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Program summary

| <i>Tuesday 8</i> | <i>Wednesday 9</i> | <i>Thursday 10</i> | <i>Friday 11</i> |
|--|--|--|--|
| 8:15 Registration | | | |
| 8:40 Opening Session | | | |
| 9:00-9:45 PL1 | 9:30-10:15 PL3 | 9:00-9:45 PL5 | 9:30-10:15 PL7 |
| 9:45-10:45 Oral Session 1 | 10:15-10:55 Oral Session 3 | 9:45 -10:45 Oral Session 6 | 10:15-10:55 Young Scientists Oral Session 8 |
| 10:45-11:30 Coffee Break & Poster Exhibition | 10:55-11:40 Coffee Break & Poster Exhibition | 10:45-11:30 Coffee Break & Poster Exhibition | 10:55-11:25 Coffee Break |
| 11:30-12:15 PL2 | 11:40-12:25 PL4 | 11:30-12:15 PL6 | 11:25-12:05 Oral Session 9 |
| 12:15-13:15 Oral Session 2 | 12:25-13:25 Oral Session 4 | 12:15-13:15 Oral Session 7 | 12:05-12:25 Flash Poster Session 4 |
| 13:15-13:25 Flash Poster Session 1 | 13:25-13:40 Flash Poster Session 2 | 13:15-13:35 Flash Poster Session 3 | 12:25-13:05 Oral Session 10 |
| 13:25-13:55 Young Scientists Oral Session 1 | 13:40-14:00 Young Scientists Oral Session 4 | 13:35-13:55 Young Scientists Oral Session 6 | 13:05-13:30 Closing Lecture |
| 14:00-15:00 Lunch | 14:00-15:00 Lunch | 14:00-15:00 Lunch | 13:30-14:00 Closing Session & Awards |
| 15:00-15:30 Technical Seminar 1 & Poster Exhibition | 15:00-15:30 Technical Seminar 3 & Poster Exhibition | 15:00-15:30 Technical Seminar 4 & Poster Exhibition | 14:00 Farewell cocktail |
| 15:30-16:00 Young Scientists Oral Session 2 | 15:30-16:30 Oral Session 5 | 15:30-16:30 Oral Session 8 | |
| 16:00-16:30 Coffee Break | 16:30-17:00 Coffee Break & Poster Exhibition | 16:30-17:00 Coffee Break & Poster Exhibition | |
| 16:30--17:00 Young Scientists Oral Session 3 | 17:00-17:30 Young Scientists Oral Session 5 | 17:00-17:20 Young Scientists Oral Session 7 | |
| 17:00-17:30 Technical Seminar 2 & Poster Exhibition | | 17:20-17:45 EU-FT-ICR Project | |
| 17:30-19:30 SEEM Meeting & Poster Exhibition | 17:30-19:30 SECyTA Meeting & Poster Exhibition | | |
| 20:30-1:30 Welcome cocktail & Dancing party | 19:30-21:30 Compostela City Walk | 21:30-00:30 Gala Dinner | |

Welcome

Dear Colleagues:

On behalf of the organizing committee, it is our pleasure to welcome you to the "1st Iberian Meeting in Separation Sciences and Mass Spectrometry" and to the city of Santiago de Compostela, a city declared World Heritage by UNESCO thanks to its monumental beauty, and for being the goal of a millenary pilgrimage route: the Camino de Santiago, which since the ninth century transformed this place of the *finis terrae* into a meeting point of the western world.

It is indeed a great place for us to meet for this international conference bringing together in the same event the "IX conference of the Spanish Society of Mass Spectrometry", the "VI conference of the Mass Spectrometry Group of the Portuguese Society of Chemistry", and the "XIX Conference of the Spanish Society of Chromatography and Related Techniques".

Last several decades have witnessed the continued evolution and scientific advances in development in the fields of separation sciences and mass spectrometry. The scientific program of the "1st Iberian Meeting in Separation Sciences and Mass Spectrometry" presents an outstanding spectrum of research papers from multidisciplinary areas to focus on the challenges of developing technologies and methodologies for biomedical, environmental, food control, and so many other applications.

We are proud to bring you a great synergy of expertise from internationally renowned scientists in separation sciences and mass spectrometry through seven plenary lectures. Sessions throughout the meeting are focused on addressing the current and future trends and challenges in scientific research, technology development, and practice applications. The scientific program is targeted to provide tangible benefits and networking opportunities to current researchers, and the most important, it provides a tremendous environment for younger scientists to learn about future prospects and professional development activities.

We would like to acknowledge the companies that have given a so important support to this meeting, presenting their latest advances and products.

In addition to the outstanding scientific program, we hope that you will enjoy the social program that we have prepared so that, practically from day one, we will have the opportunity not only to strengthen scientific ties but also friendship in the best monumental and gastronomical environments. Find also time to explore Santiago de Compostela, which is a great place to explore on your own.

With our best wishes for your participation in the "1st Iberian Meeting in Separation Sciences and Mass Spectrometry", welcome to Santiago de Compostela!

Marta Lores Aguíñ & Carmen García Jares

Chairwomen

Committees

Conference Chairwomen

Marta Lores Aguín and Carmen García Jares (USC)

Organizing Committee

Francisco J. Santos Vicente
(President of SECyTA)
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Carlos Cordeiro (University of Lisbon)
Jordi Díaz Ferrero (IQS-Universidad Ramón Llul)
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Begoña Jiménez Luque (IQOG–CSIC)
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Encarnación Moyano Morcillo (Univ. Barcelona)
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Hugo Osório (University of Porto)
Deborah Penque (INSA Lisboa)
Sandra Pérez (IDAEA–CSIC)
Pablo Rodríguez (Universidad de Oviedo)
Juan Vicente Sancho Llopis (Universitat Jaume I)
Francisco J. Santos Vicente (Univ. de Barcelona)
Marta Sousa Silva (University of Lisbon)
Rosa Ventura (Fundació IMIM Barcelona)
Óscar Yanes (Universitat Rovira i Virgili)

Invited Speakers



Prof. Dr. Adrian Covaci

University of Antwerp, Belgium

adrian.covaci@uantwerpen.be

PL1 *Trends in mass spectrometry for human biomonitoring and exposomics.*



Prof. Dr. Rosario Pereiro

University of Oviedo, Spain

mrpereiro@uniovi.es

PL2 *Laser ablation ICP-MS for simultaneous quantitative imaging of elements and biomolecules in biological studies: achievements and trends.*



Prof. Dr. Valerie Gabelica

National Institute of Health and Medical Research (Inserm), France

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PL3 *Ion mobility mass spectrometry: principles of separation and applications in the DNA structural characterization.*



Prof. Dr. Jane Thomas-Oates

University of York, United Kingdom

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PL4 *Alternative chromatographic and mass spectrometric approaches to metabolomic challenges.*



Prof. Dr. Frantisek Svec

University Hradec Kralove, Czech Republic

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PL5 *Porous polymer monoliths: Versatile materials for numerous applications.*



Prof. Dr. Miguel Herrero

Institute of Food Science Research (CIAL-CSIC), Spain

m.herrero@csic.es

PL6 *Application of comprehensive two-dimensional liquid chromatography to characterize very complex food-related samples.*



Prof. Dr. Cristina Barrocas Dias

University of Évora, Portugal

cmbd@uevora.pt

PL7 *Unveiling the secrets of the past using hyphenated chromatographic techniques.*

Scientific and Social Program

| Tuesday 8 | |
|---|---|
| 8:15 | REGISTRATION |
| 8:40 | OPENING SESSION: Authorities, Chairs of Scientific Societies, Chairwomen |
| 9:00 Plenary Lecture PL1 | <p style="text-align: center;"><i>Trends in mass spectrometry for human biomonitoring and exposomics.</i> Adrian Covaci, University of Antwerp, Belgium</p> <p>Session chairs: <i>Francisco Javier Santos, Universidad de Barcelona</i> <i>Marta Lores, Universidade de Santiago de Compostela</i></p> |
| 9:45-10:45 Oral Session 1 | <p><i>Omics & Other applications</i></p> <p>Session chairs: <i>Francisco Javier Santos, Universidad de Barcelona</i> <i>Montserrat Carrascal, IIBB-CSIC, Barcelona</i></p> |
| 9:45 | O1 <i>Evaluation of the anticancer potential golden berry calyx under a foodomics perspective.</i> Gerardo Álvarez-Rivera. CIAL-CSIC, Madrid. |
| 10:05 | O2 <i>Glycoproteomic profile of extracellular vesicles in cancer.</i> Hugo Osório. University of Porto. |
| 10:25 | O3 <i>Extreme make-up and cosmetic applicators: are they safe?</i> María Celeiro. University of Santiago de Compostela. |
| 10:45-11:30 | Coffee Break Poster Exhibition |
| 11:30 Plenary Lecture PL2 | <p style="text-align: center;"><i>Laser ablation ICP-MS for simultaneous quantitative imaging of elements and biomolecules in biological studies: achievements and trends.</i> Rosario Pereiro, Universidad de Oviedo, Spain</p> <p>Session chairs: <i>Pablo Rodríguez, Universidad de Oviedo</i> <i>Carmen García Jares, Universidade de Santiago de Compostela</i></p> |
| 12:15-13:15 Oral Session 2 | <p><i>Omics</i></p> <p>Session chairs: <i>Pablo Rodríguez, Universidad de Oviedo</i> <i>Hugo Osório, University of Porto</i></p> |
| 12:15 | O4 <i>Untargeted metabolomics of full scan MS hyphenated data – mining for minor peaks with finnee, risks and benefits.</i> Guillaume L. Erny. University of Porto. |

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| 12:35 | O5 Profiling the skin volatilome as powerful tool to the neurodegenerative diseases diagnosis. Jorge Pereira. University of Madeira. | |
| 12: 55 | O6 A metabolomics-based workflow for adductomics studies. Alexandra M.M. Antunes. IST Lisbon. | |
| 13:15-13:25 Flash Poster Session 1 | Flash Poster Session 1 | |
| | Session chairs: <i>Belén Gómara Moreno, IQOG–CSIC, Madrid</i> <i>Juan Francisco García Reyes, Universidad de Jaén</i> | |
| 13:15 | P1 Advanced membrane assisted solvent extraction (MASE) for isolating new psychoactive substances from urine before HPLC-MS/MS determination. Cristian Suárez-Oubiña. University of Santiago de Compostela. | |
| 13:20 | P2 Analytical challenges associated to essential oils and their individual components in cosmetics. Laura Rubio. University of Santiago de Compostela. | |
| 13:25-13:55 Young Scientists Oral Session 1 | Clinical & Toxicological applications | |
| | Session chairs: <i>Belén Gómara Moreno, IQOG–CSIC, Madrid</i> <i>Juan Francisco García Reyes, Universidad de Jaén</i> | |
| 13:25 | OY1 Synthesis and characterization of isotopically labelled ¹⁵N-3-monoiodotyrosine and ¹³C-3,5-diiodotyrosine for their use as internal standards in urine analysis by LC-ESI-MS/MS. Jesús Nicolás Carcelén. University of Oviedo. | |
| 13:35 | OY2 Sustainable extraction and characterization of bioactive peptides and polyphenols from brewer's spent grain: evaluation of synergic effects. Estefanía González García. University of Alcalá. | |
| 13:45 | OY3 Volatolomics approach for the identification of pup pheromones promoting maternal care in mice. Leticia Lacalle-Bergeron. Universtiy Jaume I. | |
| 14:00-15:00 | Lunch | |
| 15:00-15:30 | Technical Seminar 1 LECO | Poster Exhibition |
| 15:30-16:00 Young Scientists Oral Session 2 | Clinical & Toxicological applications | |
| | Session chairs: <i>Núria Fontanals Torroja, University of Rovira i Virgili</i> <i>José A. González Pérez, IRNAS-CSIC, Sevilla</i> | |
| 15:30 | OY4 Determination of syntethic cathinones in meconium by LC-MS/MS. Ángela López-Rabuñal. University of Santiago de Compostela. | |
| 15:40 | OY5 State-of-the-art of analytical methods for aflatoxin human biomonitoring. Beatriz Arce-López. University of Navarra. | |

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| 15:50 | OY6 Analytical considerations for the LC-MS/MS determination of endogenous steroids. Alex Gomez-Gomez. Fundación IMIM. | |
| 16:00-16:30 | Coffee Break | |
| 16:30-17:00 Young Scientists Oral Session 3 | Clinical & Toxicological applications <u>Session chairs:</u> <i>Núria Fontanals Torroja, University of Rovira i Virgili</i> <i>José A. González Pérez, IRNAS-CSIC, Sevilla</i> | |
| 16:30 | OY7 A LC-MS/MS method for determination of antipsychotic drugs in nails. María Cobo Golpe. University of Santiago de Compostela. | |
| 16:40 | OY8 Multiclass method for the determination of endocrine disrupting chemicals in human nails using alkaline digestion prior to UPLC-MS. Laura Martín Pozo. University of Granada. | |
| 16:50 | OY9 Determination of synthetic cathinones in oral fluid by LC-MS-MS. Sergi Pascual. University Rovira i Virgili. | |
| 17:00-17:30 | Technical Seminar 2 IZASA-SHIMADZU | Poster Exhibition |
| 17:00-19:30 | SEEM Meeting | |
| 20:30-1:30 | Welcome cocktail & Dancing party | |

Wednesday 9

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| 9:30 Plenary Lecture PL3 | <p style="text-align: center;"><i>Ion mobility mass spectrometry: principles of separation and applications in the DNA structural characterization.</i></p> <p style="text-align: center;">Valérie Gabelica, Inserm, France</p> <p>Session chairs: <i>Encarnación Moyano, Universidad de Barcelona</i> <i>Juan Vicente Sancho Llopis, Universitat Jaume I</i></p> | |
| 10:15-10:55 Oral Session 3 | <p style="text-align: center;"><i>Clinical & Toxicological applications</i></p> <p>Session chairs: <i>Encarnación Moyano, Universidad de Barcelona</i> <i>Juan Vicente Sancho Llopis, Universitat Jaume I</i></p> | |
| 10:15 | <p>O7 <i>Mass spectrometry contribution to metabolic studies: new insights into montelukast metabolism.</i> Gonçalo C. Justino. IST, Lisbon.</p> | |
| 10:35 | <p>O8 <i>Combination of multiple heart-cutting two dimensional LC and isotope dilution ESI-MS/MS for the accurate quantification of clinical biomarkers.</i> Pablo Rodríguez-González. University of Oviedo.</p> | |
| 10:55-11:40 | Coffee Break | Poster Exhibition |
| 11:40 Plenary Lecture PL4 | <p style="text-align: center;"><i>Alternative chromatographic and mass spectrometric approaches to metabolomic challenges.</i></p> <p style="text-align: center;">Jane Thomas-Oates, University of York, United Kingdom</p> <p>Session chairs: <i>Maria Helena Florêncio, Universidade de Lisboa</i> <i>Marta Lores, Universidade de Santiago de Compostela</i></p> | |
| 12:25-13:25 Oral Session 4 | <p style="text-align: center;"><i>Clinical & Toxicological applications</i></p> <p>Session chairs: <i>Juan Vicente Sancho Llopis, Universitat Jaume I</i> <i>Sandra Pérez, IDAEA-CSIC, Barcelona</i></p> | |
| 12:25 | <p>O9 <i>Quantification of related synthetic cathinones in rat brain by UHPLC-MS/MS. Relationship between structure and blood-brain barrier permeability.</i> David Fabregat-Safont. University Jaume I.</p> | |
| 12:45 | <p>O10 <i>Identification of growth hormone-releasing hormones in urine doping controls by immunoaffinity purification and LC-MS.</i> Éldia Alechaga. Catalanian Anti-doping Laboratory.</p> | |
| 13:05 | <p>O11 <i>HPLC-ESI-MS/MS as a valuable tool to unravel the metabolism of new psychoactive substances.</i> Noélia Duarte. University of Lisbon.</p> | |

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| 13:25-13:40 Flash Poster Session 2 | Flash Poster Session 2 | |
| | <u>Session chairs:</u> <i>Juan Vicente Sancho Llopis, Universitat Jaume I</i> <i>Sandra Pérez, IDAEA-CSIC, Barcelona</i> | |
| 13:25 | P3 Comparison of two chemometric approaches for the identification by LC-QTOF based untargeted metabolomics of potential plasma biomarkers in pediatric chronic kidney disease. Sandra Benito. University of the Basque Country. | |
| 13:30 | P4 Time-series proteomic study of diabetic nephropathy in human proximal tubular HK-2 cells by UHPLC-ORBITRAP MS/MS. María Castro-Puyana. University of Alcalá. | |
| 13:35 | P5 Annotation of oxidized phospholipids in metabolomics guided cancer study Ángeles López-López University CEU San Pablo. | |
| 13:40-14:00 Young Scientists Oral Session 4 | Food analysis | |
| | <u>Session chairs:</u> <i>Begoña Jiménez Luque, IQOG-CSIC, Madrid</i> <i>Jordi Díaz Ferrero, IQS-Universidad Ramón Llull</i> | |
| 13:40 | OY10 Simple and effective method for the determination of neonicotinoid residues in honeys and cereals by capillary LC. Laura Carbonell Rozas. University of Granada. | |
| 13:50 | OY11 GC-MS characterisation of novel pectic-oligosaccharides derived from artichoke pectin using machine learning and competitive fragmentation modelling (CFM-ID). Carlos Sabater. CIAL-CSIC-UAM. | |
| 14:00-15:00 | Lunch | |
| 15:00-15:30 | Technical Seminar 3 AGILENT | Poster Exhibition |
| 15:30-16:30 Oral Session 5 | Food analysis | |
| | <u>Session chairs:</u> <i>Antonia Carro, University of Santiago de Compostela</i> <i>Maria da Conceição Oliveira, IST, Lisboa</i> | |
| 15:30 | O12 Preliminary identification of specific markers to guarantee the authenticity of Galicia's honey by a non-target HRMS approach. Thierry Dagnac. AGACAL. | |
| 15:50 | O13 Chemical profile of coffee varieties by FT-ICR-MS. Ana Marques. University of Lisbon. | |
| 16:10 | O14 LC-MS/MS confirmation of the emerging pinnatoxins and high levels of esterified OA group toxins in commercial mollusks from the Atlantic coast of Spain. Paz Otero. University of Santiago de Compostela. | |
| 16:30-17:00 | Coffee Break | Poster Exhibition |

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| 17:00-17:30 Young Scientists Oral Session 5 | Food analysis <u>Session chairs:</u> <i>Begoña Jiménez Luque, IQOG-CSIC, Madrid</i> <i>Jordi Díaz Ferrero, IQS-Universidad Ramón Llull</i> | |
| 17:00 | OY12 <i>New procedure for the selective isolation of mercaptans using copper extraction. Application to the determination of three ultratrace odorants in wine by dual GC-MS/MS.</i> Elena Bueno Aventín. University of Zaragoza. | |
| 17:10 | OY13 <i>Detection and quantitation of almond adulterations by UHPLC-HRMS polyphenolic profiles.</i> Guillem Campmajó. University of Barcelona | |
| 17:20 | OY14 <i>Determination of the food exposure to bisphenol A and its analogs with obesogenic activity in the school population.</i> Yolanda Gálvez Ontiveros. University of Granada. | |
| 17:30-19:30 | SECyTA Meeting | Poster Exhibition |
| 19:30-21:30 | Compostela City Walk | |

Thursday 10

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| 9:00 Plenary Lecture PL5 | <p style="text-align: center;"><i>Porous polymer monoliths: Versatile materials for numerous applications.</i> Frantisek Svec, University Hradec Kralove, Czech Republic</p> <p><u>Session chairs:</u> <i>Ana M^a García Campaña, University of Granada</i> <i>Carmen García Jares, Universidade de Santiago de Compostela</i></p> | |
| 9:45-10:45 Oral Session 6 | <p style="text-align: center;"><i>Environmental analysis</i></p> <p><u>Session chairs:</u> <i>Joan Grimalt, IDAEA-CSIC, Barcelona</i> <i>Cristina Barrocas Dias, University of Évora, Portugal</i></p> | |
| 9:45 | <p>O15 <i>Evaluating plant uptake of pharmaceuticals and their metabolites from water reuse with UPLC-QTOF-MS.</i> Nicola Montemurro. IDAEA-CSIC.</p> | |
| 10:05 | <p>O16 <i>Passive sampling: calibration, detection and quantification of POPs in high-mountain lakes from the Aigüestortes National Park.</i> Raimon M. Prats. IDAEA-CSIC.</p> | |
| 10:25 | <p>O17 <i>Fate and occurrence of micro and nanoplastics in the Ebro Delta.</i> Marta Llorca. CSIC.</p> | |
| 10:45-11:30 | Coffee Break | Poster Exhibition |
| 11:30 Plenary Lecture PL6 | <p style="text-align: center;"><i>Application of comprehensive two-dimensional liquid chromatography to characterize very complex food-related samples.</i> Miguel Herrero, CIAL-CSIC, Spain</p> <p><u>Session chairs:</u> <i>Francisco Javier Santos, Universidad de Barcelona</i> <i>Marta Lores, Universidade de Santiago de Compostela</i></p> | |
| 12:15-13:15 Oral Session 7 | <p style="text-align: center;"><i>Environmental análisis</i></p> <p><u>Session chairs:</u> <i>Esteban Abad, IDAEA-CSIC, Barcelona</i> <i>Rosa Antonia Lorenzo, Universidade de Santiago de Compostela</i></p> | |
| 12:15 | <p>O18 <i>SPE-UPLC-HRMS suspect screening method for the identification of pharmaceuticals and their transformation products in surface water after photolysis.</i> Sandra Pérez. IDAEA-CSIC.</p> | |
| 12:35 | <p>O19 <i>Direct compound specific isotope analysis ($\delta^2\text{H}$, $\delta^{13}\text{C}$) of biomass components using analytical pyrolysis (Py-CSIA).</i> Layla M. San Emeterio. IRNAS-CSIC.</p> | |
| 12:55 | <p>O20 <i>Occurrence of pharmaceuticals and toxic elements in well water samples collected in Galicia.</i> Carolina Nebot. University of Santiago de Compostela.</p> | |

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| 13:15-13:35 Flash Poster Session 3 | Flash Poster Session 3 | |
| | <u>Session chairs:</u> <i>Esteban Abad, IDAEA-CSIC, Barcelona</i> <i>Rosa Antonia Lorenzo, Universidade de Santiago de Compostela</i> | |
| 13:15 | P6 Visible light photocatalytic degradation of trazodone using different modified titanate nanowires. Rodrigo Osawa. University of Lisbon. | |
| 13:20 | P7 Analysis of palytoxin and its analogues (ovatoxins) produced by <i>Ostreopsis cf. ovata</i> microalgae. Noemí-Inmaculada Medina Pérez. University of Barcelona. | |
| 13:25 | P8 Microplastics adsorption capacity and transport of cocontaminants in seawater. Albert Vega. IDAEA-CSIC. | |
| 13:30 | P9 Chiral analysis of amphetamine-related drugs in wastewater. Andrea Estévez Danta. University of Santiago de Compostela. | |
| 13:35-13:55 Young Scientists Oral Session 6 | Environmental analysis | |
| | <u>Session chairs:</u> <i>Belén Gómara Moreno, IQOG-CSIC, Madrid</i> <i>Sandra Pérez, IDAEA-CSIC, Barcelona</i> | |
| 13:35 | OY15 Fabric phase sorptive extraction for the determination of fungicides in environmental waters by GC-MS/MS. Lúa Vázquez. University of Santiago de Compostela. | |
| 13:45 | OY16 A high-sensitivity method for analysis of a mixture of relevant anthropogenic emerging organic contaminants in waters from remote areas. Ester López-García. IDAEA-CSIC. | |
| 14:00-15:00 | Lunch | |
| 15:00-15:30 | Technical Seminar 4 BRUKER | Poster Exhibition |
| 15:30-16:30 Oral Session 8 | Instrumental I | |
| | <u>Session chairs:</u> <i>Sandra Pérez, IDAEA-CSIC, Barcelona</i> <i>Antonio Moreda, Universidade de Santiago de Compostela</i> | |
| 15:30 | O21 High sensitivity applications in High Resolution MS QTOF. Javier López. Bruker | |
| 15:50 | O22 Determination of pyrrolizidine alkaloids in plant material using SFC-MS/MS. Diego Esteban-Fernández. Iza Scientific. | |

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| 16:10 | O23 Quantitation and Non-Target Detection of Pesticides in Spinach Extract with Pegasus BT 4D. Improvement to Targeted & Untargeted Pesticide Residue Analysis: Fast and Flexible Analyte Finding For GC-MS and GCxGC-MS Julio Lluch. LECO Sep Science. | |
| 16:30-17:00 | Coffee Break | Poster Exhibition |
| 17:00-17:20 Young Scientists Oral Session 7 | Food analysis <u>Session chairs:</u> <i>Begoña Jiménez Luque, IQOG-CSIC, Madrid</i> <i>Jordi Díaz Ferrero, IQS-Universidad Ramón Llull</i> | |
| 17:00 | OY17 UHPLC-API-MS/MS for the determination of azo-dyes in red spices. Ane Arrizabalaga Larrañaga. University of Barcelona. | |
| 17:10 | OY18 GC-MS analysis of six lipid peroxidation products with DNPH derivatization using a new GDME-DLLME procedure. Jorge Antonio Custodio-Mendoza. University of Santiago de Compostela. | |
| 17:20-17:45 | EU-FT-ICR project C. Cordeiro. University of Lisbon. | |
| 21:30-00:30 | Gala Dinner | |

Friday 11

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| 9:30 Plenary Lecture PL7 | <i>Unveiling the secrets of the past using hyphenated chromatographic techniques.</i> Cristina Barrocas Dias, University of Évora, Portugal <u>Session chairs:</u> <i>Maria Helena Florêncio, Universidade de Lisboa</i> <i>Encarnación Moyano, Universidad de Barcelona</i> |
| 10:15-10:55 Young Scientists Oral Session 8 | <i>Environmental análisis</i> <u>Session chairs:</u> <i>Francisco Javier Santos, Universidad de Barcelona</i> <i>Juan Vicente Sancho Llopis, Universitat Jaume I</i> |
| 10:15 | OY19 Atmospheric pressure photoionization for GC-HRMS analysis of PCDD/Fs and dioxin-like PCBs in food and environmental samples. Juan Francisco Ayala Cabrera. University of Barcelona. |
| 10:25 | OY20 Potential of micro-liquid chromatography for the determination of psychoactive substances in wastewater. Alberto Celma. Research Institute for Pesticides and Water, University Jaume I. |
| 10:35 | OY21 High throughput analysis of medium to highly polar pesticides in surface and ground water from agriculture-impacted areas of Catalonia using on-line SPE-LC-MS/MS. Maria Vittoria Barbieri. IDAEA-CSIC. |
| 10:45 | OY22 Enantiomeric determination of cathinones in environmental water sample. Yandi Fu. University Rovira i Virgili. |
| 10:55-11:25 | Coffee Break |
| 11:25-12:05 Oral Session 9 | <i>Other applications</i> <u>Session chairs:</u> <i>María Llopart, Universidade de Santiago de Compostela</i> <i>Rosario Pereiro, Universidad de Oviedo, Spain</i> |
| 11:25 | O24 Miniaturized SPE follow by GC-MS for the determination of UV filters in water. Piyaluk Nurerk. Prince of Songkla University. |
| 11:45 | O25 Evolution and developments of proton transfer reaction-mass spectrometry for security applications. Ramón González Méndez. Coventry University / University of Birmingham. |

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| <p>12:05-12:25 Flash Poster Session 4</p> | <p>Flash poster session 4</p> <p><u>Session chairs:</u> <i>María Llopart, Universidade de Santiago de Compostela</i> <i>Rosario Pereiro, Universidad de Oviedo, Spain</i></p> |
| <p>12:05</p> | <p>P10 Capsule phase microextraction with mixed-mode properties to selectively determine acidic or basic compounds from environmental water. Joan Carles Nadal. University Rovira i Virgili.</p> |
| <p>12:10</p> | <p>P11 Application of multivariate analysis to identify peptides responsible for the hypocholesterolemic capacity of protein hydrolysates released from olive seeds. Isabel M. Prados. University of Alcalá.</p> |
| <p>12:15</p> | <p>P12 Evaluation of vermicompost biofertilization on the aroma and polyphenolic composition of Albariño musts and wines. Perla Ferrer. University of Santiago de Compostela.</p> |
| <p>12:20</p> | <p>P13 Isotopic pattern as filtering rule for the screening of authorized green colorants in foods. María Roca. Instituto de la Grasa (CSIC), Sevilla.</p> |
| <p>12:25-13:05 Oral Session 10</p> | <p>Instrumental II</p> <p><u>Session chairs:</u> <i>Juan Francisco García Reyes, Universidad de Jaén</i> <i>Marta Lores, Universidade de Santiago de Compostela</i></p> |
| <p>12:25</p> | <p>O26 Development and Application of a Cyclic ion mobility mass spectrometer. Emma Marsden-Edwards. Waters Corporation.</p> |
| <p>12:45</p> | <p>O27 Does your dog have anxiety after a rough day at the mountain: analysis of CDB extracts for dogs treat. Jose Rivero. Agilent Technologies.</p> |
| <p>13:05</p> | <p>Closing Lecture</p> <p>“Año Internacional de la Tabla Periódica de los Elementos Químicos”: ¿Cómo se mide el tiempo con la tabla periódica? Joan Grimalt, IDAEA–CSIC, Barcelona</p> |
| <p>13:30</p> | <p>Closing session & Awards</p> |
| <p>14:00</p> | <p>Farewell cocktail</p> |

List of contributions

ORAL COMMUNICATIONS

- 01. Evaluation of the anticancer potential goldenberry calyx under a foodomics perspective.** Gerardo Álvarez-Rivera, Diego Ballesteros-Vivas, Alberto Valdés, Fabián Parada-Alfonso, Elena Ibañez, Alejandro Cifuentes.
- 02. Glycoproteomic profile of extracellular vesicles in cancer.** Hugo Osório, Daniela Freitas, Ana Magalhaes, Celso Reis.
- 03. Extreme make-up and cosmetic applicators: are they safe?** María Celeiro, Carmen García-Jares, Marta Lores.
- 04. Untargeted metabolomics of full scan MS hyphenated data – mining for minor peaks with finnee, risks and benefits.** Guillaume L. Erny, Arminda Alves.
- 05. Profiling the skin volatilome as powerful tool to the neurodegenerative diseases diagnosis.** Jorge Pereira, Beatriz Andrade, José Câmara.
- 06. A Metabolomics-based Workflow for Adductomics Studies.** João Nunes, Catarina Charneira, Sofia Gouveia-Fernandes, Jacinta Serpa, Judit Morello, Alexandra M.M. Antunes.
- 07. Mass spectrometry contribution to metabolic studies: new insights into montelukast metabolism.** Cátia F. Marques, Gonçalo C. Justino, M. Matilde Marques.
- 08. Combination of multiple heart-cutting two dimensional liquid chromatography and isotope dilution ESI-MS/MS for the accurate quantification of clinical biomarkers.** Pablo Rodríguez-González, Amanda Suárez Fernández, Adriana González Gago, Héctor González Iglesias, Adela Cortés Giménez-Coral, Belén Prieto García, Carlos Manuel López López, Maria Funes Menéndez, J. Ignacio García Alonso.
- 09. Quantification of related synthetic cathinones in rat brain by UHPLC-MS/MS. Relationship between structure and blood-brain barrier permeability.** David Fabregat-Safont, Manuela Barneo-Muñoz, Ferran Martínez-García, Juan Vicente Sancho, Félix Hernández, María Ibañez.
- 010. Identification of growth hormone-releasing hormones in urine doping controls by immunoaffinity purification and Liquid Chromatography Mass Spectrometry.** Élide Alechaga, Laura Pont, Alejandro Terrero, Núria Monfort, Rosa Ventura.
- 011. HPLC-ESI-MS/MS as a valuable tool to unravel the metabolism of new psychoactive substances.** Joana Carrola, Cristina Sampayo, M. Jesus Perry, Pedro Florindo, Rui Moreira, Álvaro Lopes, M. Rosário Bronze, Noélia Duarte.
- 012. Preliminary identification of specific markers to guarantee the authenticity of Galicia's honey by a non-target HRMS approach.** Thierry Dagnac, Lúa Vázquez, Meruyert Sergazina, María Celeiro, María Llompart.
- 013. Chemical profile of coffee varieties by FT-ICR-MS.** Mariana Pereira, Carlos Cordeiro, Ana Marques.
- 014. LC-MS/MS confirmation of the emerging pinnatoxins and high levels of esterified OA group toxins in commercial mollusks from the Atlantic coast of Spain.** Paz Otero, Luis Botana.
- 015. Evaluating plant uptake of pharmaceuticals and their metabolites from water reuse with UPLC-QTOF-MS.** Nicola Montemurro, Sandra Pérez.
- 016. Passive sampling: calibration, detection and quantification of persistent organic pollutants in high-mountain lakes from the Aigüestortes national park.** Raimon M. Prats, Barend L. van Drooge, Pilar Fernández, Joan O. Grimalt.
- 017. Fate and occurrence of micro and nanoplastics in the Ebro Delta.** Marinella Farré, Marta Llorca, Gabriella Schirinzi, Manuela Ábalos, Esteban Abad.
- 018. SPE-UPLC-HRMS suspect screening method for the identification of pharmaceuticals and their transformation products in surface water after photolysis.** Enelton Fagnani, Nicola Montemurro, Sandra Pérez.
- 019. Direct compound specific isotope analysis ($\delta^2\text{H}$, $\delta^{13}\text{C}$) of biomass components using analytical pyrolysis (Py-CSIA).** Layla M. San Emeterio, Nicasio T. Jiménez-Morillo, José M. de la Rosa, Francisco J. González-Vila, José-A González-Pérez.

- O20. Occurrence of pharmaceuticals and toxic elements in well water samples collected in Galicia.** Carolina Nebot, Elena Falqué, Benita Pérez, María Veiga, Carlos Franco.
- O21. High sensitivity applications in High Resolution MS QTOF.** Javier López.
- O22. Determination of pyrrolizidine alkaloids in plant material using SFC-MS/MS.** Diego Esteban-Fernández, Raymond Wong, Anja Grüning, Gesa J. Schad, Jan Stenzler.
- O23. Quantitation and non-target detection of pesticides in spinach extract with Pegasus BT 4D. Improvement to targeted & untargeted pesticide residue analysis: Fast and flexible analyte finding for GC-MS and GCxGC-MS.** Julio Lluch.
- O24. Miniaturized solid-phase extraction follow by Gas Chromatography-tandem Mass Spectrometry for the determination of UV filters in water.** Piyaluk Nurerk, Pajaree Donkhampa, Opas Bunkoed, Thierry Dagnac, Maria Llompart.
- O25. Evolution and developments of proton transfer reaction-mass spectrometry for security applications.** Ramón González Méndez.
- O26. Development and application of a cyclic ion mobility mass spectrometer.** Dale A. Cooper-Shepherd, Martin Palmer, Jakub Ujma, Kevin Giles, Emma Marsden-Edwards, James I. Langridge.
- O27. Does your dog have anxiety after a rough day at the mountain: analysis of CDB extracts for dogs treat.** Jose Juan Rivero.

YOUNG SCIENTISTS ORAL COMMUNICATIONS

- OY1. Synthesis and characterization of isotopically labelled ^{15}N -3-monoiodotyrosine and ^{13}C -3,5-diiodotyrosine for their use as internal standards in urine analysis by LC-ESI-MS/MS.** Jesús Nicolás Carcelén^{1*}, Pablo Rodríguez González¹, Alfredo Ballesteros Gimeno², Juan Manuel Marchante Gayón¹, José Ángel Cocho de Juan³, J. Ignacio García Alonso.¹
- OY2. Sustainable extraction and characterization of bioactive peptides and polyphenols from brewer's spent grain: evaluation of synergic effects.** Estefanía González García, María Luisa Marina, María Concepción García.
- OY3. Volatolomics approach for the identification of pup pheromones promoting maternal care in mice.** Leticia Lacalle-Bergeron, Carlos Sales-Martínez, Tania Portolés-Nicolau, Juan V Sancho-Llopis, Joaquim Beltrán-Arandes, Rafael Goterris-Cerisuelo, Cinta Navarro-Moreno, Fernando Martínez-García.
- OY4. Determination of synthetic cathinones in meconium by LC-MS/MS.** Ángela López-Rabuñal, Elena Lendoiro, Marta Concheiro, Manuel López-Rivadulla, Angelines Cruz, Ana de Castro.
- OY5. State-of-the-art of analytical methods for aflatoxin human biomonitoring.** Beatriz Arce-López, Elena González-Peñas, Ariane Vettorazzi, Elena Lizarraga.
- OY6. Analytical considerations for the LC-MS/MS determination of endogenous steroids.** Alex Gomez-Gomez, Olha Khymenets, Oscar J Pozo.
- OY7. A LC-MS/MS method for determination of antipsychotic drugs in nails.** María Cobo Golpe, Ana de-Castro-Ríos, Angelines Cruz, Manuel López-Rivadulla, Elena Lendoiro.
- OY8. Multiclass method for the determination of endocrine disrupting chemicals in human nails using alkaline digestion prior to Ultrahigh Performance Liquid Chromatography tandem Mass Spectrometry.** Laura Martín-Pozo, Samuel Cantarero-Malagón, Alberto Navalón, Alberto Zafra-Gómez.
- OY9. Determination of synthetic cathinones in oral fluid by Liquid Chromatography-tandem Mass Spectrometry.** Sergi Pascual, Núria Fontanals, Francesc Borrull, Carme Aguilar, Marta Calull.
- OY10. Simple and effective method for the determination of neonicotinoid residues in honeys and cereals by capillary liquid chromatography.** Laura Carbonell Rozas, Alex Rizo-Zapata, Francisco J. Lara, Monsalud del Olmo-Iruela, Ana M. García-Campaña.
- OY11. GC-MS characterisation of novel pectic-oligosaccharides derived from artichoke pectin using machine learning and competitive fragmentation modelling (CFM-ID).** Carlos Sabater, Antonia Montilla, Nieves Corzo.
- OY12. New procedure for the selective isolation of mercaptans using copper extraction. Application to the determination of three ultratrace odorants in wine by dual Gas Chromatography-tandem Mass Spectrometry.** Elena Bueno Aventín, Ignacio Ontañón, Vicente Ferreira.

- OY13. Detection and quantitation of almond adulterations by UHPLC-HRMS polyphenolic profiles.** Guillem Campmajó, Javier Saurina, Oscar Núñez.
- OY14. Determination of the food exposure to bisphenol A and its analogs with obesogenic activity in the school population.** Yolanda Gálvez Ontiveros, Laura Martín-Pozo, Victoria Martín-Laguna, Samuel Cantarero-Malagón, Margarita Aguilera, Celia Monteagudo, Lourdes Rodrigo, Ana Rivas, Alberto Zafra-Gómez.
- OY15. Fabric phase sorptive extraction for the determination of fungicides in environmental waters by GC-MS/MS.** Lúa Vázquez, Maria Celeiro, Piyaluk Nurerk, Abuzar Kabir, Thierry Dagnac, Maria Llompart.
- OY16. A high-sensitivity method for analysis of a mixture of relevant anthropogenic emerging organic contaminants in waters from remote areas.** Ester López-García, Cristina Postigo, Luis Moreno-Merino, Miren López de Alda.
- OY17. UHPLC-API-MS/MS for the determination of azo-dyes in red spices.** Ane Arrizabalaga-Larrañaga, S. Epigmenio, F.J. Santos, E. Moyano.
- OY18. GC-MS analysis of six lipid peroxidation products with DNPH derivatization using a new GDME-DLLME procedure.** Jorge Antonio Custodio-Mendoza, J. Aja-Macaya, I. Valente, R. Ramos, J. A. Rodriguez, A. M. Carro, R. A. Lorenzo.
- OY19. Atmospheric pressure photoionization for GC-HRMS analysis of PCDD/Fs and dioxin-like PCBs in food and environmental samples.** Juan Francisco Ayala Cabrera, M. Ábalos, E. Abad, E. Moyano, F. J. Santos.
- OY20. Potential of micro-liquid chromatography for the determination of psychoactive substances in wastewater.** Alberto Celma, Juan V. Sancho, Noelia Salgueiro-González, Sara Castiglioni, Ettore Zuccato, Félix Hernández, Lubertus Bijlsma.
- OY21. High throughput analysis of medium to highly polar pesticides in surface and ground water from agriculture-impacted areas of Catalonia using on-line SPE-LC-MS/MS.** Maria Vittoria Barbieri, Cristina Postigo, Vinyet Sola, Miren López de Alda.
- OY22. Enantiomeric determination of cathinones in environmental water samples.** Yandi Fu, Francesc Borrell, Núria Fontanals, Rosa Maria Marcé.

POSTERS

SELECTED FOR FLASH PRESENTATION

- P1. Advanced membrane assisted solvent extraction (MASE) for isolating new psychoactive substances from urine before HPLC-MS/MS determination.** Cristian Suárez-Oubiña, Ana María Bermejo, Pilar Bermejo-Barrera, Antonio Moreda-Piñeiro.
- P2. Analytical challenges associated to essential oils and their individual components in cosmetics.** Laura Rubio, Marta Lores, Carmen García-Jares.
- P3. Comparison of two chemometric approaches for the identification by LC-QTOF based untargeted metabolomics of potential plasma biomarkers in pediatric chronic kidney disease.** Sandra Benito, Nora Unceta, Alicia Sánchez, Alberto Gómez, M^a Aránzazu Goicolea, Ramón J. Barrio.
- P4. Time-series proteomic study of diabetic nephropathy in human proximal tubular HK-2 cells by UHPLC-ORBITRAP MS/MS.** Alberto Valdés, Coral García-Pastor, María Castro-Puyana, Francisco J. Lucio-Cazaña, María Luisa Marina.
- P5. Annotation of oxidized phospholipids in metabolomics guided cancer study.** Ángeles López-López, Joanna Godzien, Vanesa Alonso-Herranz, Anna La Salvia, Genoveva Gómez-Esteves, Beatriz Soldevilla, Rocío García-Carbonero, Ángeles López-González, Coral Barbas.
- P6. Visible light photocatalytic degradation of trazodone using different modified titanate nanowires.** Rodrigo Osawa, Beatriz Barrocas, Olinda Monteiro, M. Conceição Oliveira, M. Helena Florêncio.
- P7. Analysis of palytoxin and its analogues (ovatoxins) produced by *Ostreopsis cf. ovata* microalgae.** Noemí-Inmaculada Medina Pérez, E. Berdalet, E. Moyano.

- P8. ***Microplastics adsorption capacity and transport of cocontaminants in seawater.*** Albert Vega, Marta Llorca, Gabriella Schirinzi, Manuela Ábalos, Esteban Abad, Marinella Farré.
- P9. ***Chiral analysis of amphetamine-related drugs in wastewater.*** Andrea Estévez-Danta, Vanessa Guttmann, Rosa Montes, Iria González-Mariño, Rosario Rodil, Ailette Prieto, Manuel Miró, Rafael Cela, José Benito Quintana.
- P10. ***Capsule phase microextraction with mixed-mode properties to selectively determine acidic or basic compounds from environmental water.*** Joan Carles Nadal, Francesc Borrull, Kenneth G. Furton, Abuzar Kabir, Rosa Maria Marcé, Núria Fontanals.
- P11. ***Application of multivariate analysis to identify peptides responsible for the hypocholesterolemic capacity of protein hydrolysates released from olive seeds.*** Isabel M. Prados, Merichel Plaza, María Luisa Marina, María Concepción García.
- P12. ***Evaluation of vermicompost biofertilization on the aroma and polyphenolic composition of Albariño musts and wines.*** Perla Ferrer, María Celeiro, Hugo Martínez-Cordeiro, Tamara Vázquez, Carmen García-Jares, Marta Lores, Jorge Domínguez.
- P13. ***Isotopic pattern as filtering rule for the screening of authorized green colorants in foods.*** María Roca, Isabel Viera, Antonio Pérez.

FUNDAMENTALS ON CHROMATOGRAPHY AND ELECTRO-DRIVEN SEPARATION TECHNIQUES

- P14. ***Dual retention behavior of benzalkonium chloride in core-shell column with biphenyl groups.*** María Carmen Prieto-Blanco, Angela Planas-Franco, Soledad Muniategui-Lorenzo, María José González-Castro.
- P15. ***Statistical comparison of the retention mechanism of polychlorinated biphenyls in different gas chromatography stationary phases.*** J. Escobar-Arnanz, J. Sanz, Belén Gómara, L. Ramos

MASS SPECTROMETRY FUNDAMENTALS, STATE-OF-THE ART, APPLICATIONS AND INNOVATIONS

- P16. ***Applicability of atmospheric pressure photoionization for the determination of dechlorane plus and analogues by GC-HRMS.*** Juan Francisco Ayala-Cabrera, E. Ayvazyan-Arutyunyan, E. Moyano, F. J. Santos.

MS HYPHENATED TECHNIQUES, APPLICATIONS AND NEW DEVELOPMENTS

- P17. ***Combining in vitro bioanalysis and High Resolution Mass Spectrometry for a refined non-target screening workflow using surface waters from mediterranean littoral (Spain) as a case study.*** Alberto Celma, Geeta Mandava, Agneta Oskarsson, Frank Menger, Foon Yin Lai, Oksana Golovko, Juan V. Sancho, Félix Hernández, Lutz Ahrens, Johan Lundqvist, Lubertus Bijlsma.
- P18. ***$\delta^{13}\text{C}$ and $\delta^{18}\text{O}$ isotope signature of *Spondyliosoma cantharus* otoliths.*** Ana Isabel Janeiro, Ana Neves, Miguel Gaspar, Ana Rita Vieira, Vera Sequeira, Jorge M. R. S. Relvas, Leonel Serrano Gordo.
- P19. ***Hormones and their metabolites as prehistoric shepherds' activities and milk storage biomarkers.*** Alicia Sanchez, Blanca Navarro, Ane Gorostizu, Asier Vallejo, Josep María Vergés, Juan Antonio Quiros, Nora Unceta, Maria Aranzazu Goicolea, Ramón J. Barrio.

P20. **Determination of melatonin and its metabolites by different quantification approaches using liquid chromatography and tandem mass spectrometry (LC-MS/MS).** Adriana González Gago, Amanda Suarez Fernández, Javier García Calleja, Juan Carlos Mayo, Rosa María Sáinz, Pablo Rodríguez González, José Ignacio García Alonso.

P21. **Development of a MS/MS spectral library of phenolic compounds using electrospray ionization and triple-quadrupole mass spectrometer.** Noélia Duarte, Andreia Bento da Silva, Joana Carrola, Beatriz T. Martins, João Mota, M. Rita Ventura, M. Rosário Bronze.

P22. **Building a collision cross section (CCS) database for environmental organic micropollutants screening under travelling wave ion mobility spectrometry coupled to high resolution mass spectrometry.** Alberto Celma, Lubertus Bijlsma, Félix Hernández, Juan V. Sancho.

P23. **GC meets VION IMS-QTOF. Facilitating ion mobility measurements for GC-amenable compounds in food and environmental analysis.** Tania Portolés, David Fabregat, Juan V. Sancho, Félix Hernández.

NEW ADVANCES AND DEVELOPMENTS IN CHROMATOGRAPHY AND RELATED TECHNIQUES

P24. **Optimization and validation of a method based on capillary electrophoresis coupled to laser induced fluorescence detection (CE-LIF) for chiral analysis and absolute quantitation of 3 amino acids: L and D-ASP, L and D-GLU and L and D-SER. Application to osteocyte and osteoblast cell lines.** M^a Paz Lorenzo, Luis Valiente, Antonia García.

P25. **Pyrolysis compound-specific nitrogen isotope analysis ($\delta^{15}\text{N}$ PY-CSIA): novel analytical approach for archaeological studies.** Nicasio T. Jiménez-Morillo, José M. De la Rosa, Ana Z. Miller, Francisco J. González-Vila, Cristina Dias, Anne-France Maurer, José A. González-Pérez.

P26. **Optimization of microwave assisted extraction of bioactive carbohydrates from alfalfa.** Andrea Martín-Ortiz, Alejandra Daniela Solarte-Sarasty, Maite Rada-Mendoza, Ana Isabel Ruiz-Matute, María Luz Sanz.

SAMPLE PREPARATION, HANDLING AND TRACE ANALYSIS

P27. **Effect of the purification steps of glycoproteins from biological fluids on their recovery.** Angel Puerta, Sergio Lopez-Duque, Raquel Saez-Brox, Laura Gomez Ruiz, Jose Carlos Diez-Masa, Mercedes de Frutos.

P28. **Development of a rapid method to confirm contamination by mineral oils through SPE-GC-MS.** Janira Jaén, Celia Domeño, Chiara Gajotti, Cristina Nerín.

P29. **Application of dispersive liquid liquid micro extraction (DLLME) for determination of aflatoxins B1, B2, G1 and G2 in fish.** G.D. Thilini Madurangika Jayasinghe, Raquel Domínguez-González, Pilar Bermejo-Barrera, Antonio Moreda-Piñeiro.

P30. **Application of molecularly imprinted polymer micro solid phase extraction (MIMSPE) for determination of aflatoxins B1, B2, G1, G2 and M1 in fish.** G.D. Thilini Madurangika Jayasinghe, Raquel Domínguez-González, Pilar Bermejo-Barrera, Antonio Moreda-Piñeiro.

P31. **Identification of peptides in the olive seed responsible for in vitro and in vivo hypolipidemic capacity.** Isabel M. Prados, José María Orellana, María Luisa Marina, María Concepción García.

P32. **Molecularly imprinted polymers for solid-phase extraction of aryloxyphenoxypropionate herbicides from water samples.** Sagrario Torres-Cartas, Susana Meseguer-Lloret, Carmen Gómez-Benito, Mónica Catalá-Icardo, Natalia Prima Margiotta, José Manuel Herrero-Martínez, Ernesto Francisco Simó-Alfonso.

- P33. **Development and application of a molecularly imprinted polymer for the extraction of phenoxy herbicides from water samples.** Susana Meseguer-Lloret, Sagrario Torres-Cartas, Carmen Gómez-Benito, Mónica Catalá-Icardo, Roberto Beltrán Martí, Ernesto Francisco Simó-Alfonso, José Manuel Herrero-Martínez.
- P34. **Development of stir bar sorptive extraction directly on polytetrafluoroethylene magnets modified with monoliths.** Carmen Gómez-Benito, Mónica Catalá-Icardo, Adrián Torres-Prades, Sagrario Torres-Cartas, Susana Meseguer-Lloret, Ernesto Francisco Simó-Alfonso, José Manuel Herrero-Martínez.
- P35. **Potential of cationic carbosilane dendrimers for sustainable protein sample preparation.** Estefanía González-García, Javier Sánchez-Nieves, Francisco Javier de la Mata, M. Luisa Marina, M. Concepción García.
- P36. **Immobilization of proteolytic enzymes on silica supports functionalized with carbosilane and pamam dendrimers and evaluation of their potential in successive hydrolysis.** Ester Hernández-Corroto, María Sánchez-Milla, Javier Sánchez-Nieves, Francisco Javier de la Mata, M. Luisa Marina, M. Concepción García.
- P37. **Miniaturized Solid-Phase Microextraction followed by GC-MS for the identification of compounds with organoleptic characteristics in honey.** Lúa Vázquez, Meruyert Sergazina, María Celeiro, Thierry Dagnac, María Llompart.
- P38. **Ultrasound assisted extraction for the determination of toxic substances in surfaces made of recycled rubber by GC-MS/MS.** Daniel Armada, María Celeiro, Thierry Dagnac, María Llompart.
- P39. **Development and application of polymeric sorbents with Zwitterionic character.** Joan Carles Nadal, Francesc Borrull, Peter A. G. Cormack, Rosa Maria Marcé, Núria Fontanals.

OMICS

- P40. **Mass Spectrometric Immunoassay of proteoforms of Apolipoprotein A and C in individuals with obstructive sleep apnea.** Ana Margarida Pereira, Amelia Feliciano, Olgica Trenchevska, Fatima Vaz, Dobrin Nedelkov, Randal Nelson, Paula Pinto, Cristina Barbara, Marilia Antunes, Deborah Penque, Vukosava Milic Torres.
- P41. **Carbon isotopic fractionation of urinary metabolites in transgenic mice during the development of prostate cancer.** Laura Covadonga Rodas Sánchez, Pablo Rodríguez-Gonzalez, Pedro Gonzalez-Menéndez, Juan Carlos Mayo Barrallo, Rosa M^a Sainz Menéndez, J. Ignacio García Alonso.
- P42. **Biosynthesis and characterization of isotopically labelled DNA and RNA methylated nucleosides for the quantification of global DNA and RNA methylation by isotope dilution LC-ESI-MS/MS.** Jesús Nicolás Carcelén, Juan Manuel Marchante Gayón, Luis Valledor, Pablo Rodríguez González, M^a Jesús Cañal, J. Ignacio García Alonso.
- P43. **Survey of α -synuclein protein variants using extreme resolution Fourier-Transform Ion cyclotron Resonance Mass Spectrometry.** Vukosava Milic Torres, Margarida Isidro, Marta Sousa Silva, Joana S. Cristovão, Cláudio M. Gomes, Carlos Cordeiro.
- P44. **Study of an in vitro model of high glucose-induced changes in human proximal tubular HK-2 cells using a CE-MS metabolomic strategy.** Samuel Bernardo-Bermejo, Elena Sánchez-López, María Castro-Puyana, Selma Benito-Martínez, Francisco Javier Lucio-Cazaña, María Luisa Marina.
- P45. **A LC-MS metabolomic-based strategy for the search of potential markers of cocoa powder adulteration.** Maider Greño, Merichel Plaza, María Luisa Marina, María Castro-Puyana.

P46. **An extensive phosphoproteomic analysis suggests an up-regulation of SFK-related signalling pathways in platelets from obese patients.** Maria N. Barrachina, Irene Izquierdo, Lidia Hermida-Nogueira, Aurelio M. Sueiro, Vanessa Casas, Felipe F. Casanueva, Maria Pardo, Joaquin Abian, Montserrat Carrascal, Ángel García.

P47. **Discovering chemical processes driving wine reductive problems using a UPLC-QTOF-based metabolomic approach.** Ignacio Ontañón, Diego Sánchez, Fulvio Mattivi, Vicente Ferreira, Panagiotis Arapitsas.

P48. **Posttranslational modification differences in brachyspira hyodysenteriae and B. pilosicoli. A proteomics study.** Vanessa Casas, Joaquin Abian, Montserrat Carrascal.

P49. **Establishment of urinary volatilome of distant human populations. A useful approach to detect potential lung cancer biomarkers.** Jorge Pereira, Beatriz Andrade, José Câmara.

P50. **Estimation of the most appropriate urine sampling period based on the urinary volatome profile.** Priscilla Porto-Figueira, José Figueira, Jorge Pereira, Valdemar Máximo, José S. Câmara.

P51. **Application of novel automated data dependent acquisition (DDA) in untargeted metabolomics.** Leticia Lacalle-Bergeron, Kathleen Rousseau, Tania Portolés-Nicolau, Juan V. Sancho, Christophe Junot, François Fenaille.

PHARMACEUTICALS

P52. **Development of a QuEChERS-based method for the analysis of PPCPs in vegetal matrices and agricultural soils.** Adrià Sunyer Caldú, Pablo Gago Ferrero, M. Silvia Díaz Cruz.

P53. **Compatibility and physical-chemical stability of intravenous mixtures for multimodal analgesia by UHPLC-DAD.** Marina Bellot-Pulido, J. Báguena-Polo, F. Broto-Puig, C. López-Cabezas, D. Soy-Muner.

P54. **Comparative degradation of two highly consumed antihypertensives in water by sonochemical process.** María Ibáñez, Efraim A. Serna-Galvis, Laura Izasa-Pineda, Alejandro Moncayo-Lasso, Félix Hernández, Ricardo A. Torres-Palma.

P55. **Development of a modified QuEChERS protocol to improve extraction efficiencies of pharmaceuticals from lettuce irrigated with reclaimed water.** Sandra Perez, A. Orfanoti, N. Montemurro.

P56. **Development and validation of a LC-ESI-MS/MS method for the simultaneous quantification of aflatoxins B₁, B₂, G₁, and G₂ in medicinal plants.** Mar Mulero, Gemma Gotor, Francesc Broto.

CLINICAL, TOXICOLOGICAL AND FORENSICS ANALYSIS

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- P60. **Metabolic profiling of the novel indanyl-cathinone 5-PPDI after human hepatocyte incubation.** María Ibañez, David Fabregat-Safont, Marie Mardal, Juan Vicente Sancho, Félix Hernández, Kristian Linnet.
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- P62. **An overview of synthetic cannabinoids consumption patterns in València over 2018.** David Fabregat-Safont, Carmen Ripoll, Teresa Orengo, Juan Vicente Sancho, Félix Hernández, María Ibañez.
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- P72. **Determination of pharmaceuticals and pesticides/transformation products in the Mijares River (Spain) by UHPLC-MS/MS.** Eddie Fonseca, José Marín, Lubertus Bijlsma, Carlos Sales, Elena Pitarch, Félix Hernández.
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- P95. **Determination of nine cyanotoxins in saline water samples by using salting-out assisted Liquid-Liquid extraction and UHPLC with UV and MS/MS detection.** Monsalud del Olmo-Iruela, Maryam Hemmati, Carmen Tejada-Casado, Francisco J. Lara, Ana M. García-Campaña, M. Carmen Contreras-Morales.
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- P97. **Determination of organophosphate flame retardants in fish samples using quechers extraction followed by GC-MS/MS.** Óscar Castro, Rosa Maria Marcé, Eva Pocurull, Francesc Borrull.
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- P99. **Functionalized mesostructured silica in sample preparation for the analysis of hydroxymethyl furfural in cereal and insect bars.** Lorena González, Sonia Morante-Zarcelo, Damián Pérez-Quintanilla, Isabel Sierra.
- P100. **Determination of polycyclic aromatic hydrocarbons in complex dry vegetal extracts using QuEChERS and MIP-SPE followed by gas chromatography coupled to tandem mass spectrometry.** Antonio Garballo Rubio, J. Soto-Chinchilla, Laura Martín-Pozo, Alberto Zafra-Gómez.
- P101. **Evaluation of functionalized ordered mesoporous silicas for strong cation-exchange solid-phase extraction of tropane alkaloids in flours.** Judith Gañán, Lorena González, Sonia Morante-Zarcelo, Damián Pérez-Quintanilla, Isabel Sierra.
- P102. **Isolation of proteins from spent coffee ground. Identification of peptides in the protein hydrolysates by RP-HPLC-ESI-Q-TOF.** Alberto Valdés, María Castro-Puyana, María Luisa Marina.
- P103. **Development and optimization of a method for determination of organochlorine pesticides in mussel based on miniaturized Matrix Solid-Phase Dispersion combined with Gas Chromatography-tandem Mass Spectrometry.** Nieves Carro, A. Lopez, J. Cobas, I. García, M. Ignacio, A. Mouteira.
- P104. **A novel method to determine fipronil and fipronil sulfone in eggs by capillary electrophoresis and salting-out assisted liquid-liquid extraction.** M. Mar Aparicio-Muriana, Ivona Lhotská, Francisco J. Lara and Ana M. García-Campaña.
- P105. **Authentication of Garcinia cambogia supplements by GC-MS.** Adal Mena-García, Angie J. Belleizac, Diana M. Chito, Maite P. Rada-Mendoza, Ana C. Soria, María L. Sanz, Ana I. Ruiz-Matute.
- P106. **Olive ripeness as a tool to modulate phenolic composition of oils and in vitro inhibition of α -glucosidase.** María Figueiredo-González, Patricia Reboledo-Rodríguez, Laura Castro Sobrino, Lucía Olmo-García, Alegría Carrasco-Pancorbo, Jesús Simal-Gándara, Carmen González-Barreiro, Beatriz Cancho-Grande.
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- P108. **Alterations in Mediterranean mussel (Mytilus galloprovincialis) composition exposed to cyanotoxins as revealed by nalytical pyrolysis.** Leticia Diez-Quijada, Flavio L. de Oliveira, Ángeles Jos, Ana M. Cameán, Ramón Aparicio-Ruiz, Víctor Vasconcelos, Alexandre Campos, Francisco J. González-Vila, José A. González-Pérez.
- P109. **Multi-mycotoxin determination in unifeed by (D)SPE-QuEChERS-HPLC-HRMS.** Rocío Facorro, María Llompant, Thierry Dagnac.
- P110. **Development of a HPLCS-DAD-MS method for the quality evaluation of guarana (paullinia cupana) supplements.** Andrea Martín-Ortiz, Belén Gonzalo-Martínez, Ana Cristina Soria, María Luz Sanz, Ana Isabel Ruiz-Matute.

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P116. **Analysis and quantification of *Sambucus Nigra* extracts for potential skin application.** Ana Henriques Mota, Noélia Duarte, Maria Rosário Bronze, Andreia Bento Silva, Elias Fattal, António José Almeida, Catarina Pinto Reis.

P117. **Extraction of bioactive compounds from pomegranate seeds using High Intensity Focussed Ultrasounds and Pressurized Liquids.** Miriam Guzmán-Lorite, Estefanía González-García, María Luisa Marina, María Concepción García.

P118. **Analytical platform for the analysis of variability introduced by 10 *S. Cerevisiae* strains in tempranillo wines.** Marie Denat, Dolores Perez, Amparo Querol, Vicente Ferreira.

P119. **Natural pigments-based tattoos: analytical approaches for their safety control.** Laura Rubio, Carmen Garcia-Jares, Marta Lores.

P120. **Chromatographic insights for tracking bioactive compounds in woody by-products.** María Celeiro, J.Pablo Lamas, Rosa Arcas, Marta Lores.

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P123. **Driving proteomic nanoLC-MS to new crossroads, are we heading towards extra sensitive or increased throughput applications?** Gilles Jaouen, R. van Ling, C. Mitterer, G. van Raemdonck, J. Op De Beeck.

P124. **Maximize the output of routine proteome analyses by using micro pillar array column technology.** Geert Van Raemdonck, Jeff Op de Beeck, Kurt Van Mol, Bo Claerebout, Natalie Van Landuyt, Wim De Malsche, Gert Desmet, Paul Jacobs, Gilles Jaouen.

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- P126. **Assessment of a new derivatization reagent for the analysis of glyphosate and aminomethylphosphonic acid.** Juan M Sánchez, Clàudia Fontàs.
- P127. **A HPLC-FLD method for the simultaneous quantification of mycotoxins in animal feed using solid phase combined with dispersive liquid-liquid extraction.** Borja Muñoz Solano, Elena González-Peñas.
- P128. **LC-MS analysis of ISRIB in plasma and brain samples.** Argitxu Esquivel, Elías Marlin, Obdulia Rabal, Tomas Aragón, Montserrat Arrasate, Antonio Pineda-Lucena.
- P129. **Lipid analysis of beef meat: can MALDI-TOF mass spectrometry be used to define differential profiles for bovine breeds fed under distinct fact content diet?** Newton V. Verbisck, A.A. Perestrello, A.L.J. Ferraz, L.C. De Paula, M.N. Bonin, S.R. Medeiros, M. Mele, R.G. Almeida, G.L.D. Feijó.
- P130. **Extraction of mycotoxins from edible insects using natural deep eutectic solvents: A green alternative to conventional methods.** Fernando Pradanas-González, Gerardo Álvarez-Rivera, Elena Benito-Peña, Miguel Herrero, Fernando Navarro-Villoslada, María Cruz Moreno-Bondi.
- P131. **Photo-transformation products from halogenated pharmaceuticals.** Enelton Fagnani, Nicola Montemurro, Sandra Pérez.

TECHNICAL SEMINARS

TS1. LECO Sep Science

TS2. IZASA-Shimadzu

TS3: Agilent

TS4: Waters

TS5. Bruker

Full paper publication

Participants are invited to submit manuscripts based on presentations at the 1st Iberian Meeting in Separation Sciences & Mass Spectrometry (IMSS&MS) to be held in Santiago de Compostela, Spain, 8-11 October 2019 for possible publication in [Journal of Chromatography A](#), with the intention of publishing in an online Special Issue (VSI) that is dedicated to this meeting.

The Special Issue rules out possible delays in publication for contributors to the special issue and will make the conference special issue more complete and accessible than it has ever been. Please see below its advantageous characteristics:

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All manuscripts will be subjected to the regular selection process for the journal, including the strict peer review procedure; therefore acceptance for presentation at the meetings is not a guarantee for publication in the journal.

Thanks in advance for your contribution!

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General information

Venue

Facultad de Medicina
Rúa de San Francisco, s/n
15782 Santiago de Compostela

Conference language

*The official language of the Meeting is **English**.*

Oral Presentations

Plenary lectures (PL): 45 min.

Oral communications (O): 20 min.

Young scientists oral communications (OY): 10 min.

Posters flash presentations: 5 min.

Authors should provide a copy of their presentation PowerPoint file to the organization at least two hours before the session starts (ideally the day before the presentation).

Poster presentations

Posters are displayed from Tuesday 8 to Thursday 10.

Authors must be in attendance at their poster boards during the Poster Exhibition sessions.

Social program

Tuesday 8

20:30-1:30h. Wellcome cocktail and dancing party. San Francisco Hotel Monumento. (50 m from the Meeting Venue)

Wednesday 9

19:30-21:30h. Compostela City Walk. Departure from the Facultad de Medicina (Meeting venue)

Thursday 10

21:30-12:30h. Gala dinner. Hostal de los Reyes Católicos. Plaza do Obradoiro (50 m from the meeting Venue)

Friday 11

14:00h. Farewell cocktail. Facultad de Medicina (Meeting Venue)