

Italian Chemical Society
Division of Mass Spectrometry

*12th European Fourier
Transform Mass
Spectrometry Workshop*

MATERA (Italy)

April 5 – 8, 2016



*12th European Fourier Transform
Mass Spectrometry Workshop*

SCIENTIFIC PROGRAMME

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Organised by



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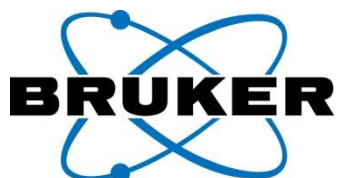
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Julia Chamot-Rooke Institut Pasteur, Paris, France
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SCIENTIFIC PROGRAMME

Tuesday, April 5	
1:00 p.m. – 2:15 p.m.	Registration and poster installation
2:15 p.m.– 2:45 p.m.	Welcome and opening ceremony
	Session 1: FT instrumentation
	Chairpersons: Peter B. O'Connor, Julia Chamot-Rooke
2:45 p.m. – 3:15 p.m.	<p>PL1: 21 Tesla Fourier transform ion cyclotron resonance mass spectrometry: instrumentation and applications <i>Alan G. Marshall, John P. Quinn, Lissa C. Anderson, Nathan K. Kaiser, Donald F. Smith, Greg T. Blakney, Tong Chen, Steven C. Beu, Christopher L. Hendrickson</i> National High Magnetic Field Laboratory and Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida, USA</p>
3:15 p.m. – 3:45 p.m.	<p>PL2: Orbitrap mass spectrometry: new frontiers <i>Alexander Makarov</i> Thermo Fisher Scientific, Bremen, Germany</p>
3:45 p.m. – 4:15 p.m.	<p>PL3: Towards the era of phase-centric FTMS <i>Yury O. Tsybin, Konstantin O. Nagornov, Anton N. Kozhinov</i> Ecole Polytechnique Fédérale de Lausanne, Biomolecular Mass Spectrometry Laboratory, Lausanne, Switzerland</p>
4:15 p.m. – 5:00 p.m.	Coffee break and poster session
5:00 p.m. – 5:30 p.m.	<p>PL4: Ion clouds micromotion in FT ICR mass-spectrometer in ultrahigh resolution mode of operation <i>Eugene Nikolaev, Gleb Vladimirov, Oleg Kharybin, Pavel Chuvakhov, Goekhan Baykut, Roland Jertz</i> Institute for Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russia</p>
5:30 p.m. – 5:45 p.m.	<p>OR1: Enabling routine isotopic fine structure analysis <i>Roland Jertz, Claudia Kriete, Matthias Witt, Jochen Friedrich, Christopher Thompson, Michael Easterling, Eugene Nikolaev, Goekhan Baykut</i> Bruker Daltonik GmbH, Bremen, Germany</p>
5:45 p.m.	End of session
7:00 p.m.	Welcome cocktail with guided tour of Sassi di Matera

Wednesday, April 6

8:30 a.m. – 9:00 a.m.	Registration
	Session 2: Two-dimensional mass spectrometry
	Chairpersons: Yury O. Tsybin, Filomena Lelario
9:00 a.m. – 9:30 a.m.	<p>PL5: Using 2-dimensional mass spectrometry (2DMS) for proteomics <i>Maria van Agthoven, Pui Yiu Lam, Chris Wootton, Federico Floris, Alice Lynch, Marc-André Delsuc, Peter B. O'Connor</i> Department of Chemistry, University of Warwick, Coventry, UK</p>
9:30 a.m.– 9:45 a.m.	<p>OR2: Principles, details, and pitfalls of the implementation of 2D FT-ICR MS Spectroscopy <i>Lionel Chiron, Christian Rolando, Marc-André Delsuc</i> I.G.B.M.C. Université de Strasbourg, Illkirch, France</p>
9:45 a.m. – 10:00 a.m.	<p>OR3: Getting the best performance out of 2-D FTICRMS <i>Maria A. van Agthoven, Federico Floris, Alice Lynch, Christopher Wootton, Lionel Chiron, Mark Barrow, Marc-André Delsuc, Christian Rolando, Peter B. O'Connor</i> Department of Chemistry, University of Warwick, Coventry, UK</p>
10:00 a.m.– 10:15 a.m.	<p>OR4: Bidimensional FT-ICR MS using non uniform sampling (NUS): a fully data independent acquisition (DIA) for complex mixture analysis at high resolution on both precursor and fragment ions <i>Fabrice Bray, Lionel Chiron, Matthias Witt, Marc-André Delsuc, Christian Rolando</i> Chemistry Department, Université Lille 1, Villeneuve d'Ascq, France</p>
10:15 a.m. – 11:00 a.m.	Coffee break and poster session
	Session 3: Ion activation & dissociation
	Chairperson: Evan Williams
11:00 a.m. – 11:30 a.m.	<p>PL6: Fourier Transform ion cyclotron resonance and infrared multiphoton dissociation (IRMPD) mass spectrometry for structural characterization of bioactive molecules <i>Giuliana Bianco</i> Dipartimento di Scienze, Università degli Studi della Basilicata, Potenza, Italy</p>

11:30 a.m. – 11:45 a.m.	<p>OR5: A Comparative study of electron ionization dissociation and ultraviolet photodissociation for characterizing native proteins and protein complexes <i>Huilin Li, Yuewei Sheng, Jennifer S. Brodbelt, Joseph A. Loo</i> Department of Biological Chemistry, University of California, Los Angeles, USA</p>
11:45 a.m. – 12:00 p.m.	<p>OR6: Electron capture dissociation and ion mobility mass spectrometry of biologically relevant phosphopeptides <i>Andrea F. Lopez-Clavijo, Carlos A. Duque-Daza, Andrew J. Creese, Peter Winn, Helen J. Cooper</i> College of Life & Environmental Sciences, The University of Birmingham, Edgbaston, UK</p>
	Session 4: Nucleic acids & informatics
	Chairperson: Alessandro Buchicchio
12:00 p.m. – 12:30 p.m.	<p>PL7: Dissociation of ribonucleic acids (RNA) and RNA-peptide complexes by FT-ICR MS <i>Heidelinde Glasner, Eva-Maria Schneeberger, Jovana Vusurovic, Kathrin Breuker</i> Institute of Organic Chemistry, University of Innsbruck, Innsbruck, Austria</p>
12:30 p.m. – 12:45 p.m.	<p>OR7: ΦSDM (Phased Spectrum Deconvolution Method) – a super-resolution algorithm for Fourier transform mass spectrometry <i>Konstantin Aizikov, Dmitry Grinfeld, Arne Kreuzman, Eugen Damoc, Alexander Makarov</i> Thermo Fisher Scientific, Bremen, Germany</p>
12:45 p.m. – 1:00 p.m.	<p>OR8: Sequence Protein IDentification by Randomized sequence Transcriptomic-database and Mass Spectrometry (SPIDER-TMS): a transcriptomic-proteomic integrated software for rapid identification of proteins by FTMS <i>Giuliana Bianco, Renzo Calace Sarli, Gabriele Cruciani, Patrizia Falabella, Gerarda Grossi, Raffaella Pascale</i> Dipartimento di Scienze, Università degli Studi della Basilicata, Potenza, Italy</p>
1:00 p.m. – 2:30 p.m.	Lunch

Session 5: Proteomics & Glycans	
	Chairpersons: Joseph A. Loo, Donatella Caruso
2:30 p.m. – 3:00 p.m.	<p>PL8: Orbitrap FTMS - challenges and opportunities in proteomics <i>Roman Zubarev</i> Department of Medicinal Biochemistry and Biophysics, Karolinska Institutet, Stockholm, Sweden</p>
3:00 p.m. – 3:15 p.m.	<p>OR9: Improving the sensitivity of proteome analyses using high resolution FTMS by iterative exclusion of identified peptides <i>Simion Kreimer, <u>Lev Levitsky</u>, William F. Danielson, Mikhail E. Belov, Barry L. Karger, Mikhail V. Gorshkov, Alexander R. Ivanov</i> Moscow Institute of Physics and Technology State University, Dolgoprudny, Moscow Region, Russia</p>
3:15 p.m. – 3:45 p.m.	<p>PL9: Innovations in the FTMS analysis of glycans and glycoconjugates <i>Yi Pu, Liang Han, Deborah Leon, Edwin Motari, John Haserick, Andrea Carpentieri, Giulia Bandini, Rebecca Glaskin, Kshitij Khatri, Yiqun Huang, Joseph Zaia, Phillips W. Robbins, John Samuelson, Cheng Lin, <u>Catherine E. Costello</u></i> Center for Biomedical Mass Spectrometry, Boston University School of Medicine, Boston, USA</p>
3:45 p.m. – 4:00 p.m.	<p>OR10: The molecular clock of islet amyloid polypeptide: from dimerization to deamidation <i><u>Yuko P.Y. Lam</u>, Christopher A. Wootton, Juan Wei, Mark Barrow, Peter B. O'Connor</i> Department of Chemistry, University of Warwick, Coventry, UK</p>
4:00 p.m. – 4:30 p.m.	<p>PL10: FTMS approaches for rapid sequencing of glycosaminoglycans <i>I. Jonathan Amster</i> Department of Chemistry, University of Georgia, Athens, USA</p>
4:30 p.m. – 5:00 p.m.	Coffee break and poster session

	Session 6: Top down proteomics & microbiology
	Chairperson: Roman Zubarev
5:00 p.m. – 5:30 p.m.	PL11: Top-down proteomics: the next step in clinical microbiology? <i>Julia Chamot-Rooke</i> Structural Mass Spectrometry and Proteomics Unit, Institut Pasteur, Paris, France
5:30 p.m. – 5:45 p.m.	OR11: Typing <i>Pseudomonas aeruginosa</i> strains using ultrahigh resolution MALDI-FTICR MS <i>Frank Fleurbaaij, Margriet E.M. Kraakman, Eric C. J. Claas, Wilco C. Knetsch, Hans C. van Leeuwen, Yuri E.M. van der Burgt, Karin Ellen Veldkamp, Margreet C. Vos, Wil Goessens, Bart J. Mertens, Ed J. Kuijper, Paul J. Hensbergen, Simone Nicolardi</i> Leiden University Medical Center, Leiden, The Netherlands
5:45 p.m. – 6:00 p.m.	OR12: A combined approach of top-down FT-ICR and native mass spectrometry to investigate the molecular details of oncogenic p53 reactivation <i>Sam Hughes, Jenna Scotcher, C. Logan Mackay, Pat. R. Langridge-Smith, Ted Hupp, David J. Clarke</i> School of Chemistry, University of Edinburgh, UK
6:00 p.m.	End of session

Thursday, April 7

Session 7: HRMS in characterizing food	
Chairpersons: Tommaso R. I. Cataldi, Laura Scranò	
9:00 a.m. – 9:30 a.m.	<p>PL12: FT-ICR-MS for the metabolomic profiling of wines and champagnes <i>C. Roullier-Gall, S. Heinzmann, M. Witting, F. Moritz, P. Jeandet, D. Steyer, M. Gonsior, R. Gougeon, <u>Philippe Schmitt-Kopplin</u></i> Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum Muenchen, Neuherberg, Germany</p>
9:30 a.m. – 9:45 a.m.	<p>OR13: Characterization of native and oxidized fatty acids in mussels by liquid chromatography-electrospray ionization-Fourier transform mass spectrometry <i><u>Ilario Losito</u>, Laura Facchini, Alessandra Valentini, Tommaso R.I. Cataldi, Francesco Palmisano</i> Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Bari, Italy</p>
9:45 a.m. – 10:00 a.m.	<p>OR14: Foodomics: Fourier transform mass spectrometry based characterization of <i>sparus aurata</i> phospholipidome <i><u>Sara Granafei</u>, Pietro Azzone, Ilario Losito, Francesco Palmisano, Tommaso R.I. Cataldi</i> Dipartimento di Chimica & Centro SMART, Università degli Studi di Bari Aldo Moro, Italy</p>
10:00 a.m. – 10:45 a.m.	Coffee break and poster session
Session 8: Residues in food	
Chairperson: Sabino A. Bufo	
10:45 a.m. – 11:15 a.m.	<p>PL13: Liquid chromatography coupled to high resolution mass spectrometry within pesticide residue control in food <i>Amadeo R. Fernández-Alba</i> European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables. University of Almería, Almería, Spain</p>

11:15 a.m. – 11:30 a.m.	<p>OR15: <i>Advances in Orbitrap™ based analytical methods for food allergen management</i> <i>Rosa Pilolli, Elisabetta De Angelis, Linda Monaci</i> Institute of Sciences of Food Production, National Research Council, ISPA-CNR, Bari, Italy</p>
11:30 a.m. – 11:45 a.m.	<p>OR16: <i>Target analysis and retrospective screening of fusarium mycotoxins and their modified forms in cereals and derived products by liquid chromatography – high resolution mass spectrometry</i> <i>Biancamaria Ciasca, Michelangelo Pascale, Valerio Guido Altieri, Francesco Longobardi, Michele Suman, Veronica M.T. Lattanzio</i> Institute of Sciences of Food Production, National Research Council, ISPA-CNR, Bari, Italy</p>
	<p>Session 9: Top-down MS of proteins and their complexes</p>
	<p>Chairperson: Michael Przybylski</p>
11:45 a.m. – 12 :15 p.m.	<p>PL14: <i>Top-Down mass spectrometry of proteins and protein complexes</i> <i>Joseph A. Loo</i> Department of Biological Chemistry, David Geffen School of Medicine at UCLA, University of California Los Angeles, USA</p>
12:15 p.m. – 12: 30 p.m.	<p>OR17: <i>Top-down analysis of calmodulin using 2D FT-ICR MS</i> <i>Federico Floris, Maria van Agthoven, Lionel Chiron, Christopher Wootton, Mark Barrow, Marc-André Delsuc, Peter B. O'Connor</i> Department of Chemistry, University of Warwick, Coventry, UK</p>
12:30 p.m. – 2:00 p.m.	<p>Lunch</p>
	<p>Session 10: Ultra high resolution MS, biomolecular recognition, MS imaging</p>
	<p>Chairpersons: Kathrin Breuker, Patrizia Falabella</p>
2:00 p.m.– 2:30 p.m.	<p>PL15: <i>Using ultra-high resolution mass spectrometry to find what lies beneath the surface</i> <i>Ljiljana Paša-Tolić, Jared Shaw, Nikola Tolić, Malak Tfaily, Lawrence Walker, Rosalie Chu, Yufeng Shen, Errol Robinson, David Koppelaar, Nancy J Hess</i> Environmental Molecular Sciences Laboratory (EMSL),</p>

	Pacific Northwest National Laboratory (PNNL), Richland, USA
2:30 p.m. – 3:00 p.m.	<p>PL16: Combining bioaffinity tools with high resolution mass spectrometry: new perspectives for biomedical and biomolecular recognition analysis <i>Michael Przybylski, Loredana Lupu, Hendrik Rusche, Zdenek Kukacka, Yannick Baschung, Stefan Slamnoiu, Adrian Moise, Mary Murphy, Jeff Bornheim</i> Steinbeis Center for Biopolymer Analysis & Biomedical Mass Spectrometry and University of Konstanz, Department of Chemistry, Konstanz, Germany</p>
3:00 p.m. – 3:15 p.m.	<p>OR18: Structural characterization of individual compound in complex mixtures by FTICR MS combined with in ESI-source H/D exchange <i>Alexey Kononikhin, Yury Kostyukevich, Alexander Zherebker, Igor Popov, Oleg Kharybin, Irina Perminova, Eugene Nikolaev</i> Moscow Institute of Physics and Technology, Moscow, Russia</p>
3:15 p.m.– 3:45 p.m.	<p>PL17: High resolution MSI: increased information content and specificity <i>Liam A. McDonnell</i> Fondazione Pisana per la Scienza ONLUS and Leiden University Medical Center, Pisa, Italy</p>
3:45 p.m.– 4:00 p.m.	<p>OR19: Dissociation behavior of a bifunctional TEMPO-benzyl active ester for peptide structure analysis by free radical initiated peptide sequencing (FRIPS) mass spectrometry <i>Christoph Hage, Christian Ihling, Mathias Schäfer, Andrea Sinz</i> Department of Pharmaceutical Chemistry & Bioanalytics, Martin Luther University Halle-Wittenberg, Halle/Saale, Germany</p>
4:00 p.m.– 11:00 p.m.	Excursion: discover the magnificence of Taranto and Gala Dinner

Friday, April 8

	Session 11: Nanodrops, sources, clusters
	Chairperson: Ilario Losito
9:15 a.m. – 9:45 a.m.	<p>PL18: The chemistry of ions in aqueous nanodrops <i>Evan R. Williams</i> Department of Chemistry, University of California, Berkeley, California, USA</p>
9:45 a.m. – 10:00 a.m.	<p>OR20: Supercharging of analytes via a novel modified ion source <i>Christopher A. Wootton, Haytham E. M. Hussein, Mang ying Wong, Cookson K. C. Chiu, Lewis A. Baker, Scott Habershon, Anthony J. Stace, Mark P. Barrow, Peter B. O'Connor</i> Department of Chemistry, University of Warwick, Coventry, UK</p>
10:00 a.m. – 10:15 a.m.	<p>OR21: Tandem Cryo Trap FT-MS for kinetics and spectroscopy of transition metal clusters <i>Jennifer Mohrbach, Sebastian Dillinger, Gereon Niedner-Schatteburg</i> Fachbereich Chemie and Forschungszentrum OPTIMAS, TU Kaiserslautern, Germany</p>
10:15 a.m. – 10:45 a.m.	Coffee break
	Session 12: Petroleomics, bio-oil, hydrocarbons
	Chairperson: Alan G. Marshall
10:45 a.m. – 11:15 a.m.	<p>PL19: High performance analysis of complex mixtures by high-field FT-Orbitrap MS: exploring the carbon space <i>Wolfgang Schrader, Alessandro Vetere</i> Max-Planck Institut für Kohlenforschung, Mülheim an der Ruhr, Germany</p>
11:15 a.m. – 11:30 a.m.	<p>OR22: Advanced automated processing of data from gas chromatography/ultrahigh-resolution mass spectrometry for petroleum analyses <i>Christopher P. Rüger, Theo Schwemer, Martin Sklorz, Peter B. O'Connor, Mark P. Barrow, Ralf Zimmermann</i> Institute for Chemistry, University of Rostock, Rostock, Germany</p>

11:30 a.m. – 11:45 a.m.	OR23: Development of a robust methodology for the characterization of biomass pyrolysis bio-oil by electrospray ionization <i>Jasmine Hertzog, Vincent Carré, Anthony Dufour, Frédéric Aubriet</i> Lorraine University, LCP-A2MC, METZ, France
11:45 a.m. – 12:00 p.m.	OR24: Understanding tridimensional structural changes of hydrocarbon during oxygenation in the ocean using SA-TIMS-FT-ICR MS <i>Paolo Benigni, Rebecca Marin, Kathia Sandoval, Christopher Thompson, Mark E. Ridgeway, Melvin A. Park, Piero Gardinali, Francisco Fernandez-Lima</i> Florida International University, Miami, USA
12:00 p.m.	Closing remarks and farewell

LIST OF POSTER COMMUNICATIONS

- P1 CHARACTERIZATION OF A QUADRUPOLEAR-DETECTION NADEL ICR CELL FOR FT-ICR MS AT THE CYCLOTRON FREQUENCY**
Konstantin O. Nagornov, Anton N. Kozhinov, Christophe Masselon, Yury O. Tsybin
Spectroswiss Sàrl, Lausanne – Switzerland
- P2 STATIC HARMONIZATION OF DYNAMICALLY HARMONIZED FT ICR CELL. HIGH ORDER CONTRIBUTIONS TO THE ELECTRIC FIELD**
Ekaterina Zhdanova, Yury Kostyukevich, Eugene Nikolaev
Institute for Energy Problems of Chemical Physics Russian Academy of Sciences Leninskij, Moscow - Moscow Institute of Physics and Technology, Dolgoprudnyi, Russia
- P3 AGC TARGET-DEPENDENT EFFECTS IN LTQ-FT SIGNAL ACQUISITION AND CONSEQUENCES ON DATA QUALITY**
Konstantin Nagornov, Anton Kozhinov, Yury O. Tsybin, Christophe Masselo
Laboratoire de Biologie à Grande Echelle - CEA Grenoble, INSERM U0138, Université Grenoble Alpes, Grenoble- France
- P4 ADVANCED DATA ACQUISITION ELECTRONICS FOR FTMS**
Anton N. Kozhinov, Konstantin O. Nagornov, Kristina Srzentić, Yury O. Tsybin
Spectroswiss Inc, Lausanne, Switzerland
- P5 LEAST-SQUARES FITTING FOR FTMS APPLICATIONS**
Yury O. Tsybin, Anton N. Kozhinov, Konstantin O. Nagornov
Spectroswiss Sarl, Lausanne – Switzerland
- P6 TIME-DEPENDENT FREQUENCY OF ION MOTION, TRANSIENT MODULATION, AND SPECTRAL COMPOSITION IN FT-ICR MS**
Oleg Tsybin, Konstantin Nagornov, Anton Kozhinov, Yury Tsybin
Peter the Great St. Petersburg Polytechnic University, Saint-Petersburg - Russia

- P7 **STATIC HARMONIZATION OF DYNAMICALLY HARMONIZED FT ICR CELL. HIGH ORDER CONTRIBUTIONS TO THE ELECTRIC FIELD****
Ekaterina Zhdanova, Yury Kostyukevich, Eugene Nikolaev
Institute for Energy Problems of Chemical Physics Russian Academy of Sciences Leninskij Moscow - Russia Moscow Institute of Physics and Technology, Dolgoprudnyi, Russia
- P8 **IDENTIFICATION OF N-TERMINAL ENDOGENEOUS FRAGMENTS OF TAU PROTEIN IN HUMAN CEREBROSPINAL FLUID BY ONLINE NANOFLOW LC-ESI-Q/ORBITRAP MS****
Gunnar Brinkmalm, Claudia Cicognola, Erik Portelius, Henrik Zetterberg, Kaj Blennow, Kina Höglund
Department of Psychiatry and Neurochemistry, Sahlgrenska Academy at University of Gothenburg, Mölndal, Sweden
- P9 **TARGETING CANCER-RELATED PROTEOFORMS UNCOVERED WITH PROTEOGENOMICS****
Marialaura Dilillo, Avinash Yadav, Erik de Graaf, Paolo Aretini, Liam McDonnell
Fondazione Pisana per la Scienza – ONLUS, Dipartimento di Chimica e Chimica Industriale – Università di Pisa
- P10 **PROTEOMIC APPROACHES FOR A DIAGNOSIS OF PARASITIC CONGENITAL INFECTIONS****
A. Alexandra Emmanuel, Chiara Giangrande, Florence Migot-Nabias, Joëlle Vinh
UMR216 – IRD/UPD - MERIT « Mère et enfant face aux infections tropicales », USR3149 – SMBP « Spectrométrie de Masse Biologique et Protéomique », ESPCI ParisTech
- P11 **IDENTIFICATION OF TWO SERINE PROTEASES FROM LEPTOMASTIX DACTYLOPII VENOM BY DIRECT INFUSION (+)-ESI-FTICR-MS****
Giuliana Bianco, Patrizia Falabella, Gerarda Grossi, Cristiana Labella, Simona Laurino, Raffaella Pascale, Philippe Schmitt-Kopplin, Heiko Vogel
University of Basilicata, Potenza, Italy

P12 DE NOVO SEQUENCING OF PEPTIDES DERIVED FROM SCORPION VENOM

Meng Li, Yuko P. Y. Lam, Christopher A. Wootton, Peng Chen, Mark P. Barrow, Hongzheng Fu, Peter B. O'Connor
University of Warwick, Coventry, United Kingdom

P13 CYSTEINE OXIDATION PROBED BY IRMPD SPECTROSCOPY OF KEY INTERMEDIATES

Debora Scuderi, Enrico Bodo, Barbara Chiavarino, Simonetta Fornarini, Maria Elisa Crestoni
Dipartimento di Chimica e Tecnologie del Farmaco, Università degli Studi di Roma La Sapienza, Roma, Italy

P14 FTMS AS A TOOL TO DEVELOP A CLINICAL ASSAY FOR MEASURING CEREBROSPINAL FLUID LEVELS OF PRE-SYNAPTIC PROTEINS

Ann Brinkmalm, Gunnar Brinkmalm, Henrik Zetterberg, Kaj Blennow, Annika Öhrfelt
Institute of neuroscience and physiology, Sahlgrenska Academy, University of Gothenburg

P15 SUPERMETALLIZATION OF PEPTIDES AND PROTEINS STUDIED BY FTICR MS COUPLED WITH ECD AND CID

Yury Kostyukevich, Alexey Kononikhin, Maria Indeykina, Igor Popov, Eugene Nikolaev
Moscow Institute of Physics and Technology, Moscow - Skolkovo Institute of Science and Technology, Skolkovo, Russia

P16 HIGH-RESOLUTION ORBITRAP™-BASED MASS SPECTROMETRY FOR RAPID DETECTION OF PEANUTS IN NUTS

Elisabetta De Angelis, Simona L. Bavaro, Rosa Pilolli, Linda Monaci
Institute of Sciences of Food Production, National Research Council (ISPA-CNR)

P17 ASPECTS OF METABOLIC PROFILING AND QUALITY CONTROL OF OLIVE OIL USING FT-ICR MS DIRECT INFUSION METHOD

Theodwra Nikou, Matthias Witt, Maria Laloti, Panagiotis Stathopoulos, Aiko Barsch, Leandros A Skaltsounis, Maria Halabalaki
Bruker Daltonik GmbH, Bremen, Germany

P18 FEASIBILITY STUDY OF INCLUSION OF MIXTURES OF PESTICIDES IN WHITE WINE MATRIX

Francesca Mottola, Paolo Fanizzi, Cosimo Mario Stefanelli, Veronica M.T. Lattanzio, Biancamaria Ciasca, Angelo Visconti
Lab.Instruments S.r.l., Castellana Grotte (BA), Italy

P19 CHARACTERIZATION OF NON-INTENTIONALLY ADDED SUBSTANCES (NIAS) AND ZINC OXIDE NANOPARTICLE RELEASE FROM NEW ANTIMICROBIAL FOOD PACKAGING MATERIALS BY BOTH LIQUID AND GAS CHROMATOGRAPHY HYPHENATED TO TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF-MS AND GC-QTOF-MS) AND INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY (ICP-MS)

M.J. Martínez-Bueno, S. Cimmino, C. Silvestre, A.I. García, J.L. Tadeo, A. R. Fernández-Alba, M.D. Hernando
University of Almería, Department of Physical and Chemistry & European Reference Laboratory for Pesticide Residue in Fruits and Vegetables, Almería, Spain

P20 MULTICLASS SCREENING METHOD TO DETECT 64 ANTIBIOTICS IN FEED BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY COUPLED TO HYBRID HIGH RESOLUTION MASS SPECTROMETRY

Rosanna Rossi, Simone Moretti, Sara Romanelli, Giorgio Saluti, Roberta Galarini
Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche

P21 MULTICLASS DETECTION OF ANABOLIC AGENTS IN BOVINE BILE BY LC-HR-MS/MS

Simone Moretti, Sara Romanelli, Rosanna Rossi, Giorgio Saluti, Roberta Galarini
Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche

P22 FOLLOW-UP OF INCLUSION STUDIES OF XENOBIOTICS IN WHITE WINE MATRIX BY THE AID OF GC-APPI-HRMS, LOW AND HIGH RESOLUTION MS ANALYTICAL TECHNIQUES

Francesca Mottola, Paolo Fanizzi, Cosimo Mario Stefanelli, Veronica M.T. Lattanzio, Biancamaria Ciasca, Angelo Visconti, Helmut Münster
Lab.Instruments S.r.l., Castellana Grotte (BA), Italy

- P23 APPLICATION OF LC-FTICR MS AND TANDEM MS PERFORMED BY IRMPD AND CID FOR THE IDENTIFICATION OF MAIN INTERMEDIATES AND DEGRADATION PATHWAY OF MEPANIPYRIM UNDER DIFFERENT ADVANCED OXIDATION PROCESSES (AOPs)**

F. Lelario, M. Brienza, S.A. Bufo., L. Scranò

Department of Science (DiS) and Department of European Cultures (DICEM), University of Basilicata, Potenza, Italy

- P24 A NEW PROTOCOL FOR TRACING SEDIMENT PORE WATER DISSOLVED ORGANIC MATTER DURING ANAEROBIC RESPIRATION**

Juliana Valle, Michael Gonsior, Mourad Harir, Philippe Schmitt-Kopplin, Norbert Hertkorn, David Bastviken, Ralf Conrad, Alex Enrich-Prast

Helmholtz Zentrum Munich, German Research Center for Environmental Health, Neuherberg, Germany

- P25 POTENTIAL OF DIRECT ANALYSIS IN REAL TIME-HIGH RESOLUTION MASS SPECTROMETRY FOR UNTARGETED INVESTIGATION OF ATMOSPHERIC PARTICULATE MATTER**

Maxime Bridoux, Roland Sarda-Estève, Dominique Baisnée, Sébastien Schramm

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- P27 LASER DESORPTION/IONIZATION FOURIER TRANSFORM ION CYCLOTRON RESONANCE MASS SPECTROMETRY, A POWERFUL TOOL TO INVESTIGATE INORGANIC SYSTEMS**

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- P28 OPTIMIZATION OF THE ACQUISITION PARAMETERS FOR A Q-EXACTIVE HIGH RESOLUTION MASS SPECTROMETER COUPLED TO AN ULTRA HIGH PERFORMANCE LIQUID CHROMATOGRAPHY SYSTEM TO CHARACTERIZE COMPLEX PHYTOCHEMICAL MIXTURES**
Giorgia La Barbera, Annalaura Capriotti, Chiara Cavaliere, Susy Piovesana, Valentina Trionfera, Riccardo Zenezini Chiozzi, Aldo Laganà
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Vincent Carre, Loïc Becker, Gregory Hamm, Patrick Chaimbault
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P35 STUDYING THE INTERACTIONS AND THE BINDING SITES OF AN ORGANO-OSMIUM (II) ANTICANCER COMPLEX TO BIOMOLECULES USING ULTRA-HIGH RESOLUTION FT-ICR TANDEM MASS SPECTROMETRY

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P36 DETERMINATION OF TERNARY CRUDE OIL MIXTURES BY FOURIER TRANSFORM ION CYCLOTRON RESONANCE MASS SPECTROMETRY AND STATISTICAL METHODS

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P37 THIN-LAYER CHROMATOGRAPHY OF CRUDE OIL: DIRECT ANALYSIS OF COMPOUND CLASSES BY LASER DESORPTION/IONIZATION FOURIER TRANSFORM ION CYCLOTRON RESONANCE MASS SPECTROMETRY

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