



XXIII MEETING OF THE SPANISH SOCIETY OF CROMATOGRAPHY AND RELATED TECHNIQUES

Pamplona, 23-25 October 2024

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WELCOME

Dear colleagues and friends,

Welcome, everyone, to Pamplona and to the XXIII Meeting of the Spanish Society of Chromatography and Related Techniques (SECyTA). We are also pleased to welcome you to the School of Pharmacy and Nutrition at the Universidad de Navarra.

This event provides us with the opportunity to once again share days filled with science, collaboration, and friendship. We have organized this meeting with great enthusiasm, and the members of the Organizing and Scientific Committees are confident that it will be both interesting and stimulating for all of you.

The topics to be addressed at the conference are as follows: T1: New developments in analytical instrumentation/detection systems, T2: Fundamentals on chromatography and electro-driven separations, T3: Sample preparation methods, T4: Environmental and industrial analysis, T5: Biological, toxicological, and forensic analysis, T6: Food and nutritional analysis and T7: Chemometrics, data processing, and omics techniques.

In addition, a special session has been organized to discuss the potential, possibilities, and opportunities that Artificial Intelligence offers for chromatographic techniques.

For all of us dedicated to chromatography and related techniques, this is a chance to share our latest research and connect with national and international speakers, as well as company representatives who will present new tools to address current challenges. Additionally, we will have opportunities to discuss, ask questions, learn, and conceive new lines of research, collaborations, and projects.

A special welcome goes to our early-career researchers, who represent the future of our field. We trust that these meeting days will offer them new perspectives, ideas, and professional connections.

We extend our gratitude to the companies supporting us and to everyone who has contributed in various ways to the organization of this event.

In addition to the scientific program, we have organized social activities that will allow you to experience the city and, of course, its rich gastronomy.

For all these reasons, we hope everyone takes full advantage of and enjoys these days in Pamplona.

On behalf of the local organizing committee

Elena González Peñas and Elena Lizarraga Pérez

ORGANIZING COMMITTEE

Elena González Peñas, *Chairwoman*

Universidad de Navarra

Elena Lizarraga Pérez, *Chairwoman*

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(IRNASE-CSIC)

Mario Fernández Martín

Instituto de Química Orgánica
General (IQOG-CSIC)

Marta Lores Aguilín

Universidad de Santiago de
Compostela

INVITED SPEAKERS



JOSÉ BERNAL DEL NOZAL

University of Valladolid

Determination of contaminants in bee products by using chromatographic techniques

José Bernal del Nozal is full Professor in Analytical Chemistry and head of TESEA group, University of Valladolid, has contributed for expanding the knowledge about some relevant issues such as food safety and quality, including the analysis of contaminants and bioactive compounds, and in development of new analytical strategies, especially those that involved green chemistry. In the last years, he has mainly worked in the apiculture area, especially in developing new strategies for determining pesticides and bioactive compounds in bee products.

During his scientific career, he has worked with several analytical separation techniques as HPLC, GC, CE and SFC. He has also contributed as author/co-author to more than 120 scientific publications (H-index of 29), 90 congress presentations, 6 book chapters, and 1 patent. In addition, he has also participated as Principal Researcher/Researcher in 17 research projects or contracts with various industries and government agencies. He is also an Associate Editor of Food Analytical Methods, and member of the Editorial Board of several journals as Journal of Food Composition and Analysis, Foods, Separations, Measurement: Food, and Molecules. Finally, he has also have supervised 4 PhD thesis, and he is currently supervising three more, and he has been also selected for the evaluation of national and international projects.

INVITED SPEAKERS



JENNIFER KIRWAN

Charité University Hospital

The metabolome and the immune system; why good chromatography matters!

Dr. Kirwan started her career as a clinical veterinarian where she became increasingly interested in translational and evidence based medicine before undertaking a PhD in metabolomics. She now heads the Berlin Institute of Health Metabolomics Platform at Charité University Hospital in Berlin, where she focuses on translational health-related metabolomics, especially on its quality management aspects. She is particularly interested in the gut-brain-heart health triad and how the microbiome influences health.

She is a founding member of the German Metabolomics Society, a Central Committee member of the international Metabolomics quality assurance and quality control consortium (MQACC) and is an active member of the Precision Medicine and Pharmacogenomics working group of the International Metabolomics Society.

INVITED SPEAKERS



GABRIEL VIVÓ-TRUYOLS

Tecnometrix

Chromatographic big data analysis using Bayesian statistics: finding alternative ways to automation

Gabriel Vivó-Truyols (1975) studied analytical chemistry at the University of Balearic Islands (Spain) and graduated in 1998. In 2004 he obtained his PhD with honours from University of Valencia (Spain) on chemometrics methods for optimization and data treatment of HPLC. His PhD dealt with the development of novel methods for optimization and data treatment in HPLC, and was awarded with the D.L. Massart award in chemometrics from the Belgian Chemometrics society in 2006, given every two years to the best PhD thesis in chemometrics, world-wide. In 2004 he joined the team of Peter Schoenmakers (University of Amsterdam), where he developed a research program focused on chemometric techniques for optimization, calibration and data-treatment of two-dimensional chromatographic methods. In 2007 he joined the analytical chemistry team at BP in Sunbury (London area). He worked as chemometric specialist developing algorithms and software for GCxGC analysis of petroleum subproducts, as well as developing chemometrics methods for on-line infra-red analysis. In 2009 he re-joined the analytical-chemistry group of Peter Schoenmakers at University of Amsterdam as assistant professor. He left in 2017, establishing his own consultancy (based in Spain) in data analysis for chromatography and spectroscopy. With 20+ years of teaching experience at 4 different universities in this subject, Gabriel is currently scientific consultant for major multinationals in the area of data analysis, including BP, Castrol, BASF, Merck and Agilent technologies, as well as a collaborator with the university of Pardubice (Holcapek group) and member of the United States Pharmacopeia (where he is chair of the chemometrics joint subcommittee). Gabriel Vivó-Truyols has co-authored more than 60 papers, besides a book (in the making) covering the interface of chemometrics & chromatography.

INVITED SPEAKERS



FREDERIC BÉEN

Vrije Universiteit and KWR Water Research Institute

Novel developments to monitor environmental contaminants and their transformation products in the aquatic environment using high-resolution mass spectrometry and data science

Dr. Frederic Béen is an Assistant Professor in the Chemistry for Environment & Health research group at the Amsterdam Institute for Environment and Health (A-LIFE) of Vrije Universiteit Amsterdam. He also serves as a Senior Scientist at KWR Water Research Institute in the Water Quality and Health research group. Frederic's work focuses on developing and enhancing suspect and non-target screening applications to monitor a wide range of environmental contaminants.

His research explores how chromatography (LC and GC) and HRMS, along with data analysis pipelines, to better understand the source, fate, and impact of contaminants on humans and the environment. This involves developing cheminformatics and data analysis tools, such as chemometrics and machine learning, to analyse large sets of chemical and mass spectrometric data. Frederic's research includes applying these techniques to human biomonitoring, effect-directed analysis (EDA), and micro- and nanoplastic analysis. He also explores wastewater-based epidemiology (WBE) to monitor and assess community health through wastewater analysis.

Frederic co-leads the effect-directed analysis working group in the NORMAN network and is the deputy co-leader of Task 4.3 in the European Partnership for the Assessment of Risk from Chemicals (PARC), focusing on innovative methods to monitor contaminants in humans and the environment.

INVITED SPEAKERS



CECILIA GAGLIERO

Univerità degli Studi di Torino

Going greener in analytical extraction for a sustainable characterization of natural products

Cecilia Cagliero (Scopus h-index 28) is Associate Professor in Pharmaceutical Biology at the Department of Drug Science and Technology of the University of Turin (Italy). She obtained her BSc degree in Drug Chemistry and Technology from the University of Turin in 2006 and the PhD degree in Science and High Technology from the same University in 2010.

In 2016, she was a Visiting Professor at the Chemistry Department of Iowa State University (USA). Her research focuses on the development of advanced approaches for the characterization of volatile and non-volatile fractions from plants and natural products.

At the 2016 International Symposium on Capillary Chromatography, she received the Leslie Etre award (given to a scientist 35 years of age or younger who presented the most interesting original research in the field of capillary gas chromatography) for her presentation on the measurement of acrylamide in coffee powder using gas chromatography/mass spectrometry (GC/MS). In October 2018, she was included in The Analytical Scientist magazine's «Top 40 Under 40 Power List», which aims to identify talented young scientists who are making waves in analytical science.

PROGRAM

WEDNESDAY, 23th October 2024

08:30-09:00 **Registration**

09:00-09:30 **Opening Ceremony**

09:30-10:15 **Opening Plenary Lecture**

Chairs:

Ana María García Campaña, University of Granada

Elena González-Peñas, Universidad de Navarra

PL-1: José Bernal del Nozal

University of Valladolid

Determination of contaminants in bee products by using chromatographic techniques (T6)

10:15-11:00 **Oral Communications (OC-Session 1)**

Chairs:

Ana María García Campaña, University of Granada

Elena González-Peñas, Universidad de Navarra

10:15-10:30 Edmondo Messinese (OC-01)

Optimization of an innovative approach for green extraction of bioactive compounds from artichoke and tomato by-products (T6)

University of Parma

10:30-10:45 Jaume C. Morales (OC-02)

Quantitation of over 1,000 pesticide residues in tomato according to SANTE 11312/2021 guideline (T6)

Agilent Technologies

10:45-11:00 Teresa Páramo-Soto (OC-03)

Comprehensive analysis of (poly)phenols in artichoke hearts, stems, bracts and leaves as a base for agro-industrial by product revalorization (T6)

Universidad de Navarra

11:00-12:00 **Poster Session 1 (P1-P15) & Coffee Break & Exhibition**

12:00-13:00 Oral Communications (OC-Session 2)*Chairs:**Mario Fernández Martín, Institute of General Organic Chemistry
Jordi Díaz Ferrero, Chemical Institute of Sarriá, Ramon Llull University***12:00-12:15** Julio Lluch (OC-04)

One analyzer, multiple solutions: from MOSH, MOAH, pesticides, and beyond (T6)

*LECO Spain&Portugal***12:15-12:30** Eva Gallego (OC-05)

Evaluation of potential sample contamination during volatile organic compounds (VOCs) active air sampling (T4)

*Universitat Politècnica de Catalunya***12:30-12:45** Águeda Sánchez-Martín (OC-06)

Adsorption capacity of emerging organic pollutants by activated biocarbons from agricultural waste (T4)

*Instituto de Recursos Naturales y Agrobiología de Sevilla (IRNAS-CSIC)***12:45-13:00** Núria Fontanals (OC-07)

Wastewater based epidemiology approach to assess pharmaceutical consumption in Spain (T4)

*Universitat Rovira i Virgili***13:00-13:45 Plenary Lecture***Chairs:**Mario Fernández Martín, Institute of General Organic Chemistry
Jordi Díaz Ferrero, Chemical Institute of Sarriá, Ramon Llull University***PL-2: Jennifer Kirwan***Charité University Hospital*

The metabolome and the immune system; why good chromatography matters! (T7)

13:45-15:15 Lunch Break

15:15-16:15 Oral Young Researchers Communications (OY-Session 1)

Chairs:

Juan Vicente Sancho Llopis, University Jaume I

Francisco Javier Santos Vicente, University of Barcelona

15:15-15:25 Mikaela Rajchman (OY-01)

Chemical characterization of the valorized winery by product *Vitis vinifera* L. cv. Tannat pomace by comprehensive two-dimensional liquid chromatography (LC x LC) (T6)

Institute of Food Science Research - CIAL (CSIC-UAM)

15:25-15:35 Marta Rivas Piña (OY-02)

Extraction of safranal and crocins from *Crocus sativus* using neoteric solvents (T6)

Instituto de Química Orgánica General (IQOR-CSIC)

15:35-15:45 Miriam González-Hernández (OY-03)

Untargeted lipidomics by UHPLC-IMS-QTOF MS for diet intake biomarkers discovery in *Sparus aurata* fish (T6)

Research Institute for Pesticides and Water, University Jaume I

15:45-15:55 Sergi Gregorio-Lozano (OY-04)

Assessment of persistent, mobile and toxic compounds uptake in escarole and tomato plants irrigated with contaminated water in a greenhouse (T6)

Research Institute for Pesticides and Water, University Jaume I

15:55-16:05 Cristian González-Jiménez (OY-05)

Study of whey proteins and caseins behaviour in a nades aqueous biphasic system. Resolving discrepancies in UV and Capillary Electrophoresis results (T3)

Instituto de Química Orgánica General (IQOG- CSIC)

16:05-16:15 Melis Cokdinleyen (OY-06)

Sustainable red seaweed biorefinery: ultrasound, pressurized liquid extraction, and natural deep eutectic solvents integration (T3)

Instituto de Investigación en Ciencias de la Alimentación CIAL (CSIC-UAM)

16:15-17:15 **Poster Session 2 (P16-P29) & Coffee Break & Exhibition**

17:15-17:40 **Poster Flash Discussion Session (PF-Session 1)**

Chairs:

Joan O. Grimalt Obrador, Institute of Environmental Assessment and Water Research

Belén Gómara Moreno, Institute of General Organic Chemistry

17:15-17:20 Araceli Rivera-Pérez (P53)

Identification of key markers revealing the sterilization impact on paprika: Liquid-Chromatography-High-Resolution Mass Spectrometry as a powerful tool (T7)

Universidad de Almería

17:20-17:25 Albert Sales-Alba (P19)

Development of an analytical method of PBDD/Fs in emissions samples (T4)

IQS School of Engineering (URL)

17:25-17:30 Natalia Rodriguez Murillo (P20)

Development of analytical techniques for monitoring PFAS in aquatic environments (T4)

Institut Químic de Sarrià

17:30-17:35 Francisco Soria Prieto (P21)

Method development to the determination of gadolinium contrast agents in peat samples (T4)

Research Institute for Pesticides and Water, University Jaume I

17:35-17:40 Pol Clivillé Cabré (P26)

Chiral determination of amphetamine-type substances in environmental waters by Solid Phase Extraction followed by Capillary Electrophoresis-tandem Mass Spectrometry (T4)

Universitat Rovira i Virgili

17:45-19:30 **SECyTA General Assembly**

20:30 **Welcome Cocktail**

THURSDAY, 24th October 2024

09:00-09:45 **Plenary Lecture**

Chairs:

José A. González Pérez, IRNAS-CSIC

Iziar A. Ludwig Sanz-Orrio, Universidad de Navarra

PL-3: Frederic Béen

Vrije Universiteit and KWR Water Research Institute

Novel developments to monitor environmental contaminants and their transformation products in the aquatic environment using high-resolution mass spectrometry and data science (T4)

09:45-11:00 **Oral Communications (OC-Session 3)**

Chairs:

José A. González Pérez, IRNAS-CSIC

Iziar A. Ludwig Sanz-Orrio, Universidad de Navarra

09:45-10:00 Monsalud del Olmo-Iruela (OC-08)

Toxic cyanopeptide monitoring in thermal spring water by capillary electrophoresis tandem mass spectrometry (T4)

University of Granada

10:00-10:15 Pedro Cano (OC-09)

From known to unknown in Mass Spectrometry: an example with PFAS challenge (T1)

Bruker Española S.A.

10:15-10:30 Enriqueta Anticó (OC-10)

New polymeric films and advanced configurations for in-situ extraction of organic pollutants (T3)

Universitat de Girona

10:30-10:45 Michael Soll (OC-11)

“Up in the air, deep on the ground” quantification & identification of microplastics in marine sediments and air by Pyrolysis-GC/MS (T1)

Frontier Laboratories Europe

10:45-11:00 Borja Peris-Camarasa (OC-12)
 Fast and eco-friendly analytical method to determine bisphenols, parabens, benzophenone-3 and triclosan in human urine by Ultra-Performance Liquid Chromatography coupled to Mass Spectrometry (T3)
Foundation for the Promotion of Health and Biomedical Research in the Valencian Region, FISABIO – Public Health

11:00-12:00 Poster Session 3 (P30-P43) & Coffee Break & Exhibition

12:00-12:45 Oral Communications (OC-Session 4)

Chairs:

Núria Fontanals Torroja, Universitat Rovira i Virgili

Elena Lizarraga Pérez, Universidad de Navarra

12:00-12:15 Santiago Nicolás Otaiza-González (OC-13)
 Antibiotic occurrence and environmental risks assessment in a recirculating aquaculture system (T4)
Institut Català de Recerca de l'Aigua (ICRA-CERCA)

12:15-12:30 Jaap de Zeeuw (OC-14)
 Liner selection in Gas Chromatography (T2)
CreaVisions

12:30-12:45 Martí Rosés (OC-15)
 Characterization of HPLC sorbents and solvents: a comparison of Tanaka and Abraham methods (T2)
Universitat de Barcelona

12:45-13:45 Round Table on Artificial Intelligence and Chromatography

Chair:

Ángel Irigoyen Barrio, Universidad de Navarra

Panelists:

Ivan Cordón Medrano, DATAI, Universidad de Navarra

Ángel Ursúa Sesma, Tairtel Data

Jaume C. Morales, Agilent Technologies

Marta Burrull, Waters

13:45-15:15 Lunch Break

15:15-16:00 Plenary Lecture

Chairs:

Begoña Jiménez Luque, Institute of General Organic Chemistry

Marta Lores Aguín, University of Santiago de Compostela

PL-4: Gabriel Vivó-Truyols

Tecnometrix

Chromatographic big data analysis using Bayesian statistics: finding alternative ways to automation (T7)

16:00-16:25 Poster Flash Discussion Session (PF-Session 2)

Chairs:

Begoña Jiménez Luque, Institute of General Organic Chemistry

Marta Lores Aguín, University of Santiago de Compostela

16:00-16:05 Sandra Adámez-Rodríguez (P05)

L-Arginine based chiral ionic liquids for the enantiomeric analysis of amino acids by Electrokinetic Chromatography and Ligand Exchange Capillary Electrophoresis. A comparative study (T2)

Universidad de Alcalá

16:05-16:10 Patricia González Palacios (P31)

Determination of obesogens in biological samples and their relationship to childhood overweight/obesity (T5)

University of Granada

16:10-16:15 Cristian González Jiménez (P32)

Therapeutic monoclonal antibodies analyzed by Capillary Electrophoresis with SDS (T5)

Instituto de Química Orgánica General (IQOG-CSIC)

16:15-16:20 Águeda M. Sánchez-Martín (P36)

Chromatographic analysis of the impact of organic amendments on the composition of soil and fruit in superintensive olive orchards (T6)

Instituto de Recursos Naturales y Agrobiología de Sevilla (IRNAS-CSIC)

16:20-16:25 Marta Díez (P46)

Extraction and characterization of bioactive carbohydrates and phenolics from phytoplankton holobionts (T6)

Instituto de Química Orgánica General (IQOG-CSIC)

16:25-17:25 **Poster session 4 (P44-P56) & Coffee Break & Exhibition**

17:25-18:05 **Oral Young Researchers Communications (OY-Session 2)**

Chairs:

Núria Fontanals Torroja, Rovira i Virgili University

Jordi Díaz Ferrero, Chemical Institute of Sarrià, Ramon Llull University

17:25-17:35 Irene Romero-Alfano (OY-07)

Optimization of large volume solid phase extraction (LV-SPE) for toxicological assessment of pharmaceuticals in treated waters from Costa Brava (T5)

Institut Químic de Sarrià

17:35-17:45 Aly Castillo (OY-08)

Transit and bioconversion of polyphenols in the digestive and circulatory systems of broilers fed on grape marc-feed (T5)

Universidade de Santiago de Compostela

17:45-17:55 Laura Solé-Domènech (OY-09)

Determination of high production volume chemicals and polycyclic aromatic hydrocarbons in particulate matter by thermal desorption coupled to gas chromatography and mass spectrometry (T4)

Universitat Rovira i Virgili

17:55-18:05 Antonia Merola (OY-10)

Analytical approach for determination of tire rubber additives and their transformation products in silicone bands (T3)

Institute of Environmental Assessment and Water Research (IDAEA-CSIC)

19:45 **Conference Dinner**

FRIDAY, 25th October 2024

09:30-10:15 Oral Communications (OC-Session 5)

Chairs:

Begoña Jiménez Luque, Institute of General Organic Chemistry

Juan Vicente Sancho Llopis, University Jaume I

09:30-09:45 Pere Colomer-Vidal (OC-16)

Long-term evaluation (2003-2022) of PFAS regulation through Scopoli's Shearwaters (*Calonectris diomedea*) from the Western Mediterranean Basin (T4)

Institute of Organic Chemistry (IQOG-SCIC)

09:45-10:00 Xavier Ortíz Almirall (OC-17)

Calibration and deployment of SPATT passive samplers for cyanotoxins analysis in freshwater by isotope dilution-direct water injection LC-MS/MS (T4)

IQS - Universitat Ramon Llull

10:00-10:15 José A. González-Pérez (OC-18)

A strategy to assess soil organic matter quality and explore processes and humification drivers by Direct Analytical Pyrolysis (PY-GC/MS) and Evolved Gas Analysis (EGA-MS) (T4)

IRNAS-CSIC

10:15-11:00 Plenary Lecture

Chairs:

Begoña Jiménez Luque, Institute of General Organic Chemistry

Juan Vicente Sancho Llopis, University Jaume I

PL-5: Cecilia Cagliero

University of Turin

Going greener in analytical extraction for a sustainable characterization of natural products (T3)

11:00-11:30 **Coffee Break**

11:30-12:45 **Oral Communications (OC-Session 6)**

Chairs:

Ana María García Campaña, University of Granada

Elena González-Peñas, Universidad de Navarra

11:30-11:45 Sara Moreno-Talavera (OC-19)

Systematic evaluation of the metabolome of polar compounds in two sepsis liver models using multiplatform chromatographic techniques coupled to high-resolution mass spectrometry (T7)

Universidad San Pablo-CEU

11:45-12:00 Mercè Garí (OC-20)

Occurrence of tire rubber additives in a natural environment characterized by high wheel traffic (T5)

Institute of Environmental Assessment and Water Research (IDAEA-CSIC)

12:00-12:15 Raúl Alva (OC-21)

Simplified methodology for the analysis of polycyclic aromatic hydrocarbons metabolites in urine. Exposure assessment in children and firefighters (T5)

Institute of Environmental Assessment and Water Research (IDAEA-CSIC)

12:15-12:30 Araceli Rivera-Pérez (OC-22)

Metabolomics based on Liquid-Chromatography-High-Resolution Mass Spectrometry reveals key markers to authenticate the botanical origin of honey (T7)

Universidad de Almería

12:30-12:45 Lucas L. Alonso (OC-23)

Occurrence of wastewater-derived contaminants in two irrigation water systems, and their fate into agricultural soils: spatial analysis and soil risk assessment (T4)

Institut Català de Recerca de l'Aigua (ICRA-CERCA)

12:45-13:45 **Closing and Awards Ceremony**

13:45 **Farewell Lunch**

T1. New developments in analytical instrumentation/detection systems

P01-Upgrading an analytical method for the determination of PMT and vPvM substances in groundwater

N. Sáez-Rosique, J. Ma, T. Garrido, M. Exposito, J. Fraile, J. Mas-Pla, J. Radjenovic, M. Gros, S. Rodriguez-Mozaz
Catalan Institute for Water Research (ICRA)

T2. Fundamentals on chromatography and electro-driven separations

P02-Understanding the partition of solutes in columns that mimic biological processes through the Abraham solvation parameter model

Susana Amézqueta, Ana Lucía Valdez, Elisabeth Fuguet, Martí Rosés
Universitat de Barcelona

P03-Chromatographic selectivity in reversed phase and HILIC columns

Xavier Subirats, Ester Lopera, Martí Rosés
Universitat de Barcelona

P04-Biomimetic chromatography: characterization of micellar and microemulsion electrokinetic systems by a fast LFER approach

Rabia Idrees, Xavier Subirats, Susana Amézqueta, Martí Rosés
Universitat de Barcelona

P05-L-Arginine based chiral ionic liquids for the enantiomeric analysis of amino acids by electrokinetic chromatography and ligand exchange capillary electrophoresis. A comparative study

Sandra Adámez-Rodríguez, María Luisa Marina, María Castro-Puyana
Universidad de Alcalá

P06-Global versus individual models to describe retention with isocratic and gradient experiments in RPLC

J.R. Torres-Lapasió, P. Peiró-Vila, M. Blázquez-Mateu, M.C. García-Alvarez-Coque
Universitat de València

P07-Use of individual and global retention models in serial coupling of columns for enhanced selectivity in RPLC

M.C. García-Alvarez-Coque, P. Peiró-Vila, M. Blázquez-Mateu, J.R. Torres-Lapasió
Universitat de València

P08-Combination of sodium dodecylsulfate and 1-hexyl-3-methylimidazolium chloride as mobile phase additives

M.C. García-Alvarez-Coque, C.J. Tereba-Mamani, M.J. Ruiz-Ángel
Universitat de València

T3. Sample preparation methods

P09-Application of the theory of solubility of Hansen to the selection of green solvents for the selective extraction of polychlorinated biphenyls from complex biotic samples

Belén Gómara, Lourdes Ramos
Instituto de Química Orgánica General (IQOG-CSIC)

P10-Natural eutectic solvent screening by Cosmo-RS for the selective bisphenol extraction from soft drinks

Luz Alonso-Dasques, Plácido Galindo-Iranzo, Rosa Lebrón-Aguilar, Belén Gómara, Jesús E. Quintanilla-López
Instituto de Química Física Blas Cabrera (IQF-CSIC)

P11-Efficient removal of natural deep eutectic solvents in extracts: Enhancing purity and bioactivity of bioactive compounds

Victor M. Amador-Luna, Miguel Herrero, Carlos Pajuelo, Elena Ibañez, Lidia Montero
Institute of Food Science Research - CIAL (CSIC-UAM)

P12- Comprehensive analysis of pesticide and fungicide levels in air and urine samples in agricultural areas. Pilot study

Natalia Bravo, Clara Jaén, Barend van Drooge, Joan O. Grimalt
Dept. Environmental Chemistry. Institute of Environmental Assessment and Water Research (IDAEA-CSIC)

P13-Hypercrosslinked sulfonated core shell particles for the selective extraction of pharmaceuticals in environmental samples

Rosa M. Marcé, Alberto Moral, Francesc Borrull, Peter A. G. Cormack, Núria Fontanals
Universitat Rovira i Virgili

P14-Unveiling the role of char incorporated in a poli ϵ -caprolactone polymer thin film for steroid hormones microextraction

Francesca Merlo, Vincenzo Cerviani, Antonella Profumo, Andrea Speltini, Alba Cabrera, Clàudia Fontàs, Enriqueta Anticó
University of Girona

P15-Computational assessment of monoterpenoids for a sustainable remediation of sulfonamides in water

Ana Ariza-Díez, Plácido Galindo-Iranzo, Rosa Lebrón-Aguilar, Belén Gómara, Jesús E. Quintanilla-López
Instituto de Química Física Blas Cabrera (IQF-CSIC)

T4. Environmental and industrial analysis

P16-Bioaccumulation and depuration of three common antibiotics in benthic organisms: sea cucumber, snakelocks anemone and beadlet anemone

Alberto Zafra-Gómez, María del Carmen Gómez-Regalado, Julia Martín, Félix Hidalgo, Juan Luis Santos, Irene Aparicio, Esteban Alonso
University of Granada

P17-Analytical method for the accurate determination of polycyclic aromatic hydrocarbons in black tattoo ink

Juan José Ramos, Sara González, Oscar Fernández, Cristina Grande, Ana Rodríguez, Marta Esteban-López, Ana Cañas-Portilla
Centro Nacional de Sanidad Ambiental, Instituto de Salud Carlos III (ISCIII)

P18-Strategies and routine analysis of PFASs by UHPLC tandem Mass Spectrometry UHPLC-MS/MS during drought periods

Guillem Carrera Ruiz, Aniol Roca Rodríguez, Maria Rosa Boleda Vall-Llobera
Aigües de Barcelona EMGCIA

P19-Development of an Analytical Method of PBDD/Fs in Emissions Samples

Albert Sales-Alba, Xavier Ortiz Almirall, Jordi Díaz-Ferrero
IQS School of Engineering (URL)

P20-Development of analytical techniques for monitoring PFAS in aquatic environments

Natalia Rodriguez Murillo, Marc Marín-García, Núria Agulló Chaler, Jordi Díaz-Ferrero, Cristian Gómez-Canela
Institut Químic de Sarrià, Universitat Ramon Llull

P21-Method development to the determination of gadolinium contrast agents in peat samples

Francisco Soria Prieto, Antoni Francesc Roig i Navarro, Raúl García Cubedo
Research Institute for Pesticides and Water, University Jaume I

P22-Pharmaceutically active compounds (PhACs) in wastewater treatment plants

Silvia Royano, Adrián De la Torre, Irene Navarro, M^a Ángeles Martínez
CIEMAT

P23-Occurrence and transference of pharmaceutically active compounds (PhACs) in sediments and fish from Tagus river basin

Silvia Royano, Adrián De la Torre, Irene Navarro, M^a Ángeles Martínez
CIEMAT

P24-Identification of molecular biomarkers linked to hydrophobicity of crops using High-Resolution Mass Spectrometry

Nicasio T. Jiménez-Morillo, Dalton Everette, Dara Park, Gonzalo Almendros, José A. González-Pérez
IRNAS-CSIC

P25-Bioaccumulation and transformation of plastic additives in hydroponically grown plants: Implications for safe water reuse

M.P. Garcia-Moll, H. Beral, L. Alonso, L.H.M.L.M. Santos, G. Buttiglieri, S. Rodriguez-Mozaz
Catalan Institute for Water Research (ICRA-CERCA)

P26-Chiral determination of amphetamine-type substances in environmental waters by solid phase extraction followed by capillary electrophoresis-tandem mass spectrometry

Pol Clivillé-Cabré, Francesc Borrull, Carme Aguilar, Marta Calull, Núria Fontanals
Universitat Rovira i Virgili

P27-Per- and poly-fluoroalkyl substances (PFAS) in follicular fluid from women undergoing *in vitro* fertilization (IVF) during oocyte retrieval procedure

Pere Colomer-Vidal, Weronika Marynowicz, Anna Ptak, Juan Muñoz-Arnanz, Begoña Jiménez
Instituto de Química Orgánica General (IQOG-CSIC)

P28-Flow-modulation comprehensive two-dimensional gas chromatography for non-target analysis of organic pollutants in environmental samples

Francisco Javier Santos, Pol Chacón, Encarnación Moyano
University of Barcelona

P29-High resolution analysis of biogenic volatile organic compounds (BVOCs) emitted by intact tomato plants using SPE/GC-TOF-MS

Federico Rodrigo, Nicasio T. Jiménez-Morillo, Carmen Rossini, José M^a de la Rosa, José A. González-Pérez
IRNAS-CSIC

T5: Biological, toxicological, and forensic analysis

P30-Gas chromatography–tandem mass spectrometry method for the determination of selected endocrine disruptors in human faeces

Alberto Zafra-Gómez, Inmaculada Moscoso-Ruiz, Samuel Cantarero-Malagón, Ana Rivas
University of Granada

P31-Determination of obesogens in biological samples and their relationship to childhood overweight/obesity

Patricia González-Palacios, Vega Almazán, Cristina Samaniego, Ana Rivas, Alberto Zafra-Gómez
University of Granada

P32-Therapeutic monoclonal antibodies analyzed by capillary electrophoresis with SDS

Rula Rostom-Ajlani, Cristian Gonzalez-Jimenez, Angel Puerta, Mercedes de Frutos
Instituto de Química Orgánica General (IQOG-CSIC)

P33-Risk assessment in analytical method development procedure according to ICH Q14 guideline. Application example

Ángel Irigoyen Barrio, Ana Lobo González, Elena Lizarraga Pérez, Elena González-Peñas
Universidad de Navarra

T6: Food and nutritional analysis

P34-Determination of obesogens in food and their relationship to childhood overweight/obesity

Yolanda Gálvez-Ontiveros, Viviana Ramírez, Lourdes Rodrigo, Ana Rivas, Alberto Zafra-Gómez
University of Granada

P35-Exploring co-exposure of mycotoxins and pesticides through human biomonitoring: effects of conventional and organic diets

Jose A. Gallardo-Ramos, Jesús Marín-Sáez, Vicente Sanchis, Laura Gámiz-Gracia, Ana M. García-Campaña, Maykel Hernández-Mesa, German Cano-Sancho
University of Granada

P36-Chromatographic analysis of the impact of organic amendments on the composition of soil and fruit in superintensive olive orchards

José María De la Rosa, Águeda M. Sánchez-Martín, Jorge Márquez-Moreno, Sara M. Pérez-Dalí, Paloma Campos, Nicasio T. Jiménez-Morillo, Jose Antonio González-Pérez
Instituto de Recursos Naturales y Agrobiología de Sevilla (IRNAS-CSIC)

P37-Simultaneous determination of pesticides and mycotoxins in fish feed by UHPLC-HRMS

María Álvarez-Romero, Jesús Marín-Sáez, Laura Gámiz-Gracia, Ana M. García-Campaña, Antonia Garrido Frenich, Maykel Hernández-Mesa
University of Granada

P38-Analytical method implementation for the determination of total amino acids in samples of chickpea flour by High Resolution Liquid Chromatography

María Teresa Murillo-Arbizu, Asier Bazán, José Miguel González, Paloma Virseda, María José Beriain
ISFOOD Research Institute, Public University of Navarra

P39-GC-MSMS 200+ Multi-residue Pesticide Screening Workflow - comparison of conventional 30 m column and LPGC kit

Fernando Rodriguez, Jana Hepner, Joseph Konschnik, and Chris English
Restek Corporation

P40-Liquid chromatography coupled to mass spectrometry as a tool for the design of a novel smoothie formulation with a highly diversified (poly)phenolic profile

Cristina Matías, Cristina del Burgo-Gutiérrez, María-José Sáiz-Abajo, María-Paz De Peña, Iziar A. Ludwig, Concepción Cid
Universidad de Navarra

P41-Optimization of a new SPME GC-MS method for oregano authentication

Sergio Rivas, Ignacio Jimenez-Amezcuca, Ainhoa Charles, Ana I. Ruiz, Ana C. Soria
Instituto de Química Orgánica General (IQOG-CSIC)

P42-A novel approach for the green extraction of forskolin from *Coleus forskohlii* root by the use of bio-solvents

Juan J. Matute-Pinos, Ignacio Jimenez-Amezcuca, Ana I. Ruiz-Matute, Jesús E. Quintanilla-López
Instituto de Química Orgánica General (IQOG-CSIC)

P43-FIA-MS methodology for the fast detection of adulterants in Damiana (*Turnera diffusa*) extracts

Adal Mena-García, Marina Díez-Municio, Ana I. Ruiz-Matute
Instituto de Química Orgánica General (IQOG-CSIC)

P44-In-Depth analysis of the phytochemical and bioactive profile of 12 species of Adriatic algae by MSPD-UHPLC-QTOF

Aly Castillo, María Celeiro, Diego Iglesias-Gonzalez, Carmen Garcia-Jares, Marta Lores, Kristina Perišić, Krunoslav Aladić, Stela Jokić
Universidade de Santiago de Compostela

P45-Recovery of proteins from grapefruit peels as a source of bioactive peptides: ultrasound assisted extraction, natural deep eutectic solvents and pressurized liquid extraction

Samuel Bernardo-Bermejo, María Luisa Marina, María Castro-Puyana
Universidad de Alcalá

P46-Extraction and characterization of bioactive carbohydrates and phenolics from phytoplankton holobionts

Marta Díez, Juan Pablo de la Roche, Pilar Águila, Ana Cristina Soria, Ana Isabel Ruiz Matute, María Luz Sanz

Instituto de Química Orgánica General (IQOG-CSIC)

P47-Subcritical water extraction combined with enzymatic assisted extraction for protein recovery from lime peels. Characterization of protein hydrolysates

Rosa María Palma-Manrique, María Concepción García, María Castro-Puyana, María Luisa Marina

Universidad de Alcalá

P48-Comparison of chromatographic methods for the analysis of hidroxycitric acid in *Garnicia cambogia* extracts

Inmaculada Luque-Jurado, Adal Mena-García, Angie Julieth Bellaizac-Riascos, Ana Cristina Soria, María Luz Sanz

Instituto de Química Orgánica General (IQOG-CSIC)

P49-Determination of MOSH and MOAH by CGxCG-TOFMS

Julio Lluch, Sebastiano Pantò

LECO SPAIN&PORTUGAL

P50-Profiling black oat avenanthramides and polyphenols

Marta Lores, María Celeiro, Miguel Otero-Otero, Carmen García-Jares, Bernardo Ordás

Universidade de Santiago de Compostela

P51-Phytochemical and antioxidant composition of *Quercus* acorn extracts obtained by Matrix Solid-Phase Dispersion

Diego Gonzalez-Iglesias, Laura Rubio, Francisco Martinez-Vazquez, Aly Castillo, Maria Celeiro, Carmen Garcia-Jares, Marta Lores

Universidade de Santiago de Compostela

P52-Novel Triple Quad approaches for robust and reliable analysis of PFAS in food matrices with Ultimate Sensitivity

Pedro Cano, Miguel Angel Pérez, Juan Gómez, Diego Martin

Bruker Española S.A.

T7: Chemometrics, data processing, and omics techniques

P53-Identification of key markers revealing the sterilization impact on paprika: Liquid-Chromatography-High-Resolution Mass Spectrometry as a powerful tool

Araceli Rivera-Pérez, Manuel Acosta Motos, Antonia Garrido French

Universidad de Almería

P54-Non-Targeted metabolomics for the authentication and differentiation of honey types: A comparative study of commercial and open-source data processing techniques

Juan V. Sancho, Zeinab Tarchichi, Samia Mokh, Tania Portolés

University Jaume I

P55-Enhanced classification of tea varieties using high-performance liquid chromatography and global retention models

J.R. Torres-Lapasió, P. Peiró-Vila, C. Pérez-Gracia, M.C. García-Alvarez-Coque

Universitat de València

P56- Application robustness of the 6495 triple quadrupole LC/MS system for non-stop pesticide analysis in black tea matrix

Jose J. Rivero, Peter Weidner, Patrick Batoon, Behrooz Zekavat, Anabel Fandino

Agilent Technologies

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