



**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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Thursday, October 15, 2020

ROOM A

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 OCURRENCE IN RADISHES IRRIGATED WITH RECLAIMED WASTEWATER BY LC-SWATH-HRMS ANALYSIS

Francesc labad

IDAEA-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 Núñez

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 Núñez

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 GCxGC-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 leave 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

18,30 Fadi Moussa

Faculty of Bioscience and Technology for Food, Agriculture and Environment, University of Teramo, Italy

LC-MS/MS Method for the Detection of Hormones: Development, Validation, and Application in Various Bovine Matrices

18,50 Julian Campo

Centro de Investigaciones sobre Desertificación-CIDE

Comparison and validation of three multi-residue methods in mussels

19,10 Maria Murcia-Morales

University of Almería, Department of Physics and Chemistry, Almería, Spain

APIStrip: environmental monitoring through honeybees based on a new passive sampler

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

Lilianna 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 Almería, Department of Physics and Chemistry, Almería, 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

Idea-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

Letricia 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

IDAEA-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, Uppsala, Sweden

Pesticide transformation products in surface water: A suspect screening approach for a better understanding

17,40 Cristina Postigo

IDAEA-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 metabolites 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

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