

15th INSTRUMENTAL ANALYSIS CONFERENCE

GRAN VIA VENUE. OCTOBER 3rd - 5th 2017

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15^{as} JORNADA DE ANÁLISIS INSTRUMENTAL

RECINTO GRAN VIA 3- 5 OCTUBRE 2017

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FINAL PROGRAM

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BIENVENIDA

En nombre del Comité Organizador de las 15^{as} JORNADAS DE ANÁLISIS INSTRUMENTAL (JAI) tenemos el placer de daros una calurosa bienvenida a todos los asistentes a esta reunión. Esta edición, organizada por la Sociedad Española de Cromatografía y Técnicas Afines (SECyTA) en colaboración con la Sociedad de Espectroscopía Aplicada (SEA), la Sociedad Española de Espectrometría de Masas (SEEM) y la Sociedad Española de Proteómica (SEProt), ofrece una oportunidad única para conocer de primera mano los últimos avances en el campo de la Química Analítica y el Análisis Instrumental, tanto desde un punto de vista fundamental como aplicado, y proporciona un punto de encuentro imprescindible para investigadores y profesionales del sector.

En esta edición, seguimos apostando por una reunión científica que integre los intereses de las diferentes Sociedades participantes con el objetivo de enriquecer y potenciar el intercambio de experiencias y conocimientos desde diferentes puntos de vista manteniendo el análisis instrumental como denominador común. La organización de estas Jornadas ha sido una apuesta difícil que asumimos en su momento con ilusión y convencidos de que con el trabajo y la colaboración de todos podríamos ser capaces de ofrecer una reunión científica atractiva y de calidad, a la altura de las expectativas.

Como en Jornadas anteriores, el programa científico recoge los últimos avances de las técnicas instrumentales en áreas como medio ambiente, alimentos, tratamiento de muestra, desarrollos instrumentales nuevos, miniaturización, bioanálisis, proteómica y control antidopaje. En esta edición vamos a contar con conferenciantes de prestigio internacional reconocido que nos presentaran las últimas novedades de las técnicas y el análisis instrumental en diferentes campos de aplicación. El programa científico consta de 140 comunicaciones, estructurado en ocho conferencias plenarias e invitadas, 33 comunicaciones orales y casi 100 pósteres, de los cuales se han seleccionado 12 para su presentación en formato corto o flash. En esta ocasión, seguimos apostando por los jóvenes investigadores, dedicando sesiones específicas dentro del programa científico para la presentación de sus trabajos, y concediendo becas de inscripción y ayudas de viaje para facilitar su asistencia al congreso.

La organización de un evento de estas características es siempre complicada, por ello quiero agradecer sinceramente a todas las Sociedades implicadas, SEA, SEEM y SEProt, su inestimable colaboración y apoyo prestado en todo momento. También quiero agradecer a Expoquímica y a la Secretaría Técnica de las Jornadas su asistencia y disponibilidad para poder organizar esta reunión.

Finalmente, en nombre del Comité Organizador quiero agradecer vuestra asistencia a esta reunión y transmitiros nuestra más cordial bienvenida a Barcelona. Esperamos que estas Jornadas sean científicamente muy productivas y provechosas.

Francisco Javier Santos Vicente
Presidente del Comité Organizador

Joan Grimalt Obrador
Vicepresidente del Comité Organizador



WELCOME

On behalf of the Organizing Committee of the 15th INSTRUMENTAL ANALYSIS CONFERENCE (JAI), we have the pleasure to warmly welcome you. This Conference edition is organized by the Spanish Society of Chromatography and Related Techniques (SECyTA) in collaboration with the Society of Applied Spectroscopy (SEA), the Spanish Society of Mass Spectrometry (SEEM) and the Spanish Society of Proteomics (SEProt). It offers an unique opportunity to be updated on the latest advances in Analytical Chemistry and Instrumental Analysis, from both the fundamental and applied viewpoints, in a context that has become a reference meeting for researchers and professionals of the sector.

This edition integrates the interests of the participating societies and is aimed to create high scientific profile synergies based on the exchange of experiences and knowledge from different perspectives, keeping instrumental analysis as a common denominator. On this occasion, the organization of the Conference has been a difficult bet due to external factors. We assumed this bet with enthusiasm, convinced that the community working with instrumental analysis deserved the continuation of the JAI meeting series that combines high quality presentations with a chemical fair (EXPOQUIMIA) that shows the latest advances in instrumental analytical techniques. With the collaboration of all participant societies we hope to have fulfilled the expectations and offer an attractive and high quality scientific meeting.

As in previous Conferences, the scientific program gathers the latest advances in instrumental techniques and their applications in different areas, such as environment, food, sample treatment, miniaturization, bioanalysis, proteomics and anti-doping control. We will have speakers of recognized international prestige who will present their latest innovations on techniques and instrumental analysis in these fields. The scientific program consists of 140 communications, structured into eight plenary and invited conferences, 33 oral communications and almost 100 posters, of which 12 communications have been selected for presentation in flash format. As in previous meetings, support the participation of young researchers is a main issue. We devote specific sessions to the presentation of their work, and grant registration and travel grants to facilitate their attendance.

We thank all the Societies involved in the organization of the Meeting together with SECyTA, SEA, SEEM and SEProt, for their invaluable collaboration and support provided as in previous JAI events. I also want to thank Expoquimia and the Technical Secretary of the Conference for their assistance and readiness to help with the organization.

On behalf of the Organizing Committee, I also thank you for attending this meeting and convey our warmest welcome to Barcelona. We hope these days will be very productive and profitable from both the scientific and technical perspectives.

Francisco Javier Santos Vicente
Chair of Organising Committee

Joan Grimalt Obrador
Co-chair of Organising Committee

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ORGANISING COMMITTEE

Francisco Javier Santos Vicente (Chairman)	Universidad de Barcelona
Joan Grimalt Obrador (Co-Chairman)	IDAEA-CSIC, Barcelona
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CONFERENCIANTES INVITADOS / INVITED SPEAKERS



Bruno Le Bizec

Laboratoire d'Etude des Résidus et Contaminants dans les Aliments (LABERCA/Oniris).

Ecole Nationale Vétérinaire, Agroalimentaire et de l'Alimentation Nantes Atlantique (Oniris), Nantes, France

An ever-increased confidence in chemical food safety driven by latest analytical innovations



Stuart Harrad

Environmental Health Science. School of Geography, Earth and Environmental Sciences,
University of Birmingham, UK

The environmental fate and behaviour of halogenated flame retardants



Daniel W. Armstrong

Department of Chemistry and Biochemistry, College of Science, University of Texas at Arlington, TX, USA
Chromatographic separations at sensor speeds: practice, consequences and advantages



Govert W. Somsen

Division of BioAnalytical Chemistry, Vrije Universiteit Amsterdam, 1081 HV, Amsterdam, The Netherlands

Probing intact protein heterogeneity with LC-MS and CE-MS



Rosa Maria Marcé

Department of Analytical Chemistry and Organic Chemistry. Universitat Rovira i Virgili, Tarragona, Spain
Role of the extraction techniques in environmental analysis



Jorge Pisonero

Department of Physics, Faculty of Science, University of Oviedo, Oviedo, Spain

Fast elemental depth profile analysis of nano and micro layers with high sensitivity using Pulsed Glow Discharge Mass Spectrometry



Rosa Ventura

Barcelona Anti-Doping Laboratory. Doping Control Research Group. IMIM Foundation, Barcelona, Spain

Latest developments in doping control in sports



Félix Elortza

Proteomics Platform Manager, CIC bioGUNE, CIBERehd, ProteoRed-ISCIII, Derio, Spain

Endogenous peptidomics: from peptide profiling to molecular histology



PROGRAM AT A GLANCE

TUESDAY, OCTOBER 3 - CONFERENCE ROOM 4.1

08:30 - 09:00	Conference Secretary Opening & Registration
09:00 - 09:30	Opening Ceremony
09:30 - 10:30	Opening Plenary Lecture: An ever-increased confidence in chemical food safety driven by latest analytical innovations Bruno Le Bizec Laboratoire d'Etude des Résidus et Contaminants dans les Aliments (LABERCA), Nantes, France
10:30 - 11:00	Coffee break
11:00 - 13:00	Oral Session 1 (Food Analysis & New developments in sample preparation)
13:00 - 14:00	Lunch (Restaurant Antara-Hall Annex 4/6)
14:00 - 15:00	Poster Session 1
15:00 - 15:30	Poster Flash Presentation Session 1 (Room 4.1. Conference Room)
15:30 - 16:30	Plenary Lecture: The environmental fate and behaviour of halogenated flame retardants Stuart Harrad Environmental Health Science. School of Geography, Earth and Environmental Sciences, University of Birmingham, UK
16:30 - 17:00	Coffee break
17:00 - 18:20	Oral Session 2 (Environmental analysis)
18:20 - 19:00	Young Scientists Oral Session 1



PROGRAM AT A GLANCE

WEDNESDAY, OCTOBER 4 - CONFERENCE ROOM 4.1

09:00 - 10:00	Plenary Lecture: Chromatographic separations at sensor speeds: practice, consequences and advantages Daniel W. Armstrong Department of Chemistry and Biochemistry, College of Science, University of Texas at Arlington, TX, USA.
10:00 - 10:30	Invited Lecture: Role of the extraction techniques in environmental analysis Rosa Maria Marcé Department of Analytical Chemistry and Organic Chemistry. University Rovira i Virgili, Tarragona, Spain
10:30 - 11:00	Coffee break
11:00 - 13:00	Oral Session 3 (Environmental analysis, Developments in analytical instrumentation & Other fields of analytical chemistry and instrumental analysis)
13:00 - 14:00	Lunch
14:00 - 15:00	Poster Session 2
15:00 - 15:30	Poster Flash Presentation Session 2 (Room 4.1. Conference Room)
15:30 - 16:00	Invited Lecture: Fast elemental depth profile analysis of nano and micro layers with high sensitivity using Pulsed Glow Discharge Mass Spectrometry Jorge Pisonero Department of Physics, Faculty of Science, University of Oviedo, Spain
16:00 - 16:40	Oral Session 4 (Developments in analytical instrumentation & Other fields of analytical chemistry and instrumental analysis)
16:40 - 17:10	Coffee break
17:10 - 17:40	Young Scientists Oral Session 2
17:45 - 19:00	General Assembly of SECyTA
21:00	Social Event: Conference Dinner



PROGRAM AT A GLANCE

THURSDAY, OCTOBER 5 - CONFERENCE ROOM 4.1

09:30 - 10:30	Oral Session 5 (Nanotechnology & Omics Techniques)
10:30 - 11:00	Coffee break
11:00 - 11:30	Invited Lecture: Latest developments in doping control in sports Rosa Ventura Barcelona Anti-Doping Laboratory. IMIM Foundation. Hospital del Mar Medical Research Institute, Barcelona, Spain
11:30 - 12:00	Invited Lecture: Endogenous peptidomics: from peptide profiling to molecular histology Félix Elortza Proteomics Platform Manager, CIC bioGUNE, Science and Technology Park of Bizkaia, Derio, Spain
12:00 - 12:40	Young Scientists Oral Session 3
12:45 - 13:45	Plenary Lecture: Probing intact protein heterogeneity with LC-MS and CE-MS Govert W. Somsen Department of Chemistry and Pharmaceutical Sciences. Faculty of Sciences, Vrije Universiteit Amsterdam, The Netherlands
13:45 - 14:15	Closing Ceremony & Announcement of Young Scientists Awards
14:15 - 15:30	Farewell Cocktail

Communication codes:

PL: Plenary Lecture

IL: Invited Lecture

O: Oral Communication

O-YS: Young Scientists Oral Communication

P: Poster Communication



SCIENTIFIC PROGRAM

TUESDAY, OCTOBER 3 - CONFERENCE ROOM 4.1

08:30 Conference Secretary opening and Registration

OPENING CEREMONY

OPENING PLENARY LECTURE

Session Chairs: Ana M^a García-Campaña – University of Granada
Francisco Javier Santos – University of Barcelona

09:30 **PL-01 An ever-increased confidence in chemical food safety driven by latest analytical innovations**

Bruno Le Bizec

Laboratoire d'Etude des Résidus et Contaminants dans les Aliments (LABERCA/Oniris).

Ecole Nationale Vétérinaire, Agroalimentaire et de l'Alimentation Nantes Atlantique (Oniris),
Route de Gachet, Atlantopôle la Chantrerie, 44307 Nantes Cx 3, France

10:30 Coffee Break & Poster Placement

ORAL SESSION 1

(FOOD ANALYSIS & NEW DEVELOPMENTS IN SAMPLE PREPARATION)

Session Chairs: Rosa Maria Marcé – University Rovira i Virgili, Tarragona
Francisco Javier Santos – University of Barcelona

11:00 **O-01 Semi-quantification of tylosin residues in honey in a non-targeted workflow: using the known to quantify the unknown**

Annie Von Eyken, Stéphane Bayen

Department of Food Science and Agricultural Chemistry, McGill University,
Sainte Anne De Bellevue, Canada

11:20 **O-02 Simultaneous stereoselective separation of aspartame and its degradation products by electrokinetic chromatography**

Laura Sánchez-Hernández, María Castro-Puyana, María Luisa Marina

Departamento de Química Analítica, Química Física e Ingeniería Química, Universidad
de Alcalá, Ctra. Madrid-Barcelona Km. 33.600, 28871-Alcalá de Henares (Madrid), Spain

11:40 **O-03 Determination of fusarium toxins in functional vegetable milks applying salting out assisted liquid-liquid extraction combined with ultra-high performance liquid chromatography tandem mass spectrometry**

Ahmed Mohammed Hamed ⁽¹⁾, Natalia Arroyo-Manzanares ⁽²⁾, Laura Gámiz-Gracia ⁽²⁾,
Ana M. García-Campaña ⁽²⁾

⁽¹⁾ Dept. Dairy Science, Cairo University, Faculty of Agriculture, 12613-Giza, Egypt;

⁽²⁾ Dept. Analytical Chemistry, University of Granada, Campus Fuentenueva, Av. Fuente Nueva s/n, 18071-Granada, Spain
Av. Fuente Nueva s/n, E-18071, Granada, Spain



SCIENTIFIC PROGRAM

TUESDAY, OCTOBER 3 - CONFERENCE ROOM 4.1

- 12:00 **O-04 Modulation strategies in comprehensive two-dimensional liquid chromatography: focusing and non-focusing approaches for the metabolic profile of complex food matrices**
Lidia Montero ⁽¹⁾, Elena Ibáñez ⁽¹⁾, Mariateresa Russo ⁽²⁾, Luca Rastrelli ⁽³⁾, Alejandro Cifuentes ⁽¹⁾, Miguel Herrero ⁽¹⁾
⁽¹⁾ Laboratory of Foodomics, Institute of Food Science Research (CIAL-CSIC), Madrid, Spain;
⁽²⁾ Dipartimento di Agraria, Università Mediterranea di Reggio Calabria, Reggio Calabria, Italy;
⁽³⁾ Dipartimento di Farmacia, Università di Salerno, Salerno, Italy
- 12:20 **O-05 Study of different extraction solvents used as support liquid membranes on miniaturised systems for sample pre-treatment**
Maria Ramos Payán ⁽¹⁾, Elia Santigosa Murillo ⁽²⁾, Rut Fernández Torres ⁽¹⁾, Miguel Ángel Bello López ⁽¹⁾
⁽¹⁾ Departamento de Química Analítica, Facultad de Química, Universidad de Sevilla, Campus Reina Mercedes, 41001-Sevilla, Spain;
⁽²⁾ Unitat de Analítica, Departamento de Química, Facultad de Ciencias, Universitat Autònoma de Barcelona, 08193-Cerdanyola del Vallès (Barcelona), Spain
- 12:40 **O-06 A new method based on ultra-high performance liquid chromatography with fluorescence detection for the analysis of benzimidazole compounds in farmed fish samples**
Carmen Tejada-Casado, Francisco J. Lara, Monsalud del Olmo-Iruela, Ana M. García-Campaña
Dept. of Analytical Chemistry, University of Granada, Av. Fuente Nueva s/n, 18071-Granada, Spain
- 13:00 Lunch (Restaurant Antara - Hall Annex 4/6)

14:00 POSTER SESSION 1

POSTER FLASH PRESENTATION SESSION 1 - (Room 4.1. Conference Room)

Session Chairs: Belén Gómara– IQOG-CSIC, Madrid
Marta Lores – University of Santiago de Compostela

- 15:00 **P-03 Multi-residue analysis of pesticides in virgin olive oil by nanoflow liquid chromatography high resolution mass spectrometry**
Jaime Alcántara-Durán ⁽¹⁾, Silvina M. Addona ⁽²⁾, David Moreno-Gonzalez ⁽¹⁾, Juan F. García-Reyes ⁽¹⁾, Antonio Molina-Díaz ⁽¹⁾
⁽¹⁾ Analytical Chemistry Research Group, Department of Physical and Analytical Chemistry, University of Jaén, Campus Las Lagunillas, 23071 Jaén, Spain;
⁽²⁾ Instituto de Ciencias Veterinarias del Litoral, Consejo Nacional de Investigaciones Científicas y Técnicas, Santa Fe, Argentina



SCIENTIFIC PROGRAM

TUESDAY, OCTOBER 3 - CONFERENCE ROOM 4.1

- 15:05 **P-15 Establishment of an integrated authenticity profile for quality control of artichoke dietary supplements for overweight control**

Adal Mena, Estela Nogales, Samuel Garrido, Sonia Rodríguez, Ana I. Ruiz-Matute, Ana C. Soria, Belén Gómara, Mario A. Fernández, Lourdes Ramos, María L. Sanz
Instituto de Química Orgánica General (IQOG-CSIC), Juan de la Cierva 3, 28006 Madrid, Spain.

- 15:10 **P-18 Identification of bioactive peptides in protein hydrolyzates from edible macroalgae by LC-ESI-QTOF**

Raquel Pérez-Míguez, María Castro-Puyana, Merichel Plaza, María Luisa Marina
Universidad de Alcalá, Departamento de Química Analítica, Química Física e Ingeniería Química,
Ctra. Madrid-Barcelona Km. 33.600, 28871 Alcalá de Henares (Madrid), Spain

- 15:15 **P-23 Atmospheric pressure ionization of pigments and dyes in edible oils**

Ane Arribalaga⁽¹⁾, Pilar Rodríguez⁽²⁾, Mireia Medina⁽²⁾, Encarnación Moyano⁽¹⁾

⁽¹⁾ University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Av. Diagonal 645, 08028 Barcelona, Spain;

⁽²⁾ Laboratori Agroalimentari, Carretera de Vilassar de Mar a Cabrils, s/n, 08348 Cabrils (Barcelona), Spain

- 15:20 **P-30 Localization of ferroportin in brain tissues with Alzheimer's disease using gold nanoclusters bioconjugated antibodies and LA-ICP-MS**

María Cruz-Alonso⁽¹⁾, Vanesa Ramírez⁽¹⁾, Aurora Astudillo⁽²⁾, Ana Navarro⁽³⁾, Beatriz Fernández⁽¹⁾, Rosario Pereiro⁽¹⁾

⁽¹⁾ Department of Physical and Analytical Chemistry, Faculty of Chemistry, University of Oviedo, Julián Clavería, 8, 33006, Oviedo, Spain;

⁽²⁾ Hospital Universitario Central de Asturias, 33011 Oviedo, Spain; ⁽³⁾ Department of Morphology and Cellular Biology, University of Oviedo, 33006 Oviedo, Spain

- 15:25 **P-46 Use of dielectric barrier discharge ionization-mass spectrometry for determination of multiclass explosives and related compounds**

David Moreno-González⁽¹⁾, José Robles-Molina⁽¹⁾, Felipe J. Lara-Ortega⁽¹⁾, Bienvenida Gilbert-López⁽¹⁾

Alexander Schütz⁽²⁾, Sebastian Brandt⁽²⁾, Joachim Franzke⁽²⁾, Juan F. García-Reyes⁽¹⁾

Antonio Molina-Díaz⁽¹⁾

⁽¹⁾ Analytical Chemistry Research Group, Department of Physical and Analytical Chemistry, University of Jaén, 23071 Jaén, Spain;

⁽²⁾ ISAS-Leibnitz Institut für Analytische Wissenschaften, Dortmund, Germany



SCIENTIFIC PROGRAM

TUESDAY, OCTOBER 3 - CONFERENCE ROOM 4.1

PLENARY LECTURE

Session Chairs:

Esteban Abad – IDAEA-CSIC, Barcelona

Jordi Diaz – IQS–Universidad Ramón LLull, Barcelona

15:30 **PL-02 The environmental fate and behaviour of halogenated flame retardants**

Stuart Harrad

Environmental Health Science. School of Geography, Earth and Environmental Sciences, University of Birmingham, Birmingham, B15 2TT, UK

16:30 Coffee Break

ORAL SESSION 2 (ENVIRONMENTAL ANALYSIS)

Session Chairs:

Esteban Abad – IDAEA-CSIC, Barcelona

Sandra Pérez – IDAEA-CSIC, Barcelona

17:00 **O-07 Exposure to PFASs in Antarctic seabirds according to their distribution, movements and trophic ecology**

Jose L. Roscales ⁽¹⁾, Alba Vicente ⁽¹⁾, Peter G. Ryan ⁽²⁾, Jacob González-Solís ⁽³⁾, Begoña Jiménez ⁽¹⁾

⁽¹⁾ Dept. of Instrumental Analysis and Environmental Chemistry, Institute of General Organic Chemistry, CSIC (IQOG-CSIC), Juan de la Cierva 3, 28006-Madrid, Spain;

⁽²⁾ Fitz Patrick Institute of African Ornithology, DST-NRF Centre of Excellence, University of Cape Town, University of Cape Town, Rondebosch 7701, South Africa;

⁽³⁾ Dept. of Animal Biology (Vertebrates), University of Barcelona, Av. Diagonal 645, 08028-Barcelona, Spain

17:20 **O-08 Determination of priority pollutants and PPCPs in reclaimed waters from metropolitan area of Barcelona**

Maria Huerta-Fontela, Mercè Aceves

Laboratori de l'Àrea Metropolitana de Barcelona (AMB), Autovia Castelldefels Km 187.9, 08840-Viladecans (Barcelona), Spain

17:40 **O-09 Twenty years measuring PCDD/Fs in ambient air in Catalonia**

Jordi Parera ⁽¹⁾, Beatriz Aristizabal ⁽²⁾, María Generosa Martrat ⁽¹⁾, Miquel Àngel Adrados ⁽¹⁾,

Jordi Sauló ⁽¹⁾, Manuela Ábalos ⁽¹⁾, Esteban Abad ⁽¹⁾

⁽¹⁾ Laboratory of Dioxins, Environmental Chemistry Dept., IDAEA-CSIC, C\ Jordi Girona 18-26, 08034-Barcelona, Spain;

⁽²⁾ Hydraulic Engineering and Environmental Research Group, Universidad Nacional de Colombia, Sede Manizales, Ctra. 27 # 64-60 Manizales, Caldas, Colombia



SCIENTIFIC PROGRAM

TUESDAY, OCTOBER 3 - CONFERENCE ROOM 4.1

18:00 **O-10 Multivariate geostatistical analysis of compound-specific isotope ratios obtained by direct pyrolysis of a xerophytic species from a volcanic valley in Tenerife Island**

José A. González-Pérez ⁽¹⁾, Nicasio T. Jiménez-Murillo ⁽¹⁾ Francisco J. González-Vila ⁽¹⁾, Gonzalo Almendros ⁽²⁾

⁽¹⁾ IRNAS-CSIC, Av. Reina Mercedes 10, 41012-Seville, Spain;

⁽²⁾ MNCN-CSIC, C/ Serrano 115b, 28006-Madrid, Spain

YOUNG SCIENTISTS ORAL SESSION 1

Session Chairs: Juan Vicente Sancho – University Jaume I, Castellón
Marta Lores – University of Santiago de Compostela

18:20 **O-YS-01 Development of a new method for the determination of benzotriazoles, benzothiazoles and benzenesulfonamides in environmental water samples by UHPLC-HRMS**

Míriam Hidalgo-Serrano, Rosa María Marcé Recasens, Eva Pocurull Aixalà

Dept. Química Analítica i Química Orgànica, Universitat Rovira i Virgili, C/ Marcel·lí Domingo s/n, 43007-Tarragona, Spain

18:30 **O-YS-02 Study of bioaccumulation of perfluorinated compounds in marine echinoderms (*Holothuria Tubulosa*) by liquid chromatography–tandem mass spectrometry analysis**

María Teresa García-Córdcoles ⁽¹⁾, Morsina Ćipa ⁽²⁾, Julia Martín ⁽³⁾, Félix Hidalgo ⁽⁴⁾, Alejandro J. Ibáñez-Yuste ⁽⁵⁾, Alberto Zafra-Gómez ⁽¹⁾

⁽¹⁾ Department of Analytical Chemistry, University of Granada, Av. Fuente Nueva s/n, Granada, Spain;

⁽²⁾ Department of Chemistry, University of Tirana, St. Bulevardi Zogu I, Tirana, Albania;

⁽³⁾ Department of Analytical Chemistry, University of Seville, St. Virgen de Africa 7, Seville, Spain;

⁽⁴⁾ Department of Zoology, University of Granada, Av. Fuente Nueva s/n, Granada, Spain;

⁽⁵⁾ Agriculture and Fisheries Management Agency of Andalusia (AGAPA), Ronda de los Alunados s/n, Jerez de la Frontera, Cadiz, Spain

18:40 **O-YS-03 Development of new methodology for the extraction and analysis of pharmaceutical in fish muscle**

Juan Manuel Peña Herrera, Sandra Pérez, Damià Barceló

Institute of Environmental Assessment and Water Research, IDAEA-CSIC, C/ Jordi Girona 18-26, 08034-Barcelona, Spain.

18:50 **O-YS-04 Multivariate appraisal of soil organic carbon storage from the patterns of nitrogen-containing pyrolytic compounds**

Marco A. Jiménez-González ⁽¹⁾, Gonzalo Almendros ⁽¹⁾, Ana M. Álvarez ⁽²⁾, Francisco J. González-Vila ⁽³⁾, José M. de la Rosa ⁽³⁾

⁽¹⁾ Museo Nacional de Ciencias Naturales (MNCN-CSIC), C/ Serrano 115-B, Madrid, Spain;

⁽²⁾ Universidad Autónoma de Madrid (UAM), C/ Francisco Tomás y Valiente 7, Madrid, Spain;

⁽³⁾ Instituto de Recursos Naturales y Agrobiología de Sevilla (IRNAS-CSIC), Av. Reina Mercedes 10, Sevilla, Spain



SCIENTIFIC PROGRAM

WEDNESDAY, OCTOBER 4 - CONFERENCE ROOM 4.1

PLENARY AND INVITED LECTURES

Session Chairs: Joan Grimalt – IDAEA-CSIC, Barcelona
Juan Vicente Sancho – University Jaume I, Castellón

PLENARY LECTURE

- 09:00 **PL-03 Chromatographic separations at sensor speeds: Practice, Consequences & Advantages**
Daniel W. Armstrong
Department of Chemistry and Biochemistry, College of Science, University of Texas at Arlington, TX 76019, USA

INVITED LECTURE

- 10:00 **IL-01 Role of the extraction techniques in environmental analysis**
Rosa Maria Marcé
Department of Analytical Chemistry and Organic Chemistry. Universitat Rovira i Virgili,
C/ Marcel·lí Domingo s/n, 43007- Tarragona, Spain

- 10:30 Coffee Break

ORAL SESSION 3 (ENVIRONMENTAL ANALYSIS, DEVELOPMENTS IN ANALYTICAL INSTRUMENTATION & OTHER FIELDS OF ANALYTICAL CHEMISTRY AND INSTRUMENTAL ANALYSIS)

Session Chairs: M^a José González – IQOG-CSIC, Madrid
M^a Teresa Galceran – University of Barcelona

- 11:00 **O-11 Patterns of organic particulate air pollutants in subway stations in Barcelona**
Barend L. van Drooge⁽¹⁾) Raimon M. Prats ⁽¹⁾, Joan O. Grimalt (1), Teresa Moreno ⁽²⁾

⁽¹⁾Institute of Environmental Assessment and Water Research (IDAEA-CSIC). Dept. Environmental Chemistry, C/Jordi Girona 18-26, 08034-Barcelona, Spain;

⁽²⁾ Institute of Environmental Assessment and Water Research (IDAEA-CSIC). Dept. Environmental Geochemistry and Atmospheric Research, C/Jordi Girona 18-26, 08034-Barcelona, Spain

- 11:20 **O-12 Levels of PCDD/Fs and PCBs in fish samples from the Sava River basin**
Manuela Ábalos⁽¹⁾, Damià Barceló ⁽¹⁾), Jordi Parera (1), Esteban Abad ⁽¹⁾, Tea Zuliani ⁽²⁾, Predrag Simonovic ⁽³⁾, Marina Piria ⁽⁴⁾, Momir Paunovic ⁽⁵⁾

⁽¹⁾ Environmental Chemistry Dept., IDAEA-CSIC, C\ Jordi Girona 18-24, 08034-Barcelona, Spain;

⁽²⁾ Department of Environmental Sciences, Jožef Stefan Institute, Ljubljana, Slovenia;

⁽³⁾ Institute for Biological Research, Faculty of Biology, University of Belgrade, Belgrade, Serbia;

⁽⁴⁾ Faculty of Agriculture, University of Zagreb, Croatia; (5) University of Belgrade, Institute for Biological Research, Belgrade, Serbia



SCIENTIFIC PROGRAM

WEDNESDAY, OCTOBER 4 - CONFERENCE ROOM 4.1

- 11:40 **0-13 Single and mixture toxicity of organic and inorganic UV-filters and parabens on Daphnia magna and Phaeodactylum tricornutum**
Ana Cristina Soler de la Vega, Daniel Molins Delgado, Damià Barceló Culleres, Silvia Díaz-Cruz
Institute of Environmental Assessment and Water Research-Spanish Council for Scientific Research (IDAEA-CSIC), Department of Environmental Chemistry, Jordi Girona 18-26, 08034-Barcelona, Spain
- 12:00 **0-14 Determination of low concentrations of synthetic cathinones in river and sewage samples using weak-cation-exchange solid-phase extraction followed by liquid chromatography-high resolution mass spectrometry**
Núria Fontanals, Rosa María Marcé, Francesc Borrull
Departament de Química Analítica i Química Orgànica, Universitat Rovira i Virgili, Marcel·lí Domingo, 1, 43007-Tarragona, Spain
- 12:20 **0-15 Accumulation of pharmaceutically active compounds through the soil-root-leaf system**
Nicola Montemurro ⁽¹⁾, Cristina Postigo ⁽¹⁾, Antonio Lonigro ⁽²⁾ Sandra Pérez ⁽¹⁾ Damià Barcelò ⁽¹⁾
⁽¹⁾ IDAEA-CSIC, Water and Soil Quality Research Group - Department of Environmental Chemistry, 08034-Barcelona, Spain;
⁽²⁾ Dept. of Agricultural and Environmental Science – University of Bari, Bari, Italy
- 12:40 **0-16 A rapid method for the chromatographic analysis of volatile organic compounds in smoke and exhaled breath of standard and non-combusted tobacco cigarette and electronic cigarette smokers**
Joan Grimalt, Esther Marco
Institute of Environmental Assessment and Water Research-Spanish Council for Scientific Research (IDAEA-CSIC), Department of Environmental Chemistry, Jordi Girona 18-26, 08034-Barcelona, Spain
- 13:00 Lunch (Restaurant Antara - Hall Annex 4/6)



WEDNESDAY, OCTOBER 4 - CONFERENCE ROOM 4.1

14:00 POSTER SESSION 2

POSTER FLASH PRESENTATION SESSION 2 (Room 4.1. Conference Room)

Session Chairs: Belén Gómara – IQOG-CSIC, Madrid
Sandra Pérez – IDAEA-CSIC, Barcelona

- 15:00 **P-47 Pollution transport by marine microplastics – POPs accumulation rate on polyethylene microparticles**
Daura Vega-Moreno ⁽¹⁾, Bárbara Abaroa-Pérez ⁽²⁾, Nerea Beltrán ⁽²⁾, José Joaquín Hernández-Brito ⁽²⁾
⁽¹⁾ Universidad de Las Palmas de Gran Canaria, Dept. Química, Las Palmas de Gran Canaria, Spain;
⁽²⁾ Plataforma Oceánica de Canarias, Telde, Spain
- 15:05 **P-71 Bioaccumulation of C60 fullerene and its transformation products in river biofilms**
Josep Sanchis ⁽¹⁾, Anna Freixa ⁽²⁾, Vicenç Acuña ⁽²⁾, Sergi Sabater ⁽²⁾, Damià Barceló ⁽²⁾,
Esteban Abad ⁽¹⁾, Marinella Farré ⁽¹⁾
⁽¹⁾ Institut de Diagnosi Ambiental i Estudis de l'Aigua, C/ Jordi Girona, 18-26, 08034, Barcelona, Spain;
⁽²⁾ Institut Català de Recerca de l'Aigua, C/ Emili Grahit Nº 101, 17003, Girona, Spain
- 15:10 **P-72 Ionization of short-chain chlorinated paraffins by atmospheric pressure sources**
Juan Francisco Ayala Cabrera, María Teresa Galcerán, Francisco Javier Santos, Encarnación Moyano
Department of Chemical Engineering and Analytical Chemistry, University of Barcelona, Av. Diagonal 645, E-08028, Barcelona, Spain
- 15:15 **P-86 Separation and identification of mouse transferrin glycan isomers by μZIC-HILIC-MS. Application to rheumatoid arthritis diagnosis**
Montserrat Mancera-Arteu ⁽¹⁾, Laura Pey ⁽¹⁾, Estela Giménez ⁽¹⁾, Jaime Sancho ⁽²⁾, José Barbosa ⁽¹⁾,
Victòria Sanz-Nebot ⁽¹⁾
⁽¹⁾University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Diagonal 645, Barcelona, Spain;
⁽²⁾ CSIC, Instituto de Parasitología y Biomedicina "López-Neyra" (IPBLN), Av. del Conocimiento 17, Granada, Spain
- 15:20 **P-92 Quantification of sulfated steroids in human urine by LC-MS/MS to improve the detection of endogenous anabolic steroids**
Argitxu Esquivel López, Élida Alechaga Silva, Nuria Monfort Mercader, Rosa Ventura Alemany
Barcelona Antidoping Laboratory, Doping Control Research Group, Carrer Doctor Aiguader 88, Barcelona, Spain
- 15:25 **P-94 Effect of the storage conditions on the stability of prostate specific antigen (PSA) from urine studied by capillary electrophoresis**
Diana Navarro ⁽¹⁾, Angel Puerta ⁽¹⁾, Eduardo Albers-Acosta ⁽²⁾, Inmaculada Fernandez ⁽²⁾
Carlos Olivier ⁽²⁾, José Carlos Díez-Masa ⁽¹⁾, Mercedes de Frutos ⁽¹⁾
⁽¹⁾ Institute of Organic Chemistry (IQOG-CSIC), Madrid, Spain; (2) Department of Urology, Hospital La Princesa, Madrid, Spain

**WEDNESDAY, OCTOBER 4 - CONFERENCE ROOM 4.1****INVITED LECTURE**

Session Chairs:

Encarnación Moyano – University of Barcelona

Maria del Mar Puyol – Universitat Autònoma de Barcelona

- 15:30 **IL-02 Fast elemental depth profile analysis of nano and micro layers with high sensitivity using Pulsed Glow Discharge Mass Spectrometry**

Jorge Pisonero

Department of Physics, Faculty of Science, University of Oviedo, 33007-Oviedo, Spain

ORAL SESSION 4 (DEVELOPMENTS IN ANALYTICAL INSTRUMENTATION & OTHER FIELDS OF ANALYTICAL CHEMISTRY AND INSTRUMENTAL ANALYSIS)

Session Chairs: Encarnación Moyano – University of Barcelona

Maria del Mar Puyol – Universitat Autònoma de Barcelona

- 16:00 **O-17 Development of a new interface for a low pressure PGD-TOFMS for VOCs analysis**

Jonatan Fandino ^{(1)*}, Marcos Bouza ⁽²⁾, Jorge Pisonero ⁽¹⁾, Nerea Bordel ⁽¹⁾⁽¹⁾ Department of Physics - University of Oviedo, Oviedo, Spain;⁽²⁾ School of Chemistry and Biochemistry - Georgia Institute of Technology, Atlanta, United States

- 16:20 **O-18 Angular projection synchronous fluorescence**

José Antonio Murillo Pulgarín, Pablo Fernández López, Elisa Jiménez García

Dept. Analytical Chemistry and Foods Technology, Faculty of Sciences and Chemical Technology, University of Castilla-La Mancha, Av. Camilo José Cela 10, 13071-Ciudad Real, Spain

- 16:40 Coffee Break

YOUNG SCIENTISTS ORAL SESSION 2

Session Chairs: Begoña Jiménez – IQOG-CSIC, Madrid

Jordi Díaz – IQS–Universidad Ramón LLull, Barcelona

- 17:10 **O-YS-05 Use of nanoflow liquid chromatography high resolution mass spectrometry for the determination of pesticides in specific part of bees, pollen and nectar**

David Moreno-González ⁽¹⁾, Jaime Alcántara-Durán ⁽¹⁾, Juan F. García-Reyes ⁽¹⁾Antonio Molina-Díaz ⁽¹⁾, Victor Cutillas ⁽²⁾, Amadeo R. Fernández-Alba ⁽²⁾⁽¹⁾ Analytical Chemistry Research Group, Department of Physical and Analytical Chemistry, University of Jaén, Campus Las Lagunillas, 23071-Jaén, Spain;



SCIENTIFIC PROGRAM

WEDNESDAY, OCTOBER 4 - CONFERENCE ROOM 4.1

⁽²⁾ Agrifood Campus of International Excellence (ceiA3), European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables, Department of Chemistry and Physics, University of Almeria, 04120-Almeria, Spain

- 17:20 **0-YS-06 Chemical characterization of Phlebodium Decumanum by using high-performance liquid chromatography coupled with mass spectrometry time-of-flight analyzer**

Laura Martín Pozo, Alberto Zafra Gómez, José Luis Vilchez Quero

Research Group of Analytical Chemistry and Life Sciences, Department of Analytical Chemistry,
University of Granada, Campus of Fuentenueva, Av. Fuente Nueva s/n, E-18071, Granada, Spain

- 17:30 **0-YS-07 Study of Cocoa procyanidins: extraction, characterization and purification**

Said Toro-Uribe ⁽¹⁾, Luis López-Giraldo ⁽¹⁾, Lidia Montero ⁽²⁾, Elena Ibáñez ⁽²⁾, Miguel Herrero ⁽²⁾

⁽¹⁾ Centro de Investigación en Ciencia y Tecnología de Alimentos, Universidad Industrial de Santander
(CICTA-UIS), Bucaramanga, Colombia;

⁽²⁾ Foodomics Laboratory, Institute of Food Science Research (CIAL, CSIC), Madrid, Spain

- 17:45 **XVIIth GENERAL ASSEMBLY OF SECYTA**

- 21:00 **Social Event:** Gala Dinner
RESTAURANTE VISUAL - TORRE CATALUNYA





SCIENTIFIC PROGRAM

THURSDAY, OCTOBER 5 - CONFERENCE ROOM 4.1

ORAL SESSION 5 (NANOTECHNOLOGY & OMICS TECHNIQUES)

Session Chairs: Francisco Javier Santos – University of Barcelona
Francisco Javier Moreno – CIAL-CSIC, Madrid

- 09:30 **O-19 Bioimaging of specific proteins in ocular tissue sections by LA-ICP-MS with bioconjugated metal nanoclusters as a promising sensitive and selective tool**
María Cruz-Alonso ⁽¹⁾, **Eva Valencia-Agudo** ⁽¹⁾, **Lydia Álvarez** ⁽²⁾, **Héctor González-Iglesias** ⁽²⁾, **Beatriz Fernández** ⁽¹⁾, **Rosario Pereiro** ⁽¹⁾
⁽¹⁾Department of Physical and Analytical Chemistry, Faculty of Chemistry, University of Oviedo, Julián Clavería, 8, 33006-Oviedo, Spain;
⁽²⁾ Instituto Oftalmológico Fernández-Vega, Av. Dres. Fernández-Vega, 34, 33012-Oviedo, Spain
- 09:50 **O-20 Highly surface enhancement Raman scattering substrate based on gold nanoparticles and sulfonamides for the determination and quantification of multi walled carbon nanotubes**
Virginia Moreno ^(1,2), **A. Adnane** ^(2,3), **R. Salghi** ³, **M. Zougagh** ^(2,4) and **A. Ríosa** ⁽²⁾
⁽¹⁾Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, Av. Camilo José Cela, 10. 13071-Ciudad Real, Spain;
⁽²⁾ Regional Institute for Applied Chemistry Research (IRICA), 13004-Ciudad Real, Spain;
⁽³⁾ Laboratoire d'Ingénieries des Procédés de l'Energie et de l'Environnement, ENSA, B.P. 1136, Agadir, Morocco;
⁽⁴⁾ Castilla-La Mancha Science and Technology Park., 20006-Albacete, Spain
- 10:10 **O-21 Untargeted HILIC-LC-MS metabolomic analysis for the assessment of endocrine disruptors effects on Zebrafish embryos**
Elena Ortiz Villanueva, Joaquim Jaumot, Laia Navarro-Martín, Benjamín Piña, Romà Tauler
Department of Environmental Chemistry, IDAEA-CSIC, C/ Jordi Girona 18-26, 08034 Barcelona, Spain
- 10:30 Coffee Break

INVITED LECTURES

Session Chairs: Encarnación Moyano – University of Barcelona
Eliandre de Oliveira – Parc Científic de Barcelona (PCB)

- 11:00 **IL-03 Latest developments in doping control in sports**
Rosa Ventura
Barcelona Anti-Doping Laboratory. Doping Control Research Group. IMIM Foundation. Doctor Aiguader 88, 08003- Barcelona, Spain
- 11:30 **IL-04 Endogenous peptidomics: from peptide profiling to molecular histology**
Félix Elortza
Proteomics Platform Manager, CIC bioGUNE, CIBERehd, ProteoRed-ISCIII, Derio, Spain



SCIENTIFIC PROGRAM

THURSDAY, OCTOBER 5 - CONFERENCE ROOM 4.1

YOUNG SCIENTISTS ORAL SESSION 3

Session Chairs: Begoña Jiménez – IQOG-CSIC, Madrid
Francisco Javier Moreno – CIAL-CSIC, Madrid

- 12:00 **O-YS-08 Ion Mobility Mass Spectrometry as a novel tool for supporting steroidomics studies**
Maykel Hernández-Mesa, Antoine Escourrou, Fabrice Montea, Gaud Dervilly-Pinel, Bruno Le Bizec
LUNAM Université, Oniris, Laboratoire d'Etude des Résidus et Contaminants dans les Aliments (LABERCA), Nantes, F-44307, France
- 12:10 **O-YS-09 Volatolomics approach to classify different smoke seafood products by GC-MS**
Leticia Lacalle Bergeron ⁽¹⁾, Carlos Sales Martínez ⁽¹⁾, Tania Portolés Nicolau ⁽¹⁾, M. Carmen Corell Dubón ⁽²⁾, Fernando Domínguez Trencó ⁽³⁾, Joaquim Beltrán Arandes ⁽¹⁾, Juan Vicente Sancho Llopis ⁽¹⁾ Félix Hernández Hernández ⁽¹⁾
⁽¹⁾ Research institute for Pesticides and Water (IUPA), University Jaume I, Av. Sos Baynat s/n, 12071-Castellón de la Plana, Spain;
⁽²⁾ Sea Delight Europe, S.L., C/ Sao Paulo, 14 Planta 2^a Oficina N°3-P.i. El Sebadal, 35008 Las Palmas de Gran Canaria, Spain;
⁽³⁾ Food Safety Unit, Centre of Public Health of Castellón, Av. del Mar 12, 12003-Castellón de la Plana, Spain
- 12:20 **O-YS-10 Characterization of PLE extracts from *Kalanchoe daigremontiana* by LC-UV/MS and GC-Q-TOF analysis. Evaluation of bioactive properties**
Gerardo Alvarez-Rivera ⁽¹⁾, Verónica Cortés-Avilés ⁽²⁾Alma Angélica Del Villar-Martínez ⁽²⁾, Pablo Emilio Vanegas-Espinoza ⁽²⁾ Alejandro Cifuentes ⁽¹⁾, Elena Ibáñez ⁽¹⁾
⁽¹⁾ Institute of Food Science Research (CSIC-UAM), Laboratory of Foodomics, Nicolás Cabrera 9, Madrid, Spain;
⁽²⁾ Centro de Desarrollo de Productos Bióticos - Instituto Politécnico Nacional, Morelos, México
- 12:30 **O-YS-11 A LC-ESI-QTOF metabolomic approach to search chemical markers related to the roasting process of coffee**
Raquel Pérez-Míguez, Elena Sánchez-López, Merichel Plaza, María Castro-Puyana, María Luisa Marina
Departamento de Química Analítica, Química Física e Ingeniería Química, Universidad de Alcalá, Ctra. Madrid-Barcelona Km. 33.600, 28871 Alcalá de Henares (Madrid), Spain



SCIENTIFIC PROGRAM

THURSDAY, OCTOBER 5 - CONFERENCE ROOM 4.1

PLENARY LECTURE

Session Chairs:

Joan Grimalt – IDAEA-CSIC, Barcelona

Ana María García-Campaña – University of Granada

- 12:45 **PL-04 Probing intact protein heterogeneity with LC-MS and CE-MS**
Govert W. Somsen
Division of BioAnalytical Chemistry, Vrije Universiteit Amsterdam, De Boelelaan 1085, 1081 HV, Amsterdam,
The Netherlands
- 13:45 **Closing Ceremony & Announcement of the José Antonio García Dominguez's Awards**
- 14:15 Farewell Cocktail



POSTER SESSION 1

(TUESDAY OCTOBER 3)



POSTER SESSION 1

TUESDAY, OCTOBER 3

P-01 Validation and ongoing analysis of the multi-residue method for finding and quantifying 130 pesticides in flowers, leaves and tree trunks by LC-QqQ and GC-QqQ

Laia Sanchez Costa, Judit Pujol Boira, Pilar Rodríguez Martínez, Mireia Medina Sala

Laboratori Agroalimentari, Ctra. Vilassar a Cabrils s/n, 08348-Cabrils (Barcelona), Spain

P-02 Development and validation of an analytical method for determining organochlorine pesticides in animal feed by GC-MS/MS

Laia Sanchez Costa, Pilar Rodríguez Martínez, Mireia Medina Sala

Laboratori Agroalimentari, Ctra. Vilassar a Cabrils s/n, 08348-Cabrils (Barcelona), Spain

P-03 Multi-residue analysis of pesticides in virgin olive oil by nanoflow liquid chromatography high resolution mass spectrometry

Jaime Alcántara-Durán ⁽¹⁾, Silvina M. Addona ⁽²⁾, David Moreno-González ⁽¹⁾, Juan F. García-Reyes ⁽¹⁾, Antonio Molina-Díaz ⁽¹⁾

⁽¹⁾ Analytical Chemistry Research Group, Department of Physical and Analytical Chemistry, University of Jaén, Campus Las Lagunillas, 23071-Jaén, Spain;

⁽²⁾ Instituto de Ciencias Veterinarias del Litoral, Consejo Nacional de Investigaciones Científicas y Técnicas, Santa Fe, Argentina

P-04 Evaluation of two sample treatments for multiresidue determination of veterinary drugs in milk by UHPLC-QqQ-MS/MS

Delia Castilla-Fernández, David Moreno-González, Juan F. García-Reyes, Antonio Molina-Díaz

Analytical Chemistry Research Group, Department of Physical and Analytical Chemistry, University of Jaén, Campus Las Lagunillas s/n, 23071-Jaén, Spain

P-05 Increasing water solubility of quercetin by increasing the temperature

Ante Loncaric ⁽¹⁾, Juan Pablo Lamas ⁽²⁾, Eugenia Guerra ⁽²⁾, Marta Lores ⁽²⁾

⁽¹⁾ Josip Juraj Strossmayer University of Osijek, Faculty of Food Technology Osijek, Department of Food Technologies, Franje Kuhaca 20, 31000-Osijek, Croatia;

⁽²⁾ Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Chemistry, University of Santiago de Compostela, Av. das Ciencias, s/n, 15782 Santiago de Compostela (A Coruña), Spain

P-06 A multiresidue DLLME and SPE based UHPLC-QTOF method for determining neonicotinoids in royal jelly

Silvia Valverde, Mario Arribas, Ana María Ares, José Luis Bernal, María Jesús del Nozal, José Bernal
Department of Analytical Chemistry, University of Valladolid, Paseo Belén 5, 47011-Valladolid, Spain

P-07 Trace level determination of neonicotinoid insecticides in honey by UHPLC-MS/MS

Silvia Valverde ⁽¹⁾, María Ibáñez ⁽²⁾, José Luis Bernal ⁽¹⁾, María Jesús del Nozal ⁽¹⁾, Félix Hernández ⁽²⁾, José Bernal ⁽¹⁾

⁽¹⁾ University of Valladolid, Paseo Belén 5, 47011 Valladolid, Spain;

⁽²⁾ University Jaume I, Av. Sos Baynat s/n, 12071-Castellón de la Plana, Spain



POSTER SESSION 1

TUESDAY, OCTOBER 3

- P-08 Comparison of sample treatments (QuEChERS, SPE and MISPE) applied to the monitoring of 5-nitroimidazole traces by UHPLC-MS/MS in an infant milk-based product**

Maykel Hernández-Mesa, Carmen Cruces-Blanco, Ana M. García-Campaña

Departamento de Química Analítica. Universidad de Granada, Av. Fuente Nueva s/n, 18071-Granada, Spain

- P-09 Multi-residue method for the analysis of quinolone antibiotics in raw cow milk.**

Application of polar stir-bars and ultra-high performance liquid chromatography–tandem mass spectrometry analysis

Alberto Zafra-Gómez ⁽¹⁾, María Teresa García-Córcoles ⁽¹⁾, Morsina Çipa ⁽²⁾,

Rocío Rodríguez-Gómez ⁽¹⁾, Dolores Barrón ⁽³⁾, Alberto Navalón ⁽¹⁾

⁽¹⁾ Analytical Chemistry Department, University of Granada, Granada, Spain;

⁽²⁾ Department of Chemistry, University of Tirana, Tirana, Albania;

⁽³⁾ Analytical Chemistry Department, University of Barcelona, Barcelona, Spain

- P-10 UHPLC-ESI-MS/MS for the detection of frauds in extra virgin olive oils by polyphenolic profiling and chemometrics**

Encarnación Moyano, Mohamed Said, Óscar Núñez, Javier Saurina

Department of Chemical Engineering and Analytical Chemistry, University of Barcelona,

Av. Diagonal 645, 08028-Barcelona, Spain

- P-11 Determination of pesticide residues in pollen by QuEChERS extraction and LC-MS/MS determination**

Pau Calatayud-Vernich ⁽¹⁾, Fernando Calatayud ⁽²⁾, Enrique Simó ⁽²⁾, Yolanda Picó ⁽¹⁾

⁽¹⁾ Desertification Research Centre (CIDE, UV-GV-CSIC), Carretera Moncada-Náquera, Km 4,5 (Moncada), Spain;

⁽²⁾ Agrupación de Defensa Sanitaria apícola (apiADS), Carretera Montroi – Turis s/n (Montroi), Spain

- P-12 Optimization of the data treatment steps of a non-targeted LC-MS based workflow for the identification of veterinary drugs in honey**

Annie Von Eyken ⁽¹⁾, Jean-François Roy ⁽²⁾, Jerry A. Zweigenbaum ⁽³⁾, Stéphane Bayen ⁽¹⁾

⁽¹⁾ Department of Food Science and Agricultural Chemistry, McGill University, Sainte Anne de Bellevue, Canada;

⁽²⁾ Agilent Technologies, Saint Laurent, Canada; ⁽³⁾ Agilent Technologies, Wilmington, Delaware, United States

- P-13 Determination of 16 benzimidazoles in milk by salting-out assisted liquid-liquid extraction and capillary liquid chromatography with UV-VIS detection**

Francisco J. Lara, Carmen Tejada-Casado, Monsalud del Olmo-Iruela, Ana M. García-Campaña

Department of Analytical Chemistry, University of Granada, Campus of Fuentenueva, Av. Fuente Nueva s/n, E-18071, Granada, Spain

- P-14 Differential Pulse Voltammetry determination of total phenols compounds with low oxidation potential in food**

Agustina Guiberteau ⁽¹⁾, María Gil ⁽¹⁾, Belén Godoy-Cancho ⁽²⁾, Carmen Guiberteau ⁽³⁾,

Cristina Ojalvo ⁽⁴⁾, Manuel Alejandro Martínez Cañas ⁽⁵⁾

⁽¹⁾ Dept. Analytical Chemistry, University of Extremadura, Av. de Elvas s/n, 06006- Badajoz, Spain;

⁽²⁾ Institute of Cork, Wood and Charcoal, Centre for Scientific and Technological Research in Extremadura (CICYTEX), Polígono Industrial El Prado, C/ Pamplona s/n, 06800-Mérida, Badajoz, Spain;



POSTER SESSION 1

TUESDAY, OCTOBER 3

⁽³⁾ Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, Av. Camilo José Cela s/n, 13071-Ciudad Real, Spain;

⁽⁴⁾ Department of Mechanical, Energetic and Material Engineering, University of Extremadura. Av. Elvas s/n, 06006-Badajoz, Spain;

⁽⁵⁾ Technological Agri-Food Institute (INTAEX). Centre for Scientific Research and Technology in Extremadura, (CICYTEX), Ctra. Cáceres s/n, Finca Santa Engracia, 06071-Badajoz, Spain

P-15 Establishment of an integrated authenticity profile for quality control of artichoke dietary supplements for overweight control

Adal Mena, Estela Nogales, Samuel Garrido, Sonia Rodríguez, Ana I. Ruiz-Matute, Ana C. Soria, Belén Gómara, Mario A. Fernández, Lourdes Ramos, María L. Sanz

Instituto de Química Orgánica General (IQOG-CSIC), Juan de la Cierva 3, 28006-Madrid, Spain

P-16 Study of volatile organic compounds in hydroalcoholic samples by SHS-GC-FID

Anna Domènech Tarrat, Judith Bágueda Polo, Gemma Gotor Navarra, Francesc Broto Puig

Analytical and Applied Chemistry Dept. IQS School of Engineering, Universitat Ramon Llull, Via Augusta, 390, 08017-Barcelona, Spain

P-17 Global migration test of plastic materials in fatty food simulators by total immersion

Marina Bellot Pulido, Laura Martínez Navarro, Roser Serret Puig, Lourdes Margarit Roig, Francesc Broto Puig

Analytical and Applied Chemistry Dept. IQS School of Engineering, Universitat Ramon Llull, Via Augusta, 390, 08017-Barcelona, Spain, Spain

P-18 Identification of bioactive peptides in protein hydrolyzates from edible macroalgae by LC-ESI-QTOF

Raquel Pérez-Míguez, Maria Castro-Puyana, Merichel Plaza, María Luisa Marina

Departamento de Química Analítica, Química Física e Ingeniería Química, Universidad de Alcalá, Ctra. Madrid-Barcelona Km. 33.600, 28871-Alcalá de Henares (Madrid), Spain

P-19 GC-MS analysis of oligosaccharides derived from hydrolysis of lactitol: a chemometric study

Carlos Sabater Sánchez, Paloma Delgado Fernández, Yuri Barrios Narváez, Nieves Corzo Sánchez, Antonia Montilla Corredora

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

P-20 Determination of mercury in tuna and mussels samples by cold vapor atomic absorption spectroscopy

Eduard Miret, Marta Benito, Ariadna Verdaguer, M. Josefa Blanco

Analytical and Applied Chemistry Dept. IQS School of Engineering, Universitat Ramon Llull, Via Augusta 390, 08017-Barcelona, Spain



POSTER SESSION 1

TUESDAY, OCTOBER 3**P-21 GC-FID determination of pectin monomers from industrial orange residue polymers after acid and enzymatic hydrolysis**María T. Pacheco, F. Javier Moreno, Mar Villamiel

Departamento Bioactividad y Análisis de Alimentos, Instituto de Investigación en Ciencias de la Alimentación CIAL, (CSIC-UAM), C/ Nicolás Cabrera 9, 28049-Madrid, Spain

P-22 HPLC-UV determination of short chain fatty acids produced by fermentation of pectin in a dynamic gastrointestinal modelÁlvaro Ferreira-Lazarte, F. Javier Moreno, Agustín Olano, Mar Villamiel

Departamento Bioactividad y Análisis de Alimentos. Instituto de Investigación en Ciencias de la Alimentación CIAL, (CSIC-UAM), C/ Nicolás Cabrera 9, 28049-Madrid, Spain

P-23 Atmospheric pressure ionization of pigments and dyes in edible oilsAne Arribalaga ⁽¹⁾, Pilar Rodríguez ⁽²⁾, Mireia Medina ⁽²⁾, Encarnación Moyano ⁽¹⁾⁽¹⁾ Department of Chemical Engineering and Analytical Chemistry, University of Barcelona, Av. Diagonal 645, 08028-Barcelona, Spain;⁽²⁾ Laboratori Agroalimentari, Carretera de Vilassar de Mar a Cabrils, s/n, 08348-Cabrils (Barcelona), Spain**P-24 Analysis of hordeins in barley (*Hordeum vulgare L.*) grain and malt by capillary electrophoresis mass spectrometry (CE-MS)**Irene Compte, Laura Pont, Victòria Sanz-Nebot, José Barbosa, Fernando Benavente

Department of Chemical Engineering and Analytical Chemistry, Faculty of Chemistry, University of Barcelona, Martí I Franquès 1-11, 08028-Barcelona, Spain

P-25 Determination of masked trichothecenes from cereal matrices using subcritical water extraction followed by solid-phase extractionNúria Fontanals, Eugènia Miró-Abella, Pol Herrero, Núria Canela, Lluís Arola, Rosa Ras, Francesc Borrull

Department of Analytical Chemistry and Organic Chemistry, Universitat Rovira i Virgili, Marcel·lí Domingo, 1, 43007-Tarragona, Spain

P-26 HILIC-ESI-TOF-MS-based metabolomics study of different hybrids of *Theobroma Cacao* treeRoberto Megias-Perez ⁽¹⁾, Sergio Grimbs ⁽¹⁾, Anne Grimbs ⁽¹⁾, Roy N. D'souza ⁽¹⁾, Marcello Corino ⁽²⁾, Nikolai Kuhnert ⁽¹⁾⁽¹⁾ Department of Life Sciences and Chemistry, Jacobs University Bremen, Campus Ring 1, 28759-Bremen, Germany;⁽²⁾ Barry Callebaut AG, Westpark, Pfingstweidstrasse 60, Zurich 8005, Switzerland**P-27 Identification and determination of free inositol and fructooligosaccharides in cocoa beans**Roberto Megias-Perez ⁽¹⁾, Ana Isabel Ruiz-Matutee ⁽²⁾, Anne Grimbs ⁽¹⁾, Marcello Corino ⁽³⁾, Nikolai Kuhnert ⁽¹⁾



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⁽³⁾ Barry Callebaut AG, Westpark, Pfingstweidstrasse 60, Zurich 8005, Switzerland

P-28 Development of an atmospheric glow discharge source for analytical applications

Jonatan Fandino ⁽¹⁾, Jaime Orejas ⁽²⁾, Laura Chauvet ⁽³⁾, David Blanco ⁽⁴⁾, Philippe Guillot ⁽³⁾, Jorge Pisonero ⁽¹⁾, Nerea Bordel ⁽¹⁾

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⁽²⁾ Department of Chemistry, State University of New York at Buffalo, Buffalo, United States;

⁽³⁾ DPHE Laboratory, INU Champollion, Albi, France;

⁽⁴⁾ Department of Construction and Manufacturing Engineering, University of Oviedo, Gijón, Spain

P-29 Fast chiral discrimination of DL-amino acids by trapped ion mobility spectrometry after (+) FLEC derivatization

Raquel Pérez-Míguez ^(1,2), Elena Domínguez-Vega ⁽²⁾, María Castro-Puyana ⁽¹⁾, María Luisa Marina ⁽¹⁾, Govert W. Somsen ⁽²⁾

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⁽²⁾ Division of BioAnalytical Chemistry, AIMMS research group BioMolecular Analysis, Faculty of Science, Vrije Universiteit, De Boelelaan 1085, 1081hv Amsterdam, The Netherlands

P-30 Localization of ferroportin in brain tissues with Alzheimer's disease using gold nanoclusters bioconjugated antibodies and LA-ICP-MS

Maria Cruz-Alonso ⁽¹⁾, Vanesa Ramírez ⁽¹⁾, Aurora Astudillo ⁽²⁾, Ana Navarro ⁽³⁾, Beatriz Fernández ⁽¹⁾, Rosario Pereiro ⁽¹⁾

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⁽²⁾ Hospital Universitario Central de Asturias, 33011-Oviedo, Spain; ⁽³⁾ Department of Morphology and Cellular Biology, University of Oviedo, 33006-Oviedo, Spain

P-31 Analysis of molecular interactions by surface Plasmon resonance

Sílvia Barceló-Batllo

Molecular Interactions Unit, IDIBELL, Gran Via de L'Hospitalet 199, L'Hospitalet de Llobregat, Spain

P-32 A new quality criterion to optimize separations of bioactive compounds in capillary electrophoresis

Roger Peró-Gascón ⁽¹⁾, Victòria Sanz-Nebot ⁽¹⁾, Marcos Tascon ⁽²⁾, Leonardo G. Gagliardi ⁽³⁾, Fernando Benavente ⁽¹⁾

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P-33 Chromatographic characterization of by-products from the wood processing industry

Juan Pablo Lamas⁽¹⁾, Rosa M^a Arcas ⁽²⁾, Marta Lores ⁽¹⁾

⁽¹⁾ Department of Analytical Chemistry, Nutrition and Food Science, University of Santiago de Compostela, Faculty of Chemistry, Av. de las Ciencias s/n, Campus Vida, E-15782, Santiago de Compostela (A Coruña), Spain;

⁽²⁾ Betanzos HB, E-15300, Betanzos (A Coruña), Spain

P-34 Scaling-up polyphenols extraction from grape marc

Juan Pablo Lamas ⁽¹⁾, Alicia Rosalowska ⁽¹⁾, Juan José Verdes Gómez ⁽²⁾, Marta Lores ⁽¹⁾

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⁽²⁾ i-Grape Laboratory, Emprendia, Campus Vida, E-15782, Santiago de Compostela (A Coruña), Spain

P-35 Unveiling the effects of UVA photocatalysis on soot particles deposited over lime mortars manufactured with titanium dioxide

Ana Miller ⁽¹⁾, José M. de la Rosa ⁽¹⁾, J. Santiago Pozo-Antonio ⁽²⁾, Nicasio T. Jimenez-Morillo ⁽¹⁾, José A. González-Pérez ⁽¹⁾, Amelia Dionisio ⁽³⁾

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⁽³⁾ Instituto Superior Técnico, Universidade de Lisboa. CERENA, Av. Rovisco Pais 1049, Lisbon, Portugal

P-36 Application of biorefinery concept as a green and sustainable management for cork wastewater

Francisco Javier Yuste-Córdoba, M.J. Trinidad-Lozano, T.M. Santiago-Codosero, A.I. Parralejo-Alcobendas, Luis Royano-Barroso, Jerónimo González Cortés, Raquel García-Mateos
CICYTEX, Autovía A-V, Km 372, 06187-Guadajira (Badajoz), Spain

P-37 Fast preconcentration and separation of lactalbumin and β -lactoglobulin using transient isotachophoresis with free zone electrophoresis in glass microchips

Agustín G. Crevillén ⁽¹⁾, Mercedes de Frutos ⁽²⁾, José Carlos Díez-Masa ⁽²⁾

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- P-38 In-house made light-emitting diode induced fluorescence (LEDIF) detector for microchip capillary electrophoresis (MCE) analysis of dyes and B2 vitamin in pharmaceutical formulations and urine**

Angel Puerta, Mercedes de Frutos, José Carlos Díez-Masa

Institute of General Organic Chemistry (IQOG, CSIC), C/ Juan de la Cierva 3, Madrid, Spain

- P-39 Dispersive liquid-liquid microextraction for the determination of chlorophenoxy acid herbicides by LC-QqQ-MS/MS**

Ainhoa Oller Ruiz⁽¹⁾, Natalia Campillo⁽¹⁾ Pilar Viñas⁽¹⁾, José Fenoll⁽²⁾, Manuel Hernández Córdoba⁽¹⁾

⁽¹⁾ Department of Analytical Chemistry, Faculty of Chemistry, University of Murcia, Regional Campus Of International Excellence "Campus Mare Nostrum" E-30100, Murcia, Spain;

⁽²⁾ Department of Food Quality and Warranty, IMIDA, C/ Mayor s/n, La Alberca, 30150-Murcia, Spain

- P-40 Assessment of an automated clean-up system for the simultaneous determination of PBDEs, PCBs and PCDD/Fs in environmental samples**

Juan Muñoz Arnanz, María Ros, Begoña Jiménez

Institute of General Organic Chemistry (IQOG-CSIC), Department of Instrumental Analysis and Environmental Chemistry, Madrid, Spain

- P-41 Development and validation of a method for the analysis of beta-agonists in hair by LC-MS/MS**

Silvia Termes⁽¹⁾, Jose Blanca⁽²⁾, Patricia Muñoz⁽²⁾, Pilar Rodriguez⁽¹⁾, Mireia Medina⁽¹⁾

⁽¹⁾ Agri-food Laboratory, Ministry of Agriculture, Livestock, Fisheries and Food, Government of Catalonia, Carretera de Vilassar de Mar a Cabril, s/n, 08348-Cabril (Barcelona), Spain;

⁽²⁾ Veterinary Drug Analysis Department CNA – AECOSAN, Ministry of Health, Social Services and Equality, Carretera de Pozuelo a Majadahonda, Km 5,100, 28220-Majadahonda (Madrid), Spain

- P-42 Direct determination of steroid glucuronides in human urine by UHPLC-ESI-(ID)MS/MS and isotope pattern deconvolution**

Jorge Pitarch-Motellón⁽¹⁾, Antoni F. Roig-Navarro⁽¹⁾, Oscar J. Pozo⁽²⁾, María Ibáñez Martínez⁽¹⁾, Juan V. Sancho Llopis⁽¹⁾

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⁽²⁾ Bioanalysis Research Group, IMIM, Doctor Aiguader 88, 08003-Barcelona, Spain

- P-43 Detection of small peptides in sports drug testing by LC-MS/MS**

Núria Monfort, Élida Alechaga, Cristina Pavón, Jolita Jancyte, Rosa Ventura

IMIM (Hospital del Mar Medical Research Institute), Barcelona Antidoping Laboratory, Dr Aiguader 88, 08003-Barcelona, Spain

- P-44 Cathinone derivatives identification in legal high samples by UHPLC-MS/MS using a pseudo-target screening strategy**

David Fabregat Safont, Juan Vicente Sancho Llopis, Félix Hernández Hernández, María Ibáñez Martínez
Research Institute for Pesticides and Water, Universitat Jaume I, Av. Sos Baynat s/n, Castellón, Spain



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P-45 Updating the on-going stimulants list through identification and characterisation of four novel cathinones in drug samples from European consumers

David Fabregat Safont ⁽¹⁾ Xoán Carbón Mallol ⁽²⁾, Iván Fornís Espinosa ⁽²⁾, Mireia Ventura Vilamana ⁽²⁾, Juan Vicente Sancho Llopis ⁽¹⁾, Félix Hernández Hernández ⁽¹⁾, María Ibáñez Martínez ⁽¹⁾

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⁽²⁾ Asociación Bienestar y Desarrollo, Energy Control, C/ Independència 384, Barcelona, Spain

P-46 Use of dielectric barrier discharge ionization-mass spectrometry for determination of multiclass explosives and related compounds

David Moreno-González ⁽¹⁾ José Robles-Molina ⁽¹⁾ Felipe J. Lara-Ortega ⁽¹⁾, Bienvenida Gilbert-López ⁽¹⁾, Alexander Schütz ⁽²⁾, Sebastian Brandt ⁽²⁾, Joachim Franzke ⁽²⁾, Juan F. García-Reyes ⁽¹⁾, Antonio Molina-Díaz ⁽¹⁾

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P-47 Pollution transport by marine microplastics – POPs accumulation rate on polyethylene microparticles

Daura Vega-Moreno ⁽¹⁾, Bárbara Abaroa-Pérez⁽²⁾, Nerea Beltrán ⁽²⁾, José Joaquín Hernández-Brito ⁽²⁾

⁽¹⁾ Dept. Química, Universidad de Las Palmas de Gran Canaria, Las Palmas de Gran Canaria, Spain;

⁽²⁾ Plataforma Oceánica de Canarias. Telde, Spain

P-48 PAH determination on seawater samples using a miniaturized solid phase extraction system (m-SPE)

Bárbara Abaroa-Pérez ⁽¹⁾, Daura Vega-Moreno ⁽²⁾, José Joaquín Hernández-Brito ⁽¹⁾,

Octavio Llinás ⁽¹⁾

⁽¹⁾ Plataforma Oceánica de Canarias (PLOCAN), Telde, Spain;

⁽²⁾ Dept. Química, Universidad de Las Palmas de Gran Canaria, Las Palmas de GranCanaria, Spain

P-49 1,4-Dioxane and 1,3-dioxolanes in the Llobregat River: seasonal trend and removal efficiency in a drinking water treatment plant

Guillem Carrera Ruiz, Lídia Vegué Garrich, Maria Rosa Boleda

Aigües de Barcelona (AGBAR), Barcelona, Spain

P-50 Assessment of the occurrence of pesticides in coastal waters under the influence of agriculture activities in NE Spain through on-line SPE-LC-MS/MS analysis

Luis Simón Monllor Alcaraz, Miren Lopez De Alda, Nuria Guillem Argiles, Damià Barceló, Marta Llorca, Marinella Farré

Water and Soil Quality Research Group, Institute of Environmental Assessment and Water Research, IDAEA-CSIC, C/ Jordi Girona, 18-26, 08034-Barcelona, Spain

P-51 Analysis of drugs of abuse in the environment: a review of analytical methodologies and occurrence data

Ester López-García, Cristina Postigo, Nicola Mastroianni, Miren López De Alda, Damià Barceló

Water and Soil Quality Research Group, Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research, IDAEA-CSIC, Jordi Girona 18-26, 08034-Barcelona, Spain

P-52 Effect of pyrolysis conditions on the total and bioavailable contents of polycyclic aromatic hydrocarbons (PAHs) in biochars produced from crop residues

José M. de la Rosa, Águeda Sánchez-Martín, Paloma Campos, Marta Velasco-Molina, Ana Z. Miller, Heike Knicker

Instituto de Recursos Naturales y Agrobiología de Sevilla, Consejo Superior de Investigaciones Científicas (IRNAS-CSIC), Av. Reina Mercedes 10, 41012-Seville, Spain

P-53 UHPLC-MS/MS determination of sweeteners in water samples

Marta Batriu ⁽¹⁾, Mª Rosa Boleda⁽¹⁾, Encarnación Moyano ⁽²⁾

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⁽²⁾ Department of Chemical Engineering and Analytical Chemistry, University of Barcelona, Av. Diagonal 645, E-08028, Barcelona, Spain



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- P-54** **Outdoor air 1,3-butadiene monitoring near a petrochemical industry using passive Radiello® samplers and active multi-sorbent bed tubes**

Eva Gallego ⁽¹⁾, Pilar Teixidor ⁽²⁾, José Francisco Perales ⁽¹⁾, Francisco Javier Roca ⁽¹⁾, Xavier Guardino ⁽³⁾, Enrique Gadea ⁽³⁾

⁽¹⁾ Universitat Politècnica de Catalunya, LCMA, Avd. Diagonal 647, 08028-Barcelona, Spain;

⁽²⁾ Universitat de Barcelona, Centres Científics i Tecnològics, C/ Lluís Soler Sabaris 1-3, 08028-Barcelona, Spain;

⁽³⁾ Instituto Nacional de Seguridad e Higiene en el Trabajo, CNCT, C/ Dulcet 2-10, 08034-Barcelona, Spain

- P-55** **Determination of benzothiazole, benzotriazole and benzenesulfonamide derivates present in particulate matter (PM10) of outdoor air. Estimating the inhalation intake**

Alba Maceira Torrents, Rosa María Marcé Recasens, Francesc Borrull Ballarín

Dept. Química Analítica i Química Orgànica, Universitat Rovira i Virgili, C/ Marcel·lí Domingo s/n, 43007-Tarragona, Spain

- P-56** **Characterization of DOM fractions in samples from a drinking water treatment plant by HPLC-SEC using fluorescence and UV absorption detection**

Nuria Ivars Cardona, José Luis Beltrán Abadía

Analytical Chemistry Section, Department of Chemical Engineering and Analytical Chemistry, Universitat de Barcelona, Martí I Franquès, 1-11, 08028-Barcelona, Spain

- P-57** **LC-HRMS method development for detection of antidiabetic drugs in wastewater and surface water samples based on suspect screening**

Juan Carlos Guillén Asensio, Bozo Zonja, Miren López de Alda, Damià Barceló

Water and Soil Quality Research Group, Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research, IDAEA-CSIC, Jordi Girona 18-26, 08034-Barcelona, Spain

- P-58** **Comparison of information-dependent acquisition and swath for non-target screening of contaminants of emerging concern in river sediments employing ultrahigh-performance liquid chromatography-quadrupole time-of-flight mass spectrometry**

Rodrigo Álvarez Ruiz ⁽¹⁾, Yolanda Picó García ⁽²⁾

⁽¹⁾ Centro de Investigaciones sobre Desertificación (CIDE), Carretera Moncada-Náquera, Km 4,5 46113 Moncada (Valencia), Spain;

⁽²⁾ Food and Environmental Safety Research Group (SAMA-UV), University of Valencia, Av. Vicent Andrés Estellés s/n, 46100-Burjassot, (Valencia), Spain

- P-59** **Non-target monitoring of pesticides and their transformation products in honey bees**

Pau Calatayud-Vernich ⁽¹⁾, Fernando Calatayud ⁽²⁾, Enrique Simó ⁽²⁾, Yolanda Picó ⁽³⁾

⁽¹⁾ Desertification Research Centre (CIDE, UV-GV-CSIC), Carretera Moncada-Náquera, Km 4,5 (Moncada), Spain;

⁽²⁾ Agrupación de Defensa Sanitaria apícola (apiADS), Carretera Montroi – Turis s/n (Montroi), Spain;

⁽³⁾ Food and Environmental Safety Research Group (SAMA-UV), University of Valencia, Av. Vicent Andrés Estellés s/n, 46100-Burjassot, (Valencia), Spain



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P-60 Trace determination of psychoactive drugs and their metabolites in water by liquid chromatography mass spectrometry

Mireia Oliver ⁽¹⁾, María Jesús Andrés-Costa ⁽¹⁾ Yolanda Pico ⁽²⁾

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P-61 Measuring emerging persistent organic pollutants in wastewater, surface water and sediment from L'Albufera Natural Park area (Valencia, Spain)

Maria Lorenzo ⁽¹⁾, Julian Campo ⁽²⁾, Yolanda Pico ⁽¹⁾

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P-62 Molecular descriptors of water repellency in forest fire affected soils. A chemometric approach

Nicasio T. Jiménez Morillo ⁽¹⁾, Gonzalo Almendros ⁽²⁾, Lorena M. Zavala ⁽³⁾, Antonio Jordán ⁽³⁾,

Francisco J. González-Vila ⁽¹⁾ José A. González-Pérez ⁽¹⁾

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P-63 Exposure of white stork (*Ciconia ciconia*) to perfluoroalkyl substances (PFASs): geographical and temporal variations (2006-2016) in the community of Madrid, Spain

Marta Pérez-Fernández ⁽¹⁾, Jose L. Roscales ⁽¹⁾, Jose I. Aguirre ⁽²⁾, Begoña Jiménez ⁽¹⁾

⁽¹⁾ Dept. of Instrumental Analysis and Environmental Chemistry, Institute of General Organic Chemistry, CSIC (IGOG-CSIC), Juan de la Cierva 3, 28006-Madrid, Spain;

⁽²⁾ Dept. of Zoology and Physic Anthropology, Faculty of Biology, University Complutense of Madrid, José Antonio Novais 2, Ciudad Universitaria, 2804-Madrid, Spain

P-64 Determination of polybrominated diphenyl ethers in meat samples

Meritxell Valentí, Montse Gasser, Ramon Martí, Jordi Díaz-Ferrero

IQS Environmental Laboratory, Via Augusta 390, Barcelona, Spain

P-65 Suspect screening of pharmaceuticals in lettuce leaves using QTOF LC-MS/MS system

Nicola Montemurro ⁽¹⁾, Cristina Postigo ⁽¹⁾, Antonio Lonigro ⁽²⁾, Sandra Pérez ⁽¹⁾, Damià Barcelò ⁽¹⁾

⁽¹⁾ IDAEA-CSIC, Water and Soil Quality Research Group - Department of Environmental Chemistry, Barcelona, Spain;

⁽²⁾ Dept. of Agricultural and Environmental Science – University of Bari, Bari, Italy

P-66 Study of automatic clean-up for dioxin and PCB analysis in food and feed samples

Marc Fernández, Berta Bayascas, M^a Jesús Montaña, Ramon Martí, Jordi Díaz-Ferrero

IQS Environmental Laboratory, Via Augusta 390, 08017-Barcelona, Spain



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P-67 Study of thermal desorption technique and application to the determination of volatile organic compounds (VOCs) in ambient air

Anna Ventayol Soler, Gemma Gotor Navarra, Judith Báguena Polo, Francesc Broto Puig

Analytical and Applied Chemistry Dept. IQS School of Engineering, Universitat Ramon Llull, Via Augusta, 390, 08017-Barcelona, Spain

P-68 Field burn severity indexes and its relation with soil organic matter molecular changes described by graphical statistical analysis of pyrochromatographic data

José A. Vega ⁽¹⁾, Cristina Fernández ⁽¹⁾, Teresa Fontúrbel ⁽¹⁾, Nicasio T. Jiménez-Morillo ⁽²⁾,

Gonzalo Almendros ⁽³⁾, José A. González-Pérez ⁽²⁾

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P-69 Analysis of urinary metabolites of organophosphate pesticides and its application in agricultural populations from Catalonia and Galicia

Natalia Bravo, Mercè Garí, Joan Grimalt

Institute of Environmental Assessment and Water Research, IDAEA-CSIC, Jordi Girona 18-26, 08034-Barcelona Spain

P-70 Occurrence and temporary trends of halogenated persistent organic pollutants in gull eggs from Spanish natural parks

F. Javier Santos ⁽¹⁾, Jorge Olmos ⁽¹⁾, Albert Bertolero ⁽²⁾, Sílvia Lacorte ⁽³⁾, M. Teresa Galceran ⁽¹⁾

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⁽³⁾ Department of Environmental Chemistry, IDAEA-CSIC, C/ Jordi Girona 18-26, 08034-Barcelona, Spain

P-71 Bioaccumulation of C60 fullerene and its transformation products in river biofilms

Josep Sanchís ⁽¹⁾, Anna Freixa ⁽²⁾, Vicenç Acuña ⁽²⁾, Sergi Sabater ⁽²⁾, Damià Barceló ⁽²⁾,

Esteban Abad ⁽¹⁾, Marinella Farré ⁽¹⁾

⁽¹⁾ Institut de Diagnosi Ambiental i Estudis de l'Aigua, C/ Jordi Girona, 18-26, 08034-Barcelona, Spain;

⁽²⁾ Institut Català de Recerca de l'Aigua, C/ Emili Grahit, 101, 17003-Girona, Spain

P-72 Ionization of short-chain chlorinated paraffins by atmospheric pressure sources

Juan Francisco Ayala, María Teresa Galceran, Francisco Javier Santos, Encarnación Moyano

Department of Chemical Engineering and Analytical Chemistry, University of Barcelona, Av. Diagonal 645, E-08028, Barcelona, Spain

P-73 Chemometric models for quantifying soil properties from its alkane patterns

Marco A. Jiménez-González ⁽¹⁾, Gonzalo Almendros ⁽¹⁾, Ana M. Álvarez ⁽²⁾, Pilar Carral ⁽²⁾,

José M. De La Rosa ⁽³⁾, Jesús Sanz ⁽⁴⁾

⁽¹⁾ Museo Nacional de Ciencias Naturales (MNCN-CSIC), c/ Serrano 115-B, Madrid, Spain;

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⁽⁴⁾ Instituto de Química Orgánica General (IQOG-CSIC), c/ Juan De La Cierva 3, Madrid, Spain



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P-74 Development of a multianalyte method based on solid-phase microextraction - gas chromatography-tandem mass spectrometry for the analysis of water samples

Marlene Vila ⁽¹⁾, J. Pablo Lamas ⁽¹⁾, Carmen García-Jares ⁽¹⁾ Maria Llompart ⁽¹⁾, Vera Homem ⁽²⁾

⁽¹⁾ Laboratory of Research and Development of Analytical Solutions (LDSA) Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Chemistry, Campus Vida, University of Santiago de Compostela, Avda. Das Ciencias S/n, Santiago De Compostela, Spain;

⁽²⁾ LEPABE - Laboratory for Process Engineering, Environment, Biotechnology and Energy Chemical Engineering Department Faculty of Engineering - University of Porto, Rua Dr. Roberto Frias, S/n 4200-465, Porto, Portugal

P-75 Method validation for the simultaneous determination of eleven widespread fungicides in water by solid-phase microextraction followed by gas chromatography-tandem mass spectrometry

Rocío Facorro ⁽¹⁾, María Celeiro ⁽²⁾, María Llompart ⁽²⁾, Thierry Dagnac ⁽¹⁾

⁽¹⁾ Agronomic Research Center (INGACAL-CIAM) - Organic Contaminant Unit, Apdo 10 – 15080-A Coruña, Spain;

⁽²⁾ Laboratory of Research and Development of Analytical Solutions (LDSA) - Department of Analytical Chemistry, Nutrition and Food Science, E-15782, Santiago De Compostela, Spain

P-76 Simultaneous measurement in high resolution and mass/mass mode for qualitative and quantitative analysis of emerging contaminants in river waters

Isabel López, Covadonga Alonso, Leonor Nózal, Alba Arenas, Andreu Rico, Marco Vighi

Fundación IMDEA Agua, Alcalá De Henares, Spain

P-77 Use of magnetic molecularly imprinted polymers (MMIPs) in the extraction of quinolones for their determination in raw milk by LC-UV

Javier Giménez-López, Elena Megías, Alexandra Junza, Cristina Minguillón Llombart, Dolores Barrón Bueno

Dept. of Nutrition, Food Science and Gastronomy, Food and Nutrition Torribera Campus, INSA. University of Barcelona, Av. Prat de la Riba 171, E-08921, Sta. Coloma de Gramenet (Barcelona), Spain

P-78 Study of the cyclodextrin-based materials advantages for pesticides analysis in water samples

Adela Maurí-Aucejo ⁽¹⁾ Pedro Amorós ⁽²⁾, Carolina Belenguer-Sapiña ⁽¹⁾, Enric Pellicer-Castell ⁽¹⁾

⁽¹⁾ Departament de Química Analítica, Universitat de Valencia, Dr. Moliner 50, Burjassot, Spain;

⁽²⁾ Institut Ciència dels Materials, València, Spain

P-79 Use of cyclodextrin-silica composites in the sample treatment step for environmental analysis

Carolina Belenguer-Sapiña ⁽¹⁾, Enric Pellicer-Castell ⁽¹⁾, Pedro Amorós ⁽²⁾, Jamal El Haskouri ⁽²⁾,

Ernesto Simó-Alfonso ⁽¹⁾, Adela Maurí-Aucejo ⁽¹⁾

⁽¹⁾ Departament de Química Analítica, Universitat de Valencia, Dr. Moliner 50, Burjassot, Spain;

⁽²⁾ Institut Ciència dels Materials, València, Spain



POSTER SESSION 2

WEDNESDAY, OCTOBER 4**P-80 Comparison of titanium-based materials for organophosphorus pesticides determination in environmental samples**

Enric Pellicer-Castell ⁽¹⁾, Carolina Belenguer-Sapiña ⁽¹⁾ Pedro Amorós ⁽²⁾, Jamal El Haskouri ⁽²⁾, Jose Manuel Herrero-Martínez ⁽¹⁾ Adela Mauri-Aucejo ⁽¹⁾

⁽¹⁾ Departament de Química Analítica, Universitat de València, Dr. Moliner 50, Burjassot (Valencia), Spain;

⁽²⁾ Institut Ciència dels Materials, València, Spain

P-81 Use of carbon nanotubes as adsorbent in magnetic solid phase microextraction coupled with GC-MS to analyze parabens in water samples

Marta Pastor Belda, Lidia Marín Soler, Pilar Viñas López-Pelegrín, Natalia Campillo Seva, Manuel Hernández Córdoba

Department of Analytical Chemistry, Faculty of Chemistry, University of Murcia, Campus de Espinardo 30100 Murcia, Spain

P-82 Optimization of polylactic acid (PLA) sample treatment and determination of its main oligomers

Margarita Aznar, Sara Úbeda, Nicola Dreolin, Cristina Nerín

Department of Analytical Chemistry, University of Zaragoza, María de Luna 3, Zaragoza, Spain

P-83 Comparison of two sample treatments for polyethylene terephthalate pellets analysis

Sara Úbeda Jasanada, Marga Aznar Ramos, Cristina Nerín de la Puerta

Department of Analytical Chemistry, University of Zaragoza, María de Luna 3, Zaragoza, Spain

P-84 Comparison between liquid phase microextraction and electromembranes extraction used on microfluidic devices for the determination of drugs in environmental waters

Maria Ramos Payán ⁽¹⁾, Elia Santigosa Murillo ⁽²⁾, Jordi Coello ⁽²⁾

⁽¹⁾ Departamento de Química Analítica, Universidad de Sevilla, 41012-Sevilla, Spain;

⁽²⁾ Unitat de Analítica, Departamento de Química, Facultad de Ciencias, Universidad Autònoma de Barcelona, 08193-Cerdanyola del Vallès (Barcelona), Spain

P-85 Analysis of UV filters, preservatives, fragrance allergens, plasticizers, and synthetic musks in cosmetic and personal care products by μ -matrix solid-phase dispersion gas chromatography–tandem mass spectrometry

Marlene Vila, Carmen Garcia-Jares, Maria Llompart

Laboratory of Research and Development of Analytical Solutions (LIDSA), Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Chemistry, Campus Vida, University of Santiago de Compostela, Avda. Das Ciencias S/n, Santiago De Compostela, Spain

P-86 Separation and identification of mouse transferrin glycan isomers by μ ZIC-HILIC-MS. Application to rheumatoid arthritis diagnosis

Montserrat Mancera-Arteu ⁽¹⁾, Laura Pey ⁽¹⁾, Estela Giménez ⁽¹⁾, Jaime Sancho ⁽²⁾, José Barbosa ⁽¹⁾ Victòria Sanz-Nebot ⁽¹⁾

⁽¹⁾ Department of Chemical Engineering and Analytical Chemistry, University of Barcelona, Diagonal 645, Barcelona, Spain;

⁽²⁾ CSIC, Instituto de Parasitología y Biomedicina "López-Neyra" (IPBLN), Av. del Conocimiento 17, Granada, Spain



POSTER SESSION 2

WEDNESDAY, OCTOBER 4**P-87 Variety classification of almonds by UHPLC-QTOF MS metabolomics**

Rubén Gil Solsona, Clara Boix Sales, María Ibáñez Martínez, Juan Vicente Sancho Llopis

Research Institute for pesticides and Water (IUPA), University Jaume I, Av. Sos Baynat, s/n, 12071-Castellón de la Plana, Spain

P-88 UHPLC-HRMS based metabolomics study to evaluate the inoculation of *Enteromyxum leei* in *Sparus aurata*

Leticia Lacalle Bergeron⁽¹⁾, Rubén Gil Solsona⁽¹⁾, Jaime Nácher Mestre⁽¹⁾, Josep Calduch Giner⁽²⁾, Juan Vicente Sancho Llopis⁽¹⁾, Félix Hernández Hernández⁽¹⁾, Jaume Pérez Sánchez⁽²⁾

⁽¹⁾ Research Institute for Pesticides and Water (IUPA), University Jaume I, Av. Sos Baynat, s/n, 12071-Castellón de la Plana, Spain;

⁽²⁾ Nutrigenomics and Fish Growth Endocrinology Group, Institute of Aquaculture Torre de la Sal (CSIC), 12595-Ribera de Cabanes, Castellón, Spain

P-89 On-line protein digestion by immobilised enzyme microreactor capillary electrophoresis mass spectrometry

Victoria Sanz-Nebot, Lorena Villegas, Roger Peró-Gascón, José Barbosa, Fernando Benavente

Department of Analytical Chemistry, University of Barcelona, Martí i Franquès 1-11, 08028-Barcelona, Spain

P-90 Determination of prevalent drugs and related metabolites: a comparative study of different GC-MS configurations

Jorge Sáiz⁽¹⁾, Carmen García-Ruiz⁽²⁾, Belen Gómara⁽¹⁾

⁽¹⁾ IQOG-CSIC. Institute of General Organic Chemistry, Spanish National Research Council, Juan de la Cierva, 3, 28006-Madrid, Spain;

⁽²⁾ Department of Analytical Chemistry, Physical Chemistry and Chemical Engineering, University of Alcalá, Ctra. Madrid-Barcelona Km 33.6, 28871-Alcalá de Henares (Madrid), Spain

P-91 Evaluation of the reporting level to detect budesonide misuse in sports using LC-MS/MS

Sergi Coll Camenforte⁽¹⁾, Xavier Matabosch Gerones⁽¹⁾, Katerina Papakonstantinou⁽¹⁾,

Clara Perez Maña⁽²⁾, Rosa Ventura Alemany⁽¹⁾

⁽¹⁾ Barcelona Anti-doping laboratory, IMIM, Doctor Aiguader, 88, 08003-Barcelona, Spain;

⁽²⁾ Human Pharmacology and Clinical Neurosciences Research Group, IMIM, Doctor Aiguader, 88, 08003-Barcelona, Spain

P-92 Quantification of sulfated steroids in human urine by LC-MS/MS to improve the detection of endogenous anabolic steroids

Argitxu Esquivel López, Élida Alechaga Silva, Nuria Monfort Mercader, Rosa Ventura Alemany

Barcelona Antidoping Laboratory, Doping Control Research Group, Carrer Doctor Aiguader 88, 08003-Barcelona, Spain



POSTER SESSION 2

WEDNESDAY, OCTOBER 4

P-93 CE and HPLC-MS to characterize prostate specific antigen (PSA) purification from urineAngel Puerta⁽¹⁾, Diana Navarro-Calderon⁽¹⁾, Andras Acs^(2,3), Noemi Farina-Gomez⁽¹⁾Eduardo Albers-Acosta⁽⁴⁾, Carlos Olivier⁽⁴⁾, Laszlo Drahos⁽²⁾, José Carlos Díez-Masa⁽¹⁾, Karoly Vekey^(2,5), Mercedes de Frutos⁽¹⁾⁽¹⁾ Institute of General Organic Chemistry (IQOG, CSIC), C/ Juan de la Cierva 3, Madrid, Spain;⁽²⁾ MS Proteomics Research Group, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary;⁽³⁾ Semmelweis University, Budapest, Hungary;⁽⁴⁾ Department of Urology, Hospital La Princesa, Madrid, Spain;⁽⁵⁾ Szent Istvan University, Ybl Miklos Faculty of Architecture and Civil Engineering, Budapest, Hungary**P-94 Effect of the storage conditions on the stability of prostate specific antigen (PSA) from urine studied by capillary electrophoresis**Diana Navarro⁽¹⁾, Angel Puerta⁽¹⁾, Eduardo Albers-Acosta⁽²⁾, Inmaculada Fernandez⁽²⁾,Carlos Olivier⁽²⁾, José Carlos Díez-Masa⁽¹⁾, Mercedes de Frutos⁽¹⁾⁽¹⁾ Institute of General Organic Chemistry (IQOG-CSIC), Madrid, Spain;⁽²⁾ Department of Urology, Hospital La Princesa, Madrid, Spain**P-95 Spectrofluorimetry as an essential tool for screening small molecule candidates against neurodegenerative diseases: studies on fluorene derivatives designed as fluorescent analogues of GN8**Ana Molina⁽¹⁾, Karen Xiomara Orellana⁽¹⁾, Ana I. Olives⁽¹⁾, M. Antonia Martín⁽¹⁾.José Carlos Menéndez⁽²⁾⁽¹⁾ Universidad Complutense, Facultad de Farmacia, Dept. Química Analítica, 28040-Madrid, Spain;⁽²⁾ Universidad Complutense, Facultad de Farmacia, Dept. Química Orgánica y Farmacéutica, 28040-Madrid, Spain**P-96 Verifying the efficiency of camptothecin-beta cyclodextrin nanoencapsulation.****Study of the camptothecin lactone - carboxylate equilibrium by RP-HPLC**

Karen Xiomara Orellana, Ana Molina, Ana I. Olives, M. Antonia Martín

Universidad Complutense, Facultad de Farmacia, Dept. Química Analítica, 28040-Madrid, Spain



GENERAL INFORMATION



GENERAL INFORMATION

VENUE

Fira de Barcelona

Gran Via Venue

Av. Joan Carles I, 64

08908 L'Hospitalet de Llobregat

Barcelona



DATES

October 3rd – 5th 2017

HOW TO ARRIVE

By plane



Direct access from the airport:

- **By road:** 12 kilometers away (C-31)
- **Metro:** Line L9 Sud ("Fira" and "Europa/Fira" stations)
- **Bus:** TMB Line 46 ("Pl. Europa" stop)
- **Taxi**

By road



The Gran Via venue is located in a new business development area, connected to the main motorways and roads to Barcelona: AP-7, AP-2, A-2, C-16, C-58, C-31, C-32, C-33

Metro



TMB Line: L9 Sud ("Fira" and "Europa/Fira" stations)

Bus



TMB Lines: H12 and 79

Train



Ferrocarrils Generalitat de Catalunya (FGC): Lines S8, S33, R6, R5, S4 ("Europa/Fira" station). Renfe "Barcelona-Sants" station, 4 km from the venue, is connected to a complete regional, national and international rail network.



GENERAL INFORMATION

CONFERENCE LANGUAGE

The official languages of the meeting are Spanish and English.

BOOK OF ABSTRACTS

The book of abstracts is delivered on the USB memory stick upon registration.

ORAL COMMUNICATIONS

Oral communications will be preferably in English.

Time scheduled for all the plenary lectures is 50 min and 30 minutes for the invited lectures. Time scheduled for the rest of lectures is 20 min (ideally distributed using 15 min for the presentation, plus 5 min for questions), except for the lectures of the Young Scientist Session which will be 10 min (ideally using up to 7 min for the presentation plus 3 min for questions) and must be presented in English.

Authors should provide to the organization a copy of the file of their presentation in PowerPoint format at least two hours before the session starts, although ideally should be provided the day before the presentation.

POSTER COMMUNICATIONS

Poster communications will be written in English.

Posters should have dimensions close to 150 cm high x 90 cm wide. Double adhesive tape will be provided to fix the posters to the panels. Posters are displayed during all the days of the Conference.

Poster design is free, but remember it should be clear enough to be understood on its own and sufficiently striking to attract reader's attentions. It is recommended to use a font size that allows a correct reading of the text from a distance of one meter.

Author(s) must be in attendance at their poster boards during their corresponding poster session which will be indicated in the Final Scientific Program.

The oral presentation of selected posters in flash format will have a duration of 5 min, highlighting the most relevant aspects of the research presented. Authors must provide well in advance to the organizers a copy of their presentation file (Microsoft PowerPoint format).

CONFERENCE SECRETARY OFFICE

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