, SICRIT successfully replicated the functionality of ESI by providing MS2 spectra that allowed for compound identification through library matching. Furthermore, we take 50+ other common exposomic, environmentally important components in the same method and experimental set-up and utilize the MS2 capabilities of Lab Solution to do online tandem mass spectrometry matching.

Overall, the results are highly competitive with ESI. The study showed that SICRIT could be seamlessly integrated into the existing analytical pipeline, offering additional advantages for metabolomic and exposomic analyses, particularly with non-polar compounds. Even though some compounds, such as quinolines, showed weaker comparison in terms of [M+H]+ ionization, SICRIT could still detect molecular ion peaks and oxidation products, making it a versatile tool for broader chemical analysis. Overall, the findings highlight SICRIT's capability to serve as a complementary or alternative ionization technique, expanding the scope of analysis beyond traditional ESI-optimized methods.

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S1-P22 Targeted quantitative screening pesticides in food matrices using high resolution DIA spectral library matching

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A single, generic untargeted data independent acquisition (DIA) method was developed for the analysis of extended panels of pesticides in food matrices using a fast High-Resolution LCMS QTOF system.

The high-resolution LC-MS/MS method was designed for multi-residue screening and quantitation of pesticides to meet the European Union SANTE 11312/2021 v2 guidelines capable of working with extended target pesticide panels.

The MS and DIA-MS/MS method was applied to quantify a routine panel of pesticides (>250 pesticides + 10 deuterated internal standards) but also included an additional target panel of fungicides for qualitative screening.

Several food commodity matrices were tested including apple, honey, olive oil, orange and tomato.

The single, generic TOF MS and DIA-MS/MS method results in the quantitation of >250 pesticides at or below the default MRL concentration (10 µg/kg). Pesticides are reported by high confidence using a high-resolution compound library. In addition, Suspect screening can be applied retrospectively to find pesticide compounds outside the scope of the initial target compound panel.

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S2-P01 Characterization of the non-volatile fraction focusing on the identification of oligomers in a PHA biopolymer packaging using LC-MS/MS

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Polyhydroxyalkanoates (PHA) are biobased and biodegradable polyesters naturally produced by the bacterial fermentation of lipids and sugars. In recent years, interest in these biopolymers as a sustainable alternative for food packaging has increased. Food contact materials must comply with food safety legislation. However, very little information is available on its composition, particularly on the non-intentionally added substances (NIAS). Recently, special attention has been paid to oligomers. Therefore, the aim of the present research work was to perform a preliminary non-targeted analysis to tentatively identify the non-volatile components of PHA material in two different formats: pellets and processed films.

Samples of a PHA material in pellet and film formats were analyzed. For the extraction, 1 g of each sample was placed in glass vials and extracted with 5 mL of acetonitrile for 24 hours at 70°C under sealed conditions. Each sample was analyzed in triplicate. An aliquot of the extract was filtered and analyzed by liquid chromatography tandem-mass spectrometry (LC-MS/MS) using a Gemini C18 reverse-phase column (150 mm x 3 mm, 5 μm) at 35°C. The mobile phase consisted of water and acetonitrile, both with 0.1% formic acid (v/v) in a gradient elution mode at 0.40 mL/min. The mass spectrometer was operated in positive electrospray ionization mode (ESI) and mass spectra were acquired in full scan mode (m/z 100-1000).

Oligomers of linear and cyclic nature were tentatively identified in both material formats. Since no toxicological data were available for the oligomers, Cramer's rules were used to estimate the theoretical toxicity of the identified compounds based on their molecular structure. Results showed that the identified cyclic oligomers mostly belonged to Cramer Class III, while the linear ones showed lower toxicological levels (Cramer Class I).

Acknowledgement: The study was financially supported by the Ministerio de Ciencia e Innovación, Agencia Estatal de Investigación and by Fondo Europeo de Desarrollo Regional (FEDER). Ref.Nº. PID2021-124729NB-I00 "MIGRABIOQUANT" (MCIN/AEI/ 10.13039/501100011033/FEDER, UE). Authors are grateful to "Ministerio de Ciencia, Innovación y Universidades" for the Predoctoral fellowship (ref. PRE2022- 105027) awarded to CVG.

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S2-P02 Development of analytical methods for the determination of lifestyle and dietary biomarkers in municipal wastewater

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This work focuses on the development of analytical methods for the determination of more than 50 lifestyle and dietary biomarkers in raw municipal wastewater. These include biomarkers of alcoholic beverages, nicotine/tobacco, caffeine, artificial sweeteners, vitamins and a range of food constituents, particularly plant-based, that indicate healthy dietary habits, such as flavonoids, lignans and phenylethanoids. The method will be used to assess lifestyle and dietary habits in Croatian regions using a wastewater-based epidemiology approach.

Selected biomarkers were analyzed by ultra-high performance liquid chromatography − tandem mass spectrometry (UHPLC-MS/MS) using electrospray ionization in negative and positive polarity. A C18 HSS T3 column (2.1 x 100 mm; 1.8 µm) and gradient elution with 0.1 % acetic acid and acetonitrile were used to separate the target compounds, while detection and quantification were performed in multiple reaction monitoring (MRM) mode on a triple quadrupole mass spectrometer. The total run time was 13.5 minutes with negative ionization polarity and 8.5 minutes with positive ionization polarity.

During method development, various solid-phase extraction (SPE) sorbents and protocols were tested. Optimal recovery for most analytes was achieved with hydrophilic-lipophilic balance (HLB) cartridges at a pH of 2. However, some target compounds, such as B vitamins, could not be extracted efficiently with HLB cartridges, so mixed-mode cation-exchange (MCX) cartridges were also used. The analytes were quantified using more than 20 isotopically labeled analogs as internal standards, which allowed accurate and reliable determination of most target compounds in a complex wastewater matrix in the low ng/L range.

The applicability of the method was tested using real samples collected at the inlet of the wastewater treatment plant of the city of Zagreb. Most of the target biomarkers could be quantified in these samples, with concentrations typically ranging from high ng/L to low µg/L.

Acknowledgments: This work was supported by the Croatian Science Foundation under the project number HRZZ-IP-2022-10-5332.

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S2-P03 Simultaneous analysis of pesticides and mycotoxins in primary processed foods: the case of bee pollen

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Primary processed foods are a class of food items that are ready for consumption after minimal processing in the supply chain. These products are ubiquitous in our daily diet, but so far a limited number of studies dealt with the optimization of quality control methods to check their content of contaminants. Among primary processed foods, bee pollen is a nutritionally acclaimed food supplement, whose safety is still largely debated. In fact, extensive evidence has been collected on its contamination with a variety of health threatening compounds, including pesticides and mycotoxins. For this reason, the present study aimed at optimizing for the first time a comprehensive mass spectrometry-based method capable of analyzing simultaneously 282 pesticides and 8 mycotoxins in bee pollen. To allow the detection of these contaminants, often present at traces level, a thorough process of extraction optimization was conducted by comparing the classical QuEChERS method, with a new QuEChERS approach including a fully automated clean up, combining various sorbents in a single micro cartridge. For a further improvement of the analytical performance, different chromatographic gradients and columns were also tested. The optimized methodology comprehended a new and effective extract clean up, followed by an analytical method including inert LC column technology. The method was fully validated and applied to a sample set of 34 bee pollens. The analyzed samples collectively showed the presence of 41 pesticides and 1 mycotoxin. The optimized analytical methodology showed good performance and allowed the extraction and analysis of the main contaminants found in bee pollen in a very short time. Such analytical approach represent a first step in the development of a routine procedure to ensure bee pollen's safety.

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S2-P04 Pesticide water dynamics and prioritization: The first steps to improve water management strategies in irrigation hydro-agricultural areas

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The presence of pesticides in aquatic ecosystems poses significant risks to non-target organisms, necessitating monitoring and environmental risk assessment. This study aimed to evaluate the dynamics and environmental risk of pesticides in a hydro-agricultural area with intensive agricultural practices, in the Mediterranean region (South of Portugal). Seasonality and location influenced pesticide numbers and concentrations, with the highest levels observed during the dry season. Triazines, phenylureas, and organophosphates were the predominant pesticide classes, with terbuthylazine, bentazone, terbutryn, diazinon, and metolachlor exhibiting the highest detection frequencies (68 % to 72 %). Notably, 44 % of the quantified pesticides are no longer authorized in Portugal, with 33 % posing a high environmental risk. Irgarol, an algicide used in irrigation canals, presented high risk (RQ≥ 1) in 91 % of the analysed samples. Imidacloprid, methiocarb, and malathion were occasionally detected at concentrations that posed high risks to the aquatic ecosystem. The study's distribution profile of pesticides revealed a significant transport of these compounds from reservoirs to irrigation hydrants, establishing them as a secondary source of crop and environmental contamination. Additionally, the assessment of environmental risk allowed for the identification of specific pollutants in different locations, prioritizing them based on their ecotoxicological risk to aquatic ecosystems. These findings reinforce the importance of implementing management measures at the level of hydro-agricultural areas, helping to stop the cycle of pesticide contamination.

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S2-P05 Static and dynamic flow biochar systems for the remediation of per- and polyfluoroalkyl substances in contaminated stormwater

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Pyrolyzed organic matter, also known as biochar, has recently shown strong potential as a treatment solution for sorption of organic micropollutants in contaminated water. Biochar generally consists of a complex structure of carbonaceous fibers with different chemical composition and physical properties depending on the feeding material used for the pyrolysis. Due to its intrinsic hydrophobic characteristics as well as a variety of chemical moieties on its surface, biochar has been proved valuable for soil function improvement, by retaining nutrients and contaminants. In this study, we aim to evaluate the potential sorption of per- and polyfluoroalkyl substances (PFAS) into biochar structure as a green remediation strategy for PFAS-polluted stormwater systems. To that end, different biochar materials (both commercial and research-based), as well as different feeding materials for biochar production have been tested. At first, batch sorption tests (static system) were carried out over 7 days in a set of 12 different biochar materials to identify the best performing ones. Later on, 5 selected materials were subjected to filter tests in a constant-flow column experimental set-up. With the final goal of identifying retention rates as well as breakthrough levels for the 15 PFAS tested, the columns were constantly running over a period of 90 days. Our observations indicate that there are large differences in the biochar performance when it comes to the retention rates of the tested PFAS contaminants. Thus, biochar performance for removal of PFAS depends on both the feeding material and production conditions. Correlation with physico-chemical properties of the investigated materials will help elucidate the sorption mechanisms. Overall, static flow tests, i.e. batch tests, showed a very promising application of biochar as a remediation tool for PFAS with some materials reaching removal efficiencies up to 99% in static systems. Also, long-chain PFAS showed a stronger sorption to the biochar compared to short-chain PFAS. For the dynamic flow system, similar observations were achieved. Short-chain PFAS tended to remain in the aqueous phase and, thus, column breakthrough occurred at an earlier stage. However, overall biochar has been proven as a promising and green strategy for the removal of PFAS from polluted stormwater.

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S2-P06 Urban Stormwater Contamination: LC-QTOF-MS Analysis of PMTs in Barcelona

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Persistent, mobile, and toxic (PMT) chemicals are emerging contaminants of concern for urban water quality, increasingly threatened by urbanization and extreme weather events. Although legacy and regulated contaminants (e.g., pesticides, drugs, anti-corrosion agents, plasticizers) are already detected in various water sources, there is still limited scientific knowledge on the source, transport, and fate of new chemicals of concern due to the absence of comprehensive monitoring in the urban water cycle. Standard water treatments often fail to remove these chemicals, leading to their presence in both ground and surface waters. In 2019, the German environmental authority UBA issued a list of PMT substances registered under REACH, providing a prioritization based on preliminary emission assessments. Stormwater catchment and reuse present a promising resource, especially in densely populated arid regions facing water scarcity. However, stormwater is also a significant source of contamination, particularly in "sponge cities" where urban planning and design strategies are essential for sustainable rainwater management. Installing stormwater blue-green infrastructures (BGI) is a promising practice to mitigate contamination, recharge urban aquifers, and manage combined sewer overflows (CSOs).

This study focuses on urban stormwater "first flushes" from various sites across three districts in Barcelona, collected from March to April 2022. The sampling design included conventional and pedestrian street runoff and BGI effluents. Grab samples were analyzed using an evaporative enrichment methodology. 34 PMTs of urban interest, including 18 reported in the UBA list, were quantified using a targeted LC-QTOF method with a HSS T3 UHPLC column coupled with a Bruker QTOF mass spectrometer in bbCID data acquisition mode. All target chemicals were detected in at least one sample, with benzenesulfonamide, 1,3 diphenylalanine, di-n-butyl phosphate, tolytriazole, and TCPP being the most abundant and ubiquitous, with median concentrations exceeding 100 ng L-1. Additionally, BGI effluent samples showed reduced contamination loads compared to street runoff. Monitoring PMTs in urban stormwaters is crucial to prevent their spread into surface and ground waters and to ensure the safe use of water supplies.

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S2-P07 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.

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S2-P08 Polybrominated diphenyl ethers in household dust of breastfeeding mothers: Exposure levels and health risk assessment

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Polybrominated diphenyl ethers (PBDEs) are a group of synthetic organo-bromine compounds that can be distinguished in 209 structurally similar compounds, referred to as PBDE congeners. They are industrially used as mixtures acting as flame retardants in foams, plastics, resins, and other materials usually applied in electrical equipment.

In the last years, associations between PBDEs levels and neurological disorders, reproductive disorders, and endocrine disruption, have been demonstrated. Moreover, several studies conducted in rats during pregnancy and lactation identified the transfer of BDE-47 and BDE-209 from fat stores to milk and demonstrated that BDE-209 was able to cross the placenta barrier. Thus, human exposure to these pollutants has raised special concern for the scientific community.

In this work, an analytical method has been developed and validated for the determination of 18 PBDE congeners, including BDE-209, in household dust of breastfeeding mothers. Sample extraction and purification procedures were studied and optimized based on microwave assisted extraction (MAE), acid digestion, and solid phase extraction (SPE), respectively. The analyses were performed using gas chromatography coupled to high-resolution mass spectrometry (GC-HRMS), using a Thermo Q-Exactive GC Orbitrap MS system.

A total of 54 household dust samples of breastfeeding mothers from the Valencian Region (Spain) were analyzed. BDE-207, BDE-206, and BDE-209 congeners were detected in all samples, the last showing the highest levels (50-39220 ng•g-1dust). Futhermore, BDE-47, BDE-99, BDE-153, BDE-183, and BDE-196 congeners were also found in concentrations ranged from 1 to 10 ng•g-1dust. After that, PBDEs exposure risk assessment was performed and house characteristics were statistically evaluated to set correlations between them and PBDEs levels.

This is the first work in which PBDEs have been monitored in household dust of breastfeeding mothers and exposure risk assessment has been performed.

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S2-P09 Presence and Quantification of Per- and Polyfluoroalkyl Substances (PFAS) in Surface Water of the Miccosukee Reservation and Coastal Environment of Miami, FL, US

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PFAS have a long history of negative human health implications studied in urban environments, and have been found as well in sparsely populated rural environments. Their widespread presence, transport, and persistence make them particularly relevant in environmental regulation locally and nationally given their stability as an environmental contaminant. PFAS are of environmental and health concern in both the urban coastal environment of the city, but also in the wetlands of the Everglades, potentially impacting agriculture, and wildlife. In this study, three canals discharging into the Biscayne Bay in Miami, FL and canals and marshes in the Everglades National Park were monitored to compare urban and rural environments' PFAS contamination levels. Surface water samples (250 mL) were collected and processed through solid phase extraction (SPE) using Strata-AW-XL cartridges and analyzed for a total of 40 PFAS by liquid chromatography tandem mass spectrometry (LC-MS/MS). Preliminary results showed an average of the sum of PFAS (∑40PFAS) to be 29.80 ng/L in the Everglades area, which was the first time PFAS levels were recorded to date in the Miccosukee Tribe Reservation. PFAS concentrations and compound compositions vary in the Everglades compared to Miami River, which has an average of ∑40PFAS to be 78.05 ng/L. The sum of PFAS at each Everglades site ranged from 18.36- 37.06 ng/L and ranged from 18.71- 140.99 ng/L in Miami River. PFAS concentrations, compound and chain length compositions, and locations will give rise to potential point sources in South Florida which could potentially cause a threat to human health by consumption of fish from these areas.

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S2-P10 Determination of highly polar anionic pesticides in foods using ion chromatography coupled to tandem mass spectrometry

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Among the highly polar pesticides, some of the most widely used worldwide include the herbicide glyphosate "group". However, monitoring residues of these contaminants in food has been limited compared to other pesticide groups, likely due to the need for specific residue methods for accurate quantitation in food samples. Thus, ongoing research and advancements in analytical methodologies are essential for the comprehensive monitoring and regulation of highly polar pesticide residues.

Ion chromatography has become a potent technique for the direct analysis of these pesticides. Coupling ion chromatography with tandem mass spectrometry detection significantly improves selectivity and sensitivity, enabling the achievement of low quantitation limits critical for regulatory compliance. A methanol/water-based method was employed as the sample preparation strategy for extracting 13 compounds (glyphosate, AMPA, glufosinate, their N-acetyl metabolites, MPPA, ethephon, HEPA, fosetyl-Al, phosphonic acid, chlorate and perchlorate). Final extracts were diluted with water (20x for fruits, vegetables, and cereals; 50x for green coffee beans). For method validation, SANTE/11312/2021 guidelines were followed. Recovery studies on grapes, onions, rice, and rye at concentrations of 0.005, 0.010, and 0.050 mg/kg resulted in absolute average recoveries ranging from 70% to 120%, with relative standard deviation values below 20% for almost all tested pesticides. Quantitation limits ranged from 0.005 to 0.010 mg/kg. Linearity was assessed from 0.002 to 0.500 mg/kg, and matrix effects showed medium to low signal suppression for most compounds, with AMPA exhibiting the highest signal suppression. Proficiency test samples were analyzed to evaluate the method's performance.

Additionally, 105 fruit and vegetable samples, 22 cereal samples, and 19 green coffee bean samples were analyzed, demonstrating the occurrence of highly polar pesticides in real samples. At least one evaluated compound was present in 85% of the samples, with residue concentrations ranging from 0.005 to 8.2 mg/kg. Chlorate, perchlorate, and phosphonic acid were the most frequently detected compounds in fruits and vegetables, while glyphosate residues were ubiquitously found in green coffee bean samples.

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S2-P11 Levels and risk assessment of dl-PCBs and dioxins in soils surrounded by cement plants from industrial areas of Colombia and Spain

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Chlorinated organic compounds such as polychlorinated dibenzo-p-dioxins (PCDDs), polychlorinated dibenzofurans (PCDF), and dioxin-like polychlorinated biphenyls (dl-PCBs), are a threat to both humans and the environment because of their toxicity, persistence and their capacity for long-range atmospheric transport. This study investigates concentrations of 17 PCDD/Fs and 12 dl-PCBs congeners in soil samples collected at industrial areas of Cartagena de Indias (Colombia) and Valencia (Spain), to assess the characteristic distribution patterns and the possible risk around cement plants inside the selected locations due to a lack of information regarding PCDD/Fs and dl-PCBs in soil from both areas studied. Soil samples were analysed using gas chromatography coupled to high-resolution mass spectrometry (GC-HRMS). The PCDD/Fs concentrations varied from 0.01 pg g-1 dw to 520.43 pg g-1 dw in Colombia and from 0.01 pg g-1 dw to 150.48 pg g-1 dw in Spain. For dl-PCBs, levels ranged from 0.03 pg g-1 dw to 1611.83 pg g-1 dw in Colombia and from 0.06 to 189.64 pg g-1 dw in Spain. Despite the differences observed in concentration terms between the two areas studied, the same pattern of congeners was observed. The hazard index (HI) values for exposure of adults and children in soil were, in overall, smaller than one (HI<1), while the total cancer risk (TCR) values exceeded the acceptable risk value of 10−6, which indicate probable non-carcinogenic and carcinogenic risks resulting from exposure to PCDD/Fs and dl-PCBs in these areas.

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S2-P12 Pesticide Pathways Revealed: Combining Complementary Analytical Methods for Comprehensive Multi-compound Monitoring in Urban and Agricultural Catchments

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The ecotoxicological risk posed by pesticides (plant protection products and biocides) to aquatic organisms and humans has driven research progress in recent decades. Pesticides can be introduced into surface waters through runoff from agricultural fields or through wastewater. In order to develop effective mitigation measures, it is crucial to investigate their entry pathways to the environment. However, the presence of a large variety of pesticides and their differing seasonal use makes thorough assessment challenging. In addition, studies have shown that non-polar pesticides such as pyrethroids exhibit toxic effects already in the low pg/L range, tend to sorb to particles and potentially bioaccumulate due to their hydrophobicity. For a comprehensive characterisation of the complex aquatic pollution, it is indispensable to combine sensitive and complementary analytical methods to determine the total concentration (i.e., the dissolved and the particle-bound fractions) and the concentration in the dissolved fraction only. Few studies include a broad spectrum of different pesticides with a wide range of physicochemical properties and continuous river and wastewater sampling beyond the application period.

Hence, the present study collected time-proportional two-week composite river and effluent wastewater samples from February to November 2023 at five different sites with varying proportions of agricultural and urban areas in Switzerland. The combination of three analytical methods resulted in an extensive screening: The quantification of about 240 pesticides in the ng/L range was based on enrichment by vacuum-assisted evaporative concentration and subsequent analysis by liquid chromatography coupled to high-resolution tandem mass spectrometry (Mechelke et al., 2019). The total concentration of around 70 non-polar pesticides (log P > 4) was quantified in the pg/L range using liquid-liquid-extraction followed by extract splitting and then simultaneous analysis by gas chromatography and liquid chromatography, both coupled to triple-quadrupole mass spectrometry (Rösch et al., 2019).

The most frequently detected pesticides, their entry pathways, and their concentrations dynamics before, during and after the application period will be described in detail. This work emphasises the need for a robust monitoring program and combined analytical methods to effectively manage the ecotoxicological risk of pesticides and ensure the long-term health of our ecosystems.

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S2-P13 First study on the impact of plastic greenhouses on airborne microplastics presence

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Given the current dearth of knowledge regarding the impact of plastic pollution from greenhouses, this study presents preliminary findings with the aim of advancing scientific understanding of airborne microplastics (MPs) in arid regions, such as southwestern Spain. To this end, a portable active sampling device was developed and validated, enabling the collection of comparable data on the quantity and types of MPs detected in areas heavily influenced by intensive agriculture. These measurements, expressed as MPs/m3, were gathered using a standardised sampling protocol to evaluate and compare various environmental compartments, including the Campo de Dalías, which has the highest concentration of greenhouses globally, an urban area, and a nearby nature park.

No statistically significant differences in the total number of MPs/m3 of air inside of greenhouses, surrounding areas, and urban locations, were observed with mean values of 35, 25, and 39 items/m3, respectively. However, the concentration was somewhat lower in the natural park, at 19 items/m3. In all scenarios, fibres constituted 70-80% of the MPs, with blue fibres being the predominant type (50%), except in Cabo de Gata nature park, where black fibres were the most prevalent (56%). Polyethylene terephthalate (PET) was the most common synthetic polymer identified in both fibres and fragments across all scenarios, except inside the greenhouse, where the majority of fragments were identified as polypropylene (PP). The findings from this preliminary study indicated that plastic greenhouses do not significantly impact the concentration of airborne MPs. Nevertheless, further research is essential to thoroughly understand these new atmospheric pollutants and to evaluate the potential effects of weather conditions on their distribution.

This study was conducted as part of the projects PID2023-147846OB-C21 and PLEC2021-007693 which was financed by the MICINN.

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S2-P14 Metabolomic profiling for European eel exposed to contaminants of emerging concern

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One of the factors under consideration regarding the presence of contaminants in aquatic environments pertains to their potential impact on highly endangered species, such as the European eel (Anguilla anguilla). Metabolomic profiling is an important tool for assessing fish health and optimal physiological function. Therefore, our research aims to identify biomarkers indicative of exposure to these contaminants and to investigate their toxicokinetic. To this end, a laboratory study was conducted using realistic environmental concentrations of tebuconazole (1 µg/L) or a combination of tebuconazole (1 µg/L) and other emerging contaminants, including diclofenac, venlafaxine, carbamazepine, caffeine, difenoconazole, acetamiprid, PFOS, and PFOA (0.125 µg/L each, 1 µg/L total), administered to European eels via water exposure for 34 days. Following the exposure phase, the water was replaced, and the eels underwent a 22-day depuration period. Sampling occurred on days 0, 2, 8, 15, 28, 34, 36, 44 and 55, encompassing plasma, liver, and muscle tissues for metabolomic analysis. Plasma, liver, and muscle samples were extracted using QuEChERS, while plasma samples were extracted using Phree™ Phospholipid Removal cartridges. All samples were analyzed using liquid chromatography coupled to mass spectrometry (LC-MS/MS). Discrepancies were observed between the exposure to only tebuconazole and the combination of tebuconazole and the mixture of contaminants in the liver and plasma, in terms of metabolites that exhibited differences between control and treated fish. European eels were exposed to only 10 CECs but are generally exposed to hundreds of these compounds in contaminated aquatic environments. These data allowed an exploration of key metabolites and altered metabolic pathways that may provide greater insights into the physiological function and mechanisms underlying the observed responses.

Acknowledgments: This work has been supported by Grant CIPROM/2021/032 funded by the Conselleria de Cultura, Educació, Universitats i Ocupació (Generalitat Valenciana).

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S2-P15 Use of ceramic passive samplers and HR-MS for the analysis of pharmaceuticals in groundwater samples

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Determining water quality is becoming increasingly important due to the EU's efforts towards environmental protection and the threats to water availability posed by global warming and environmental change. Traditional sampling methods for river and groundwater include grab sampling and the use of autosampler devices. However, these methods only provide a snapshot of contamination at the time of sampling, making them susceptible to spikes and dips in concentration and thus requiring repeated sampling over time. This necessitates exploring alternative sampling methods to obtain a more representative or averaged value of contamination.

One such alternative is the use of ceramic passive samplers (CPSs). These samplers consist in porous ceramic cylinders filled with sorbent material and are deployed for periods ranging from weeks to months in river water or groundwater. Contaminants diffuse slowly through the ceramic membrane and are retained in the sorbent. When the CPS is retrieved, the analytes are extracted and their concentration measured using liquid chromatography-high-resolution mass spectrometry (LC-HRMS). The result is expressed as absolute mass of each analyte in the CPS extract, which corresponds to the amount accumulated during the deployment period. This mass can be converted to ng/L considering the sampling rate of each contaminant.

In this study, CPSs were deployed at 2 well locations in the basin of the Besòs River in Barcelona. The deployment period ranged from 15 to 40 days. The samplers were then extracted and analyzed using targeted LC-HRMS, measuring the uptake of 99 pharmaceuticals, anticorrosion inhibitors, artificial sweeteners and their transformation products. Where diffusion rates were available in the literature, the average concentration in well water was also calculated.

The results show the presence of several contaminants in the groundwaters of Barcelona, among which pharmaceuticals and benzotriazole-based anticorrosion inhibitors stand out. The accumulation of the contaminants increased with deployment time, reaching its maximum after 40 and 28 days in the 2 wells studied, for the majority of contaminants. This shows that the CPSs have high capacity under field conditions, and can be effectively used for extended periods of time as a tool to measure contamination.

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S2-P16 Identification of bisphenol A diglycidyl ether derivatives after *in vitro* digestion process by LC-MS/MS

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Epoxy-based resins, obtained by polymerization between bisphenol A (BPA) and epichlorohydrin, are well-known compounds used for coating applications in canned food (1). Despite their frequent appearance in packaging, this chemical group has arisen as a public concern because of the endocrine disruptor character of their monomer, BPA, along with the possible health effects that their major derivatives may pose on consumers (2).

The objective of this work was to study the gastrointestinal fate of bisphenol A diglycidyl ether (BADGE), the main constituent of the cited resins. An accelerated stability test was performed, simulating the industry storage process of the cans. Moreover, the in vitro digestion protocol INFOGEST (3) was applied to olive oil and tuna samples spiked with BADGE to evaluate the bioaccessibility of the contaminant and analyze its biotransformation into known products as well as non-identified substances.

A suitable chromatographic method was optimized to determine the compounds of interest, using liquid chromatography coupled to tandem mass spectrometry

(LC-MS/MS) to confirm the identity of BADGE and its derivatives in the samples formed after the digestion process using selected reaction monitoring (SRM). The preliminary results revealed the presence of BADGE products with chloride (BADGE.HCl and BADGE.2HCl) as well as water molecules (BADGE.2H2O). Further research should be undertaken to study the effect of different food matrices on the transformation of BADGE, together with the tentative identification of other substances yet unknown.

Acknowledgements:

BACFood4Expo project (PID2020-114569RJ-I00) funded by Spanish Ministry of Science and Innovation under the competitive State R&D Program Oriented to the Challenges of the Society, "R&D Projects 2020" - Modalities "Research Challenges and Knowledge Generation" and ACHED (CNS2022-135887) funded by Spanish Ministry of Science (10.13039/50110001103) and European Union NextGenerationEU/PRTR. Lara Pazos-Soto is grateful to ACHED project for her pre-doctoral contract.

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S2-P17 Risk assessment of the exposure to bisphenols, parabens, benzophenone-3 and triclosan in the Spanish adult population by urinary human biomonitoring

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Bisphenols, parabens, benzophenone-3 and triclosan, synthetic chemicals well-known as potential endocrine-disrupting chemicals (EDCs), are commonly used in various products such as cosmetics, pharmaceuticals and food items. This leads to human exposure through ingestion, dermal contact and inhalation. After entering the body, they are rapidly absorbed, metabolised and excreted predominantly in urine due to their short half-lives. This study employs human biomonitoring (HBM) to assess the internal exposure and associated risks of nine potential EDCs within the Spanish population. The EDCs include three bisphenols (bisphenol A (BPA), bisphenol F (BPF) and bisphenol S (BPS)), four parabens (methyl paraben (MP), ethyl paraben (EP), propyl paraben (PP) and butyl paraben (BP)), benzophenone-3 (BP-3) and triclosan (TCS). This study was conducted within the framework of the BIOMOVAL project, a HBM cross-sectional project (2021) involving a representative sample of the adult population (aged 18 – 65 years) residing in the Valencian Region (Spain). First-morning urine samples were analysed using a dilute-and-shoot method followed by ultra-performance liquid chromatography coupled to tandem mass spectrometry (UHPLC-MS/MS) analysis. The limit of quantification (LoQ) ranged from 0.2 to 0.5 ng/mL. MP exhibited the highest detection frequency (84.5%), followed by BP-3 (78.2%) and BPF (73.8%). In contrast, BP was only found in around 2% of the samples. The highest urinary concentration levels were also presented by MP, with a geometric mean (GM) and 95th percentile (P95) of 1.88 and 54.7 ng/mL, respectively. Finally, the estimated daily intakes (EDIs) were calculated to interpret urinary levels in the context of risk assessment. These were then compared to health-based reference values to determine the corresponding values of the hazard quotient (HQ) or margin of exposure (MOE). According to the obtained values, exposure to BPA and its substitute BPF is considered to pose a public health risk.

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S2-P18 Inexpensive and low-tech sampler to collect time-integrated samples for multi-residue LC-MS analysis of organic contaminants in water

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The TIMFIE (Time-Integrating, Micro-Flow, In-situ Extraction) sampler is an inexpensive and low-tech device designed and optimized to collect time-proportional water samples (50 mL) over one week that is currently in use to monitor pesticides in surface water by the SLU Centre for Pesticides in the Environment. This work aimed to adapt and validate the TIMFIE device for the collection of ≈100 mL water samples over one and three days. For this, temperature-controlled experiments were conducted in the lab with water matrices of different turbidity and total suspended solid concentrations (milli-Q water, surface water, and influent and effluent wastewater) to assess the flow rate entering the device and the reproducibility of the system. Then, the one-day optimized approach was validated for the in-situ extraction of ≈100 emerging organic contaminants, including pharmaceuticals, personal care products, illicit drugs, pesticides, and industrial contaminants, and subsequent analysis with liquid chromatography-tandem mass spectrometry (LC-MS/MS). The results obtained in these experiments will be shown.

Acknowledgments: CP acknowledges grant RYC2020-028901-I funded by MCIN/AEI/10.13039/501100011033 and “ESF investing in your future”. This work is supported by grant PID2022-138229NB-I00 funded by MICIU/AEI/10.13039/501100011033 and ERDF/EU.

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S2-P19 Suspected and non-targeted analysis of environmental contaminants in water and sediments of L'Albufera Natural Park using liquid chromatography-high resolution mass spectrometry

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The widespread release of anthropogenic chemical compounds has significantly contaminated freshwater resources, posing a challenge for detecting contaminants of emerging concern (CECs). Over the past decade, high-resolution mass spectrometry (HRMS) has proven effective in non-target screening (NTS) for analyzing multiple contaminants and identifying CECs. This technique has been especially useful in environmental chemistry for analyzing urban waters, surface water, wastewater, and reclaimed water.

This study aimed to evaluate the presence of pesticides, as they are key contaminants, through target analysis and to identify other CECs and potential transformation products using NTA. Sampling took place in L'Albufera Natural Park in Valencia, Spain, a Mediterranean wetland mainly used for rice cultivation. Monitoring was conducted at 51 points during two campaigns (May-June and September-October) to collect data on pesticides and other CECs in water and sediments. Pesticides were extracted from water samples using solid-phase extraction (SPE) and from sediments using the citrate-buffered QuEChERS method. Analysis was performed using liquid chromatography-HRMS (LC-HRMS) with an Orbitrap Exploris 120 mass spectrometer. Both target and non-target screenings were performed, with the latter utilizing data-dependent MS2 (ddMS2) to the four most intense ions in each cycle.

Quantitative analysis revealed that fungicides constituted a significant portion of detected CECs, accounting for approximately 50% of the total quantified pesticides. Tebuconazole emerged as the predominant fungicide, exhibiting the highest mean concentration (>16935 ng L^{-1}), followed by azoxystrobin and tricyclazole. Non-target screening tentatively identified 16 pesticides, 43 pharmaceuticals and personal care products (PPCPs), 24 industrial compounds, and 12 other CECs with high confidence. Moreover, risk assessment, evaluated through risk quotient calculations based on parent compound concentrations, indicated a decreasing trend towards the outlet, suggesting the wetland's degradation capacity. Nonetheless, significant risk levels persist throughout much of the Natural Park, underscoring the urgent need for mitigation measures to protect the integrity of this vital ecosystem.

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S2-P20 Surveillance of commercial frauds in honey sold in the Italian market by isotope ratio mass spectrometry

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Honey is a natural food product highly appreciated by consumers, as confirmed by the high market demand. However, reduced production and growing costs raise numerous concerns about the authenticity of honey regarding its botanical or geographical origin, as well as adulteration through the addition of sugars.

This study aims to evaluate the incidence of honey frauds in the Italian market through the analysis of carbon isotope ratios δ13C to detect the addition of exogenous sugar. Stable isotope ratio measurement has become a powerful tool in food control, particularly in combating food fraud.

A total of 40 honey samples were analyzed according to the Association of Analytical Communities (AOAC) method 998.12. The honey samples were collected as part of a regular veterinary monitoring plan and represented various types of honey: multifloral and monofloral such us rhododendron, cherry and acacia.

The IRMS DELTA V hyphenate EA IsoLink system (ThermoFisher) was used for isotope analysis. Approximately 1.0-1.4 mg of honey and extracted proteins were loaded into a tin capsule, which were dropped via an autosampler into the reactor where they were burned in the presence of pure oxygen to form CO2 for isotope analysis.

While data analysis is still ongoing, preliminary results indicate compliance with expected values. Specifically, the difference between the δ13C values of proteins and honey is less than 1‰, suggesting the absence of adulteration and confirming the authenticity of the honey samples.

The growing consumer demand of honey needs the constant monitoring of its quality. Through the use of isotope ratio mass spectrometry it is possible to evaluate the incidence of commercial fraud which can negatively affect producers and consumers of honey

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S2-P21 Removal and accumulation of pharmaceutical compounds in sediments and biota of a full-scale constructed wetland

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Pharmaceutically active compounds (PhACs) are emerging pollutants present in several environmental compartments. Constructed wetlands (CW) offer a cost-efficient and eco-friendly solution to remove them from wastewaters. However, few studies have addressed PhACs accumulation in sediments and their uptake by the biota inhabiting CW at full-scale level. The objective of this study was to evaluate the distribution and bioaccumulation of PhACs in a full-scale CW. Sampling was conducted in summer 2023 in Empuriabrava free water surface FWS – CW (Girona, Spain), which operates as tertiary treatment of the municipal wastewater treatment plant. Water, sediments and biota (zooplankton and common reed-Phragmites australis) were collected at 5 treatment stages. Following extraction, 65 PhACs from 9 families (mostly antibiotics, psychiatrics and beta-blockers), were analyzed by liquid chromatography coupled to tandem mass spectrometry. In water, antibiotics concentration significantly decreased along the treatment chain, with total removal of 97%. Psychiatrics showed opposite patterns, reaching a total 46% removal, while beta blockers removal was acceptable (76%). Sediments concentration decreased 78% at final step and they accumulated mostly psychiatrics (moderate to hardly mobile PhACs, according to logKoc). P. australis accumulated PhACs mostly in roots and from the psychiatric family, followed by beta-blockers and then antibiotics. Roots concentrated 10 PhACs when comparing to sediments, and metronidazole, carbamazepine, trazodone, propranolol and levamisole translocated from roots to aerial leaves and stem. In zooplankton, most antibiotics decreased accumulation following treatment chain, but psychiatrics and beta-blockers increased at the final step. Nevertheless, bioaccumulation factors (zooplankton/water concentration) were lower than 1000 L/kg wet weight. The FWS – CW improves the removal of PhACs as tertiary treatment of conventional WWTP, reaching acceptable values for most families and improving treated wastewater quality. Sediments accumulate mostly psychiatrics, decreasing its concentration throughout the treatment chain. P. australis accumulate PhACs mostly in roots and translocate 5 compounds to aerial tissues, which proves the usefulness of the macrophyte in this system. Zooplankton bioaccumulate higher concentrations of PhACs in the final step of CW, which raises concern on possible risk of trophic transfer. However, this topic should be further evaluated, and it was not part if this study.

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S2-P22 NG(A) CASTORE XL iQ: Advanced On-Site Nitrogen Generation for LC-MS Applications

Filippo Bonadonna, *LNI Swissgas Srl*

The NG(A) CASTORE XL iQ nitrogen generator by LNI Swissgas is an advanced system designed for LC-MS (Liquid Chromatography-Mass Spectrometry) applications, providing an innovative solution for laboratories requiring a reliable and efficient nitrogen supply. This poster presents an overview of the generator's key features, benefits, and operating principles.

The generator incorporates a scroll compressor with inverter control to ensure a continuous, on-demand nitrogen supply. This system offers several advantages over traditional nitrogen generators, including reduced energy consumption and maintenance costs. It achieves energy efficiency by generating high-purity nitrogen with lower heat output and reduced air consumption. Additionally, the NG(A) CASTORE XL iQ is oil-free and operates at low noise levels (<50 dB(A)), making it ideal for laboratory environments where quiet operation and minimal vibrations are crucial.

One of the standout features of this generator is its long service intervals, which contribute to lower overall maintenance costs. The compact size of the NG(A) CASTORE XL iQ ensures it can fit easily into laboratory spaces and onto lab benches, allowing for convenient placement near LC-MS instruments.

In terms of methodology, the nitrogen generator uses a scroll compressor design, where two interleaving scrolls—one fixed and the other orbiting eccentrically—create the pressure needed for nitrogen generation. This design, coupled with inverter control, allows the generator to adjust its output according to demand, ensuring an efficient and reliable nitrogen supply for various applications.

The NG(A) CASTORE XL iQ is also equipped with combined outputs, providing nitrogen, dry air, and ultra-high-purity (UHP) nitrogen for collision cells, making it highly versatile for different LC-MS requirements. By delivering precise gas flow and pressure control, this generator addresses the specific needs of LC-MS users, optimizing performance and reducing operational costs.

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