

# Program

## Thursday, November 18

### 8:45 h Opening Ceremony

Ana M. García-Campaña, Juan V. Sancho

### 9:00 h Keynote Lecture: Environmental Analysis

*Chairs: Joan Grimalt, Begoña Jiménez*

**BAREND L. VAN DROOGE**

*Trace-level analysis of molecular organic compounds in atmospheric PM by Q Exactive Orbitrap GC/MS*

### 09:45 h Oral Session 1: Environmental Analysis (I)

*Chairs: Joan Grimalt, Begoña Jiménez*

### 09:45 h O-E1: Wastewater reuse for agricultural irrigation in real crops: analytical tools and difficulties in the investigation of pharmaceutical transformation products

Patricia Plaza-Bolaños<sup>(1),(2)\*</sup>, Ana Belén Martínez-Piernas<sup>(2),(3)</sup>, Ana Agüera<sup>(1),(2)</sup>

<sup>(1)</sup> Dept. Chemistry and Physics, University of Almeria; <sup>(2)</sup> CIESOL (Center for Solar Energy Research), Joint Centre University of Almeria–CIEMAT, Almería, Spain; <sup>(3)</sup> Dept. Physical Chemistry and Analytical Chemistry, University of Jaén, Spain

### 09:55 h O-E2: Analysis of uv filters and uv stabilisers adsorbed in microplastics from canary islands beaches

Sarah Montesdeoca-Esponda<sup>\*</sup>, Sergio Santana-Viera, Zoraida Sosa-Ferrera, José Juan Santana-Rodríguez

*Instituto Universitario de Estudios Ambientales y Recursos Naturales (i-UNAT), Universidad de Las Palmas de Gran Canaria, Spain*

### 10:05 h O-E3: Ultra-high performance liquid chromatography-mass spectrometry analysis of ultraviolet filters in human nails

Laura Martín-Pozo<sup>(1)\*</sup>, María del Carmen Gómez-Regalado<sup>(1)</sup>, Samuel Cantarero-Malagón<sup>(2)</sup>, Alberto Navalón<sup>(1)</sup>, Alberto Zafra-Gómez<sup>(1,3)</sup>

<sup>(1)</sup> Analytical Chemistry and Life Sciences, Department of Analytical Chemistry, University of Granada, Spain; <sup>(2)</sup> Center for Scientific Instrumentation, University of Granada, Spain; <sup>(3)</sup> Instituto de Investigación Biosanitaria ibs, Granada, Spain

### 10:15 h Discussion

### 10:30 h Oral Session 1: Environmental Analysis (I)

*Chairs: Ana Agüera, Juan V. Sancho*

### OY-E1: Vertical distribution of volatile organic compounds and their influence on tropospheric ozone formation in Vic by using aerostatic balloons

Isabel Díez<sup>(1)</sup>, Clara Jaen<sup>(1)</sup>, Esther Marco<sup>(1)</sup>, Barend van Drooge<sup>(1)</sup>, Joan Grimalt<sup>(1)</sup>, Pilar Fernández<sup>(1)</sup>

<sup>(1)</sup> Institute of Environmental Assessment and Water Research, Barcelona, Spain

### 10:38 h OY-E2: NOVEL MULTICLASS CYANOTOXIN ANALYSIS BASED ON A DUAL CARTRIDGE SOLID-PHASE EXTRACTION SYSTEM FOLLOWED BY HYDROPHILIC INTERACCIÓN LIQUID CHROMATOGRAPHY- MASS SPECTROMETRY

M. Mar Aparicio-Muriana<sup>\*</sup>, Rocío Carmona-Molero, Francisco J. Lara, Ana M. García-Campaña, Monsalud del Olmo-Iruela

*Dept. of Analytical Chemistry, University of Granada, Spain*

### 10:46 h OY-E3: Suspect screening of micro(nano)plastics in the drinking water supply system of the Barcelona metropolitan area

Albert Vega-Herrera<sup>(1)</sup>, Marta Llorca<sup>(1)</sup>, Xavier Borrell-Díaz<sup>(1)</sup>, Katerina Savva<sup>(1)</sup>, Cristina Villanueva<sup>(2)</sup>, Esteban Abad<sup>(1)</sup>, Marinella Farré<sup>(1)\*</sup>

<sup>(1)</sup> Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Barcelona, Spain;

<sup>(2)</sup> Barcelona Institute for Global Health (ISGlobal), Barcelona, Spain

**10:54 h OY-E4: Development, validation, and uncertainty assessment of a gas chromatography – electron ionization – Orbitrap mass spectrometry targeted method for POPs and PAHs in avian blood**

Bernat Oró-Nolla<sup>(1)</sup>, Letizia Campioni<sup>(2)</sup>, Sílvia Lacorte<sup>(1)</sup>

<sup>(1)</sup> Department of Environmental Chemistry, IDAEA-CSIC, Jordi Girona 18-26, 08034 Barcelona, Spain;

<sup>(2)</sup> MARE - Marine and Environmental Sciences Centre, ISPA, Instituto Universitário, Lisbon, Portugal

**11:02 h OY-E5: Investigation of antibiotics in wastewater by large-volume direct injection uhplc-ms/ms. importance of chromatography optimisation**

Elisa Gracia-Marín<sup>\*</sup>, David Fabregat-Safont, María Ibáñez, Lubertus Bijlsma, Elena Pitarch, Félix Hernández

Environmental and Public Health Analytical Chemistry, Research Institute for Pesticides and Water (IUPA), University Jaume I, Castellón, Spain

**11:10 h Discussion**

**11:20 h Break & Exhibition**

**12:00 h Oral Session 2: Environmental Analysis (II)**

Chairs: Ana Agüera, Juan V. Sancho

**12:00 h OY-E6: Analysis of molecular compounds in organic aerosols from low-volume samples collected during meteorological balloon flights**

Clara Jaén<sup>(1),\*</sup>, Isabel Díez<sup>(1)</sup>, Esther Marco<sup>(1)</sup>, Barend L. van Drooge<sup>(1)</sup>, Joan O. Grimalt<sup>(1)</sup>, Pilar Fernández<sup>(1)</sup>

<sup>(1)</sup>Institute of Environmental Assessment and Water Research (IDAEA), CSIC, Barcelona, Spain

**12:08 h OY-E7: Sweeping-micellar electrokinetic chromatography - tandem mass spectrometry as a novel approach to determine neonicotinoid and boscalid residues in pollen and honeybee samples**

Laura Carbonell-Rozas<sup>(1),\*</sup>, Marcos Rodríguez-Vela<sup>(1)</sup>, Burkhard Horstkotte<sup>(2)</sup>, Francisco J. Lara<sup>(1)</sup>, Ana M. García-Campaña<sup>(1)</sup>

<sup>(1)</sup> Faculty of Sciences, University of Granada, Spain; <sup>(2)</sup> Faculty of Pharmacy, Charles University, Hradec Králové, Czech Republic

**12:16 h OY-E8: Analysis of steroid hormones sorbed on microplastics by ultrasonic assisted extraction and ultra-high performance liquid chromatography tandem mass spectrometry**

Rayco Guedes-Alonso<sup>(1),\*</sup>, Zoraida Sosa-Ferrera<sup>(1)</sup>, José Juan Santana-Rodríguez<sup>(1)</sup>

<sup>(1)</sup> Instituto Universitario de Estudios Ambientales y Recursos Naturales (i-UNAT), Universidad de Las Palmas de Gran Canaria, Spain

**12:24 h Discussion**

**12:34 h Web communications**

Chairs: Belén Gómara, F. Javier Santos

**12:34 h Session A: Environmental Analysis**

**13:04 h Session B: Clinical and Pharmaceutical Analysis/Omics Techniques**

**13:35 h Lunch**

**15:00 h Keynote Lecture: Clinical & Pharmaceutical Analysis**

Chairs: Elena González, Ana M. García-Campaña

**JOSEP RUBERT**

*Could gut microbial metabolites serve as a Rosetta Stone to promote gut health?*

**15:45 h Oral Session 3: Clinical & Pharmaceutical Analysis/Omics Techniques**

Chairs: Elena González, Nuria Fontanals

**15:45 h O-CF1: Tackling protein biomarkers through targeted bottom-up analysis by on-line aptamer affinity solid-phase extraction-immobilized enzyme microreactor capillary electrophoresis-mass spectrometry**

Hiba Salim, Roger Pero-Gascon, Estela Giménez, Fernando Benavente<sup>\*</sup>

Department of Chemical Engineering and Analytical Chemistry, Institute for Research on Nutrition and Food Safety (INSA·UB), University of Barcelona, Spain

- 15:55 h O-CF2: Solute Interactions In Microemulsion Liquid Chromatography With Ionic Liquids**  
 María José Ruiz-Ángel\*, Nitaben Pankajkumar-Patel, Ester Peris-García, María Celia García-Álvarez-Coque  
*Departament de Química Analítica, Universitat de València, Burjassot, Spain*
- 16:05 h O-O1: In vitro study of the neuroprotective potential of a supercritical extract obtained from dunaliella salina microalgae**  
 Rocío Gallego, José David Sánchez-Martínez, Zully J. Suárez-Montenegro, Elena Ibáñez, Alejandro Cifuentes, Miguel Herrero, Alberto Valdés\*  
*Laboratory of Foodomics, Institute of Food Science Research (CIAL, CSIC-UAM), Madrid, Spain*
- 16:15 h Discussion**
- 16:30 h Oral Session 3: Clinical & Pharmaceutical Analysis/Omics Techniques**  
 Chairs: Ana M. García-Campaña, Mario Fernández
- OY-O1: The Role of Oxidized Lipids in Fungal Mediated Diseases Using Ion Mobility-Mass Spectrometry**  
María Morán-Garrido<sup>(1),\*</sup>, Jorge Sáiz<sup>(1)</sup>, Coral Barbas<sup>(1)</sup>  
<sup>(1)</sup> CEMBIO, Facultad de Farmacia, Universidad San Pablo-CEU, Madrid, Spain
- 16:38 h OY-O2: Differential Modulation of the Central and Peripheral Monoaminergic Neurochemicals by Deprenyl in Zebrafish Larvae**  
Marina Bellot<sup>(1),\*</sup>, Helena Bartolomé<sup>(1)</sup>, Melissa Faria<sup>(2)</sup>, Cristian Gómez-Canela<sup>(1)</sup>, Demetrio Raldúa<sup>(2)</sup>, Jordi Díaz-Ferrero<sup>(1),(2)</sup> *Department of Analytical and Applied Chemistry, School of Engineering, Institut Químic de Sarrià-Universitat Ramon Llull, Barcelona, Spain;* <sup>(2)</sup> *Institute for Environmental Assessment and Water Research (IDAEA-CSIC), Barcelona, Spain*
- 16:46 h OY-CF1: Simultaneous determination of 40 drugs of abuse and some metabolites in human urine by SPE followed by LC-MS/MS**  
Sergi Pascual-Caro<sup>(1),\*</sup>, Francesc Borrull<sup>(1)</sup>, Carme Aguilar<sup>(2)</sup>, Marta Calull<sup>(1)</sup>  
<sup>(1)</sup> *Department of Analytical Chemistry and Organic Chemistry, Universitat Rovira i Virgili, Tarragona, Spain;* <sup>(2)</sup> *Serra Hunter Professor, Department of Analytical Chemistry and Organic Chemistry, Universitat Rovira i Virgili, Tarragona, Spain*
- 16:54 h OY-CF2: Simultaneous enantiomeric separation of licarbazepine and licarbazepine acetate by electrokinetic chromatography. Determination in pharmaceutical formulations and urine samples**  
Sandra Salido-Fortuna<sup>(1),\*</sup>, María Luisa Marina<sup>(1,2)</sup>, María Castro-Puyana<sup>(1,2)</sup>  
<sup>(1)</sup> *Universidad de Alcalá. Departamento de Química Analítica, Química Física e Ingeniería Química, Alcalá de Henares (Madrid), Spain;* <sup>(2)</sup> *Universidad de Alcalá. Instituto de Investigación Química Andrés M. del Río., Alcalá de Henares (Madrid), Spain*
- 17:02 h Discussion**
- 17:30 h SECYTA GENERAL ASSEMBLY**

## Friday, November 19

- 8:45 h Keynote Lecture: New development Instrumentation & Applications**  
 Chairs: F. Javier Santos, Jordi Díaz  
**JUAN VICENTE SANCHO LLOPIS**  
*Benefits of Collision Cross Section (CCS) data obtained by UPLC-ESI-IMS-QTOFMS and GC-APGC-IMS-QTOFMS for the identification of small molecules in screening applications*
- 09:30 h Oral Session 4: Sample Prep. / New Develop. Instrumentation / Fundamentals/Chemometrics**  
 Chairs: F. Javier Santos, Jordi Díaz
- 09:30 h O-F1: DEVELOPMENT AND VALIDATION OF A METHOD FOR THE COMPREHENSIVE INSPECTION OF EXPERIMENTAL DESIGNS IN HPLC**  
María Celia García-Álvarez-Coque, José Ramón Torres-Lapasió, Adrián Gisbert-Alonso, José Antonio Navarro-Huerta  
*Departament de Química Analítica, Universitat de València, Burjassot, Spain*

- 09:40 h O-ND1: Controlled atmosphere flexible microtube plasma soft ionization source: a promising tool for the determination of small molecules by GC-MS in the field of clinical and food analysis**  
David Moreno-González<sup>(1,2),\*</sup>, Delia Castilla-Fernández<sup>(1)</sup>, Pascal Vogel<sup>(2)</sup>, Sebastian Brandt<sup>(2)</sup>, Constantinos Lazarou<sup>(3)</sup>, Odhisea Gazeli<sup>(3)</sup>, Juan F. García-Reyes<sup>(1)</sup>, Antonio Molina-Díaz<sup>(1)</sup>, Joachim Franzke<sup>(2)</sup>  
<sup>(1)</sup> Analytical Chemistry Research Group, Department of Physical and Analytical Chemistry, University of Jaén, Spain; <sup>(2)</sup> ISAS-Leibniz-Institut für Analytische Wissenschaften, Dortmund Germany; <sup>(3)</sup> FOSS Research Centre for Sustainable Energy, PV Technology, University of Cyprus
- 09:50 h O-ND2: Insights of tube plasma as a new ion source for gc-ms coupling**  
Juan F. Ayala-Cabrera<sup>(1,2),\*</sup>, Jasmin Heine<sup>(1,2)</sup>, Lidia Montero<sup>(1,2)</sup>, Sven W. Meckelmann<sup>(1,2)</sup>, Florian Uteschil<sup>(1,2)</sup>, Oliver J. Schmitz<sup>(1,2)</sup>  
<sup>(1)</sup> Applied Analytical Chemistry, University of Duisburg-Essen, Germany; <sup>(2)</sup> Teaching and Research Center for Separation, University of Duisburg-Essen, Germany
- 10:00 h Discussion**
- 10:10 h Oral Session 4: Sample Prep. / New Develop. Instrumentation / Fundamentals/Chemometrics**  
 Chairs: Juan V. Sancho, José Antonio González
- OY-S1: Combining microfluidic paper based platform and metal-organic frameworks in a single device for phenolic content assessment in fruits**  
H. Martínez-Pérez-Cejuela<sup>1,\*</sup>, Raquel B. R. Mesquita<sup>2</sup>, E.F. Simó-Alfonso<sup>1</sup>, J.M. Herrero-Martínez<sup>1</sup>, António O. S. S. Rangel<sup>2</sup>  
<sup>1</sup>Department of Analytical Chemistry, University of Valencia, Burjassot, Spain; <sup>2</sup>Universidade Católica Portuguesa, CBQF - Centro de Biotecnologia e Química Fina- Laboratório Associado, Escola Superior de Biotecnologia, Porto, Portugal
- 10:18 h OY-S2: Determination of veterinary drugs and pesticides in salmon using liquid chromatography/tandem mass spectrometry using a specific sample cleanup**  
Delia Castilla-Fernández<sup>\*</sup>, David Moreno-González, Marcos Bouza, Evaristo Ballesteros, Juan F. García-Reyes, Antonio Molina-Díaz  
 Analytical Chemistry Research Group, Department of Physical and Analytical Chemistry, University of Jaén, Spain
- 10:26 h OY-ND1: Hand-held diode laser for on-site analysis using transportable mass spectrometry**  
Ane Arrizabalaga-Larrañaga<sup>(1,2),\*</sup>, Michel W.F. Nielen<sup>(2)</sup>, Marco H. Blokland<sup>(2)</sup>  
<sup>(1)</sup> Department of Chemical Engineering and Analytical Chemistry, University of Barcelona, Spain; <sup>(2)</sup> Wageningen Food Safety Research (WFSR), Wageningen University & Research, The Netherlands
- 10:34 h OY-ND2: Exploring GC-APCI-IMS-HRMS possibilities for the screening of organic-micropollutants**  
David Izquierdo-Sandoval<sup>(1),\*</sup>, David Fabregat-Safont<sup>(1)</sup>, Leticia Lacalle-Bergeron<sup>(1)</sup>, Juan Vicente Sancho<sup>(1)</sup>, Félix Hernández<sup>(1)</sup>, Tania Portolés<sup>(1)</sup>  
<sup>(1)</sup> Environmental and Public Health Analytical Chemistry, Research Institute for Pesticides and Water (IUPA), University Jaume I, Castellón, Spain
- 10:42 h Discussion**
- 10:50 h Break & Exhibition**
- 11:20h Web communications**  
 Chairs: Nuria Fontanals, Marta Lores
- 11:20 h Session A: Sample Preparation / New Develop. Instrumentation / Fundamentals/Chemometrics**
- 11:50 h Session B: Food Analysis**
- 12:20 h Oral Session 5: Food Analysis**  
 Chairs: Belén Gómara, Mario Fernández
- 12:20 h O-FA1: Determination of intact glucosinolates in bee pollen by using ultra-high performance liquid chromatography coupled to a quadrupole time-of-flight mass detector**  
Ana María Ares<sup>(1),\*</sup>, David Sánchez<sup>(1)</sup>, Jesús Tapia<sup>(2)</sup>, Mariano Higes<sup>(3)</sup>, Amelia Virginia González Porto<sup>(3)</sup>, Raquel Martín-Hernández<sup>(3)</sup>, María Teresa Martín<sup>(1)</sup>, José Bernal<sup>(1)</sup>  
<sup>(1)</sup> I.U. CINQUIMA, GRUPO TESEA, Universidad de Valladolid, España; <sup>(2)</sup> Departamento de Estadística e Investigación Operativa, Universidad de Valladolid, España; <sup>(3)</sup> Instituto Regional de Investigación y Desarrollo Agroalimentario y Forestal de Castilla La Mancha (IRIAF), Centro de Investigación Apícola y Agroambiental, Guadalajara, España

- 12:30 h O-FA2: New solvents for bioactive compounds extraction from blueberry leaves**  
María Santos-Martín<sup>(1),\*</sup>, Ana Sayago<sup>(1,2)</sup>, Raúl González-Domínguez<sup>(1,2)</sup>, Juan Urbano<sup>(1,2)</sup>, Ángeles Fernández-Recamales<sup>(1,2)</sup>  
<sup>(1)</sup> AgriFood Laboratory, Faculty of Experimental Sciences, University of Huelva, Spain; <sup>(2)</sup> International Campus of Excellence Ceia3, University of Huelva, Spain
- 12:40 h O-FA3: Beyond the established limit: capillary gel electrophoresis of human immunoglobulin a from serum and colostrum**  
Angel Puerta<sup>(1),\*</sup>, Daniel Garcia-Lopez<sup>(1)</sup>, Paula Tejedor-Matellanes<sup>(1)</sup>, Laura Gomez-Ruiz<sup>(1)</sup>, Mercedes de Frutos<sup>(1)</sup>  
<sup>(1)</sup> Institute of Organic Chemistry (IQOG-CSIC), Madrid, Spain
- 12:50 h O-FA4: A label-free shotgun proteomics approach for the characterization and differentiation of quinoa seed varieties**  
Laura Pont<sup>1,\*</sup>, Rocío Galindo-Luján<sup>1</sup>, Victoria Sanz-Nebot<sup>1</sup>, Zoran Minic<sup>2</sup>, Maxim V. Berezovski<sup>2</sup>, Fernando Benavente<sup>1</sup>  
<sup>(1)</sup> Department of Chemical Engineering and Analytical Chemistry, Institute for Research on Nutrition and Food Safety (INSA-UB), University of Barcelona, Spain; <sup>(2)</sup> Department of Chemistry and Biomolecular Sciences, University of Ottawa, Canada
- 13:00 h O-FA5: Comprehensive analysis of odour-active wine volatiles by heart-cutting bidimensional gas chromatography coupled to mass spectrometry and flame ionization detection**  
O. Castejón-Musulén<sup>[1]</sup>, I. Ontañón<sup>[1]</sup>, R. Lopez<sup>[1]</sup>, V. Ferreira<sup>[1]</sup>  
<sup>[1]</sup> Laboratorio de Análisis del Aroma y Enología (LAAE), Department of Analytical Chemistry, Universidad de Zaragoza, Instituto Agroalimentario de Aragón (IA2) (UNIZAR-CITA), Associate Unitto Instituto de las Ciencias de la Vid y del Vino (ICVV), Spain
- 13:10 h Discussion**
- 13:25 h Oral Session 5: Food Analysis**  
 Chairs: Marta Lores, José Antonio González
- OY-FA1: Fast non-aqueous capillary electrophoresis–mass spectrometry: an efficient alternative to determine emerging mycotoxins in food**  
María del Mar Delgado-Povedano<sup>\*</sup>, Francisco J. Lara, Emilio Borrego-Marín, Laura Gámiz-Gracia, Ana M. García-Campaña  
 Department of Analytical Chemistry, Faculty of Sciences, University of Granada, Spain
- 13:33 h OY-FA2: Differentiation of two industrial hemp varieties by comprehensive two-dimensional liquid chromatography (lcxlc)**  
Lidia Montero<sup>(1,2),\*</sup>, Hyerin Kim, Juan F. Ayala-Cabrera<sup>(1,2)</sup>, Sven W. Meckelmann<sup>(1,2)</sup>, Oliver J. Schmitz<sup>(1,2)</sup>  
<sup>(1)</sup> Applied Analytical Chemistry, University of Duisburg-Essen, Germany; <sup>(2)</sup> Teaching and Research Center for Separation, University of Duisburg-Essen, Germany
- 13:41 h Discussion**
- 13:45 h Keynote Lecture: Sample Preparation**  
 Chairs: Juan V. Sancho, Ana M. García-Campaña  
**VERÓNICA PINO**  
*Microextraction using novel solvents and sorbents: from green to white analytical sample preparation*
- 14:30 h Closing Ceremony & Awards**