

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



**MONDAY, 2<sup>nd</sup> July 2012**

**8.45 – 9.15 Registration**

**9.15 – 9.30 Welcome and Introduction**

**David Serrat**, President of the Science and Technology Section, Institut d'Estudis Catalans, Barcelona, Spain

**Damià Barceló**, IDAEA-CSIC, Barcelona and ICRA, Girona, Spain

**Session 1: Analytical challenges and new trend in LC-MS-MS**

*Chair: Damià Barceló*

**9.30 – 10.00** Novel micro and nano bioaffinity mass spectrometry tools for the detection of emerging contaminants in food and environment

**Michel W.F. Nielen**, RIKILT-Institute of Food Safety and Wageningen University, Wageningen, The Netherlands

**10.00 – 10.30** Harnessing the potential of ion-mobility mass spectrometry for the development and characterization of a multi-residue method for the determination of veterinary antibiotics in crude extracts

**Sandra Rontree**, Waters Corporation, Manchester, UK

**10.30 – 11.30 Poster session/Coffee break**

*Chair: Sandra Rontree*

**11.30 – 12.00** Reference Materials for Environmental and Food Analyses – LC/MS/MS in Their Development and Use

**Stephen A. Wise**, National Institute of Standards and Technology (NIST), Gaithersburg, USA

**12.00 – 12.30** Strategies for the Effective Integration of Reference Data and Reference Materials for MS Applications in Health and Environment

**Carlos Gonzalez**, National Institute of Standards and Technology (NIST), Gaithersburg, USA

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



**12.30 – 13.00** Doping for sensitivity: evaluation of atmospheric pressure photoionization (APPI) for the detection of wastewater related chemicals in aqueous samples

**Piero R. Gardinali**, Florida International University, Miami, Florida, USA.

**13.00 – 13.30** Analytical challenges in high performance liquid chromatography tandem mass spectrometry for accurate determination of primary and secondary phthalate metabolites in real samples

**Maria Jose Gonzalez**, General Organic Chemistry Institute (CSIC), Madrid, Spain

**13.30 – 15.30 Lunch**

**Session 2: Target analysis, non-target analysis, screening**

*Chair: Diana Aga*

**15.30 – 16.00** Enantiomeric profiling of chiral drugs in the environment with the usage of Chiral-LCMS/MS

**Barbara Kasprzyk-Hordern**, Department of Chemistry, University of Bath, UK

**16.00 – 16.30** From target to non-target screening of micropollutants in the aquatic environment by HPLC combined with high resolution mass spectrometry

**Juliane Hollender**, EAWAG, Dübendorf, Switzerland

**16.30 – 17.00** Significance of “known unknowns” analysis in water treatment

**Jelena Radjenovic**, The Advanced Water Management Centre (AWMC), Brisbane, Australia

**17.00 – 17.40 Poster session/Coffee break**

*Chair: Frank L. Dorman*

**17.40 – 18.00** Liquid chromatography coupled to tandem mass spectrometry: triple quadrupole (QqQ) or quadrupole-time of flight (QTOF) detection for environmental applications?

**Margoum Christelle**, Irstea, Saint Quentin, France

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



- 18.00 – 18.20** Determination of endocrine disruptors and related compounds in river sediments by Turbulent-Flow Chromatography-LC-MS/MS  
**Marina Gorga**, IDAEA-CSIC, Barcelona, Spain
- 18.20 – 18.40** Determination of pharmaceuticals in fish: method optimization and occurrence in different species from Mediterranean rivers  
**Belinda Huerta**, ICRA, Girona, Spain
- 18.40 – 19.00** Development of analytical method based on ultra performance liquid chromatography (UPLC) tandem QTRAP mass spectrometry for determination of antihelmintic drugs in surface waters  
**Mirta Zrnčić**, FKIT, University of Zagreb, Croatia

**TUESDAY, 3<sup>rd</sup> July 2012**

**Session 3: Applications in environmental analysis**

*Chair: Amadeo Rodríguez Fernández-Alba*

- 9.00 – 9.30** Occurrence and Fate of Pharmaceuticals and Personal Care Products in Municipal Wastewater Treatment Systems  
**Mehran Alaee**, National Water Research Institute, Burlington, Canada
- 9.30 – 10.00** Solid-phase extraction - UHPLC-MS-MS for the analysis of polar organic persistent pollutants in coastal and marine waters for the implementation of the European Water Framework and Marine Strategy Framework Directives,  
**Robert Loos**, European Commission - DG Joint Research Centre (JRC) Institute for Environment and Sustainability (IES), ISPRA, Italy
- 10.00 – 10.30** Investigation of pharmaceutical metabolites/transformation products in urban waste- water by LC-QTOF MS  
**Juan Vicente Sancho Llopis**, University Jaume I, Castellón, Spain

**10.30 – 11.30** **Poster session/Coffee break**

*Chair: Mira Petrovic*

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



- 11.30 – 12.00** Identification of Pharmaceutical By-products After Advanced Oxidation and Biofiltration of Wastewater  
**Diana S. Aga**, Chemistry Department, University at Buffalo, Buffalo, NY, USA
- 12.00 – 12.30** Identifying the photoproducts of (demethyl)sildenafil: electrospray-high resolution MS/MS alone is not enough  
**Sandra Perez**, IDAEA-CSIC, Barcelona, Spain
- 12.30 – 12.50** HILIC in service of low detection limits for X-ray contrast media  
**Bozo Zonja**, IDAEA-CSIC, Barcelona, Spain
- 12.50 – 13.10** Comprehensive bioaffinity mass spectrometry approach for thyroid transporter agonists  
**Payam Aqai**, RIKILT- Institute of Food Safety, Wageningen, The Netherlands
- 13.10 – 15.00** **Lunch**
- Chair: Mehran Alaee*
- 15.00 – 15.30** Perfluorinated compounds determination by quadrupole time of flight mass time-of-spectrometry in environmental and food matrices  
**Yolanda Picó**, Faculty of Pharmacy, University of Valencia, Spain
- 15.30 – 16.00** On-line SPE optimisation for the analysis of perfluorocarboxylic and perfluorosulfonic acids in surface and drinking waters by LC/MS/MS  
**Stefano Polesello**, Water Research Institute CNR-IRSA, Brugherio (MB), Italy
- 16.00 – 16.20** Analysis of perfluoroalkyl substances in waters from Germany and Spain  
**Marta Llorca**, IDAEA-CSIC, Barcelona, Spain
- 16.20 – 16.40** Distribution of fluoroalkyl substances on human body  
**Francisca Pérez**, IDAEA-CSIC, Barcelona, Spain
- 16.40 – 17.00** Simultaneous determination of HBCD isomers and TBBPA in biota  
**Guillaume ten Dam**, RIKILT – Institute of Food Safety, Wageningen, The Netherlands

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



**17.00 – 17.40 Poster session/Coffee break**

*Chair: Marinella Farré*

**17.40 – 18.00** Exact mass measurement at high resolution for identification, quantification and confirmation of poly(amidoamine) dendrimers (pamam) by LC-ESI-TRIPLE-TOF mass spectrometer

**Maria Malgorzata Ulaszewska**, IMDEA-Agua (Instituto Madrileño De Estudios Avanzados- Agua), Alcalá de Henares, Madrid, Spain

**18.00 – 18.20** Analysis of volatile dimethylsiloxanes in wastewater, surface water, river sediment and biota samples

**Josep Sanchís**, IDAEA-CSIC, Barcelona, Catalonia, Spain

**18.20 – 19.00** Micro pollutants as chemical markers for environmental forensics applications: Differentiating sewage and manure

**Cecilia Fenech**, School of Biotechnology, Dublin City University, Dublin, Ireland,

**21.00 Joint dinner**

**WEDNESDAY, 3<sup>rd</sup> July 2012**

**Session 4: Applications in food analysis and forensics**

*Chair: Yolanda Picó*

**9.00 – 9.30** Benefits and pitfalls in the evaluation of pesticide residues in food by LC-QTOF-MS

**Amadeo Rodríguez Fernández-Alba**, University of Almeria, Almeria, Spain

**9.30 – 10.00** Challenges in the Analysis of Residues from Packaging Materials in Food

**Maria Teresa Galceran**, University of Barcelona, Barcelona, Spain

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



**10.00 – 10.30** New Ultra Performance Convergence Chromatography UPC2 combined with Analytical SFE for Food Safety  
**Helene Boiteux**, Waters Corporation, St-Quentin, France

**10.30 – 11.30** **Poster session/Coffee break**

*Chair:*

**11.30 – 12.00** Utilizing Serially-Coupled HPLC Columns and Elevated Temperature to Increase the Separation Efficiency of Cacao Metabolites  
**Frank L. Dorman**, The Pennsylvania State University and Restek Corporation, USA

**12.00 – 12.20**

**12.20 – 12.40** Utilizing QTOF Screening for Pesticide Residue Analysis  
**Antonietta Gledhill**, Waters Corporation, Manchester, UK

**12.40 - 13.10** Chromatographic Analysis of Synthetic Amphetamine Street Samples  
**Amanda Leffler**, The Pennsylvania State University, USA

**13.10 – 13.30** Discussion + student awards

**13.30** End of workshop

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



**Posters**

**Environmental**

- 1. Nanomaterials in the environment: Analysis of fullerenes in environmental matrixes and assessment of their acute toxicity effects in environmentally relevant conditions. Evidences of Trojan Horse Effect.**

Josep Sanchís<sup>1</sup>, Naiara Berrojalbiz<sup>1</sup>, Gemma Caballero<sup>1</sup>, Jordi Dachs<sup>1</sup>,  
Naif Abdullah Al-Harbi<sup>3</sup>, Marinella Farré<sup>1</sup>, Damià Barceló<sup>1,2,3</sup>

<sup>1</sup> Department of Environmental Chemistry, IDAEA-CSIC, Barcelona, Catalonia, Spain

<sup>2</sup> Catalan Institute for Water Research (ICRA), Girona, Catalonia, Spain

<sup>3</sup> King Saud University, P.O. Box 2455, 11451, Riyadh, Saudi Arabia

- 2. Multi-component quantitative analysis of pharmaceuticals and personal care products in the environment by LC-MS/MS with fast polarity switching**

<sup>1</sup>Natsuyo Asano; <sup>1</sup>Kiyomi Arakawa; <sup>1</sup>Shinjiro Fujita; <sup>1</sup>Kazuo Mukaibatake; <sup>1</sup>Ichiro Hirano; <sup>2</sup>Yuka Fujito

<sup>1</sup>Shimadzu Corporation: 1, Nishinokyo-Kuwabaracho Nakagyo-ku, Kyoto 604-8511, Japan

<sup>2</sup>Shimadzu Analytical and Measuring Center Inc.: 1, Shimoaicho Nishinokyo Nakagyo-ku, Kyoto 604-8436, Japan

- 3. Application of mass spectrometry techniques for the determination of organic contaminants on food-processing industry effluents**

M.M Gómez-Ramos, M. Mezcuca, C. Ferrer, S. Uclés, A.R. Fernandez-Alba, A. Agüera

Pesticide Residue Research Group, University of Almería, Spain

- 4. Simultaneous quantitative/qualitative screening of PPCPs in river water by LC-QTOF-MS and direct sample injection**

Sonia Herrera<sup>1</sup>, Maria M. Ulaszewska<sup>1</sup>, M<sup>a</sup>Jesús Martínez Bueno<sup>1,2</sup>, Amadeo R. Fernández-Alba<sup>1,2</sup>

<sup>1</sup> Fundación IMDEA-Agua, C/ Punto Net 4, 2<sup>a</sup> planta, Edificio ZYE, Parque Científico Tecnológico de la Universidad de Alcalá. 28805, Alcalá de Henares. Madrid (Spain)

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



<sup>2</sup> Pesticide Residues Research Group, Department of Hydrogeology and Analytical Chemistry, University of Almería, 04120 La Cañada de San Urbano, Almería (Spain)

**5. Towards more accurate environmental measurements. A case study on LC-MS<sup>2</sup> pesticides quantification in water**

Lardy-Fontan S., Le Diouron V., Lalere B., Vaslin-Reimann S.

**Laboratoire National De Metrologie D'essais Lne, 1 Rue Gaston Boissier, 75724 Paris Cedex 15, France**

**6. Analysis of trace level phthalate esters in environmental water samples by using online-SPE-LC coupled to a high speed triple quadrupole mass spectrometer**

<sup>1</sup>Ichiro Hirano, <sup>1</sup> Tairo Ogura, <sup>2</sup>Yuka Fujito

<sup>1</sup>Shimadzu Corporation: 1, Nishinokyo-Kuwabaracho Nakagyo-ku, Kyoto 604-8511, Japan

<sup>2</sup>Shimadzu Analytical and Measuring Center Inc.: 1, Shimoaicho Nishinokyo Nakagyo-ku, Kyoto 604-8436, Japan

**7. Characterization and estimation of sulfaquinoxaline metabolites in residue analysis using liquid chromatography coupled to tandem mass spectrometry**

Rodrigo Barcellos Hoff\*<sup>1,2</sup>, Fabiano Barreto<sup>1</sup>, Jéssica Melo<sup>1</sup>, Louise Jank<sup>1</sup>, Maria do Carmo Ruaro Peralba<sup>2</sup>, Tânia Mara Pizzolato<sup>2</sup>

1 - Laboratório Nacional Agropecuário do Rio Grande do Sul (LANAGRO/RS), Porto Alegre, RS, Brazil.

2 Instituto de Química - Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil.

**8. Antibiotics degradation by photolytic process in different water matrices**

Carla Sirtori<sup>a,b</sup>, Louise Jank<sup>a</sup>, Flávia Justina Costa<sup>a</sup>, Tânia Mara Pizzolato<sup>a</sup>  
a Instituto de Química, Universidade Federal do Rio Grande do Sul (UFRGS), Av. Bento Gonçalves, 9500, Porto Alegre - RS, Brasil;

b Universidade Federal da Integração Latino-Americana (UNILA), Av. Tancredo Neves, 6731 - Bloco 4, Caixa Postal 2044 - CEP 85867-970, Foz do Iguaçu - PR, Brasil.

**9. Multiresidue trace determination of UV-absorbing compounds in fish using HPLC-(ESI)-QqLIT-MS<sup>2</sup>**

Pablo Gago-Ferrero<sup>1\*</sup>, M.Silvia Díaz-Cruz<sup>1</sup>, Damià Barceló<sup>1,2</sup>.



8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



<sup>1</sup>Dept. Environmental Chemistry, IDAEA-CSIC, Jordi Girona 18-26, E-08034 Barcelona, Spain.

<sup>2</sup>Catalan Institute for Water Research (ICRA), Emili Grahit 101, Edifici H2O, Parc Científic i Tecnològic de la Universitat de Girona, 17003 Girona, Spain

**10. Hospital effluents as source of pharmaceuticals: characterization and contribution of four different hospitals**

L.H.M.L.M. Santos<sup>1\*</sup>, M. Gros<sup>2</sup>, S. Rodriguez-Mozaz<sup>2</sup>, D. Barceló<sup>2,3</sup>, C. Delerue-Matos<sup>4</sup>, A. Pena<sup>5</sup>, M.C.S.M.B. Montenegro<sup>1</sup>

<sup>1</sup>REQUIMTE, Departamento de Ciências Químicas, Faculdade de Farmácia da Universidade do Porto, Rua de Jorge de Viterbo, n.º 228, 4050-313 Porto, Portugal

<sup>2</sup>Catalan Institute for Water Research (ICRA), C/Emili Grahit 101, 17003 Girona, Spain

<sup>3</sup>IDAEA-CSIC: Department of Environmental Chemistry, IDAEA-CSIC, C/ Jordi Girona 18-26, 08034 Barcelona, Spain

<sup>4</sup>REQUIMTE, Instituto Superior de Engenharia do Porto, Rua Dr. António Bernardino de Almeida 431, 4200-072 Porto, Portugal

<sup>5</sup>Group of Health Surveillance, Center of Pharmaceutical Studies, University of Coimbra, Health Sciences Campus, Azinhaga de Santa Comba, 3000-548 Coimbra, Portugal

11. Selective pressurized liquid extraction and liquid chromatography tandem mass spectrometry for the analysis of alkylphenols and bisphenol a in mussels  
N. Salgueiro-González, M. I. Turnes-Carou, S. Muniategui-Lorenzo, P. López-Mahía, D. Prada-Rodríguez. Department of Analytical Chemistry. University of A Coruña. Campus da Zapateira. E-15071 A Coruña, Spain

**12. Direct injection with triple quadrupole LC/MS system: rapid method for the analysis of PFOS and PFOA in water**

Laura Díaz Esplá, , Lorena Sanjuan Tortosa, Julio Llorca Pórcel  
LABAQUA S.A. c/ del Dracma, Parcelas 16-18 03114-Alicante, Spain

**13. Study of Diclofenac metabolic biotransformation pathways to its nitrified microbial metabolites and development of an LC-MS/MS method for their determination in wastewater.**

Victoria Osorio<sup>1</sup>, Marta Imbert-Bouchard<sup>1</sup>, Asunción Navarro<sup>1</sup>, Jose Luis Abad<sup>2</sup>, Antoni Ginebreda<sup>2</sup>, Sandra Pérez<sup>1</sup>, Damià Barceló<sup>1,3</sup>

<sup>1</sup> IDAEA-CSIC, Department of Environmental Chemistry, Jordi Girona 18-26,

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



Barcelona (Spain),

<sup>2</sup> RUBAM-IIQAC-CSIC Department of Biomedical Chemistry, Jordi Girona 18-26, Barcelona (Spain),

<sup>3</sup> Catalan Institute for Water Research (ICRA), Parc Científic i Tecnològic de la Universitat de Girona, Edifici Jaume Casademont, Porta A, Planta 1, Despatx 13C/ Pic de Peguera, 15E-17003 Girona, Spain

**14. Novel amide polar-embedded reversed-phase column for the fast liquid chromatography-tandem mass spectrometry determination of polyether ionophores in sewage and river waters**

Pol Herrero, Francesc Borrull, Rosa M<sup>a</sup> Marcé and Eva Pocurull

Department of Analytical Chemistry and Organic Chemistry, Faculty of Chemistry, Universitat Rovira i Virgili, C/ Marcel·lí Domingo s/n, 43007, Tarragona, Catalonia, Spain

**15. Residues and organic contaminants in agricultural soils in intensive agricultural areas from Spain: a three years survey**

Lucía Alcarraz Farall<sup>1,2</sup>, Juan Antonio Padilla-Sánchez<sup>2</sup>, Roberto Romero-González<sup>2</sup>, Patricia Plaza-Bolaños<sup>2,3</sup>, José Luis Martínez Vidal<sup>2</sup>, Antonia Garrido Frenich<sup>2</sup>

<sup>1</sup>Tecnological Laboratory of Uruguay (LATU), Avenida Italia 6201, 11500. Montevideo (Uruguay)

<sup>2</sup>Research Group "Analytical Chemistry of Contaminants", Department of Hydrogeology and Analytical Chemistry, Research Centre for Agricultural and Food Biotechnology (BITAL), University of Almería, Agrifood Campus of International Excellence, ceiA3, Carretera de Sacramento s/n, E-04120, Almería (Spain)

<sup>3</sup>Department of Analytical Chemistry, University of Granada, E-18071, Granada (Spain)

**16. Screening and quantifying anti-cancer drugs and metabolites in hospital's wastewaters and rivers by online SPE – LC-MS/MS.**

Mikaël Levi<sup>2</sup>, Claude Villard<sup>1</sup>, Thérèse Schembri<sup>1</sup>, Marcus Mreyen<sup>4</sup>, Anja Grüning<sup>4</sup>, Stéphane Moreau<sup>2</sup>, Pierre Boissery<sup>3</sup>, Daniel Lafitte<sup>2</sup>

<sup>1</sup>Aix Marseille Université, Inserm UMR 911 CRO2 faculté de pharmacie 27 bd jean moulin 13385 Marseille, France.

<sup>2</sup> SHIMADZU France SAS, Le Lizard 2, Boulevard Salvador Allende, 77448 Marne la Vallée Cedex 2, France.

<sup>3</sup> Agence de l'Eau Rhône Méditerranée & Corse, délégation de Marseille, 62 immeuble Le Noaille, 13001 Marseille, France.

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



4 SHIMADZU Europa GmbH, Albert-Hahn-Str. 6-10, D-47269 Duisburg, Germany.

**17. Simultaneous determination of ten different pharmaceuticals and three sulfonamide metabolites by high performance liquid chromatography -tandem mass spectrometry**

Martina Periša, Sandra Babić

Department of Analytical Chemistry, Faculty of Chemical Engineering and Technology, Marulićev trg 19, 10000 Zagreb, Croatia

**18. Enantiomeric profiling of chiral drugs from environmental solid matrices with the use of microwave assisted extraction and chiral LC-MSMS**

Sian Evans, Paul Davies, Anneke T. Lubben and Barbara Kasprzyk-Hordern

University of Bath, Department of Chemistry, Faculty of Science, Bath, BA2 7AY, UK

**19. Trametes versicolor degrades the antiepileptic carbamazepine: Identification of intermediates formed in an air pulsed fluidized bed bioreactor**

Aleksandra Jelic<sup>a</sup>, Carles Cruz-Morato<sup>b</sup>, Ernest Marco-Urrea<sup>b</sup>, Monserrat Sarrà<sup>b</sup>, Sandra Perez<sup>a</sup>, Teresa Vicent<sup>b</sup>, Mira Petrovic<sup>c, d</sup>, Damia Barcelo<sup>a, d</sup>

<sup>a</sup> Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research (IDAEA), Spanish Council for Scientific Research (CSIC), 08034 Barcelona, Spain

<sup>b</sup> Departament d'Enginyeria Química, Universitat Autònoma de Barcelona (UAB), Bellaterra, Spain

<sup>c</sup> Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

<sup>d</sup> Catalan Institute for Water Research (ICRA), H2O Building, Scientific and Technological Park of the University of Girona, Girona, Spain

**20. Rapid screening and confirmation of emerging contaminants in UK river waters by UHPLC-IT-TOF**

David R. Baker<sup>1</sup>, John Bagnall<sup>2</sup>, Alan J. Barnes<sup>1</sup>, Barbara Kasprzyk-Hordern<sup>2</sup>, Neil J. Loftus<sup>1</sup>

<sup>1</sup>Shimadzu, Manchester, UK; <sup>2</sup>University of Bath, Bath, UK

**21. Liquid chromatography-tandem mass spectrometry to determine sweeteners in wastewater and surface water**

P. Arbeláez, F. Borrull, E. Pocurull, R. M. Marcé

Department of Analytical Chemistry and Organic Chemistry, Universitat Rovira i

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



Virgili, Marcel·lí Domingo s/n 43007 Tarragona, Spain

**22. LC-MS-MS to determine phosphodiesterase type V inhibitors, analogues and their metabolites in different water matrices**

Jaume Aceña<sup>1</sup>, Bianca Ferreira da Silva<sup>2</sup>, J.L. Abad<sup>3</sup>, Sandra Pérez<sup>1</sup>, Damià Barceló<sup>1,4</sup>

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

<sup>2</sup> Laboratório de Biogeoquímica Ambiental, Department of Chemistry, UFSCar, Rod. Wash. Luís km235, São Carlos, SP, Brazil

<sup>3</sup> IQAC-CSIC, Jordi Girona 18-26, Barcelona (Spain),

<sup>4</sup> Catalan Institute for Water Research- ICRA, C/Emili Grahit, 101, Edifici H2O, Parc Científic i Tecnològic de la Universitat de Girona, E-17003 Girona, Spain

**23. Simultaneous Quantitative Analysis of Pesticides Including Phenoxy-Acids in Surface Water using UPLC-MS/MS with direct injection**

Gerard Bondoux, Waters Corporation,

**24. Determination of wetland pollutants by liquid chromatography-tandem mass spectrometry**

Pablo Vazquez-Roig<sup>1</sup>, Cristina Blasco<sup>1</sup>, Vicente Andreu<sup>2</sup>, Yolanda Picó<sup>1</sup>

<sup>1</sup> Grupo de Investigación en Seguridad Alimentaria y Medioambiental (SAMA-UV), Facultat de Farmàcia, Universitat de València, Av, Vicent Andrés s/n, 46100 Burjassot, València, España.

<sup>2</sup>

**25. Levels of perfluorinated contaminants in breast milk of the Valencian community by liquid chromatography-tandem mass spectrometry**

C. Blasco<sup>1\*</sup>, Y. Picó<sup>1</sup>, A. Masiá<sup>1</sup>, M. Farré<sup>2</sup>, D. Barceló<sup>2</sup>

<sup>1</sup> Grupo de Investigación en Seguridad Alimentaria y Medioambiental (SAMA-UV), Facultat de Farmàcia, Universitat de València, Av, Vicent Andrés s/n, 46100 Burjassot, València, España.

<sup>2</sup> Department of Environmental Chemistry, IDAEA-CSIC, C/Jordi Girona 18-26, Barcelona, España

**26. Outcompeting GC for the detection of legacy chlorinated pesticides: online-SPE UPLC APCI/MSMS detection of endosulfans at part per trillion levels.**

Natalia Quinete<sup>1</sup> and Piero Gardinali<sup>1,2</sup>

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



<sup>1</sup>Southeast Environmental Research Center (SERC) and <sup>2</sup>Department of Chemistry and Biochemistry, Florida International University, 3000 NE 151 Street, Biscayne Bay Campus, North Miami, Florida, 33181 USA.

**27. Development of a liquid/electrospray chemical ionization tandem mass spectrometry analytical method for analysis of eleven hydroxylated polybrominated diphenyl ethers.**

Maria Luisa Feo<sup>1</sup>, Enrique Baron<sup>1</sup>, Diana S. Aga<sup>2</sup>, Ethel Eljarrat<sup>1</sup>, Damià Barcelò<sup>1,3</sup>.

<sup>1</sup> IDEA CSIC, Analytical Chemistry Department, Jordi Girona 18-26, 08034 Barcelona, Spain.

<sup>2</sup>Department of Chemistry, University at Buffalo, State University of New York, Buffalo, New York 14260.

<sup>3</sup> Catalan Institute for Water Research (ICRA), Parc Científic i Tecnològic de la Universitat de Girona, Pic de Peguera 15, 17003 Girona, Spain

**28. The stereo-selective biodegradation of amphetamine and methamphetamine in river water using chiral-LC-(QTOF)MS**

John Bagnall, Louis Malia, Anneke Lubben and Barbara Kasprzyk-Hordern  
University of Bath, Department of Chemistry, Faculty of Science, Bath, BA2 7AY, UK

**29. Analysis of Synthetic Cannabinoids using GC-MS and LC-MS/MS**

Sharyn E. Miller, The Pennsylvania State University

**30. Selection of a Column and Optimization of a method for the Analysis of Antidepressants in Aqueous Samples using Liquid Chromatography-Tandem Mass Spectrometry**

Kenton Chodara, The Pennsylvania State University

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



**Food and forensics**

**31. Rapid method for the detection of metabolite of nerve agents in urine by liquid chromatography–negative electrospray-tandem mass spectrometry**

Arkady Braun<sup>1</sup>, Igor Rodin<sup>1</sup>, Oleg Shpigun<sup>1</sup>, Andrey Stavriani<sup>1</sup>, Igor Rybalchenko<sup>2</sup>

1. Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia.

2. Lumex Ltd, Moscow, Russia

**32. Quick target scan of LC screening method for pesticides analysis in fruits and vegetables**

Samanta Uclés, Ana Uclés, Carmen Ferrer, Ana Agüera, Amadeo R. Fernández-Alba

Pesticide Residue Research Group, Dpt. of Hydrogeology and Analytical Chemistry  
University of Almería, Ctra. Sacramento s/n, 04120 Almería, Spain

**33. Analysis of poly(amidoamine) dendrimers (PAMAM) in biological samples by LC-QLIT-MS/MS**

Ana Uclés<sup>1,2</sup>, M<sup>a</sup>Jesús Martínez Bueno<sup>1,2</sup>, María Dolores Hernando<sup>3</sup>, Amadeo R. Fernández-Alba<sup>1,2</sup>

<sup>1</sup>Fundación IMDEA-Agua, C/ Punto Net 4, 2<sup>a</sup> planta, Edificio ZYE, Parque Científico Tecnológico de la Universidad de Alcalá. 28805, Alcalá de Henares. Madrid (Spain)

<sup>2</sup>Pesticide Residues Research Group, Department of Hydrogeology and Analytical Chemistry, University of Almería, 04120 La Cañada de San Urbano, Almería (Spain)

<sup>3</sup>Spanish National Institute for Agriculture and Food Research and Technology, INIA, Ctra. de la Coruña, km. 7,5 28040 Madrid (Spain)

**34. Rapid and Highly Sensitive Quantitative Analysis and Screening of Aflatoxins in Foods Using Liquid Chromatography Triple Quadrupole Mass Spectrometry**

<sup>1</sup>Manami Kobayashi; <sup>1</sup>Satoshi Yamaki; <sup>1</sup>Ayako Nomura; <sup>1</sup>Kyoko Watanabe;

<sup>1</sup>Yoshihiro Hayakawa; <sup>1</sup>Tsutomu Nishine; <sup>2</sup>Yuka Fujito

<sup>1</sup>Shimadzu Corporation: 1, Nishinokyo-Kuwabaracho Nakagyo-ku, Kyoto 604–8511, Japan

<sup>2</sup>Shimadzu Analytical and Measuring Center Inc.: 1, Shimoaicho Nishinokyo Nakagyo-ku, Kyoto 604-8436, Japan

**35. Identification of amoxicillin, ceftiofur and cephalixin metabolites and transformation products in chicken muscle by LC-ESI-QTOF-MS/MS**

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



P. Gómez-Rodríguez, M.P. Hermo, J.Barbosa, D. Barrón  
University of Barcelona, Faculty of Chemistry, Department of Analytical Chemistry,  
Diagonal 645, E- 08028 Barcelona (Spain)

- 36. Standard-free qualitative analysis of ginsenosides in plants by HPLC-MS/MS**  
Stavrianidi Andrey, Rodin Igor, Braun Arkady, Shpigun Oleg.  
Chemistry Department, Lomonosov Moscow State University, Moscow, Russia
- 37. Simultaneous HPLC-MS/MS determination of salidroside, rosarin and rosavin in the extracts from Rhodiola rosea**  
Rodin Igor, Stavrianidi Andrey, Braun Arkady, Shpigun Oleg  
Chemistry Department, Lomonosov Moscow State University, Moscow, Russia
- 38. LC-MS/MS method for simultaneous determination of anaplerotic dysfunction, methylmalonic acidemia and endothelial dysfunction metabolic markers in human plasma**  
A. Stavrianidi<sup>1</sup>, A. Braun<sup>1</sup>, I. Ananieva<sup>1</sup>, I. Rodin<sup>1</sup>, O. Shpigun<sup>1</sup>, A. Zhloba<sup>2</sup>  
1. Chemistry Department, Lomonosov Moscow State University, Moscow, Russia  
2. St.-Petersburg State I.P. Pavlov Medical University, Petersburg, Russia
- 39. Exploring the application of a universal method for pesticide screening in foods using a high data acquisition speed MS/MS**  
Ichiro Hirano, <sup>1</sup>Yusuke Inohana, <sup>1</sup>Kiyomi Arakawa, <sup>2</sup>Yuka Fujito  
<sup>1</sup>Shimadzu Corporation: 1, Nishinokyo-Kuwabaracho Nakagyo-ku, Kyoto 604–8511, Japan  
<sup>2</sup>Shimadzu Analytical and Measuring Center Inc.: 1, Shimoaicho Nishinokyo Nakagyo-ku, Kyoto 604-8436, Japan
- 40. Multi-class pesticides residues analysis in challenging vegetable matrices by using fast MRM with 15 msec polarity switching**  
<sup>1</sup>Ichiro Hirano, <sup>1</sup>Kiyomi Arakawa, <sup>1</sup>Yusuke Inohana, <sup>2</sup>Yuka Fujito  
<sup>1</sup>Shimadzu Corporation: 1, Nishinokyo-Kuwabaracho Nakagyo-ku, Kyoto 604–8511, Japan  
<sup>2</sup>Shimadzu Analytical and Measuring Center Inc.: 1, Shimoaicho Nishinokyo Nakagyo-ku, Kyoto 604-8436, Japan
- 41. High Throughput Quantitative Analysis of Multi-mycotoxin in Beers using UHPLC-MS/MS**  
Masayoshi Tamura <sup>1</sup>; Keiko Matsumoto <sup>2</sup>; Jun Watanabe <sup>2</sup>; Junko Iida <sup>2</sup>; Yuka Fujito<sup>3</sup>;  
Yasushi Nagatomi <sup>1</sup>; Naoki Mochizuki <sup>1</sup>;

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



1. Asahi Group Holdings, Limited, 1-1-21 Midori, Moriya, Ibaraki 302-0106, Japan
2. Shimadzu Corporation. 1, Nishinokyo-Kuwabaracho Nakagyo-ku, Kyoto 604-8511, Japan
3. Shimadzu Analytical & Measuring Center Inc. , 1, Shimoaicho Nishinokyo Nakagyo-ku, Kyoto 604-8436, Japan

**42. Simultaneous identification, confirmation and quantification of pesticides and veterinary drug residues in meat matrices applying a high resolution mass database**

María Luz Gómez-Pérez<sup>1</sup>, Patricia Plaza-Bolaños<sup>1,2</sup>, Roberto Romero-González<sup>1</sup>, José Luis Martínez Vidal<sup>1</sup>, Antonia Garrido French<sup>1</sup>

<sup>1</sup>Research Group "Analytical Chemistry of Contaminants", Department of Hydrogeology and Analytical Chemistry, Research Centre for Agricultural and Food Biotechnology (BITAL), University of Almeria, Agrifood Campus of International Excellence, ceiA3, Carretera de Sacramento s/n, E-04120, Almeria (Spain)

<sup>2</sup>Department of Analytical Chemistry, University of Granada, E-18071, Granada (Spain)

**43. Occurrence of cloxacillin and ampicillin in cow milk after the end of the withdrawal period of dry cow intramammary antibiotics**

Erja Lindfors<sup>1</sup>, Katariina Pekkanen<sup>2</sup>, Kaija-Leena Saraste<sup>3</sup>

Finnish Food Safety Authority Evira, <sup>1</sup>Chemistry and Toxicology Research Unit,

<sup>2</sup>Food and Feed Microbiology Research Unit. <sup>3</sup>Food Hygiene Unit. Mustialankatu 3, FI-00790, Helsinki, Finland

**44. Multi-residue quantitation of veterinary drugs in animal tissue using an optimised solid phase extraction protocol.**

<sup>1</sup>Alan J. Barnes, <sup>3</sup>Yuka Fujito, <sup>2</sup>Ichiro Hirano, <sup>1</sup>Neil J. Loftus

<sup>1</sup>Shimadzu Corporation, MS-BU Overseas, Manchester, United Kingdom;

<sup>2</sup>Shimadzu Corporation: 1, Nishinokyo-Kuwabaracho Nakagyo-ku, Kyoto 604-8511, Japan; <sup>3</sup>Shimadzu Analytical and Measuring Center Inc.: 1, Shimoaicho Nishinokyo Nakagyo-ku, Kyoto 604-8436, Japan

**45. Multiclass method for determination of 27 pesticides in food and soil samples by LC-MS/MS**

Virgínia C. Fernandes <sup>(1,2)\*</sup>, Steven Lehotay <sup>(3)</sup>, L. Geis-Asteggianti <sup>(3)</sup>, V.F. Domingues <sup>(1)</sup>, N. Mateus <sup>(2)</sup> and C. Delerue-Matos <sup>(1)</sup>

<sup>(1)</sup> REQUIMTE – Instituto Superior de Engenharia, Instituto Politécnico do Porto, Portugal

<sup>(2)</sup> CIQ – Centro de Investigação em Química, Universidade do Porto, Portugal



8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



<sup>(3)</sup> Eastern Regional Research Center, Agricultural Research Service, U.S.  
Department of Agriculture, Wyndmoor, PA. USA

- 46. The use of Microflow UHPLC as a way to solvent usage in pesticide screening of food samples by LC-MS/MS**  
Stephen Lock and Pam Stoddart  
AB SCIEX, Warrington, Cheshire, UK
- 47. The use of large volume injection as a way to reduce sample preparation in pesticide screening of drinking water and other beverages by LC-MS/MS**  
Stephen Lock and Pam Stoddart  
AB SCIEX, Warrington, Cheshire, UK
- 48. New approaches for Screening and Quantitation of Mycotoxins in different baby food Matrices**  
Stephen Lock, Jianru Stahl-Zeng and Kristin von Czapiewski,  
AB SCIEX, Pheonix House, Centre Park, Warrington, UK
- 49. Can LC/MS/MS be used as a routine tool for Allergens analysis including the detection of Mustard?**  
Stephen Lock  
AB SCIEX, Warrington, Cheshire, UK
- 50. Comprehensive Analysis of the B-Vitamin Complex in Food and Beverages by LC-MS/MS**  
**Stephen Lock**  
AB SCIEX, Pheonix House, Centre Park, Warrington, UK
- 51. Extraction of fluoroquinolones fom eggs using molecularly imprinted polymers**  
Cristina Blasco and Yolanda Picó, University of Valencia, Spain
- 52. Determination of plasma metabolites of thyme bioactive compounds by improved liquid chromatography coupled to tandem mass spectrometry**  
Alba Macià, Laura Rubió, Aida Serra, Maria-Paz Romero, Maria-José Motilva  
Food Technology Department, Escola Tècnica d'Enginyeria Superior Agrària, Universitat de Lleida. Av. Alcalde Rovira Roure, 191. 25198 Lleida. Spain.
- 53. Pesticide and veterinary drugs residue analysis in goat milk**

8th ANNUAL

**LC/MS/MS WORKSHOP ON ENVIRONMENTAL APPLICATIONS AND FOOD  
SAFETY**

2-4 July 2012, Barcelona, Spain



**Waters**  
THE SCIENCE OF WHAT'S POSSIBLE.™



Porto Filho JM<sup>1</sup>; Costa RG<sup>1</sup>; Cunha NA<sup>2</sup>; Silva MCC<sup>2</sup>; Silva HCM<sup>2</sup>; Albuquerque Junior EC<sup>2</sup>, Silva M<sup>2</sup>; Telles DL<sup>2</sup>, Araújo ACP<sup>2</sup>

<sup>1</sup>Federal University of Paraíba - UFPB, Areia CCA Zootecnic Doctorate Program. Areia-PB-BRAZIL.

<sup>2</sup>Pesticide Residue Laboratory - LabTox/ITEP, Av. Prof. Luis Freire 700. 50740-540. Recife-PE-BRAZIL. eden@itep.br