SECYTA 2023

XXII Meeting of the Spanish Society of Chromatography and Related Techniques

S'Arenal, Mallorca, 16-18 OCTOBER 2023

Organised by

SECYTA Sociedad Española de Cromatografía y Técnicas Afines

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WELCOME

Chromatography is a rugged analytical method that has undergone tremendous strides in recent years. Gas and liquid chromatographic methods coupled to mass spectrometry or other detectors are now capable of determining organic molecules over a wide range of volatility and polarity properties, even at trace levels. These analytical techniques provide the necessary tools to meet the societal challenges and demand for monitoring the more than 300,000 organic compounds in common use in our civilization, e.g. their occurrence in the environment, food intake, human exposure and other issues such as transformations by oxidation, photolysis, hydrolysis in the environment or metabolic processes in organisms, including humans.

However, human development is continuously increasing the number and diversity of chemical compounds to fulfill new societal requirements, which in turn increases the demand for better analytical methods with higher sensitivity, accuracy and precision for the understanding of the environmental and human threats posed by the new chemical species. Chromatography is at the cross-road of the analytical methods to meet these needs.

In this XXII Scientific Meeting of the SECyTA we provide an update on the latest advances in gas and liquid chromatography and related techniques. The topics that are welcome in this meeting include (i) developments on the theoretical fundamentals of column separation, (ii) hyphenated techniques and omics, (iii) miniaturization and automation, (iv) imaging, (v) green separation methods, (vi) chemometrics, and (vii) environmental, toxicological, forensic, food and nutritional analysis.

In collaboration with the Spanish Society of Mass Spectrometry there is a session specifically devoted to image applications of MALDI (Matrix-assisted laser desorption/ionization mass spectrometry) in which significant improvements have been reported over the past few years.

Furthermore, a special session is organized to critically discuss potential alternatives available in view of the progressive scarcity and increasing cost of helium, one of the most used gases in gas chromatography.

Last but not least, there are specific presentations devoted to the analysis and identification of micro/nanoplastics, and contaminants of emerging concern associated to them, in marine waters, freshwaters systems, biota and food commodities.

We welcome you all in Mallorca.

Joan O. Grimalt and Manuel Miró

PHILIPPE SCHMITT-KOPPLIN

Technical University of Munich

High resolution tailored metabolomics in the food-nutrition-health continuum

Prof. Ph. Schmitt-Kopplin's team performs tailored and comprehensive metabolomics in the food-health continuum. He has a strong profile in analytical chemistry with integrated approaches combining (ultra) high resolution mass spectrometry, (μ)separation sciences, NMR-spectroscopy with (bio)informatics for the description of complex organic systems on a molecular level. A focus in the last decades was to implement ultrahigh resolution mass spectrometry into cross-Omics applications and for a rapid and robust tool for deep metabotyping and small molecules profiling. His focus is the chemical understanding of microbiomes in foods, health and environments and integrating these information with existing biological Omics data. His interdisciplinary studies are related to the interface of chemistry and biology. He is director of the research unit analytical BioGeoChemistry of the Helmholtz Munich and heads the Comprehensive Foodomics Platform at the Institute of analytical Food Chemistry of the Technische University Munich Germany.

LARS WÖRMER

MARUM – Center of Marine Environmental Sciences, University of Bremen

Reading the fine print: mass spectrometry imaging of molecular fossils in geological samples

Lars Wörmer is a senior researcher at MARUM – Center of Marine Environmental Sciences, University of Bremen (Germany). He holds a MSc in Environmental Sciences and a PhD from Universidad Autónoma de Madrid (Spain). Lars is especially interested in chemical signatures archived in marine or lacustrine sediments, i.e., molecular fossils. These molecules can inform on past climate, but also on changes in terrestrial or marine ecosystems. In the last years, he has pioneered the implementation of Mass Spectrometry Imaging (MSI) in the Earth Sciences and is currently the scientific leader of the Geobiomolecular Imaging Laboratory at the University of Bremen. MSI of molecular fossils allows to map their distribution in the sedimentary archive with micrometer-resolution and thus to explore these records with unprecedented resolution and detail. As a result, climate and environmental reconstructions can now be performed at time scales (seasons to decades) extremely relevant from a human and ecosystem perspective.

PAVEL KUBÁŇ

Czech Academy of Science

Capillary electrophoresis as an all-in-one tool for the fully autonomous pretreatment and analysis of dried blood spots

Pavel Kubáň graduated in Chemistry and Mathematics from Masaryk University, Brno, Czech Republic, obtained his Doctor of Philosophy degree from Mendel University, Brno, Czech Republic, Doctor of Science degree from Palacký University, Olomouc, Czech Republic, and Researcher Professor degree from the Czech Academy of Sciences. Currently, he is the Head and the Leading Scientist at the Department of Electromigration Methods at the Institute of Analytical Chemistry of the Czech Academy of Sciences.

His work is devoted mainly to capillary electrophoresis, liquid phase microextraction techniques and their coupling for direct analyses of complex samples. Recently, his research activities focused on the analysis of dried material spots, such as dried blood and dried urine spots. He is author of more than 110 scientific papers, reviews and book chapters and 70 contributions on scientific conferences. He is a member of the editorial board of the Separation Science Plus (Wiley), Talanta Open (Elsevier), and Journal of Pharmaceutical Analysis (Elsevier) journals. He is also the Head of the Science Council of the Institute of Analytical Chemistry, a member of the Science Council of the Czech Academy of Sciences and a member of the Czech Science Foundation committee for Analytical Chemistry.

RAFAEL LUCENA

University of Cordoba

Biopolymer-based sorptive phases into stainless steel needles: microextraction and ambient mass spectrometry analysis in a single device

Dr. Rafael Lucena Rodríguez is full professor in the Department of Analytical Chemistry at the University of Córdoba and member of the "Affordable and Sustainable Sample Preparation" research group. His research lines focus on analytical sample treatment (development of new extraction techniques and materials) and their direct coupling with instrumental techniques (vibrational spectroscopic techniques and mass spectrometry). He has participated in 16 research projects being Principal Investigator in four of them. He is co-author of 124 scientific papers and 22 book chapters. He has co-edited the book "Analytical Sample Preparation with Nano- and other High-performance Materials" (Elsevier, 2021). He is the author of three patents of invention and has participated in several R&D contracts. He has actively participated in the training of new researchers, directing 9 theses already presented and 4 in progress.

He has acted as evaluator of research projects and researcher contracts for the Spanish Research Agency. He has also acted as evaluator of projects for the National Commission for Scientific and Technological Research (Chile) and the Czech Science Foundation (Czech Republic).

He is currently secretary of the Chemical Institute for Energy and Environment (IQUEMA) of the University of Cordoba and associate editor of the journal "Advances in Sample Preparation" (Elsevier).

ANA MARIA AGÜERA

University of Almeria

Target and suspect analysis of contaminants of emerging concern in water reuse practices: challenges and future perspectives

Prof. Dr. Ana Agüera is full professor in Analytical Chemistry at the University of Almería and leader of the Environmental Analysis Unit at the Solar Energy Research Centre (CIESOL). Her research focuses on the application of low and high-resolution mass spectrometry to the identification and fate of emerging contaminants and their transformation products in the aquatic environment, as well as the analytical assessment of advanced wastewater treatment processes applied to complex effluents to get their regeneration and enable their reuse. She is especially interested in the study of the impact of reclaimed water reuse in the agricultural environment (water-soil-plant nexus). She is co-author of 2 patents and 175 scientific publications (h-index 66). For her research work, she has been included in the U. Stanford world ranking "The World Scientists: World's Top 2% Scientists (in 2020 and 2022)", "Analytical Chemistry" area.

OY-7
Perfluoroalkyl substances in striped dolphins (Stenella coeruleoalba) from the NW Mediterranean Sea: Biomagnification and temporal trends (1990-2021)

Odei Garcia-Garin [1], Asunción Borrell [1], Pere Colomer-Vidal [2], Morgana Vighi [1], Núria Trilla-Prieto [3], Alex Aguilar [1], Manel Gazo [1], Begoña Jiménez [2]

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Poly- and Perfluoroalkyl Substances (PFAS) are widely recognized as a class of pollutants known for their ability to bioaccumulate and biomagnify in the environment. In this study, the objective is to determine the biomagnification rates of PFAS in sexually mature striped dolphins and assess the temporal trends of PFAS concentrations over the past three decades (1990-2021) in the North-Western Mediterranean Sea. Thirteen out of the 19 targeted PFAS compounds were detected in the digestive content of the dolphins, while all 17 PFAS compounds were detected in the liver samples. Concentrations of PFAS in the digestive content ranged from 50 to 1611 ng/g, while the liver samples showed concentrations ranging from 268 to 7014 ng/g. The most prevalent compounds found in both types of samples were linear perfluorooctanesulfonic acid (n-PFOS) and perfluorooctanesulfonamide (FOSA), which were present in all samples. Additionally, perfluoroundecanoic acid (PFUnDA), perfluorotridecanoic acid (PFTrDA), and perfluorononanoic acid (PFNA) were also detected in significant quantities. Interestingly, the study found that long-chain PFAS compounds exhibited greater biomagnification rates compared to short-chain PFAS compounds in striped dolphins. This suggests a potential impact on the health of these marine mammals due to the accumulation of long-chain PFAS in their systems. The analysis of the samples indicated that half of the digestive content samples exceeded the Environmental Quality Standards (EQS) concentrations, indicating that the consumption of polluted prey may pose health risks for striped dolphins. When examining the temporal trends, the concentrations of most long-chain PFAS compounds showed an increase from 1990 to 2004-2009. However, concentrations appeared to stabilize during the period of 2014-2021, potentially reflecting the impact of country regulations and industry initiatives aimed at reducing PFAS pollution. These findings underscore the persistent presence of banned PFAS compounds in the marine ecosystem and highlight the need for ecological risk assessments and the development of management strategies to mitigate PFAS pollution in marine environments. In conclusion, this study provides valuable insights into the biomagnification rates of PFAS in striped dolphins and highlights the persistent nature of these pollutants in the North-Western Mediterranean Sea. The identification of specific PFAS compounds and their temporal trends contribute to the understanding of PFAS pollution and support future efforts in assessing ecological risks and implementing effective management strategies in marine ecosystems.

Acknowledgements
The authors thank the MCIN/AEI/10.13039/501100011033 and FSE "El FSE invierte en tu futuro" for supporting O. Garcia-Garin with a Ph.D. FPU scholarship (FPU17/00073).

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