16th ANNUAL WORKSHOP ON EMERGING HIGH-RESOLUTION MASS SPECTROMETRY (HRMS) AND LC-MS/MS APPLICATIONS IN ENVIRONMENTAL ANALYSIS AND FOOD SAFETY

Organized by:

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https://lcmsms.activacongresos.com/
09,40 Introduction to the poster session by Damià Barceló (Chair)

09,45-12,00 POSTER SESSION 1

P1 - Cryogenically-modulated comprehensive two-dimensional gas chromatography-high resolution time-of-flight mass spectrometry: fingerprint of the unsaponifiable fraction of vegetable oils
Ivan Aloisi  
Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Messina, Italy

P2 - Accurate Identification of Chlorinated Paraffins in a Complex Environmental Sample by Using a Novel Ionization Source coupled with High Resolution Mass Spectrometry  
Scott Pugh  
LECO Corporation, St. Joseph, USA

P3 - A non-targeted metabolomic study for the characterization of honeys by UHPLC-QTOF-MS  
Iciar Beraza Gomez  
University of Almeria

P4 - HRMS for the analysis of organic contaminants in beehive matrices  
Iciar Beraza Gomez  
University of Almeria

P5 - Novel prioritization strategy of non-targeted features in archived white-tailed sea eagle muscle tissue using temporal trend analysis  
Wiebke Dürig  
Dept. of Aquatic Science and Assessment, Swedish University of Agricultural Sciences

P6 - Optimization of analytical conditions to identify transformation products (TPs) by LC-QTOF: application to monitor the wastewater treatment of a vegetation filter (VF)  
Blanca Huidobro López  
Instituto IMDEA Agua

P7 - Targeted and suspect screening of contaminants in coastal water and sediment samples in Qatar  
Lan Liu  
Department of Food Science and Agricultural Chemistry, McGill University

P8 - Non-target proteomics study of wastewater by ROIMCR procedure using polymeric passive samplers  
Carlos Pérez López  
Institute of Environmental Assessment and Water Studies (IDAEA-CSIC), Department of Environmental Chemistry, Barcelona, Spain
P9 - Nontargeted and Suspect Screening Analysis of Indoor Environmental Chemicals Using the SCIEX X500R QTOF System and SCIEX OS Software  
Jianru Stahl-Zeng  
SCIEX Germany

P10 - NON-TARGETED ANALYSIS IN POLYPROPYLENE FOR FOOD PACKAGING BY LC-MS  
Patricia Vazquez Loureiro  
USC

P11 - PHARMACEUTICALS AND THEIR METABOLITES OCCURRENCE IN RADISHES IRRIGATED WITH RECLAIMED WASTEWATER BY LC-SWATH-HRMS ANALYSIS  
Francesc labad  
IDAIA-CSIC

P12 - Quantification of bisphenol related compounds in canned food by HPLC-FLD  
Antía Lestido Cardama  
Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Pharmacy, University of Santiago de Compostela, Spain

P13 - Identification of migrants in epoxy can coatings by LC-MS/MS  
Antía Lestido Cardama  
Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Pharmacy, University of Santiago de Compostela, Spain

P14 - PLANT UPTAKE AND DISTRIBUTION OF ORGANIC CONTAMINANTS IN TOMATO CROPS IRRIGATED WITH RECLAIMED WATER: SOIL, LEAVES AND FRUIT  
Maria Jesús Martínez Bueno  
University of Almería, Department of Physics and Chemistry, Almería, Spain

P15 - LC-HRMS Polyphenolic and Capsaicinoid Profiling to Guarantee Paprika Integrity, Safety and Authenticity  
Oscar Nuñez  
University of Barcelona

P16 - Non-targeted LC-HRMS Fingerprinting Strategy for the Prevention of Frauds in Turmeric and Curry Samples  
Oscar Nuñez  
University of Barcelona

P17 - Targeted LC-HRMS and LC-MS/MS polyphenolic profiling to guarantee the integrity, safety and authenticity of different coffee varieties  
Nerea Nuñez  
Department of Chemical Engineering and Analytical Chemistry, University of Barcelona, Barcelona, Spain

P18 - Targeted LC-HRMS polyphenolic and curcuminoid profiling and Chemometrics to prevent food frauds in Turmeric and Curry Samples  
Nerea Nuñez  
Department of Chemical Engineering and Analytical Chemistry, University of Barcelona, Barcelona, Spain
P19 - Selective, rapid and simultaneous determination of ergosterol and ergocalciferol in mushrooms by UPLC-Q-TOF-MS

Cristina Roman-Hidalgo
Universidad de Sevilla

Poster discussion

12,00 Welcome and introduction by Damià Barceló (Chair) and Antoni Ginebreda (Co-chair)

12,05 David Solomon Jalajel, PRINCE SULTAN BIN ABDULAZIZ INTERNATIONAL WATER PRIZE

12,15-13,00 PLENARY LECTURE: Susan Richardson
Department of Chemistry & Biochemistry, University of South Carolina, Columbia, SC, USA
Emerging DBPs: New discoveries, potential risks, and promising solutions

13,00-13,20 Laura Righetti
Department of Food and Drug, University of Parma, Italy
Ion mobility derived collision cross section database: application and benefits for mycotoxins screening

13,20-13,50 INVITED LECTURE: Heinz Singer
EAWAG, Dübendorf, Switzerland
On-site non-target screening of water sources with a transportable Orbitrap

13,50-14,20 Albert Lebedev
Lomonosov Moscow State University, Moscow, Russia
Non-targeted analysis of environmental samples by GC×GC-HRTOFMS

14,20-14,50 Jaume C. Morales
Agilent Technologies Spain S.L.
Profiling of Environmental Contaminants in Surface Water Using GC/Q-TOF

14,50-15,30 Brunch break

15,30-16,00 INVITED LECTURE: Diana S. Aga
Chemistry Department, University at Buffalo, Buffalo, NY, USA
Retrospective Screening Reveals Previously Un-targeted Contaminants in Global Surface Waters

16,00-16,30 Jianru Stahl-Zeng
SCIEX
Suspect and non-targeted screening of Environmental Chemicals Using the SCIEX X500R QTOF System

16,30-17,00 INVITED LECTURE: Mehran Alaee
National Water Research Institute, Burlington, Canada
Sources, fate and impact of metformin on aquatic environment

17,00-17,30 Neville Llewellyn
Thermo Fisher Scientific, Hemel Hempstead, London, UK
The first Global surveillance study of organic micro-pollutants in riverine environments and drinking water using HRAM LCMSMS and Compound Discoverer
17.30 - 19.30 ORAL SESSION 1

17.30 Lucia Helena Santos
ICRA, Girona, Spain
*Revealing the impact of the antidepressant venlafaxine on fish: identification of biomarkers of exposure using target, suspect and non-target screening*

17.50 Nicola Montemurro
IDAEA-CSIC
*Earthworms impact on the uptake of selected pharmaceuticals in lettuce crops irrigated with wastewater*

18.10 Rayana Manasfi
UMR HydroSciences Montpellier, Montpellier University, Montpellier, France
*Wastewater-borne organic micropollutants accumulation in soil and lettuce leaves using QuEChERS extraction methods and LC-QTOF-MS: A field study*

18.30 Yolanda Gálvez Ontiveros
Department of Nutrition and Food Science, University of Granada, Instituto de Investigación Biosanitaria, Ibs-Granada, Granada, Spain
*DETERMINATION OF THE FOOD EXPOSURE TO BISPHENOLS AND PARABENS WITH OBESOGENIC ACTIVITY IN THE SCHOOL POPULATION*

18.50 Laura Carbonell-Rozas
Department of Analytical Chemistry, Faculty of Sciences, University of Granada
*DETERMINATION OF ERGOT ALKALOIDS IN OAT-BASED PRODUCTS USING QuEChERS COMBINED WITH UHPLC-MS/MS*

19.10 Roman Lyubimenko
Karlsruhe Institute of Technology (KIT), Institute of Microstructure Technology (IMT), Institute for Advanced Membrane Technology (IAMT), Germany
*Coupling of liquid chromatography and flow scintillation analysis for in-line detection of water-borne radiolabelled steroid hormones*

ROOM B

17.30 - 19.30 ORAL SESSION 2

17.30 Anca Baesu
McGill University
*Application of suspect screening for the identification of erythrohydrobupropion and other PPCPs in fish livers*

17.50 Nina Huynh
LEESU
*Evaluation of road runoff treatment systems performance by non-target screening combined with ecotoxicological studies*

18.10 Ruben Gil
ICRA, Girona, Spain
*Linking xenobiotic presence with metabolite alterations in wild fish from Mar Menor lagoon by xenometabolomics tools*
Friday, October 16, 2020

ROOM A

08,40 Introduction to the poster session

08.45-11,00 POSTER SESSION 2

P20 - Development of a comprehensive analytical method for determination of biomarkers of human exposure to personal care and household products in wastewater

Ivan Senta
Catalan Institute for Water Research

P21 - LC–ESI-MS/MS method for the simultaneous determination of pharmaceutical residues and caffeine in the coastal ecosystem of Southern Baltic Sea

Lillianna Sharma
Institute of Oceanology, Polish Academy of Sciences

P22 - CONTROL OF ANABOLIC SUBSTANCES IN URINE BY LC-MS/MS

Naiara Pardo Mates
Agri-food laboratory

P23 - Sensitive determination of dinitrophenols and their main metabolites in saliva and urine samples by liquid chromatography-mass spectrometry after hollow fiber liquid phase microextraction

Noemí Aranda-Merino
Universidad de Sevilla

P24 - Analysis of plant commodities employing pressurized liquid extraction as a tool to avoid sample hydration

Francisco José Díaz-Galiano
University of Almeria, Department of Physics and Chemistry, Almeria, Spain
P25 - VALIDATION OF A QUICK AND EASY EXTRACTION METHOD FOR THE DETERMINATION OF EMERGING CONTAMINANTS AND PESTICIDE RESIDUES IN AGRICULTURAL SOILS
Mar García Valverde
University of Almería, Department of Chemistry and Physics, Almería, Spain

P26 - Analytical method development using solid-phase extraction method and liquid chromatography coupled to HR and LR-MS for the detection of PMOCs in waters from intermittent rivers
Diana Patricia Manjarrés López
Idaea-CSIC

P27 - Advance sample preparation to analyses selected emerging pollutants in Anguilla anguilla by liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS).
Dyana Vitale
Food and Environmental Safety Research Group (SAMA-UV), Desertification Research Centre (CIDE, UV-CSIC-GV), University of Valencia, Spain

P28 - First determination of Carbamazepine emerging pollutant and your metabolites in Anemonia sulcata and Actinia equina species by ultra-high-performance liquid chromatography Mass Spectrometer (UHPLC-HRMS) and a quadrupole-time-of-flight (QqTOF).
Dyana Vitale
Food and Environmental Safety Research Group (SAMA-UV), Desertification Research Centre (CIDE, UV-CSIC-GV), University of Valencia, Spain

P29 - Investigation of organic sulphur compounds in coal tar by using comprehensive two-dimensional gas chromatography-high resolution time-of-flight mass spectrometry
Ivan Aloisi
Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Messina, Italy

P30 - BIOACCESSIBILITY OF BISPHENOL S DURING THE IN VITRO GASTROINTESTINAL DIGESTION
Leticia Barbosa-Pereira
Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Pharmacy, University of Santiago de Compostela

P31 - BIOMONITORING OF PHARMACEUTICAL POLLUTION IN THE EBRO RIVER: COMPARING THEIR PREVALENCE AND LEVELS IN DIFFERENT FISH TISSUES
Jose M Castaño-Ortiz
Catalan Institute for Water Research (ICRA) / Universitat de Girona

P32 - Prioritization of pharmaceutical contaminants in the environment after evaluation of 10 years in-house monitoring data for analytical method upgrade
Marc Castaño-Trias
ICRA

P33 - DETERMINATION OF ORGANOPHOSPHORUS FLAME-RETARDANT IN A DUST SAMPLE BY ON LINE REVERSED PHASE LIQUID CHROMATOGRAPHY-GAS CHROMATOGRAPHY-MASS SPECTROMETRY USING THE THROUGH OVEN TRANSFER ADSORPTION DESORPTION (TOTAD) INTERFACE
Francisco José Espinosa Pérez
University of Castilla La Mancha
P34 - Determination of residues of pharmaceuticals in crayfish (Procambarus clarkii) by LC-ESI-QTOF-MS
Rut Fernandez Torres
Universidad de Sevilla

P35 - Sitagliptin and photo-transformation products in freshwater by LC-HRMS (Orbitrap)
Olga Gómez Navarro
IDAEA-CSIC, Barcelona, Spain

P36 - Demonstrating improvements in PFAS sensitivity using a microflow LC approach for the EPA 537 panel
Daniel McMillan
SCIEX, UK

P37 - Determination of glyphosate (GLY) and aminomethylphosphonic acid (AMPA) in water by liquid chromatography with tandem mass spectrometry (LC-MS/MS)
Phuong Bich Trinh
Institute for Advanced membrane Technologies (IAMT), Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

P38 - Analysis of Captan, Folpet and their derivatives in food with APCI-LCMS-8060
Uwe Oppermann
Shimadzu Europa GmbH, Duisburg, Germany

P39 - Quantification of Glyphosate, Glufosinate, and AMPA in Food via In-vial Addition of Pairing Agent
Uwe Oppermann
Shimadzu Europa GmbH, Duisburg, Germany

Poster discussion

11.00-11,30 INVITED LECTURE: Michel Nielen
WFSR, Wageningen University & Research, Wageningen, The Netherlands
Towards on-site food analysis by (trans)portable mass spectrometry

11,30-12,00 Victor Cutillas
European Union Reference Laboratory for Pesticide Residues in Fruit and Vegetables, AgrifoodCampus of International Excellence (CeiA3), Department of Chemistry and Physics, University of Almería, Almería, Spain
Advantages of supercritical fluid chromatography for the determination of pesticide residues in fruits and vegetables

12,00-12,30 INVITED LECTURE: Yolanda Picó
University of Valencia, Valencia, Spain
Different LC-MS approaches to study occurrence, uptake and distribution of emerging contaminants in plants

12,30-13,00 Peter Q. Tranchida
Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Messina, Italy
Analytical potential of comprehensive two-dimensional gas chromatography-high resolution time-of-flight mass spectrometry within the context of environmental and food analysis
13,00-13,30 INVITED LECTURE: Amadeo Rodríguez Fernández-Alba
University of Almeria, Almeria, Spain
*Overcoming typical problems of high resolution mass spectrometry with the new Q-Orbitrap platform*

13,30-14,00 Jaume C. Morales
Agilent Technologies Spain S.L.
*Comprehensive analytical LCMS methods for measuring emerging PFAS in the Environmental and Food*

14,00-14,20 Natalia Soares Quinete
Institute of Environment, Florida, USA
*Application of a chloroform-free lipid extraction method to Staghorn Coral (Acropora Cervicornis) Lipidomics assessments*

14,20-15,00 Brunch break

15,00-15,20 Michael McCullagh
Waters Corporation (Wilmslow UK)
*Making the Unknown Known and the Invisible Visible Using Ion Mobility*

15,20-15,40 Sandra Pérez
IDAESA-CSIC, Barcelona, Spain
*Differential uptake and metabolism of wastewater-borne drugs into lettuce studied by HR-MS*

15,40-16,10 Olaf Scheibner
Thermo Fisher Scientific, Dreieich, Germany
*Analysis of perfluorinated surfactants in Environmental Matrices*

16,10-16,30 Maria José Farré
ICRA, Girona, Spain
*Impact of disinfection on dissolved organic matter fingerprint identified by high resolution mass spectrometry*

16,30-17,00 Neil Loftus
Shimadzu Corporation, Manchester, UK
*Increasing the impact of targeted and suspect screening workflows in food safety by HRMS*

17,00-17,20 Bozo Zonja
Swedish University of Agricultural Sciences, Uppsala, Sweden
*Strategies for Detection and Identification of Transformation Products of Contaminants in Aquatic Environment using High Resolution MS*

17,20 -18,20 ORAL SESSION 3

17,20 Frank Menger
SLU, Uppsal, Sweden
*Pesticide transformation products in surface water: A suspect screening approach for a better understanding*

17,40 Cristina Postigo
IDAESA-CSIC, Barcelona, Spain
*Non-target HRMS approaches to characterize complex disinfection byproduct mixtures*
18,00 Laura Martín-Pozo  
Research Group of Analytical Chemistry and Life Sciences, Department of Analytical Chemistry, University of Granada, Granada, Spain  
*Multiclass method for the determination of endocrine disrupting chemicals in human nails prior to ultra-high performance liquid chromatography–tandem mass spectrometry*

18,20 Andrzej Wnorowski  
*Invitation to LCMSMS 2021 Ottawa, Canada, October 14-15, 2021*

18,25 Closing Ceremony & Elsevier poster awards

**ROOM B**

**17.20 -18.20 ORAL SESSION 4**

17,20 Montserrat Sole  
ICM-CSIC  
*Biomarker responses and metabolite identification in Lumbricus terrestris exposed to drugs of environmental concern, an in vivo and in vitro approach*

17,40 Josep Sanchis  
ICRA, Girona, Spain  
*Characterization of dissolved organic matter by HRMS: Effects of water chlorination on molecular fingerprints and generation of disinfection by-products*

18,00 Ana Belén Martínez Piernas  
University of Almería  
*Identification of transformation products of pharmaceuticals in real-field agricultural environments irrigated with reclaimed water by retrospective analysis by LC-QTOF-MS/MS*