



# XXII International Mass Spectrometry Conference

Florence (Italy) - August 26-31, 2018



# CONFERENCE PROGRAM



## SCIENTIFIC PROGRAM

Fundamental Mass Spectrometry	Instrumentation and Methods	Food & Beverage	Organic and inorganic MS: challenges & applications	Life sciences
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### SATURDAY, August 25<sup>th</sup>, 2018

2:00 ÷ 6:00 p.m.	<b>Short Courses</b> <i>Venue: University of Florence, Via Gino Capponi, 9 - Florence</i>	
	1. <b>Fundamentals of Mass Spectrometry</b>	<i>Room 4</i>
	2. <b>Foodomics &amp; Mass Spectrometry</b>	<i>Room 9</i>
	3. <b>Mass Spectrometry Imaging</b>	<i>Room 5</i>
	4. <b>Expanded Newborn Screening by Tandem Mass Spectrometry</b>	<i>Room 3</i>
	5. <b>SPME: Comprehensive Overview of the Technology &amp; Applications to Analytical MS</b>	<i>Room 7</i>

### SUNDAY, August 26<sup>th</sup>, 2018

9:00 a.m. ÷ 1:00 p.m.	<b>Short Courses</b> <i>Venue: University of Florence, Via Gino Capponi, 9 - Florence</i>	
	1. <b>Fundamentals of Mass Spectrometry</b>	<i>Room 4</i>
	2. <b>Foodomics &amp; Mass Spectrometry</b>	<i>Room 9</i>
	3. <b>Mass Spectrometry Imaging</b>	<i>Room 5</i>
	4. <b>Expanded Newborn Screening by Tandem Mass Spectrometry</b>	<i>Room 3</i>
	5. <b>SPME: Comprehensive Overview of the Technology &amp; Applications to Analytical MS</b>	<i>Room 7</i>
5:00 p.m.	<b>IMSC 2018 Opening Ceremony</b> Gianluca Giorgi, Catherine Costello, Rector University of Florence  <b>IMSC 2018 Youth Ceremony</b> <ul style="list-style-type: none"> <li>Nico Nibbering Travel Awards</li> <li>Italian Chem. Soc., Division of Mass Spectrometry Award and fellowships</li> </ul>	<i>Plenary room</i>  <i>Level 0</i>
6:00 p.m.	<b>PL01: Plenary Lecture</b>  <b>At the intersection between chemistry and art: scientific research for the study and preservation of cultural heritage</b>  <i>Marco Leona</i> Department of Scientific Research, The Metropolitan Museum of Art, New York, USA	<i>Plenary room</i>  <i>Level 0</i>
7:00 p.m.	<b>Welcome Exhibition &amp; Mixer</b>	<i>Exhibition room</i>  <i>Level 0</i>

Sat./Sunday

MONDAY, August 27<sup>th</sup>, 2018

8:30-9:15 a.m.	<p><b>PL02: Plenary Lecture</b> <span style="float: right;"><i>Chair: Ron M. A. Heeren</i></span></p> <p><b>Advances in MALDI imaging mass spectrometry: molecular microscopy in the new age of biology and medicine</b></p> <p><i>Richard Caprioli</i> Depts. of Biochemistry, Chemistry, Pharmacology and Medicine Vanderbilt University School of Medicine, Nashville, USA</p>	<p><b>Plenary room</b> <b>Level 0</b></p>
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	<p><b>MOr.01 - Nucleic acids</b></p> <p><i>Chairs: Daniele Fabris, Giuliana Bianco</i></p>	<p><b>Plenary room</b> <b>Level 0</b></p>
9:30-10:10 a.m.	<p><b>Structures, energetics and reactivity of nucleic acids and their molecular building blocks via tandem MS and computations approaches</b></p> <p><u>M. T. Rodgers</u> Wayne State University, Detroit, USA</p>	
10:10-10:30 a.m.	<p><b>Tandem mass spectrometric sequencing of isomeric methyl nucleosides on RNA toward the understanding of epitranscriptome</b></p> <p><u>H. Nakayama</u>, Y. Yamauchi, T. Isobe, M. Taoka RIKEN Center for Sustainable Resource Science, Wako, Japan</p>	
10:30-10:50 a.m.	<p><b>TEAD1: Yin and Yang of the cell regulation</b></p> <p><u>P. Novak</u>, R. Liskova, L. Slavata, J. Cerny, K. Valis Institute of Microbiology, Laboratory of Structural Biology, Prague, Czech Republic</p>	
10:50-11:10 a.m.	<p><b>Hsa-miR-1587 G-quadruplex formation and dimerization induced by NH<sub>4</sub><sup>+</sup>, molecular crowding environment and jatrorrhizine derivatives</b></p> <p>W. Tan, L. Yi, Z. Zhu, L. Zhang, <u>J. Zhou</u>, G. Yuan Peking University, Chemistry, Beijing, China</p>	
11:10-11:30 a.m.	<p><b>Biophysical characterization of aptamer-metabolite interactions using ion mobility mass spectrometry</b></p> <p><u>S. Piccolo</u>, E. Daems, F. Sobott, V. Gabelica INSERM, CNRS &amp; University of Bordeaux (ARNA laboratory), IECB, Pessac, France</p>	
9:30-11:30 a.m.	<p><b>MOr.02 - Clinical proteomics</b></p> <p><i>Chairs: Giuseppina Maccarrone, Donatella Caruso</i></p>	<p><b>Room 1</b> <b>Level 0</b></p>
9:30-10:10 a.m.	<p><b>Immunoassays in multiplex for biomarker discovery and validation</b></p> <p><u>T. O. Joos</u> University of Tübingen, Reutlingen, Germany</p>	
10:10-10:30 a.m.	<p><b>Shedding new light on spinal cord injury</b></p> <p><u>M. Salzet</u>, J. Quanico, M. Karnoub, C. Meriaux, Z. Laouby, F. Rodet, D. Cizkova, I. Fournier, R. Assaker U1192 Inserm, PRISM Laboratory, University Lille, Villeneuve D'Ascq, France</p>	
10:30-10:50 a.m.	<p><b>Multiomeric plasma analysis of patients with hepatocellular carcinoma by mass spectrometry</b></p> <p>R. De Oliveira, R. Amaral, T. Da Silva, M. Castro, W. Fontes, C. Ricart, M. De Sousa, M. Eberlin, J. Garcia, <u>A. Martins</u> University of Brasilia, Laboratory of Biochemistry and Protein Chemistry, Brasilia, Brazil</p>	
10:50-11:10 a.m.	<p><b>Identification of proteomic and lipidomic markers in inflammatory bowel diseases by MS-based techniques and multivariate statistical analysis</b></p> <p><u>E. Robotti</u>, M. Manfredi, E. Conte, E. Barberis, A. Buzzi, V. Caneparo, D. Cecconi, J. Brandi, E. Vanni, S. Landolfo, M. Gariglio, E. Marengo, M. De Andrea University of Piemonte Orientale, Alessandria, Italy</p>	

11:10-11:30 a.m.	<b>A novel mass spectrometry based assay for the diagnosis and typing of systemic amyloidosis</b> <i>P. Boersema, T. Huang, J. Bijzet, C. Zimmerli, O. Vitek, B. Hazenberg, P. Picotti</i> ETH Zurich, Institute of Molecular Systems Biology, Zurich, Switzerland
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9:30-11:30 a.m.	<b>MOr.03 - Ion spectroscopy &amp; Photodissociation</b> <i>Chairs: Nicolas C. Polfer, Simonetta Fornarini</i>	<b>Room 2</b> <b>Level 0</b>
9:30-10:10 a.m.	<b>New frontiers for cryogenic chemistry and optical spectroscopy of mass-selected ions</b> <i>M. Johnson</i> Yale University, Department of Chemistry, New Haven, USA	
10:10-10:30 a.m.	<b>Structural characterization of ETD product ions using IR ion spectroscopy</b> <i>J. Oomens, L. Kempke, J. Martens, G. Berden</i> Radboud University, FELIX Laboratory, Nijmegen, Netherlands	
10:30-10:50 a.m.	<b>Structures and photodissociation action spectroscopy of nucleic acid cation radicals</b> <i>F. Turecek</i> University of Washington, Department of Chemistry, Seattle, USA	
10:50-11:10 a.m.	<b>Photochemistry of glyoxylate embedded in sodium chloride clusters, a laboratory model for tropospheric sea-salt aerosols</b> <i>N. K. Bersenkowitsch, M. Oncak, C. van der Linde, A. Herburger, M. K. Beyer</i> Universität Innsbruck, Ionenphysik und Angewandte Physik, Innsbruck, Austria	
11:10-11:30 a.m.	<b>Photodissociation spectroscopy of m/z-selected functionalised protonated pyridine ions: are some predictive patterns emerging?</b> <i>M. Benajmin, M. Samuel, K. Patrick, S. Blanksby, A. Trevitt</i> University of Wollongong, School of Chemistry, Wollongong, Australia	

Monday

9:30-11:30 a.m.	<b>MOr.04 - Hyphenated techniques</b> <i>Chairs: Myeong Hee Moon, Michele Suman</i>	<b>Room 3</b> <b>Level 1</b>
9:30-10:10 a.m.	<b>Hyphenation of sampling/sample preparation to mass spectrometry</b> <i>J. Pawliszyn</i> University of Waterloo, Chemistry, Waterloo, Canada	
10:10-10:30 a.m.	<b>Simultaneous quantification of sixteen polyphenols in 31 legumes by using HPLC-MS/MS Dynamic-MRM triple quadrupole</b> <i>G. Caprioli, M. Ricciutelli, S. Vittori, N. F. Kamgang, G. Sagratini</i> University of Camerino, School of Pharmacy, Camerino, Italy	
10:30-10:50 a.m.	<b>On-line coupling of Surface Plasmon Resonance to ambient mass spectrometry</b> <i>H. Liu, Y. Zhang, X. Li, H. Nie, Y. Bai</i> Peking University, College of Chemistry and Molecular Engineering, Beijing, China	
10:50-11:10 a.m.	<b>Online high pressure proteolytic biosensor- mass spectrometry (PROTEX-SPRMS): a new powerful tool for protein epitope and affinity identification and antibody characterization</b> <i>L. Lupu, P. Wiegand, Y. Baschung, F. Völklein, A. Lazarev, K. Schmitz, M. Przybylski</i> Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrom., Rüsselsheim am Main, Germany	
11:10-11:30 a.m.	<b>Chemical profiling of the human skin surface for malaria vector control using a non-invasive solvent modified sorptive sampler with GC×GC-ToFMS and UPLC-IMS-HRMS</b> <i>M. Wooding, T. Dodgen, M. Bouwer, Y. Naudé, E. Rohwer</i> University of Pretoria, Department of Chemistry, Pretoria, South Africa	

9:30-11:30 a.m.	<b>MOr.05 - Volatile molecules &amp; nose-space analysis</b>		<b>Room 4 Level 1</b>
	<i>Chairs: Egmont Rohwer, Giorgio Mellerio</i>		
9:30-10:10 a.m.	<b>Exploring food aroma release and perception using direct-injection mass spectrometry</b> <i>J. Beauchamp</i> Fraunhofer Institute for Process Engineering and Packaging IVV, Department of Sensory Analytics, Freising, Germany		
10:10-10:30 a.m.	<b>High-pressure photoionization time of flight mass spectrometry combined with dynamic purge-injection for rapid analysis of volatile metabolites in urine</b> <i>H. Lei, L. Hua, E. Li, H. Li</i> Dalian Institute of Chemical Physics, Chinese Academy of Sciences, CAS Key Laboratory of Separation Sciences for Analytical Chemistry, Dalian, China		
10:30-10:50 a.m.	<b>Nose-space of dark chocolates using PTR-ToF-MS and link to flavour perception through simultaneous Temporal Dominance of Sensations (TDS)</b> <i>Z. Deuscher, I. Andriot, S. Cordelle, M. Repoux, R. Boulanger, H. Labouré, P. Schlich, J. Le Quéré</i> INRA, Centre des Sciences du Goût et de l'Alimentation (CSGA), Dijon, France		
10:50-11:10 a.m.	<b>In nose-space analysis through Proton Transfer Reaction mass spectrometry: investigating variability in flavor release and perception during chewing gum consumption</b> <i>M. Pedrotti, I. Khomenko, V. Fogliano, F. Biasoli</i> Foundation Edmund Mach, Wageningen University FQD, Wageningen, Netherlands		
11:10-11:30 a.m.	<b>Methodology for qualitative and quantitative analysis of volatile compounds from composite materials at elevated temperatures</b> <i>C. Lourenco, S. Bergin, D. Francis, S. Staines, J. Hodgkinson, C. Walton, J. Saffell, R. Tatam</i> Cranfield University, School of Aerospace, Transport and Manufacturing, Cranfield, United Kingdom		
11:30 a.m. - 1:00 p.m.	Coffee Break		<b>Exhibition hall Level 0</b>
	<b>Poster Sessions MPS-S01 – MPS-S10</b> <i>Odd numbered abstracts</i>		
12:30 - 1:45 p.m.	<b>Lunch Symposia</b>		
	<b>BRUKER DALTONICS</b>	<b>Room 1 – Level 0</b>	
	<b>JEOL</b>	<b>Room 4 – Level 1</b>	
	<b>SCIEX</b>	<b>Room 3 – Level 1</b>	
	<b>WATERS</b>	<b>Room 2 – Level 0</b>	
1:30 - 3:00 p.m.	Coffee Break		<b>Exhibition hall Level 0</b>
	<b>Poster Sessions MPS-S01 – MPS-S10</b> <i>Even numbered abstracts</i>		
3:00-5:00 p.m.	<b>MOr.06 - Clinical chemistry</b>		<b>Plenary room Level 0</b>
	<i>Chairs: Hugo Rocha, Giancarlo la Marca</i>		
3:00-3:40 p.m.	<b>Tandem mass spectrometry in the clinical laboratory: can standardization improve operation?</b> <i>M. Pasquali</i> University of Utah, School of Medicine, Salt Lake City, USA		
3:40-4:00 p.m.	<b>A combined micro-extraction by packed sorbent-UHPLC-ESI-MS/MS procedure for the analysis of prostanoids and isoprostanoids in dried blood spots of preterm newborns with Patent Ductus Arteriosus</b> <i>D. Biagini, S. Antoni, S. Ghimenti, T. Lomonaco, F. G. Bellagambi, A. Cuttano, R. T. Scaramuzzo, M. Ciantelli, F. Di Francesco, R. Fuoco</i> University of Pisa, Department of Chemistry and Industrial Chemistry, Pisa, Italy		

4:00-4:20 p.m.	<b>Profiling of membrane lipids relevant to Alzheimer's disease pathogenesis</b> <i>Z. Spacil, E. Cechova, P. Telensky, S. Olkowicz, L. Opalka, K. Sheardova, R. Jancalek, J. Klanova, A. Hampl, J. Damborsky</i> Masaryk University, Faculty of Science, Research Centre for Toxic Compounds in the Environment, Brno, Czech Republic
4:20-4:40 p.m.	<b>The use of stable isotopes in the study of albumin metabolism in patients with acute lung disease</b> <i>M. Simonato, S. Gianbelluca, L. Vedovelli, M. Dalla, C. Ori, V. Carnielli, P. Cogo</i> Istituto di Ricerca Pediatrica "Città della Speranza", Padova, Italy
4:40-5:00 p.m.	<b>Mass-spectrometry approach for rapid intraoperative identification of brain tumor tissues - a way for online analysis</b> <i>S. Pekov, V. Eliferov, E. Zhvansky, A. Vorobyev, V. Shurkhay, A. Sorokin, I. Popov, A. Potapov, E. Nikolaev</i> Moscow Institute of Physics and Technology, Dolgoprudnyj, Russian Federation

3:00-5:00 p.m.	<b>MOr.07 - Quantitative proteomics</b> <i>Chairs: Michael Linscheid, Nathalie Norais</i>	Room 1 Level 0
3:00-3:40 p.m.	<b>Drug effects on protein homeostasis</b> <i>M. Bantscheff</i> GSK, Heidelberg, Germany	
3:40-4:00 p.m.	<b>Measuring nascent proteomics in signaling and cellular differentiation</b> <i>A. Burlingame, N. Phillips, C. Forester</i> UCSF, Pharmaceutical Chemistry, San Francisco, USA	
4:00-4:20 p.m.	<b>A chemical probe for understanding how proteome foldedness changes under proteostasis stress</b> <i>G. Reid, D. Cox, Y. Hong, D. Hatters</i> University of Melbourne, School of Chemistry, Department of Biochemistry and Molecular Biology, Parkville, Australia	
4:20-4:40 p.m.	<b>TMT quantification in MS<sup>2</sup> using high field asymmetric waveform ion mobility spectrometry</b> <i>P. Sibylle, B. Eric, P. Thibault</i> Institute for Research in Immunology and Cancer (IRIC), Université de Montreal, Montreal, Canada	
4:40-5:00 p.m.	<b>The key to big biobanks: analyzing 24 proteomes per day by micro-flow SWATH® acquisition and Spectronaut Pulsar Analysis</b> <i>J. Muntel, N. Morrice, R. Bruderer, L. Reiter</i> Biognosys AG, R&D, Schlieren, Switzerland	

3:00-5:00 p.m.	<b>MOr.08 - Chiral discrimination</b> <i>Chairs: Anne Zehnacker-Rentien, Maurizio Speranza</i>	Room 2 Level 0
3:00-3:40 p.m.	<b>Chiral recognition in protonated molecular clusters studied by mass-coupled IR-UV double resonance spectroscopy with cold ion trap</b> <i>M. Fujii</i> Laboratory for Chemistry and Life Science, Institute of Innovative Research, Tokyo Institute of Technology, Tokyo, Japan	
3:40-4:00 p.m.	<b>A new MS-based hyphenated method for analysis of hexuronic acid epimers and sulfate patterns in glycosaminoglycan oligosaccharides by MS<sup>n</sup> coupled to infrared ion spectroscopy</b> <i>G. Renois-Predelus, B. Schindler, L. Barnes, S. Chambert, A.-R. Allouche, I. Compagnon</i> Institut Lumière Matière, Université Claude Bernard Lyon 1, Lyon, France	
4:00-4:20 p.m.	<b>Chiral discrimination in collision-induced dissociation experiments: a theoretical approach of the cycloPhe-HisH<sup>+</sup> system</b> <i>A. Pérez-Mellor, R. Spezia</i> Laboratoire de Chimie Théorique, LCT, Sorbonne Université, CNRS, Paris, France	

4:20-4:40 p.m.	<b>Enantioselective reduction from quaternary copper D,L amino acid complexes: origin of the weak chiral effect observed with D/L aspartic and glutamic acids</b> <i>D. Lesage, S. Alves, E. Darii, J.-C. Tabet</i> SPI, LEMM, CEA, INRA, Université Paris Saclay, Gif-sur-Yvette, France	
4:40-5:00 p.m.	<b>Direct enantiomer-selective mass spectrometry of multi-component chiral mixtures</b> <i>M. H. M. Janssen</i> MassSpecpec D BV, R&D, Enschede, Netherlands	
3:00-5:00 p.m.	<b>MOr.09 - Ambient MS and new ionization methods</b> <i>Chairs: Jentaie Shiea, Pietro Traldi</i>	<b>Room 3 Level 1</b>
3:00-3:40 p.m.	<b>Breath metabolomics using Secondary Electrospray Ionization (SESI) - high resolution mass spectrometry</b> <i>R. Zenobi</i> ETH Zurich, Zurich, Switzerland	
3:40-4:00 p.m.	<b>Direct detection of small n-alkanes at sub-ppbv level in breath air by photoelectron induced O<sub>2</sub><sup>+</sup> cation chemical ionization mass spectrometry at kPa pressure</b> <i>Y. Wang, L. Hua, H. Li</i> Dalian Institute of Chemical Physics, Chinese Academy of Sciences, CAS Key Laboratory of Separation Sciences for Analytical Chemistry, Dalian, China	
4:00-4:20 p.m.	<b>Direct coupling of magnetic-particle-based sample preparation strategies to mass spectrometry via microfluidic open interface</b> <i>M. Tascon, V. Singh, M. Huq, J. Pawliszyn</i> University of Waterloo, Chemistry, Waterloo, Canada	
4:20-4:40 p.m.	<b>Development of the feedback control system for the advanced tapping mode scanning probe electrospray ionization (t-SPESI)</b> <i>Y. Otsuka, B. Kamihoriuchi, A. Takeuchi, F. Iwata, T. Matsumoto</i> Osaka University, Department of Chemistry, Toyonaka, Japan	
4:40-5:00 p.m.	<b>Direct mass spectrometry analysis using in-capillary ionic liquids-based dispersive liquid-liquid microextraction and sonic-spray ionization</b> <i>Q. Ma</i> Chinese Academy of Inspection and Quarantine, Beijing, China	
3:00-5:00 p.m.	<b>MOr.10 - Polymers</b> <i>Chairs: Marek M. Kowalczyk, Leopoldo Ceraulo</i>	<b>Room 4 Level 1</b>
3:00-3:40 p.m.	<b>Mass spectrometry methods for the characterization of functional materials</b> <i>C. Wesdemiotis</i> The University of Akron, Departments of Chemistry and Polymer Science, Akron, OH, USA	
3:40-4:00 p.m.	<b>Unravelling the architecture of branched polyester oligomers by combined trapped ion-mobility spectrometry – tandem mass spectrometry</b> <i>R. Voeten, P. van de Bram, J. Jordens, Y. Mengerink, R. Peters, R. Haselberg, P. Schoenmakers, G. W. Somsen</i> VU Amsterdam, Amsterdam, Netherlands	
4:00-4:20 p.m.	<b>MS/MS reading of polyurethane barcodes used as taggants in polymeric materials</b> <i>S. Poyer, S. Chimjarn, D. Karamessini, J. Lutz, L. Charles</i> Aix-Marseille Université, Institut de Chimie Radicalaire, Marseille, France	
4:20-4:40 p.m.	<b>Electrospray ionization mass spectrometry of nonpolar polyisobutylenes</b> <i>S. Kéki, L. Nagy, T. Nagy, G. Deák, A. Kuki, M. Purgel, M. Narmandakh, B. Iván, M. Zsuga</i> University of Debrecen, Department of Applied Chemistry, Debrecen, Hungary	
4:40-5:00 p.m.	<b>Analysis of polystyrene based microplastics in the environment</b> <i>G. F. Schirinzi, M. Llorca, M. Farré, D. Barcelò</i> CSIC, IDAEA, Barcelona, Spain	



5:15-7:00 p.m.	<b>Workshops</b>	
	<b>WKS-M1 - Mass spectrometry in virology</b>	ROOM 1 - Level 0
	<b>WKS-M2 - Police casework - successes and challenges from an academic perspective</b>	ROOM 2 - Level 0
	<b>WKS-M3 - Environmental Mass Spectrometry: from trace analysis to effect assessment</b>	ROOM 3 - Level 1
	<b>WKS-M4 - Are MS-based methods fit for purpose?</b>	ROOM 4 - Level 1

## TUESDAY, August 28<sup>th</sup>, 2018

8:30-9:15 a.m.	<b>Thomson Medal Award Ceremony</b> <i>Chair: Catherine E. Costello</i> <b>PL03: Plenary Lecture: THOMSON MEDALIST</b> <b>Gaining weight in mass spectrometry. From analyzing electrons to intact molecular machineries</b> <b>Albert J. R. Heck</b> Netherlands Proteomics Centre, Utrecht University, The Netherlands	<b>Plenary room</b> <b>Level 0</b>
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	<b>TOr.01 - Therapeutic drug monitoring and drug discovery</b> <i>Chairs: Gérard Hopfgartner, Fabio Garofolo</i>	<b>Plenary room</b> <b>Level 0</b>
9:30-10:10 a.m.	<b>Therapeutic drug monitoring and drug discovery: is it all known or are we innovative and game changing?</b> <i>R. M.A. Heeren, F. Cuyckens, R. J. Vreeken</i> Janssen R&D, Beerse, Belgium	
10:10-10:30 a.m.	<b>A highly selective and sensitive LC-MS/HRMS assay for Coproporphyrin-I and -III, emerging endogenous biomarkers of OATP, in first-in-human clinical trials</b> <i>R. Ramanathan</i> Pfizer, Inc, Medicine Design, Groton, USA	
10:30-10:50 a.m.	<b>Development of an ex vivo solid-phase microextraction calibration model towards in vivo quantitation of doxorubicin in lungs during a novel chemotherapeutic procedure</b> <i>A. Roszkowska, M. Tascon, B. Bojko, K. Gorynski, R. G. A. Gomez, N. Looby, S. P. Reck Dos, M. Cypel, J. Pawliszyn</i> University of Waterloo, Department of Chemistry, Waterloo, Canada	
10:50-11:10 a.m.	<b>Characterization of paclitaxel metabolites by UHPLC-MS/MS: biomedical application of the study in targeted drug delivery systems</b> <i>C. Sottani, E. Grignani, E. Studioso, D. Cottica</i> Istituti Clinici Scientifici - Maugeri, Environmental Research Center, Pavia, Italy	
11:10-11:30 a.m.	<b>The effects of low temperature storage on the structure of Herceptin®: to freeze, or not to freeze: that is the question</b> <i>R. Upton, K. Pacholarz, D. Firth, S. Estdale, P. Barran</i> Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom	

9:30-11:30 a.m.	<b>TOr.02 - Life sciences - Single cell</b> <i>Chairs: Peter Nemes, Giuliana Bianco</i>	<b>Room 1</b> <b>Level 0</b>
9:30-10:10 a.m.	<b>Single cell mass spectrometry: from qualitative to quantitative studies</b> <u>Z. Yang</u> University of Oklahoma, Department of Chemistry and Biochemistry, Norman, USA	
10:10-10:30 a.m.	<b>Analysis of single mammalian cells with SCoPE-MS with mPOP</b> <i>H. Specht, G. Harmange, D. Perlman, J. Neveu, C. Adams, N. Slavov, B. Budnik</i> Harvard University, FAS Division of Science, Cambridge, USA	
10:30-10:50 a.m.	<b>LiveCell MS methodology in the context of drug discovery</b> <u>C. Newman</u> , A. West The University of Nottingham, School of Pharmacy, Nottingham, United Kingdom	
10:50-11:10 a.m.	<b>In situ mass spectrometry unravels metabolic differences between cells of the live vertebrate embryo (<i>Xenopus laevis</i>)</b> <u>E. Portero</u> , S. Moody, P. Nemes University of Maryland, Chemistry and Biochemistry, College Park, USA	
11:10-11:30 a.m.	<b>A ToF-SIMS tandem MS Imaging method to probe the composition of cellular organelles</b> <u>G. L. Fisher</u> , C. E. Chini, B. Johnson, M. M. Tamkun, M. L. Kraft Physical Electronics, Marketing & Applications, Chanhassen, USA	
9:30-11:30 a.m.	<b>TOr.03 - Noncovalent interactions</b> <i>Chairs: Renato Zenobi, Francesco De Angelis</i>	<b>Room 2</b> <b>Level 0</b>
9:30-10:10 a.m.	<b>Membrane proteins - the lipid connection</b> <u>C. Robinson</u> University of Oxford, Physical and Theoretical Chemistry Laboratory, United Kingdom	
10:10-10:30 a.m.	<b>Aryl bis-sulfonamides bind to the active site of a homotrimeric isoprenoid biosynthesis enzyme IspF and extract the essential divalent metal cation cofactor</b> <u>K. Root</u> , K. Barylyuk, A. Schwab, J. Thelemann, B. Illarionov, M. Fischer, F. Diederich, R. Zenobi ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland	
10:30-10:50 a.m.	<b>Native MS of noncovalent RNA: protein complexes</b> <u>V. Wysocki</u> Dept of Chemistry and Biochemistry, Ohio State University, USA	
10:50-11:10 a.m.	<b>Exploring the inhibition mechanisms of amyloid protofibrils using Fourier Transform Ion Cyclotron Resonance-Mass Spectrometry (FTICR-MS)</b> <u>Y. P. Y. Lam</u> , C. K. C. Chiu, C. A. Wootton, J.-I. Song, M. Li, I. Hands-Portman, M. P. Barrow, P. B. O'Connor University of Warwick, Department of Chemistry, Coventry, United Kingdom	
11:10-11:30 a.m.	<b>Different means of solubilization of membrane proteins for native MS</b> <u>N. Morgner</u> , O. Peetz Frankfurt University, Physical Chemistry, Frankfurt, Germany	
9:30-11:30 a.m.	<b>TOr.04 - High resolution MS: instrumentation, methods &amp; applications</b> <i>Chairs: Evgeny Nikolaev, Gianluca Giorgi</i>	<b>Room 3</b> <b>Level 1</b>
9:30-10:10 a.m.	<b>Life at the frontier: 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometry</b> <u>A. Marshall</u> , P. M. L. Chacon, Y. E. Corilo, C. L. Hendrickson, L. He, S. F. Niles, J. C. Putman, S. M. Rowland, D. F. Smith, R. L. Ware, C. R. Weisbrod, R. P. Rodgers Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, USA	
10:10-10:30 a.m.	<b>Bridging the gap between images and molecules: Parallel acquisition of FTMS mass spectrometry imaging and MS/MS data coupled with automated and high confidence lipid identifications</b> <u>S. Ellis</u> , M. Paine, G. Eijkel, J. Pauling, P. Husen, M. Jervelund, M. Hermansson, C. Ejsing, R. M. A. Heeren Maastricht University, The Maastricht Multimodal Molecular Imaging Institute (M4I), Maastricht, Netherlands	

10:30-10:50 a.m.	<b>Large-scale ring trial metabolomics study of human blood plasma using diverse FT-ICR-MS systems</b> <i>S. Forcisi, F. Moritz, B. Kanawati, J. Uhl, C. Thompson, A. Barsch, G. Kruppa, M. Easterling, T. Ring, P. Schmitt-Kopplin</i> Helmholtz Zentrum München, Research Unit Analytical BioGeoChemistry, Neuherberg, Germany
10:50-11:10 a.m.	<b>Single cell metabolomics with LAESI-21T-FTICR-MS</b> <i>L. Pasa-Tolic, C. R. Anderton, D. Veličković, S. Stopka, L. Samarah, R. Khattar, J. Shaw, B. Agtuca, G. Stacey, A. Vertes</i> Pacific Northwest National Lab, Environmental Molecular Sciences Lab, Richland, USA
11:10-11:30 a.m.	<b>Comprehensive high-resolution mass spectrometric evolved gas analysis in the context of petroleomics: analysis of bitumen, heavy crude oils and asphaltenes</b> <i>C. Rüger, A. Neumann, C. Grimmer, U. Käfer, M. Sklorz, T. Gröger, T. Streibel, R. Zimmermann</i> University of Rostock, Institute of Chemistry, Rostock, Germany

9:30-11:30 a.m.	<b>TOr.05 - MS imaging: instrumentation</b> <i>Chairs: Liam McDonnell, Fulvio Magni</i>	<b>Room 4 Level 1</b>
9:30-10:10 a.m.	<b>Molecular imaging at the interface of health and disease</b> <i>R. M. A. Heeren</i> M4I, The Maastricht MultiModal Molecular Imaging institute, Maastricht University, Maastricht, The Netherlands	
10:10-10:30 a.m.	<b>Novel hyperspectral Imaging Mass Spectrometry to delineate Amyloid polymorphism</b> <i>J. Hanrieder</i> University of Gothenburg, Department of Neuroscience and Physiology, Gothenburg, Sweden	
10:30-10:50 a.m.	<b>Validation studies of phosphopeptide enrichment procedures using TiO<sub>2</sub>-attached membrane funnel-based spray ionization for Imaging Mass Spectrometry</b> <i>Y.-L. W. Hung, C. T.-W. Dominic</i> The Chinese University of Hong Kong, Chemistry Department, Hong Kong, Hong Kong	
10:50-11:10 a.m.	<b>Infrared Laser Ablation Microsampling coupled with MALDI imaging</b> <i>K. Murray, F. Donnarumma, K. Wang, T. Solouki, M. Pettit</i> Louisiana State University, Department of Chemistry, Baton Rouge, USA	
11:10-11:30 a.m.	<b>Pulsed cold plasma for post-ionization in MALDI-MS imaging</b> <i>J. Soltwisch, U. Röhling, K. Dreisewerd</i> University of Münster, Institute for Hygiene, Münster, Germany	

11:30 a.m. - 1:00 p.m.	Coffee Break <b>Poster Sessions TPS-S01 – TPS-S10</b> <i>Odd numbered abstracts</i>	<b>Exhibition hall Level 0</b>
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12:30 - 1:45 p.m.	<b>Lunch Symposia</b>	
	<b>AGILENT TECHNOLOGIES</b>	<b>Room 2 – Level 0</b>
	<b>BRUKER DALTONICS</b>	<b>Room 1 – Level 0</b>
	<b>SCIEX</b>	<b>Room 3 – Level 1</b>
	<b>THERMO FISHER SCIENTIFIC</b>	<b>Room 4 – Level 1</b>

1:30 - 3:00 p.m.	Coffee Break <b>Poster Sessions TPS-S01 – TPS-S10</b> <i>Even numbered abstracts</i>	<b>Exhibition hall Level 0</b>
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3:00-5:00 p.m.	<b>TOr.06 - Post Translational Modifications</b> <i>Chairs: Joseph A. Loo, Fulvio Magni</i>	<b>Plenary room Level 0</b>
3:00-3:40 p.m.	<b>Rapid, sensitive and quantitative phosphoproteomics for large-scale cell perturbation analysis</b> <u>J. Olsen</u> University of Copenhagen, Faculty of Health and Medical Sciences, Denmark	
3:40-4:00 p.m.	<b>Comprehensive NISTmAb reference spectral libraries for reliable and robust identification of post-translational modifications in human and recombinant IgG antibodies</b> <u>Q. Dong</u> , Y. Liang, X. Yan, S. Markey, Y. Mirokhin, D. Tchekhovskoi, T. Bukhari, S. Stein National Institute of Standards and Technology, Bimolecular Measurement Division, Gaithersburg, USA	
4:00-4:20 p.m.	<b>SEAGal: the method to fish for uncommon phosphorylations</b> <u>V. Gorshkov</u> , Y. Palarasah, K. Skjødt, F. Kjeldsen University of Southern Denmark, Department of Biochemistry and Molecular Biology, Odense, Denmark	
4:20-4:40 p.m.	<b>Proteome-wide effects of singlet oxygen produced by next generation Iridium anti-cancer metallodrugs</b> <u>C. K. C. Chiu</u> , P. Zhang, Y. P. Y. Lam, C. A. Wootton, M. P. Barrow, P. J. Sadler, P. B. O'Connor University of Warwick, Department of Chemistry, Coventry, United Kingdom	
4:40-5:00 p.m.	<b>Polyamine modifications in diatom biosilica proteomes</b> <u>A. Milentyev</u> , C. Heintze, N. Poulsen, N. Kroeger, A. Shevchenko Max Planck Institute of Molecular Cell Biology and Genetics, Shevchenko Lab, Dresden, Germany	
3:00-5:00 p.m.	<b>TOr.07 - Mass spectrometric analysis of forensic science evidence</b> <i>Chairs: Simona Francese, Gloriano Moneti</i>	<b>Room 1 Level 0</b>
3:00-3:40 p.m.	<b>Extended mass spectrometry workflow for the analysis of drugs of abuse in biological fluids and tissues</b> <u>G. Hopfgartner</u> University of Geneva, Life Sciences Mass Spectrometry, Switzerland	
3:40-4:00 p.m.	<b>The death of Thomas Chatterton - an LC-MS<sup>n</sup> investigation</b> <u>P. Gates</u> University of Bristol, School of Chemistry, Bristol, United Kingdom	
4:00-4:20 p.m.	<b>Class identification of novel psychoactive substances using mass spectral library searching with hierarchical clustering</b> A. Moorthy, <u>W. Wallace</u> , A. Kearsley, D. Tchekhovskoi, S. Stein National Institute of Standards and Technology, Mass Spectrometry Data Center, Gaithersburg, USA	
4:20-4:40 p.m.	<b>Identifying wood from protected species with DART fingerprint spectra and the software platform OMFF</b> <u>S. Martínez-Jarquín</u> , C. Lancaster, E. Espinoza, R. Winkler CINVESTAV, Biochemistry and Biotechnology, Irapuato, Mexico	
4:40-5:00 p.m.	<b>Green forensics - isotopic traceability in horticulture. Geographical origin of roses</b> <u>E. De Rijke</u> , M. Trisna, S. Verdegaal, R. Magnússon, J. Schoorl, C. Cerli, C. De Koster University of Amsterdam, Institute for Biodiversity and Ecosystem Dynamics, Amsterdam, Netherlands	
3:00-5:00 p.m.	<b>TOr.08 - Ion activation and dissociations</b> <i>Chairs: Vicki Wysocki, Gianluca Giorgi</i>	<b>Room 2 Level 0</b>
3:00-3:40 p.m.	<b>Understanding fragmentation of complex ions using Surface-Induced Dissociation experiments</b> <u>J. Laskin</u> Purdue University, Dept. of Chemistry, West Lafayette, USA	

3:40-4:00 p.m.	<b>Investigation of hemicryptophane host-guest binding energies using advanced tandem mass spectrometry</b> <i>P. Bayat, D. Gatineau, D. Lesage, V. Robert, A. Martinez, R. B. Cole</i> Sorbonne Université, IPCM, Paris, France
4:00-4:20 p.m.	<b>Tandem ToF mass spectrometry of biomolecules: from dual stage to curved field and parabolic analyzers as second stage</b> <i>E. Pittenauer, G. Allmaier</i> TU Wien, Institute of Chemical Technologies and Analytics, Wien, Austria
4:20-4:40 p.m.	<b>Specific radical-driven dissociation of hydrogen-excess and -deficient radical peptides produced by MALDI in-source decay mass spectrometry</b> <i>M. Takayama</i> Yokohama City University, Graduate School of Nanobioscience, Yokohama, Japan
4:40-5:00 p.m.	<b>Juggling fragile van der Waals complexes in an ion trap for multiplexed infrared photodissociation</b> <i>L. Tesler, M. Bell, T. Harmon, L. Bailey, N. Polfer</i> University of Florida, Dept. of Chemistry, Gainesville, USA

3:00-5:00 p.m.	<b>TOr.09 - Metal and non-metal clusters: gas phase structures and reactivity</b> <i>Chairs: Evan Williams, Pietro Traldi</i>	<b>Room 3 Level 1</b>
3:00-3:40 p.m.	<b>Tandem cryo ion trap mass spectrometry for kinetics and spectroscopy of transition metal clusters</b> <i>G. Niedner-Schatteburg</i> Fachbereich Chemie and Forschungszentrum OPTIMAS, TU Kaiserslautern, Kaiserslautern, Germany	
3:40-4:00 p.m.	<b>UV-VIS spectroscopy and photochemistry of trapped ions using FT-ICR-MS</b> <i>C. Van der Linde, M. Oncák, N. K. Bersenkovitsch, A. Herburger, T. Taxer, M. K. Beyer</i> Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik, Innsbruck, Austria	
4:00-4:20 p.m.	<b>ESI in the study of the interactions between phosphino-Cu(I) complexes and Cu(II) salts with model peptides relevant to human copper transporters (hCTR)</b> <i>F. Tisato, K. Bossak-Ahmed, M. Porchia, W. Bal, A. Bonna</i> ICMATE – CNR, Padova, Italy	
4:20-4:40 p.m.	<b>Structure and reactivity of antimonato polyoxovanates in solution and in the gas phase</b> <i>U. Warzok, L. K. Mahnke, M. Wendt, W. Bensch, C. A. Schalley</i> Free University Berlin, Institute for Chemistry and Biochemistry, Berlin, Germany	
4:40-5:00 p.m.	<b>FT-ICR MS studies of thiomolybdate clusters as model catalysts for hydrogen evolution</b> <i>A. Baloglou, M. Oncák, C. Van der Linde, M. Grutza, P. Kurz, M. K. Beyer</i> Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik, Innsbruck, Austria	

3:00-5:00 p.m.	<b>TOr.10 – Astrochemistry</b> <i>Chairs: Paul Mayer, Simonetta Fornarini</i>	<b>Room 4 Level 1</b>
3:00-3:40 p.m.	<b>Cosmic PAHs: formation and UV processing</b> <i>C. Joblin</i> University Toulouse / CNRS, Toulouse, France	
3:40-4:00 p.m.	<b>Relaxation and fragmentation dynamics of polycyclic aromatic hydrocarbons excited by an ultrashort XUV pulse</b> <i>M. Herve, P. Castellanos, G. Karras, V. Despre, A. Marciniak, E. Constant, V. Lorient, A. Kuleff, A. Tielens, F. Lepine</i> Université Lyon 1, Institut Lumière Matière (ILM), Lyon, France	
4:00-4:20 p.m.	<b>Experimental study of high-energy ion/molecule interactions relevant to planetary atmospheres</b> <i>V. Krizova, J. Zabka, I. Zymak, M. Polasek</i> Charles University in Prague, Faculty of Science, Prague, Czech Republic	

Tuesday

4:20-4:40 p.m.	<b>Investigating the possibility of forming prebiotic molecules by gas phase ion-molecule reactions. Application to glycine</b> <i>R. Spezia, Y. Jeanvoine, A. Largo, W. L. Hase, J. Lemaire, D. Scuderi</i> CNRS, Sorbonne Université, Laboratoire de Chimie Théorique, Paris, France									
4:40-5:00 p.m.	<b>The threshold displacement energy of Buckminsterfullerene C60 and formation of the endohedral defect Fullerene He@C59</b> <i>M. Stockett, M. Wolf, M. Gatchell, H. Schmidt, H. Zettergren, H. Cederquist</i> Stockholm University, Department of Physics, Stockholm, Sweden									
5:15-7:00 p.m.	<b>Workshops</b> <table border="0" style="width: 100%;"> <tr> <td style="width: 20%;"><b>WKS-T1 -</b></td> <td style="width: 60%;"><b>Careers in Mass Spectrometry</b></td> <td style="width: 20%; text-align: right;">ROOM 1 - Level 0</td> </tr> <tr> <td><b>WKS-T2 -</b></td> <td><b>Transforming Drug Discovery and Clinical Biomarker Bioanalysis: It's Time for a Paradigm Shift from SRM to HRMS</b></td> <td style="text-align: right;">ROOM 2 - Level 0</td> </tr> <tr> <td><b>WKS-T3 -</b></td> <td><b>Integration of native MS with structural biology methods</b></td> <td style="text-align: right;">ROOM 3 - Level 1</td> </tr> </table>	<b>WKS-T1 -</b>	<b>Careers in Mass Spectrometry</b>	ROOM 1 - Level 0	<b>WKS-T2 -</b>	<b>Transforming Drug Discovery and Clinical Biomarker Bioanalysis: It's Time for a Paradigm Shift from SRM to HRMS</b>	ROOM 2 - Level 0	<b>WKS-T3 -</b>	<b>Integration of native MS with structural biology methods</b>	ROOM 3 - Level 1
<b>WKS-T1 -</b>	<b>Careers in Mass Spectrometry</b>	ROOM 1 - Level 0								
<b>WKS-T2 -</b>	<b>Transforming Drug Discovery and Clinical Biomarker Bioanalysis: It's Time for a Paradigm Shift from SRM to HRMS</b>	ROOM 2 - Level 0								
<b>WKS-T3 -</b>	<b>Integration of native MS with structural biology methods</b>	ROOM 3 - Level 1								

## WEDNESDAY, August 29<sup>th</sup>, 2018

8:30-9:15 a.m.	<b>CURT BRUNNÉE AWARD Ceremony</b> <span style="float: right;"><i>Chair: Scott A. McLuckey</i></span> <b>PL04: Plenary Lecture</b> <b>Lithographically patterned electrodes for miniaturized ion trap mass spectrometers and other ion optics devices</b> <i>Daniel E. Austin</i> Brigham Young University, Department of Chemistry and Biochemistry and Department of Electrical and Computer Engineering, Provo, USA	<b>Plenary room</b> <b>Level 0</b>
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	<b>WOr.01 - Native MS and structural proteomics</b> <i>Chairs: Frank Sobott, Nathalie Norais</i>	<b>Plenary room</b> <b>Level 0</b>
9:30-10:10 a.m.	<b>Native mass spectrometry: a technique of many faces</b> <i>M. Sharon, G. Ben-Nissan, S. Vimer, J. Cveticanin</i> Weizmann Institute of Science, Department of Biomolecular Sciences, Rehovot, Israel	
10:10-10:30 a.m.	<b>Native Mass Spectrometry reveal functioning mechanism of membrane protein translocation pathway</b> <i>S. Mehmood, M. McDowell, I. Sinning, C. Robinson</i> University of Oxford, Department of Chemistry, Oxford, United Kingdom	
10:30-10:50 a.m.	<b>Charge-independent mass spectrometry of single virus capsids above 100MDa with nanomechanical resonators</b> <i>C. Masselon, S. Hentz, S. Dominguez-Medina, S. Fostner, M. Halim, M. Defoort, E. Vernhes, P. Boulanger</i> CEA, DRF/BIG/Large Scale Biology Laboratory, Grenoble, France	
10:50-11:10 a.m.	<b>A cross-linking/mass spectrometry workflow based on MS-cleavable cross-linkers and the MeroX software for mapping protein-protein interactions</b> <i>C. Iacobucci, M. Götze, A. Sinz</i> Martin-Luther-Universität Halle-Wittenberg, Institut für Pharmazie, Halle, Germany	

11:10-11:30 a.m.	<b>Can we use HDX-MS to model protein conformations?</b> <i>A. Borysik</i> King's College London, Chemistry, London, United Kingdom	
9:30-11:30 a.m.	<b>WOr.02 - JMS Award Symposium</b> <i>Chairs: Richard Caprioli, John Langley</i>	<b>Room 1 Level 0</b>
9:30-9:50 a.m.	Presentation of the JMS Award Symposium	
9:50-10:10 a.m.	<b>Anion formation in MALDI depends on matrix and target plate material choice</b> <i>G. P. Zeegers, R. Zenobi</i> ETH Zürich, Chemistry and Applied Biosciences, Zürich, Switzerland	
10:10-10:30 a.m.	<b>Combining bio-conjugation and matrix-assisted laser desorption ionisation mass spectrometry for biomolecule detection and localisation in tissues</b> <i>K. Stevens, P. Mittal, A. Abell, T. Pukala</i> University of Adelaide, Physical Sciences, Adelaide, Australia	
10:30-10:50 a.m.	<b>Histology-directed proteomics: combining autofluorescence guided micro-digestions with liquid surface extractions</b> <i>D. Ryan, N. Patterson, J. Moore, J. Spraggins, R. Caprioli</i> Vanderbilt University, Department of Chemistry, Nashville, USA	
10:50-11:10 a.m.	<b>Dual microprobe CE-ESI-HRMS for the characterization of proteins and metabolites in single embryonic cells of live frog embryos</b> <i>C. Lombard-Banek, R. Onjiko, S. Moody, P. Nemes</i> University of Maryland, Chemistry & Biochemistry, College Park, USA	
11:10-11:30 a.m.	<b>Wastewater-based epidemiology: use of adulterants to estimate cocaine consumption patterns in Brasília, Brazil by LC-QToF-MS</b> <i>K. M. Da Silva, A. O. Maldaner, S. F. Fabríz</i> Instituto de Química, Universidade de Brasília, Brasília, Brazil	

9:30-11:30 a.m.	<b>WOr.03 - Reaction mechanisms and elusive intermediates</b> <i>Chairs: Scott A. McLuckey, Francesco De Angelis</i>	<b>Room 2 Level 0</b>
9:30-10:10 a.m.	<b>Elucidating the chemistry of elusive gas phase radicals using distonic radical ions: Trying to get a good deal from a Faustian bargain</b> <i>S. Blanksby, D. L. Marshall, B. L. J. Poad, A. J. Trevitt</i> Central Analytical Research Facility (CARF), Institute for Future Environments, Queensland University of Technology, Brisbane, Australia	
10:10-10:30 a.m.	<b>Acetone as photo-initiator for disulfide reduction – Application to structural analysis of disulfide rich peptides and proteins</b> <i>Y. Xia, S. Adhikari, X. Yang</i> Tsinghua University, Chemistry, Beijing, China	
10:30-10:50 a.m.	<b>Kinetics of a click reaction in charged microdroplets with Time Resolved Reactive Laser Ablation Electrospray Ionization Mass Spectrometry</b> <i>F. van Geenen, S. Gangarapu, M. Franssen, M.W.F. Nielen, H. Zuilhof</i> Wageningen University, Laboratory of Organic Chemistry, Wageningen, Netherlands	
10:50-11:10 a.m.	<b>Amino-acids oxidation: a combined study of cysteine oxo-forms by mass spectrometry, IRMPD spectroscopy and simulations</b> <i>D. Scuderi, E. Bodo, S. Fornarini, B. Chiavarino, M. Crestoni, V. Macaluo, R. Spezia</i> Laboratoire de Chimie Physique, UMR 8000, Université Paris Sud, Orsay, France	
11:10-11:30 a.m.	<b>Loss of water from polyglycines and their [bn]<sup>+</sup> ions; imidazolones and oxazolones</b> <i>K. H. B. Lam, J. K.-C. Lau, C.-K. Lai, I. K. Chu, J. Oomens, A. C. Hopkinson, K. W. M. Siu</i> University of Windsor, Department of Chemistry and Biochemistry, Windsor, Canada	

9:30-11:30 a.m.	<b>WOr.04 – Pharmaceuticals</b> <i>Chairs: Christine Eckers, Gianluca Bartolucci</i>	<b>Room 3</b> <b>Level 1</b>
9:30-10:10 a.m.	<b>Pharmaceutical Industry Challenges with Mass Spectrometry Solutions: from Microsampling to Monoclonal Antibodies</b> <i>W. Korfmacher</i> Sanofi, Drug Metabolism & Pharmacokinetics, Waltham, USA	
10:10-10:30 a.m.	<b>Impact of centroiding and differences in data processing on quantification using high-resolution mass spectrometry</b> <i>L. Vereyken, L. Dillen, R. Vreeken, F. Cuyckens</i> Janssen R&D, Discovery Sciences, Beerse, Belgium	
10:30-10:50 a.m.	<b>LC-ICP-MS as an alternative to radioactivity in pharmacology</b> <i>C. Enjalbal, E. Cordeau, G. Subra, D. Gagne, N. Prache, C. Arnaudguilhem, B. Bouyssiere</i> IBMM, University of Montpellier, Montpellier, France	
10:50-11:10 a.m.	<b>Sub-ppm detection and identification of in-vivo metabolites of an antibody-drug conjugate by data-independent HPLC-High-Resolution tandem MS</b> <i>A. Triolo, E. Ciuti, C. Carboni, V. Chirulli</i> Menarini Ricerche, Firenze, Italy	
11:10-11:30 a.m.	<b>New QC identity testing for acellular pertussis combination vaccines using LC-MS</b> <i>H. Zhang, R. Maharajh, S. Vydelingum, L. Yin</i> Sanofi Pasteur, Analytical Process and Technology, Toronto, Canada	
9:30-11:30 a.m.	<b>WOr.05. - Food integrity, authenticity &amp; traceability</b> <i>Chairs: Ruud Peters, Michele Suman</i>	<b>Room 4</b> <b>Level 1</b>
9:30-10:10 a.m.	<b>A story on food, faith and fraud – detection of the fakes</b> <i>S. van Ruth</i> Wageningen University and Research, Wageningen, The Netherlands	
10:10-10:30 a.m.	<b>Detecting food fraud: determination of a potato´s variety and its geographical origin in one analysis via UPLC-IMS-QToF</b> <i>C. Claassen, J. Kuballa, S. Rohn</i> GALAB Laboratories GmbH, University of Hamburg, Hamburg, Germany	
10:30-10:50 a.m.	<b>Nosespace analysis by PTR-ToF-MS for the extravirgin olive oil characterization</b> <i>I. Khomenko, E. Aprea, F. Gasperi</i> Edmund Mach Foundation, Food quality and nutrition, San Michele all'Adige, Italy	
10:50-11:10 a.m.	<b>Ultra-fast identification of fish species by paperspray coupled to a benchtop Orbitrap mass spectrometer</b> <i>D. Lopez-Ferrer, G. Foster, M. Prieto</i> Thermo Fisher Scientific, San Jose, USA	
11:10-11:30 a.m.	<b>Characterization and classification of Spanish paprika with protected designation of origin by UHPLC-HRMS polyphenolic fingerprinting and chemometrics</b> <i>S. Barbosa, G. Campmajó, O. Núñez, J. Saurina, L. Puignou</i> University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain	
11:30 a.m. - 1:00 p.m.	Coffee Break <b>Poster Sessions WPS-S01 – WPS-S10</b> <i>Odd numbered abstracts</i>	<b>Exhibition hall</b> <b>Level 0</b>
12:30 - 1:45 p.m.	<b>Lunch Symposia</b> <b>AGILENT TECHNOLOGIES</b> Room 2 – Level 0 <b>BIOGNOSYS</b> Room 3 – Level 1 <b>PERKINELMER</b> Room 1 – Level 0 <b>THERMO FISHER SCIENTIFIC</b> Room 4 – Level 1	



1:30 - 3:00 p.m.	Coffee Break <b>Poster Sessions WPS-S01 – WPS-S10</b> <i>Even numbered abstracts</i>	<b>Exhibition hall</b> <b>Level 0</b>
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3:00-5:00 p.m.	<b>WOr.06 - MS tools in doping &amp; toxicology</b> <i>Chairs: Mario Thevis, Gianluca Bartolucci</i>	<b>Plenary room</b> <b>Level 0</b>
3:00-3:40 p.m.	<b>Evolution and application of mass spectrometry-based analytical methods in anti-doping analyses</b> <u>T. Kuuranne</u> Swiss Laboratory for Doping Analyses, University Center of Legal Medicine Geneva and Lausanne, Centre Hospitalier Universitaire Vaudois and University of Lausanne, Lausanne, Switzerland	
3:40-4:00 p.m.	<b>LC-HRMS/MS vs. LC-MRM: screening of covalent drug-protein adducts</b> <u>T. Geib, L. Sleno</u> Université du Québec à Montréal, Chemistry Department, Montréal, Canada	
4:00-4:20 p.m.	<b>Coupling mass spectrometry and chemometrics for structural characterization of androgenic anabolic steroids</b> <u>P. Leogrande, T. De La, F. Botrè, D. Jardines, F. Marini</u> "Sapienza" Università di Roma, Dipartimento di Chimica; Lab. Antidoping, Federazione Medico Sportiva Italiana, Rome, Italy	
4:20-4:40 p.m.	<b>Detection of chemical warfare agents-related phenylarsenic compounds in marine biota and identification of their metabolites in in vitro studies by Orbitrap HRMS</b> <u>H. Niemikoski, D. Koske, P. Vanninen</u> Finnish Institute of Verification of Chemical Weapon Convention, University of Helsinki, Helsinki, Finland	
4:40-5:00 p.m.	<b>A fit-for-purpose UHPLC-MS/MS method for routine screening of SARM residues in bovine and equine serum</b> <u>E. Ventura, A. Gadaj, T. Buckley, M. H. Mooney</u> Institute for Global Food Security, Queen's University Belfast, School of Biological Sciences, Belfast, United Kingdom	

3:00-5:00 p.m.	<b>WOr.07 - MS imaging: applications</b> <i>Chairs: Martina Marchetti-Deschmann, Fulvio Magni</i>	<b>Room 1</b> <b>Level 0</b>
3:00-3:40 p.m.	<b>Combining mass spectrometry imaging &amp; microproteomics to investigate intratumor heterogeneity</b> <u>L. McDonnell</u> Leiden University Medical Center, Leiden, Netherlands	
3:40-4:00 p.m.	<b>Multisite multimodal mass spectrometry imaging of genetically engineered mouse models containing mutations linked to bowel cancer</b> <u>C. J. Nikula, R. T. Steven, E. A. Elia, A. D. Campbell, S. A. Thomas, A. Dexter, T. Murta, S. Ling, A. K. Najumudeen, A. J. Taylor, J.-L. Vorng, G. Hamm, R. Havelund, R. Filipe-Soares, D. Gay, B. Yan, A. Al-Afeef, T. Fu, R. Phillip, K. N. Robinson, S. Barry, K. Brindle, I. S. Gilmore, R. J. A. Goodwin, J. F. Marshall, G. Poulogiannis, Z. Takats, M. O. Yuneva, O. J. Sansom, J. Bunch</u> National Physical Laboratory, NiCE-MSI, Teddington, United Kingdom	
4:00-4:20 p.m.	<b>Can 3D MALDI-MS Imaging be the missing piece for understanding the traumatic brain injury puzzle?</b> <u>K. Mallah, J. Quanico, F. Kobeissy, K. Zibara, M. Salzet, I. Fournier</u> INSERM, U1192 - Laboratoire Protéomique, Réponse Inflammatoire et Spectrométrie de Masse (PRISM), Université de Lille, Department of Biology, Lille, France	
4:20-4:40 p.m.	<b>DLEMMA-MS-imaging for identification of spatially localized metabolites and metabolic network map reconstruction</b> <u>Y. Dong, L. Feldberg, U. Heinig, I. Rogachev, A. Aharoni</u> Weizmann Institute of Science, Weizmann Institute of Science, Rehovot, Israel	

4:40-5:00 p.m.	<b>Silver-doped nano-DESI MSI for prostaglandin imaging</b> <i>K. Duncan, R. Fang, J. Yuan, R. Chu, S. K. Dey, K. Burnum-Johnson, I. Lanekoff</i> Uppsala University, Dept of Chemistry-BMC, Uppsala, Sweden	
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3:00-5:00 p.m.	<b>WOr.08 - Gas phase ion chemistry &amp; thermochemistry</b> <i>Chairs: Pan Yanjiang, Giovanni Sindona</i>	<b>Room 2</b> <b>Level 0</b>
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3:00-3:40 p.m.	<b>Progress towards enzyme-like specificity in protein fragmentation</b> <i>S. A. Mcluckey, D. J. Foreman</i> Purdue University, Department of Chemistry, West Lafayette, USA	
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3:40-4:00 p.m.	<b>Dissociation of hydrogen-abundant peptide radical formed by hydrogen attachment in gas phase</b> <i>D. Asakawa, H. Takahashi, S. Iwamoto, K. Tanaka, K. Kamiya</i> AIST, Research Institute for Measurement and Analytical Instrumentation, Tsukuba, Japan	
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4:00-4:20 p.m.	<b>One-electron reduction of isolated metallo-supramolecular aggregates</b> <i>M. Engeser</i> Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Bonn, Germany	
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4:20-4:40 p.m.	<b>Reaction dynamics of ionized 1-methylpyrene: why is the 1-methylenepyrene ion formed from H atom loss and not a tropylium-containing ion?</b> <i>P. Mayer, B. West, B. Lowe</i> University of Ottawa, Dept. of Chemistry and Biomolecular Sciences, Ottawa, Canada	
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4:40-5:00 p.m.	<b>Highly charged protein ions: The strongest acids to date</b> <i>M. Zenaidee, W. Donald</i> UNSW, School of Chemistry, Sydney, Australia	
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3:00-5:00 p.m.	<b>WOr.09 - FTMS and innovative methods for (bio)analyses</b> <i>Chairs: Ljiljana Pasa-Tolic, Giuliana Bianco</i>	<b>Room 3</b> <b>Level 1</b>
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3:00-3:40 p.m.	<b>Mative top-down Fourier Transform mass spectrometry of proteins and protein complexes as a tool for structural biology and drug development</b> <i>J. A. Loo, H. Li, W. Jung, C. Lantz, M. Nshanian</i> University of California-Los Angeles (UCLA), Los Angeles, USA	
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3:40-4:00 p.m.	<b>Advances in Orbitrap instrumentation for analysis of high-mass proteins and protein complexes</b> <i>A. Makarov, E. Damoc, E. Denisov, K. Fort, M. van de Waterbeemd, D. Boll, D. Grinfeld, M. Reinhardt-Szyba, M. Belov, A. Heck</i> Thermo Fisher Scientific, Bremen, Germany	
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4:00-4:20 p.m.	<b>Ion traps with quadratic potentials in Fourier transform based mass spectrometry. Harmonized multi-electrode Kingdon traps and FT ICR cell</b> <i>E. Nikolaev, G. Vladimirov, O. Kharybin, V. Fernando, A. Fursova, Z. Sun, M. Sudakov, A. Lioznov</i> Skolkovo Institute of Science and Technology, Transnational Medicine and Space, Moscow, Russian Federation	
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4:20-4:40 p.m.	<b>The next dimension in proteomics</b> <i>P.Y.Y. Lam, P. B. O'Connor</i> University of Warwick, Department of Chemistry, Coventry, United Kingdom	
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4:40-5:00 p.m.	<b>Ultra-high resolution Orbitrap FTMS: implementation and applications</b> <i>Y. Tsybin, K. Nagornov, D. Kilgour, N. Gasilova, L. Menin</i> Spectroswiss, Biomolecular Mass Spectrometry, Lausanne, Switzerland	
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3:00-5:00 p.m.	<b>WOr.10 - Food additives and contaminants</b> <i>Chairs: Jose Diana Di Mavungu, Roberta Galarini</i>	<b>Room 4</b> <b>Level 1</b>
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3:00-3:40 p.m.	<b>Direct food analysis by (transportable) ambient ionization mass spectrometry</b> <i>M. W. F. Nielsen, M. Blokland, A. Gerssen, M. van Dam, G. A. Gómez-Ríos, J. Pawliszyn</i> Wageningen University & Research, Wageningen, The Netherlands	
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3:40-4:00 p.m.	<b>Gum arabic characterisation and its detection in wine using high resolution mass spectrometry</b> <i>T. Nardin, G. Ferrari, R. Larcher</i> Fondazione E. Mach, CTT, San Michele all' Adige, Italy
4:00-4:20 p.m.	<b>The fragmentation behaviour of pyrrolizidine alkaloids and its implications on food analysis</b> <i>C. Czerwenka</i> Austrian Agency for Health and Food Safety, Group for Contaminant and Special Analysis, Wien, Austria
4:20-4:40 p.m.	<b>Validation of an accurate mass screening method for pesticide residue analysis in cocoa beans and evaluation of collision cross section values using ion mobility QToF mass spectrometry</b> <i>B. H. Zainudin, S. Salleh</i> Malaysian Cocoa Board, Cocoa Downstream Technology Division, Nilai, Malaysia
4:40-5:00 p.m.	<b>The sweet deal of adding ion mobility to full scan acquisitions to profile steviol glycosides knowns and known-unknowns in food matrices</b> <i>S. Goscinny, M. Herman, W. Van Hoeck, M. McCullagh</i> Sciensano, Organic Contaminants and Additives, Brussels, Belgium

5:15-7:00 p.m.	<b>Workshops</b>
	<p><b>WKS-W1 - MS-Based Techniques for the Characterization of Nanomaterials in Food, Biological and Other Complex Matrices</b> ROOM 1 - Level 0</p> <p><b>WKS-W2 - Mass spectrometry in Microbiology</b> ROOM 2 - Level 0</p> <p><b>WKS-W3 - Advances in Protein Structure Analysis with Mass Spectrometry</b> ROOM 3 - Level 1</p> <p><b>WKS-W4 - The EU_FT-ICR_MS network</b> ROOM 4 - Level 1</p>

THURSDAY, August 30 <sup>th</sup> , 2018		
8:30-9:15 a.m.	<b>PL05: Plenary Lecture - THOMSON MEDALIST</b> <i>Chair: Renato Zenobi</i> <b>Driving innovation - From a protein sequence to a proteome</b> <i>John R. Yates</i> Department of Chemical Physiology, The Scripps Research Institute La Jolla, USA	<b>Plenary room</b> <b>Level 0</b>
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	<b>ThOr.01 - Glycomics, saccharides and glycoconjugates</b> <i>Chairs: Catherine Costello, Joseph Banoub</i>	<b>Plenary room</b> <b>Level 0</b>
9:30-10:10 a.m.	<b>Hybridation of mass spectrometry and ion spectroscopy for glycoanalytics</b> <i>I. Compagnon</i> Institut Lumière Matière, Université Lyon 1/CNRS. Villeurbanne, France	
10:10-10:30 a.m.	<b>Application of a novel functionalized resin with phenylboronic acid for capturing of glycosylated and glycosylated peptides and their MS identification</b> <i>M. Wierzbicka, M. Kijewska, M. Waliczek, F. Nuti, A. Papini, P. Stefanowicz, Z. Szewczuk</i> University of Wrocław, Faculty of Chemistry, Wrocław, Poland	

Thursday

10:30-10:50 a.m.	<b>Glycan isomer differentiation using a sialic acid derivatization toolbox for higher throughput mass spectrometric glycomics</b> <i>N. De Haan, K. Reiding, S. Holst, B. Heijs, D. Falck, G. Kammeijer, V. Dotz, M. Wuhrer</i> Leiden University Medical Center, Leiden, Netherlands
10:50-11:10 a.m.	<b>HILIC MS-HCD/FT-IT and hybrid search enhance the structure elucidation of oligosaccharides in NIST human milk reference material</b> <i>C. Remoroza, T. Mak, S. Stein</i> National Institute of Standards and Technology, Mass Spectrometry Data Center, Gaithersburg, USA
11:10-11:30 a.m.	<b>Competitive Universal Proxy Receptor Assay (CUPRA) for quantitative high-throughput glycan library screening</b> <i>J. Klassen, E. Kitova, P. Kitov, L. Han, Z. Li</i> University of Alberta, Chemistry, Edmonton, Canada

9:30-11:30 a.m.	<b>ThOr.02 - Probing Protein Structure and Dynamics</b>	<b>Room 1</b> <b>Level 0</b>
	<i>Chairs: Lars Konermann, Giancarlo la Marca</i>	
9:30-10:10 a.m.	<b>Probing the structures of native and pathological <math>\alpha</math>-synuclein species by hydrogen/deuterium exchange mass spectrometry</b> <i>T. J. D. Jørgensen, J. B. Madsen, A. L. Hemdrup, C. Sahin, D. Otzen, P. H. Jensen</i> University of Southern Denmark, Department of Biochemistry and Molecular Biology, Odense M, Denmark	
10:10-10:30 a.m.	<b>HDX-MS reveals conformational changes of IL-23 in complex with IL-23R/IL-12RB1 and phage display peptides</b> <i>H. Broughton, L. Cano, J. Dodge, I. Gonzalez, C. Michael, F. Zhang, S. Afshar, A. Espada Lilly, S.A.,</i> Centro de Investigación, Alcobendas, Spain	
10:30-10:50 a.m.	<b>Mapping conformational dynamics to binding modes in TEM-1 <math>\beta</math>-lactamase using millisecond scale ESI-MS</b> <i>R. Knox, D. Wilson</i> York University, Chemistry, Toronto, Canada	
10:50-11:10 a.m.	<b>Using mass spectrometry to examine the conformational landscape of proteins – The perfect tool to report on self solvation and the effect of charge location on structure?</b> <i>P. Barran, D. Stuchfield, L. Migas, R. Beveridge, J. Ujma, B. Bellina</i> The University of Manchester, School of Chemistry, Manchester Institute of Biotechnology, Manchester, United Kingdom	
11:10-11:30 a.m.	<b>A coarse-grained computational workflow for the elucidation of biomolecular structure and dynamics by ion mobility spectrometry-mass spectrometry</b> <i>R. D'esposito, D. Fabris</i> University at Albany, Chemistry and Biological Sciences, Albany, USA	

9:30-11:30 a.m.	<b>ThOr.03 - Organic and inorganic MS: challenges &amp; applications - Natural substances and their complexes</b>	<b>Room 2</b> <b>Level 0</b>
	<i>Chairs: Pascal Gerbaux, Luisa Mattoli</i>	
9:30-10:10 a.m.	<b>Contextualizing metabolomics data through multi-informative molecular networks: metabolite annotation and bioactive natural products prioritization strategies</b> <i>P. Allard</i> School of Pharmaceutical Sciences, EPGL, University of Geneva, University of Lausanne, CMU, Geneva, Switzerland	
10:10-10:30 a.m.	<b>New approach for the structure elucidation of (acyl)polyamines in spider venoms by UHPLC-HR-ESI-MS/MS</b> <i>Y. Forster, S. Bienz, L. Bigler</i> University of Zurich, Department of Chemistry, Zurich, Switzerland	
10:30-10:50 a.m.	<b>Glycoalkaloids in plants using high resolution mass - neutral loss approach</b> <i>T. Nardin, R. Larcher</i> Fondazione E. Mach, CTT, San Michele all'Adige, Italy	

10:50-11:10 a.m.	<b>Structural investigation of natural organic matter using direct fractionation and selective isotopic labeling coupled to FTICR MS</b> <i>A. Zherebker, Y. Kostyukevich, E. Shirshin, O. Kharybin, A. Kononikhin, I. Perminova, E. Nikolaev</i> Skolkovo Institute of Science and Technology, Translational medicine, Moscow, Russian Federation	
11:10-11:30 a.m.	<b>Evaluation of cosmetic interest of the Yellow-legged hornet venom (<i>Vespa velutina nigrithorax</i>)</b> <i>N. Le Thao, D. Da Silva, C. Colas, E. Darrouzet, P. Baril, L. L. Petit, B. Maunit</i> Institut de Chimie Organique et Analytique (ICOA), UMR 7311, Université d'Orléans-CNRS, Orléans, France	
9:30-11:30 a.m.	<b>ThOr.04 - Environmental MS</b> <i>Chairs: Encarnation Moyano, Cecilia Bergamini</i>	<b>Room 3</b> <b>Level 1</b>
9:30-10:10 a.m.	<b>Emerging contaminants: state of the art and new discoveries</b> <i>S. D. Richardson</i> University of South Carolina, Department of Chemistry & Biochemistry, Columbia, USA	
10:10-10:30 a.m.	<b>Development and optimization of a membrane-inlet-photoionization mass spectrometer for real-time analysis of (poly)aromatic compounds in aquatic systems</b> <i>C. Gehm, T. Streibel, J. Passig, D. Schulz-Bull, R. Zimmermann</i> Joint Mass Spectrometry Center, University of Rostock, Rostock, Germany	
10:30-10:50 a.m.	<b>Selective and rapid quantification of atmospheric monoterpenes</b> <i>K. Sovová, P. Pásztor, V. Shestivska, A. Spesyvyi, M. Lacko, P. Španel</i> J. Heyrovský Institute of Physical Chemistry of the CAS, v. v. i., Department of Chemistry of Ions in Gaseous Phase, Prague, Czech Republic	
10:50-11:10 a.m.	<b>Comprehensive depth profiling of Staten Island soil by GC and petroleomics</b> <i>M. Thomas, E. Collinge, M. Witt, C. Vane, M. Barrow</i> MAS CDT, University of Warwick, Coventry, United Kingdom	
11:10-11:30 a.m.	<b>New pesticide metabolites in groundwater detected using high resolution mass spectrometry</b> <i>K. Kiefer, A. Müller, H. Singer, J. Hollender</i> Eawag, Environmental Chemistry, Dübendorf, Switzerland	

9:30-11:30 a.m.	<b>ThOr.05 - Safe &amp; Valuable Food</b> <i>Chairs: Michel W.F. Nielen, Emanuela Gregori</i>	<b>Room 4</b> <b>Level 1</b>
9:30-10:10 a.m.	<b>How far can we trust untargeted HRMS-based exposomics to assess food value and safety for the consumer: the case of exposure to pesticides</b> <i>L. Debrauwer</i> INRA, UMR 1331 Toxalim, Toulouse, France	
10:10-10:30 a.m.	<b>Novel identification of 3-epi-25-hydroxyvitamin D3 in pork and beef longissimus thoracis steaks confirms the presence of this metabolite in the human food chain</b> <i>K. G. Dowling, A. Hayes, K. Galvin, S. K. Duffy, A. K. Kelly, J. V. O'doherty, K. D. Cashman</i> Cork Centre for Vitamin D and Nutrition Research, School of Food and Nutritional Sciences, University College Cork, Cork, Ireland	
10:30-10:50 a.m.	<b>Artificial Intelligence enables the detection of pathogens in food and other complex biological matrices by mass spectrometric analysis of RNA modifications</b> <i>B. Toro, R. Nemati, M. Salehi, W. McIntyre, C. Aldrich, D. Fabris</i> University at Albany, Chemistry and Biological Sciences, Albany, NY, USA	
10:50-11:10 a.m.	<b>Hydrogen/deuterium exchange is an effective method for the structural resolution of isomeric proanthocyanidins in wine and other dietary sources</b> <i>V. Merkyte, E. Longo, F. Rossetti, E. Boselli</i> Free University of Bozen - Bolzano, Faculty of Science and Technology, Bolzano, Italy	
11:10-11:30 a.m.	<b>MALDI-ToF mass spectrometry identification and detection of relevant pathogens in beef cattle</b> <i>G. Bacanelli, C. Mantovani, A. Louzan, T. Pasquatti, D. Bier, G. Rosinha, F. Araujo, N. Verbisck</i> EMBRAPA Beef Cattle, Animal Health, Campo Grande, Brazil	

11:30 a.m. - 1:00 p.m.	Coffee Break <b>Poster Sessions ThPS-S01 – ThPS-S13</b> <i>Odd numbered abstracts</i>	<i>Exhibition hall Level 0</i>
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12:30 - 1:45 p.m.	<b>Lunch Symposia</b>	
	<b>AGILENT TECHNOLOGIES</b>	Room 2 – Level 0
	<b>SHIMADZU</b>	Room 3 – Level 1
	<b>THERMO FISHER SCIENTIFIC</b>	Room 4 – Level 1
	<b>WATERS</b>	Room 1 – Level 0

1:30 - 3:00 p.m.	Coffee Break <b>Poster Sessions ThPS-S01 – ThPS-S13</b> <i>Even numbered abstracts</i>	<i>Exhibition hall Level 0</i>
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3:00-5:00 p.m.	<b>ThOr.06 - Lipidomics</b> <i>Chairs: Gavin Reid, Donatella Caruso</i>	<b>Plenary room Level 0</b>
3:00-3:40 p.m.	<b>Lipidomics analysis of cells and tissues identifies therapeutic targets</b> <i>M. Wakelam, A. Nguyen, Q. Zhang, R. Solari</i> Babraham Institute, Signalling, Cambridge, United Kingdom	
3:40-4:00 p.m.	<b>Non-subjective characterization of medulloblastoma subgroup affiliation with Desorption Electro spray Ionization Mass Spectrometry</b> <i>A. Zarrine-Afsar, M. Woolman, A. Tata, I. Ferry, C. Kuzan-Fischer, M. Wu, S. Das, M. Taylor, J. Rutka, H. Ginsberg</i> University of Toronto, University Health Network, TECHNA Institute, Toronto, Canada	
4:00-4:20 p.m.	<b>Expanding the lipidome by data-independent ozone-induced dissociation to profile complex lipid isomers</b> <i>D. Marshall, B. Poad, R. Young, S. Blanksby</i> Queensland University of Technology, Institute for Future Environments, Brisbane, Australia	
4:20-4:40 p.m.	<b>Modelling cancer lipogenesis using LA-REIMS metabolic flux analysis in breast cancer cell lines</b> <i>S. Turkseven, N. Koundouros, R. Soares, L. Doria, M. Perdones-, S. Cameron, G. Poulogiannis, Z. Takats</i> Imperial College London, Department of Surgery and Cancer, London, United Kingdom	
4:40-5:00 p.m.	<b>Relative quantification of phospholipid sn-Isomers using positive doubly charged lipid-metal ion complexes</b> <i>S. Helles, S. Becher, P. Esch</i> Justus Liebig University Giessen, Analytical Chemistry, Giessen, Germany	

3:00-5:00 p.m.	<b>ThOr.07 - Developments and applications in ion mobility MS</b> <i>Chairs: Perdita Barran, Leopoldo Ceraulo</i>	<b>Room 1 Level 0</b>
3:00-3:40 p.m.	<b>IMS-MS as a means of revealing new states during the melting of proteins</b> <i>D. Clemmer, T. El Baba, D. Woodall, S. Raab</i> School of Public Health-Bloomington, Indiana University, USA	
3:40-4:00 p.m.	<b>Probing peptide conformational rearrangements with high resolution SLIM traveling wave ion mobility-MS</b> <i>R. Wojcik, I. K. Webb, Y. M. Ibrahim, S. B. V. Garimella, R. Renslow, S. Colby, D. G. Thomas, R. D. Smith</i> PNNL, Integrative Omics, Richland, USA	
4:00-4:20 p.m.	<b>Ion mobility-derived collision cross section for mycotoxins: an interlaboratory study</b> <i>L. Righetti, L. Gethings, S. Stead, C. Dall'Asta</i> University of Parma, Department of Food and Drug, Parma, Italy	

Thursday

4:20-4:40 p.m.	<b>Practical two-dimensional high-resolution ion mobility separations using FAIMS integrated with trapped IMS</b> <i>K. Jeanne Dit Fouque, J. Porter, F. Fernandez-Lima, A. Shvartsburg</i> Wichita State University, Wichita, USA
4:40-5:00 p.m.	<b>Collision cross sections of phosphoric acid cluster anions and their use as calibrants</b> <i>V. Calabrese, H. Lavanant, F. Rosu, V. Gabelica, C. Afonso</i> Normandie Univ, UNIROUEN, INSA Rouen, CNRS, COBRA, Rouen, France

3:00-5:00 p.m.	<b>ThOr.08 - Petroleomics, hydrocarbons and biofuels</b> <i>Chairs: Alan G. Marshall, Giorgio Mellerio</i>	<b>Room 2</b> <b>Level 0</b>
3:00-3:40 p.m.	<b>The compositional and structural continuum of petroleum revealed by FT-ICR mass spectrometry</b> <i>R. P. Rodgers, M. L. Chacón-Patiño, S. M. Rowland, S. F. Niles, D. F. Smith, G. T. Blakney, Y. E. Corilo, A. M. Mckenna, A. G. Marshall, C. L. Hendrickson</i> National High Magnetic Field Laboratory, Florida State University, Tallahassee, USA	
3:40-4:00 p.m.	<b>Evidence of island and archipelago structures in distillable and truly non-distillable fractions of vacuum residues</b> <i>D. C. Palacio Lozano, A. Guzman, O. E. Mejia, M. P. Barrow</i> University of Warwick, Chemistry, Coventry, United Kingdom	
4:00-4:20 p.m.	<b>Direct inlet probe - high resolution time-of-flight mass spectrometry for the description of high boiling petroleum fractions</b> <i>U. Käfer, M. Saraji, J. Wendt, T. Wilharm, R. Zimmermann, T. Gröger</i> Helmholtz Center Munich, CMA, Munich, Germany	
4:20-4:40 p.m.	<b>Characterization of asphaltenes precipitated at different solvent power conditions using Magnetic Resonance Mass Spectrometry (MRMS)</b> <i>M. Witt, M. Godejohann, S. Oltmanns, E. Rogel</i> Bruker Daltonik GmbH, MRMS Solutions, Bremen, Germany	
4:40-5:00 p.m.	<b>Detailed molecular characterization of the upgrading process of pyrolysis oil by ultrahigh resolution mass spectrometry</b> <i>Y. Xu, Z. Cao, F. Schüth, W. Schrader</i> Max-Planck Institut für Kohlenforschung, Mass Spectrometry, Mülheim an der Ruhr, Germany	

3:00-5:00 p.m.	<b>ThOr.09 - Materials &amp; nanomaterials</b> <i>Chairs: Jan Preisler, Giuseppe Avellone</i>	<b>Room 3</b> <b>Level 1</b>
3:00-3:40 p.m.	<b>Bioimaging of nanoparticles in cells and tissue by laser ablation inductively coupled plasma mass spectrometry</b> <i>N. Jakubowski, H. Traub</i> Bundesanstalt für Materialforschung und -prüfung (BAM), Inorganic Trace Analysis, Berlin, Germany	
3:40-4:00 p.m.	<b>Nanostructured tungsten oxide substrate with oxygen vacancies for efficient Surface-Assisted Laser Desorption/Ionization mass spectrometry analysis</b> <i>Q. Ma</i> Chinese Academy of Inspection and Quarantine, Chinese Academy of Inspection and Quarantine, Beijing, China	
4:00-4:20 p.m.	<b>Supramolecular nanoreactors studied by ion mobility mass spectrometry</b> <i>E. Kalenius, T. Lee, P. Barran</i> University of Jyväskylä, Department of Chemistry, Jyväskylä, Finland	
4:20-4:40 p.m.	<b>H<sub>2</sub> detection in-situ by membrane introduction mass spectrometry</b> <i>A. Rousseau, B. Luna, H. Remita, E. Louarn</i> Laboratoire de Chimie Physique, CNRS, Univ. Paris-Sud, Université Paris-Saclay, Orsay, France	
4:40-5:00 p.m.	<b>Development of isolation techniques and capillary electrophoresis mass spectrometry (CESI-MS) methods for the characterisation of nanomaterial protein coronas</b> <i>K. Faserl, A. Chetwynd, I. Lynch, J. Thorn, H. Lindner</i> AB Sciex UK Ltd, Separations, Warrington, United Kingdom	

3:00-5:00 p.m.	<b>ThOr.10 - Novel food; nanoparticles in food and beverage; future applications</b> <i>Chairs: Stefan Weigel, Giovanni Sindona</i>	<b>Room 4 Level 1</b>
3:00-3:40 p.m.	<b>Mass spectrometric detection and characterisation of nanoparticles</b> <i>R. Peters, A. Undas, M. van der Lee</i> RIKILT Wageningen University & Research, Wageningen, The Netherlands	
3:40-4:00 p.m.	<b>How to manage matrix effects for accurate nanoparticle sizing using single-particle ICP-ToF MS?</b> <i>L. Hendriks, A. Gundlach-Graham, D. Günther</i> ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland	
4:00-4:20 p.m.	<b>Use of ICP-MS-based techniques for the characterization of nanomaterials used in food-related applications</b> <i>F. Aureli, F. Ferraris, S. Savini, A. Raggi, F. Cubadda</i> Istituto Superiore di Sanità - National Institute of Health, Rome, Italy	
4:20-4:40 p.m.	<b>Translating into practice the EFSA Guidance on risk assessment of the application of nanotechnologies in the food chain: the role of mass spectrometry</b> <i>F. Aureli, F. Ferraris, S. Savini, A. Raggi, F. Cubadda</i> Istituto Superiore di Sanità - National Institute of Health, Rome, Italy	
4:40-5:00 p.m.		
8:00 p.m.	<b>Conference dinner</b>	

## FRIDAY, August 31<sup>st</sup>, 2018

8:30-9:15 a.m.	<b>PL06: Plenary Lecture</b> <b>Mass spectrometry and theoretical chemistry in service of catalysis research: a ménage-à-trois at its best</b> <i>Chair: Simonetta Fornarini</i> <b>Helmut Schwarz</b> Institut für Chemie, Technische Universität Berlin, Berlin, Germany	<b>Plenary room Level 0</b>
9:15-9:30 a.m.	Break	
9:30-11:30 a.m.	<b>FOr.01 - Life sciences - Metabolomics</b> <i>Chairs: Ulf Sommer, Donatella Caruso</i>	<b>Plenary room Level 0</b>
9:30-10:10 a.m.	<b>Metabolomics and the exposome - Application to cancer epidemiology</b> <i>A. Scalbert</i> International Agency for Research on Cancer (IARC), Biomarkers Group, Nutrition and Metabolism Section, Lyon, France	
10:10-10:30 a.m.	<b>Targeted on-line breath analysis supports the hypothesis of altered collagen turnover in idiopathic pulmonary fibrosis</b> <i>M. T. Gaugg, A. Engler, S. P. Martinez-Lozano, L. Bregy, Y. Nussbaumer-Ochsner, L. Eiffert, T. Bruderer, R. Zenobi, M. Kohler</i> ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland	
10:30-10:50 a.m.	<b>Targeted metabolomic analysis of urine for improving the diagnosis of asthma and COPD</b> <i>M. Khamis, H. Awad, K. Allen, D. Adamko, A. El-Aneed</i> University of Saskatchewan, College of Pharmacy and Nutrition, Saskatoon, Canada	



10:50-11:10 a.m.	<b>In vivo real-time monitoring system for metabolites in a living mouse brain using probe electrospray ionization/tandem mass spectrometry (PESI/MS/MS)</b> <i>K. Zaitso</i> Nagoya University, In Vivo Real-time Omics Laboratory, Institute for Advanced Research, Nagoya, Japan	
11:10-11:30 a.m.	<b>Energy metabolism in age-related diseases: focus on mitochondria</b> <i>N. Mitro, D. Caruso</i> Università degli Studi di Milano, Department of Pharmacological and Biomelecular Sciences, Milano, Italy	
9:30-11:30 a.m.	<b>FOr.02 - Informatics tools and data analysis</b> <i>Chairs: Peter O'Connor, Giuseppe Avellone</i>	<b>Room 1 Level 0</b>
9:30-10:10 a.m.	<b>Leveraging new algorithmics for better MS spectra</b> <i>M.-A. Delsuc</i> IGBMC, Illkirch, France	
10:10-10:30 a.m.	<b>Advanced mass spectrometry methods for unravelling the mechanisms of organophosphate toxicity</b> <i>H. Wang, M. Leeming, B. Cochran, W. Donald</i> University of New South Wales, School of Chemistry, UNSW, Sydney, Australia	
10:30-10:50 a.m.	<b>Algorithm for processing complex mixture data from hyphenated ultrahigh resolution mass spectrometry</b> <i>R. Gavard, H. Jones, D. Rossell, S. Spencer, M. Barrow</i> University of Warwick, MAS CDT, Coventry, United Kingdom	
10:50-11:10 a.m.	<b>LC-MS<sup>1</sup> method for protein identification and quantitation without using tandem mass spectra</b> <i>M. Ivanov, I. Tarasova, E. Solovyeva, M. Gorshkov</i> V.L. Talrose Institute for Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russian Federation	
11:10-11:30 a.m.	<b>Phase-constrained spectrum deconvolution-real time super-resolution processing of FTMS data</b> <i>K. Aizikov, D. Grinfeld, A. Kreuzmann, D. Mourad, E. Damoc, T. N. Arrey, O. Lange, A. Makarov</i> ThermoFisher Scientific, LSMS, Bremen, Germany	
9:30-11:30 a.m.	<b>FOr.03 - Cultural heritage and archaeology</b> <i>Chairs: Klaas Jan van den Berg, Giorgio Mellerio</i>	<b>Room 2 Level 0</b>
9:30-10:10 a.m.	<b>Art and cultural heritage natural polymers by bottom up and top down approaches</b> <i>C. Tokarski</i> Université de Lille 1 Sciences et Technologies, Villeneuve d'Ascq, France	
10:10-10:30 a.m.	<b>Fast analysis of modern oil paintings and dyes in textiles by surface acoustic wave nebulization-mass spectrometry (SAWN-MS)</b> <i>A. Astefanei, M. van Bommel, K. J. van den Berg, G. Corthals</i> University of Amsterdam, HIMS, Analytical Chemistry, Amsterdam, Netherlands	
10:30-10:50 a.m.	<b>Molecular signatures of protein aging in ancient human bones from the eruption area of Vesuvius</b> <i>G. Ntasi, P. Pucci, G. Marino, L. Birolo</i> University of Naples Federico II, Chemical Sciences, Naples, Italy	
10:50-11:10 a.m.	<b>Characterization of isobaric species and photo-degradation products of triarylmethane dyes within textiles</b> <i>F. Sabatini, C. Bracini, A. Quye, I. Degano, M. P. Colombini</i> University of Pisa, Department of Chemistry and Industrial Chemistry, Pisa, Italy	
11:10-11:30 a.m.	<b>Wine production and consumption in pre Roman times: residue analysis of a production structure an ceramic vessels from the Western Mediterranean</b> <i>A. Peccj, A. Zifferero, G. Giorgi, S. Mileto, R. Jornet, C. Belarte Franco, A. De Palmas, M. Vidale</i> ERAAUB, Departament Història i Arqueologia, Universitat de Barcelona, Spain	

9:30-11:30 a.m.	<b>FOr.04 - Atomic mass spectrometry: metallomics and isotope ratio mass spectrometry</b> <i>Chairs: Ryszard Lobinski, Federica Camin</i>	<b>Room 3 Level 1</b>
9:30-10:10 a.m.	<b>New ion sources for metallomic analysis and isotope-ratio mass spectrometry</b> <u>G. M. Hieftje</u> Indiana University, Department of Chemistry, Bloomington, USA	
10:10-10:30 a.m.	<b>Element analysis with thermalized laser ablation ions from solid samples</b> <u>L. Querci</u> , <u>B. Hattendorf</u> , <u>D. Günther</u> ETH Zürich, Laboratory of Inorganic Chemistry, Zurich, Switzerland	
10:30-10:50 a.m.	<b>High-resolution and tandem mass spectrometry techniques contribute to the discovery of new arsenic metabolites of toxicological importance</b> <u>Q. Liu</u> , <u>X. Lu</u> , <u>H. Peng</u> , <u>E. Leslie</u> , <u>M. Zuidhof</u> , <u>X.-F. Li</u> , <u>X. C. Le</u> University of Alberta, Analytical and Environmental Toxicology, Edmonton, Canada	
10:50-11:10 a.m.	<b>Isotopic techniques for studying the sources and processes of pollutants in the environment</b> <u>N. Ogrinc</u> Jožef Stefan Institute Department of Environmental Sciences, Ljubljana, Slovenia	
11:10-11:30 a.m.	<b>Potential use of the stable isotope ratios of bioelements and elemental composition to trace the origin of dairy products</b> <u>L. Bontempo</u> , <u>F. Camin</u> Fondazione E. Mach, Food Quality and Nutrition Department, San Michele all'Adige, Italy	

9:30-11:30 a.m.	<b>FOr.05 - Nutraceuticals directions</b> <i>Chairs: Roberto Romero Gonzalez, Roberta Galarini</i>	<b>Room 4 Level 1</b>
9:30-10:10 a.m.	<b>Medicinal extremophile plants: valuable source of "GRAS" and health promoting biomolecules with medical, nutraceutical and food applications</b> <u>K. Riadh</u> Laboratory of Aromatic and Medicinal Plants, CBBC, BP901, Hammam-Lif, Tunisia	
10:10-10:30 a.m.	<b>Ancient apple of Friuli Venezia Giulia region as potential new nutraceutical ingredients</b> <u>S. Sut</u> , <u>S. Dall'Acqua</u> University of Padova, Dept. of Pharmaceutical and Pharmacological Sciences, Padova, Italy	
10:30-10:50 a.m.	<b>Putting pigment to paper. The quantitation of bioactive anthocyanins in fruits and nutraceuticals with paper spray ionization mass spectrometry</b> <u>R. Cody</u> , <u>J. Tamura</u> , <u>K. Downard</u> University of New South Wales, Medicine, Sydney, Australia	
10:50-11:10 a.m.	<b>Reliable identification of bioactive compounds in foodstuffs through the use of a novel dual-filter mass spectral library in liquid chromatography</b> <u>F. Rigano</u> , <u>M. Oteri</u> , <u>P. Dugo</u> , <u>L. Mondello</u> Chromaleont Srl, c/o Dipartimento ChiBioFarAm, University of Messina, Messina, Italy	
11:10-11:30 a.m.	<b>Antioxidant activities and phytochemical profile of <i>Azorella glabra</i></b> <u>I. Faraone</u> , <u>D. K. Ray</u> , <u>L. Chiummiento</u> , <u>A. Choudhary</u> , <u>D. Russo</u> , <u>C. Sinisgalli</u> , <u>E. Fernandez</u> , <u>L. Milella</u> University of Basilicata, Department of Science, Potenza, Italy	
11:30-11:45 a.m.	Break	
11:45 a.m. - 12:15 p.m.	<b>Presentation of IMSC 2020</b>	
12:15-1:00 p.m.	Arrivederci & farewell drinks	

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## POSTER SESSIONS

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Odd numbers: 11:30 a.m.- 1:00 p.m.

Even numbers: 1:30 p.m.- 3:00 p.m.

Poster set up: 8:00-8:30 a.m.

Poster removal: 6:00-7:00 p.m.

MONDAY, August 27<sup>th</sup>, 2018

### MPS-S01 - Nucleic Acids

- MP-1**      **Characterization of LILBID-MS using DNA structures**  
*G. Hense, P. Young, N. Morgner*  
 AK Morgner, Physical and Theoretical Chemistry at the Goethe University, Frankfurt am Main, Germany
- MP-2**      **The simultaneous determination of intracellular nucleoside triphosphates and cyclic dinucleotides with LC-MS/MS**  
*R. Oertel, R. Behrendt, A. El-Armouche*  
 Institute of Clinical Pharmacology, GWT TU Dresden, Dresden, Germany
- MP-3**      **Semi-quantitative determination of oligonucleotide drug impurities: main and co-eluting species**  
*S. Roussis*  
 Ionis Pharmaceuticals, ADQC, Carlsbad, USA
- MP-4**      **Interactions of oxaliplatin and carboplatin with DNA building blocks as studied in the gas phase: a combined experimental and theoretical study**  
*J.-Y. Salpin, M. E. Crestoni, D. Corinti, S. Fornarini, D. Scuderi, B. Chiavarino*  
 CNRS, LAMBE - UMR 8587 - Université d'Evry Val d'Essonne, Evry, France
- MP-5**      **Development of the LC-MS method for the analysis and characterization chemically modified RNA**  
*D. Strzelecka, M. Smietanski, M. Warminski, P. Sikorski, J. Jemiellity, J. Kowalska*  
 University of Warsaw, Faculty of Physics, Warsaw, Poland
- MP-6**      **Solution and gas-phase structures of DNA G-quadruplexes: ion mobility mass spectrometry, solution spectroscopy, and collision cross section calculations**  
*A. Ghosh, F. Rosu, V. Gabelica*  
 INSERM, University of Bordeaux/IECB, Pessac, France

### MPS-S02 - Clinical Proteomics

- MP-7**      **Cluster-assembled smart surfaces for on-target processing of biological samples in MALDI-MS analysis**  
*E. Barborini, S. Vinati, G. Bertolini, M. Baumann*  
 Tethis SpA, R&D, Milan, Italy
- MP-8**      **Proteome profiling of bronchioalveolar lavage fluid after exposure to magnetic iron and cobalt oxide nanoparticles**  
*A. M. Billing, K. B. Knudsen, U. Vogel, F. Kjeldsen*  
 University of Southern Denmark, Department of Biochemistry and Molecular Biology, Odense, Denmark

- MP-9**      **Concurrent quantification of synaptotagmin-1 and SNAP-25 in clinically relevant volumes of CSF by immunoaffinity LC-MS/MS**  
*A. Brinkmalm, A. Öhrfelt, L. Frölich, L. Hausner, H. Zetterberg, K. Blennow*  
 The Sahlgrenska Academy at University of Gothenburg, Institute of Neuroscience and Physiology, Department of Psychiatry and Neurochemistry, Mölndal, Sweden
- MP-10**      **Single shot DIA profiling of >1500 plasma proteomes of the weight loss and maintenance study DiOGenes**  
*R. Bruderer, J. Muntel, S. Müller, O. M. Bernhardt, T. Gandhi, P. Mironova, O. Walter, J. Carayol, A. Astrup, W. H.M. Saris, J. Hager, A. Valsesia, L. Dayon, L. Reiter*  
 Biognosys AG, Schlieren, Switzerland
- MP-11**      **Identification of complete pool of bio active peptides in mouse brain striatum including SEPs, a novel class of non-classical bio active peptides**  
*H. Budamgunta*  
 Center for proteomics, University of Antwerp/Biology, Antwerp, Belgium
- MP-12**      **Proteomic characterization of human platelet lysate by label-free nLC-MS/MS: towards the effectors of its beneficial effect in regenerative medicine**  
*C. Chinello, F. Re, C. Almici, A. James Smith, F. Paolella, G. Lisignoli, I. Piga, M. Stella, M. Mazza, V. Denti, L. Sartore, D. Russo, F. Magni*  
 University of Milano-Bicocca, Department of Medicine and Surgery, Clinical Proteomics and Metabolomics Unit, Veduggio al Lambro, Italy
- MP-13**      **Validation of a LC-MS assay for assessment of alpha-defensin in synovial fluid**  
*R. Dall'Anese, P. Pezzati, M. Quercioli, F. Balboni, G. Balato, A. Baldini, G. Bartolini*  
 Buzzi Lab, Analytical chemistry, Prato, Italy
- MP-14**      **Mass spectrometry evaluation of circulating S100A8 and S100A9 proteins as prognosis biomarkers in sepsis**  
*C. Dubois, D. Payen, V. Faivre, S. Simon, F. Fenaille, C. Junot, N. Morel, F. Becher*  
 Service de Pharmacologie et Immunoanalyse (SPI), Laboratoire d'Etude du Métabolisme des Médicaments (LEMM), CEA, INRA, Université Paris Saclay, Gif-sur-Yvette CEDEX, France
- MP-15**      **Characterization of the PIF peptide (preimplantation factor) interactome in human serum**  
*A. Fel, P. Czaplewska, K. Macur, M. Thiel, K. Lukaszuk, S. Oldziej*  
 University of Gdansk, Intercollegiate Faculty of Biotechnology, and Medical University of Gdansk, Gdansk, Poland
- MP-16**      **Molecular fingerprinting of the interstitium proteome in the vastus lateralis muscle in women with fibromyalgia compared to healthy controls using MD-LC-MS/MS**  
*B. Ghafouri, M. Turkina, N. Christidis, K. Mannerkorpi, E. Kosek, M. Ernberg, B. Gerdle*  
 Linköping University, Department of medical and health sciences, Linköping, Sweden
- MP-17**      **Deep proteomics of saw-scaled viper (*Echis carinatus sochureki*) venom by integrated top-down and bottom-up mass spectrometric approaches**  
*P. Ghezellou, V. Garikapati, S. M. Kazemi, K. Strupat, A. Ghassempour, B. Spengler*  
 Justus Liebig Giessen University, Institute of Inorganic and Analytical Chemistry, Giessen, Germany
- MP-18**      **Differential proteome analysis of human neuroblastoma xenograft primary tumors and matched spontaneous distant metastases**  
*L. Haenel, H. Schlüter, L. Heikaus, T. Lange*  
 University Medical Center Hamburg-Eppendorf, Institute of Clinical Chemistry and Laboratory Medicine, Hamburg, Germany
- MP-19**      **Biomarker candidates for acute myocardial infarction in human serum**  
*M.-J. Kang, Y. Seong*  
 Korea Institute of Science and Technology, Molecular Recognition Research Center, Seoul, Republic of Korea
- MP-20**      **Rheumatoid factor-correlated proteins is complementary biomarker of rheumatoid arthritis**  
*H.-G. Kang, S. Mun, A. Park, A. Seok, Y. Lee, H. Kim, Y. Lee*  
 Eulji University, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Daejeon, Republic of Korea

- MP-21 Novel biomarker discovery in extracellular vesicles from plasma for colorectal cancer**  
*K. Kasahara, R. Narumi, Y. Shimizu, K. Masuda, S. Nagayama, T. Tomonaga, Y. Sakai, J. Adachi*  
 National Institute of Biomedical Innovation, Health and Nutrition, Laboratory of Proteome Research, Osaka, Japan
- MP-22 Quantitative proteomic analysis of cervicovaginal fluid proteome using a 2D-nLC-ESI-MS/MS for early detection of preterm birth**  
*Y. E. Kim, K. Kim, D. Kang*  
 Center of Bioanalysis, Korea Research Institute of Standards and Science, Daejeon, Republic of Korea
- MP-23 Antibody-free LC-MS methods for low to sub ng/mL quantification of the soluble Receptor for Advanced Glycation End-products (sRAGE) in serum**  
*F. Klont, S. D. Pouwels, M. Hadderingh, M. R. Joosten, J. Hermans, N.C. van de Merbel, P. Horvatovich, N.H.T. ten Hacken, R. Bischoff*  
 University of Groningen, Department of Analytical Biochemistry, Groningen, Netherlands
- MP-24 Proteome analysis of human neuromelanin granules and neurons in the context of dementia with Lewy bodies**  
*S. Kösters, S. Plum, C. May, K. Marcus*  
 Medizinisches Proteom-Center, Ruhr-University Bochum, Bochum, Germany
- MP-25 Proteomic profiling of melanoma cell lines and tissue using data independent acquisition mass spectrometry to predict treatment response and patient survival**  
*C. Krisp, R. Parker, D. Pascovici, N. K. Hayward, J. S. Wilmott, R. A. Scolyer, M. P. Molloy*  
 Australian Proteome Analysis Facility, Macquarie University, Sydney, Australia
- MP-26 Unveiling the outer membrane vesicle proteome of *A. salmonicida*: a physiological insight**  
*T. Kroniger, A. Otto, B. Köllner, D. Becher*  
 University of Greifswald, Institute for Microbiology, Greifswald, Germany
- MP-27 Quantitation of monoclonal antibody infliximab in human plasma by LC-MS/MS using Fab-selective limited proteolysis nSMOL technology**  
*N. Loftus, A. Barnes, A. Jaffuel*  
 Shimadzu, MS/BU, Manchester, United Kingdom
- MP-28 Top down mass spectrometry with multiple MS/MS strategies to identify age-related proteoform changes in tear fluid**  
*D. Lopez-Ferrer, R. Huguet, D. Horn, P. P. M. Raus, V. Zabrouskov, A. Huhmer, P. Dem Verhaert*  
 Thermo Fisher Scientific, San Jose, USA
- MP-29 Advances in clinical proteomics for analysis of thyroid fine needle aspiration biopsies: evaluating proteomic stability in preservative solutions**  
*I. Piga, G. Capitoli, S. Tettamanti, V. Denti, A. Smith, C. Chinello, M. Stella, D. Leni, M. Garancini, S. Galimberti, F. Magni, F. Pagni*  
 University of Milano-Bicocca, Department of Medicine and Surgery - Clinical Proteomics and Metabolomics Unit, Vedano al Lambro, Italy
- MP-30 Quantification of endogenous VEGFA levels from human plasma using nanoLC/high resolution mass spectrometry combined with immunocapture enrichment**  
*S. Pleiner, K. Koehler, J. Hoke, S. Keller*  
 Boehringer Ingelheim Pharma GmbH & Co. KG, DMPK, Biberach a. d. Riss, Germany
- MP-31 Characterization of the modification in mitochondrial proteome due to eIF6 depletion by SWATH-MS analysis and multivariate statistical tools**  
*E. Robotti, M. Manfredi, S. Martinotti, D. Brina, A. Scagliola, E. Ranzato, E. Marengo, S. Biffo*  
 University of Piemonte Orientale, Department of Sciences and Technological Innovation, Alessandria, Italy
- MP-32 Label-free proteomic analysis of urinary exosomes from patients with cc-Renal Cell Carcinoma: stage-specific differential protein profile**  
*L. Santorelli, F. Raimondo, C. Chinello, F. Magni, M. Grasso, G. Bovo, M. Pitto*  
 University of Milano-Bicocca, Department of Medicine and Surgery, Vedano al Lambro, Italy
- MP-33 Maximized throughput and analytical depth for shotgun proteomics using PASEF on a TIMS equipped QToF and a novel LC system**  
*T. Kosinsky, S. Koch, M. Lubeck, P. Schmit, N. Bache, O. Bjeld Horning, L. Falkenby, H. Koch, L. Woods*  
 Bruker France, Proteomics, Wissembourg, France

- MP-34 Targeted quantitation of proteins for discriminating obese from normal-weight adolescents by liquid chromatography-mass spectrometry**  
*H. Shin, K. Dan, S. Song, D. Han*  
Seoul National University Hospital, Biomedical Research Institute, Seoul, Republic of Korea
- MP-35 Development of a sandwich ELISA for the thrombin light chain identified by serum proteome analysis**  
*K. Sogawa, M. Miyahara, S. Yamanaka, S. Takano, H. Yoshitomi, M. Miyazaki, M. Ohtsuka, F. Nomura*  
Azabu University, Biochemistry, Kanagawa, Japan
- MP-36 Use of the MALDI BioTyper system with MALDI-ToF MS for rapid identification of microorganisms causing bacterial urinary tract infection from urine samples**  
*M. Yano, K. Sogawa, H. Maeda*  
Azabu University, Biochemistry, Kanagawa, Japan
- MP-37 Topological distribution of lipid biomarkers in adipose tissue of metabolic-healthy and unhealthy subjects**  
*R. Tans, R. Bande, A. van Rooij, B. Molloy, R. Heeren, R. Stienstra, C. Tack, H. Wessels, A. van Gool*  
Radboud University Medical Center, Translational Metabolic Laboratory, Nijmegen, Netherlands
- MP-38 LC-MS/MS-based characterization of glioblastoma cell responses to type I interferons for establishing defects in antiviral mechanisms**  
*I. Tarasova, A. Tereshkova, E. Solovyeva, J. Bubis, V. Gorshkov, F. Kjeldsen, I. Ilina, S. Moshkovskii, P. Chumakov, M. Gorshkov*  
RAS, Talrose Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation
- MP-39 Epitope identification of glycosylated HSA and the extracellular region of human RAGE by SPR and affinity-MS spectrometry**  
*A. Tamarin, M. Naldi, L. Lupu, P. Wiegand, E. Fabini, G. Degani, L. Popolo, G. Aldini, M. Przybylski, M. Bartolini*  
Alma Mater Studiorum, University of Bologna, Department of Pharmacy and Biotechnology, Bologna, Italy
- MP-40 The molecular pattern of plasma proteins and their correlation to pain intensity and sensitivity in women with fibromyalgia – a multi-center study**  
*K. Wählén, B. Gerdle, K. Mannerkorpi, E. Kosek, M. Ernberg, B. Ghafouri*  
Linköping University, Department of medical and health sciences, Linköping, Sweden
- MP-41 Therapeutic proteins in sports drug testing: detection of different ActRII inhibitors in serum by means of (immuno-)affinity purification, tryptic digestion, and LC-HRMS**  
*K. Walpurgis, A. Thomas, C. Reichel, F. Dellanna, M. Thevis*  
German Sport University Cologne, Institute of Biochemistry/Center for Preventive Doping Research, Cologne, Germany
- MP-42 A novel high-throughput antibody-free LC-MS/MS assay to quantitate Chromogranin-A in serum**  
*D. Weber, S. Goldman, M. McPhaul, M. Caulfield, N. Clarke*  
Quest Diagnostics, R&D Mass Spectrometry, San Juan Capistrano, USA
- MP-43 Exosomes purification for new biomarkers discovery in cancer**  
*F. Anastasi, M. Cecchini, L. A. McDonnell*  
Laboratorio NEST, Scuola Normale Superiore, Pisa, Italy
- MP-44 Development of a novel LC concept for clinical proteomics**  
*N. Bache, P. Geyer, C. Ravensborg, O. Hoerning, L. Falkenby, P. Treit, S. Doll, I. Paron, F. Meier, O. Vorm, M. Mann*  
Evosep, Odense, Denmark
- MP-45 Analysis and characterization of gastrointestinal metabolism of major soy allergens glycinin and  $\beta$ -conglycinin in an in-vitro model by LC-MS/MS**  
*J. Bräcker, N. Lok, J. Brockmeyer*  
University of Stuttgart, Food Chemistry, Stuttgart, Germany
- MP-46 Proteomic profiling of extracellular vesicles derived from mesenchymal stromal cells**  
*J. Brandi*  
University of Verona, Department of Biotechnology, Verona, Italy

- MP-47**     **Differentiation of hypertensive disorders during pregnancy based on urine peptidome profiling by high resolution mass spectrometry**  
*A. Bugrova, A. Kononikhin, V. Sergeeva, M. Indeykina, I. Popov, N. Starodubtseva, V. Frankevich, E. Nikolaev*  
 Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russian Federation
- MP-48**     **Comparative analysis of lectin based glycoproteins between yoga groups**  
*J. Kang, Y. Jung, W. Cho*  
 Wonkwang University, Department of Chemistry, Iksan, Republic of Korea
- MP-49**     **Serum protein classifiers of ALS for disease etiology and progression**  
*S. Filip, T. Sosnowski, I. Dervishi, Y. A. Goo, P. H. Ozdinler*  
 Northwestern University, Proteomics Center of Excellence, Chicago, USA
- MP-50**     **Blood plasma proteome and peptidome comparative screening for potential biomarkers of Alzheimer's disease**  
*M. Indeykina, A. Bugrova, N. Zakharova, A. Kononikhin, Y. Fedorova, A. Brhozovskiy, I. Popov, S. Gavrilova, E. Nikolaev*  
 Emanuel Institute of Biochemical Physics of the Russian Academy of Sciences, Laboratory for Mass Spectrometry of Biomacromolecules, Moscow, Russian Federation
- MP-51**     **A online 2D-NCFC-RP/RPLC system for comprehensive and high-throughput proteomics analysis**  
*H. Lee, S. Lee*  
 Korea University, Chemistry, Seoul, Republic of Korea

### **MPS-S03 - Ion Spectroscopy & Photodissociation**

- MP-52**     **Structural elucidation of metabolites using infrared ion spectroscopy**  
*H. Bentlage, J. Martens, G. Berden, R. Wevers, J. Oomens*  
 FELIX, Radboud University, Nijmegen, Netherlands
- MP-53**     **Infrared ion spectroscopy of metal-ligand redox pairs generated via electron transfer reduction reactions**  
*M. Munshi, J. Martens, G. Berden, J. Oomens*  
 FELIX, Radboud University, Nijmegen, Netherlands
- MP-54**     **Counter cation-dependent action spectroscopy of IR-797 and IR-806 cyanine dyes**  
*M. Herve, R. Bredy, G. Karras, B. Concina, F. Lepine, I. Compagnon*  
 University of Lyon, Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, Villeurbanne, France
- MP-55**     **Ion mobility spectrometry and gas phase spectroscopy of mass and isomer selected porphyrin anions**  
*K. Brendle, P. Weis, M. M. Kappes*  
 Karlsruhe Institute of Technology, Institute of Physical Chemistry, Karlsruhe, Germany
- MP-56**     **REMPI and MATI spectroscopy of methyl and halo pyridines**  
*N. Helle, J. Grotemeyer*  
 Institute of Physical Chemistry, CAU Kiel, Kiel, Germany
- MP-57**     **Action Spectroscopy without a trap: on-the-fly spectroscopy of IR-797 and IR-806 cyanine dyes**  
*M. Herve, R. Bredy, G. Karras, B. Concina, A. R. Allouche, F. Lepine, I. Compagnon*  
 Institut Lumière Matière (ILM), Université Lyon 1, Lyon, France
- MP-58**     **IR tagging pre-dissociation spectroscopy to reveal isomeric composition**  
*P. Jusko, A. Simon, G. Wenzel, S. Brünken, S. Schlemmer, C. Joblin*  
 Institut de Recherche en Astrophysique et Planétologie (IRAP), Université de Toulouse, CNRS, CNES, Toulouse, France
- MP-59**     **Validation of an IRMPD experimental setup and theoretical methods for IRMPD assignment**  
*A. F. Rodrigues-Oliveira, F. W. M. Ribeiro, G. Cervi, T. C. Correra*  
 University of São Paulo, Institute of Chemistry, São Paulo, Brazil
- MP-60**     **Infrared Multiple Photon Dissociation of copper formate clusters**  
*T. Pascher, M. Ončák, C. Van Der Linde, J. Lengyel, M. K. Beyer*  
 Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik, Innsbruck, Austria

- MP-61 Development of a 3D ion trap mass spectrometer for IRMPD spectroscopy**  
*T. C. Penna, G. Cervi, A. F. Rodrigues-Oliveira, J. Menegon, T. C. Correra*  
 Universidade de São Paulo, Instituto de Química, São Paulo, Brazil
- MP-62 Photoisomerization action spectroscopy of a ruthenium sulfoxide complex**  
*M. Scholz, J. Bull, E. Carrascosa, G. Kosgei, J. Rack, E. Bieske*  
 University of Melbourne, School of Chemistry, Parkville, Australia
- MP-63 Photochemistry of  $Mg^+(H_2O)_n$ ,  $n=1-5$ : experiment and theory**  
*T. Taxer, M. Oncak, C. van der Linde, E. Barwa, M. Beyer*  
 Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik, Innsbruck, Austria
- MP-64 Shedding light on structure: initial protein unfolding events revealed by 213 nm UVPD**  
*A. Theisen, R. Black, D. Corinti, J. Brown, B. Bellina, P. Barran*  
 University of Manchester, Manchester Institute of Biotechnology and Photon Science Institute, Manchester, United Kingdom
- MP-65 IRMPD spectra of protonated hydroxybenzaldehydes: the evidence of the torsional barriers in carboxonium ions**  
*B. Chiavarino, M. E. Crestoni, O. Dopfer, P. Maitre, S. Fornarini*  
 Università di Roma "La Sapienza", Dipartimento di Chimica e Tecnologie del Farmaco, Roma, Italy
- MP-66 Valence and core electron induced photoionization and dissociation dynamics of the thiazole molecule**  
*A. F. Lago, R. D. Januario, R. L. Cavasso-Filho, M. Simon, J. Z. Dávalos*  
 Federal University of ABC (UFABC), Center for Natural Sciences and Humanities (CCNH), Santo Andre, Brazil
- MP-67 Relevance of the gas-phase studies to biology: cold ion spectroscopy of the opioid peptide drugs**  
*A. Y. Pereverzev, V. N. Kopysov, I. Szabo, E. Rosta, O. V. Boyarkin*  
 EPFL, LCPM, Lausanne, Switzerland
- MP-68 The use of peptide bonds for cold ion spectroscopy**  
*A. Y. Pereverzev, V. N. Kopysov, O. V. Boyarkin*  
 EPFL, LCPM, Lausanne, Switzerland
- MP-69 Action spectroscopy of flavins**  
*M. Stockett, L. Giacomozzi, H. Zettergren, C. Kjær, J. Langeland Knudsen, L. Andersen, S. Brøndsted Nielsen, J. Bull, E. Carrascosa, E. Bieske*  
 Stockholm University, Department of Physics, Stockholm, Sweden

### MPS-S04 - Hyphenated Techniques

- MP-70 Speeding up GC-MS analysis – From few minutes down to real-time analysis**  
*A. B. Fialkov, U. Keshet, T. Alon, A. Amirav*  
 School of Chemistry, Tel Aviv University, Tel Aviv, Israel
- MP-71 Development of comprehensive steroid analysis methods using GCxGC-ToFMS**  
*V. Artaev, D. Alonso, J. Shiel, G. Tikhonov, A. Lebedev*  
 LECO Corporation, St. Joseph, USA
- MP-72 Using electrokinetic injection to increase throughput and improve sensitivity in the detection of proteins by CE-MS**  
*W. Belloni*  
 Sciex Spa, Separations CE, Milano, Italy
- MP-73 Multivariate study of matrix effect in the analysis of phytoestrogens in soy-food by LC-ESI-MS/MS**  
*B. Benedetti, M. Di Carro, E. Magi*  
 University of Genova, Department of Chemistry and Industrial Chemistry, Genova, Italy
- MP-74 Application of SPME GC-MS to explore possible differences in free-lactose milks from the market**  
*R. Bottioli, E. Aprea, E. Betta, F. Gasperi*  
 Edmund Mach Foundation, Food Quality and Nutrition Department, San Michele all'Adige, Italy



- MP-75 Post-column in-source derivatization in LC-MS: a tool for natural products characterization and metabolomics**  
*A. Cirigliano, G. M. Cabrera*  
 DQO, FCEN, Universidad de Buenos Aires, UMYMFOR-DQO, UBA-CONICET, Buenos Aires, Argentina
- MP-76 Conjugation among nucleotides and cyanocobalamin functionalized with cisplatin: a study by liquid chromatography coupled with ESI and multistage MS**  
*G. Ventura, C. D. Calvano, A. Viola, V. Cinquepalmi, F. Palmisano, T. Cataldi*  
 University of Bari, Dept. of Chemistry, Bari, Italy
- MP-77 Analytical method for quantification of bixin in extract of annatto using V-EASI(-)-LC-MS a method softer than ESI-LC-MS**  
*L. F. C. Oliveira, D. U. Tega, M. B. Coelho, D. R. Morais, M. Baptista, M. N. Eberlin*  
 UNICAMP, Chemistry Institute, Campinas, Brazil
- MP-78 Thin layer chromatography combined with Flame-Induced Atmospheric Pressure Chemical Ionization Mass Spectrometry (FAPCI/MS) for volatile and semi-volatile compound analysis**  
*S. Cheng, J. Shiea*  
 National Sun Yat-sen University, Department of Chemistry, Kaohsiung, Taiwan, Province of China
- MP-79 Evaluation of gas chromatography coupled to electrospray-atmospheric pressure photon ionization Orbitrap mass spectrometry as an advanced strategy for polyaromatic hydrocarbon analysis**  
*Y. Cho, E. Cho, S. Kim*  
 Green-Nano Material Research Center, Kyungpook National University/Chemistry, Daegu, Republic of Korea
- MP-80 Online coupling of non-denaturing chromatography to native mass spectrometry is no more an impossible marriage**  
*A. Etkirch, O. Hernandez-Alba, T. Botzanowski, S. Cianféran*  
 LSMBO/IPHC, University of Strasbourg, CNRS UMR7178, Strasbourg, France
- MP-81 Identification and time variation analysis of perfume by using GCxGC/HRTofMS with EI/FI/PI**  
*R. Cody, M. C. Long, A. Dane, K. Okuda*  
 JEOL USA, Inc., Mass Spectrometry, Peabody, USA
- MP-82 Seconds-per-sample: novel acoustic hyphenated approaches to enable truly label-free ultra high-throughput ambient mass spectrometry advancing drug discovery**  
*S. Datwani, L. Ghislain*  
 Labcyte, Inc - Chemistry, San José, USA
- MP-83 Experimental measurements of effective electric field radii of Rectilinear ion traps**  
*C. Ding, F. Xu*  
 Fudan University, Chemistry Department, Shanghai, China
- MP-84 Universal electrode for quadrupole electrode systems**  
*M. Dubkov, M. Burobin, V. Ivanov, A. Malutin, V. Gurov*  
 Ryazan State Radio Engineering University, Department of General and Experimental Physics, Ryazan, Russian Federation
- MP-85 Degradation studies of the antibiotic sulfamethoxazole utilizing HPLC/MS**  
*K. Eckey, U. Karst*  
 University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany
- MP-86 The importance of enhanced molecular ions in GC-MS**  
*A. B. Fialkov, U. Keshet, T. Alon, A. Amirav*  
 Tel Aviv University, School of Chemistry, Tel Aviv, Israel
- MP-87 GC-MS with cold EI - extending the range of compounds and applications amenable for GC-MS analysis**  
*A. Amirav, A. Fialkov, T. Alon, U. Keshet*  
 Tel Aviv University, School of Chemistry, Tel Aviv, Israel
- MP-88 Study of endocrine disrupting compound release from medical devices in plasma samples of premature newborns through an on-line SPE UHPLC-MS/MS method**  
*F. Gosetti, B. Bolfi, M. Manfredi, E. Robotti, F. Ferrero, G. Bona, E. Marengo*  
 University of Piemonte Orientale, Department of Science and Technological Innovation, Alessandria, Italy

- MP-89 Triode-type MCP-based ion detector enabling miniature mass spectrometers to operate at low vacuum up to 1Pa**  
*M. Hayashi, Y. Washiyama, K. Ishii, J. Sakakiyama*  
Hamamatsu Photonics K.K., Electron Tube Division, Hamamatsu, Japan
- MP-90 The dynamic behavior of nano liquid bridge during ambient sampling ionization in scanning probe electrospray ionization mass spectrometry**  
*B. Kamihoriuchi, Y. Otsuka, A. Takeuchi, F. Iwata, T. Matsumoto*  
Osaka Univ., Department of Chemistry, Toyonaka, Japan
- MP-91 Integration of a droplet microfluidic chip with mass spectrometry – A step towards high throughput cellular analysis**  
*E. E. Kempa, X. Li, C. A. Smith, P. E. Barran*  
University of Manchester, Manchester Institute of Biotechnology, Manchester, United Kingdom
- MP-92 Portable gas chromatography mass spectrometer with a rapid heating carbon nanotube paste**  
*B. Yi, S. Y. Kim, W. Jeong, J. Y. Eo, B. S. Lee, B. Kang, H. S. Kim*  
Korea Basic Science Institute, Mass Spectrometry & Advanced Instrumentation Group, Cheongju, Republic of Korea
- MP-93 Analytical procedure for determination of perfluoroalkyl acids, parabens and cotinine from a low volume human serum sample by LC-MS/MS**  
*J. Koponen, H. Kiviranta*  
National Institute for Health and Welfare (THL), Health Security, Kuopio, Finland
- MP-94 Cold vaporization of Tissues by Picosecond Infrared Laser Ablation (PIRL) - Unique access to the original proteoform composition**  
*M. Kwiatkowski, H. Schlüter*  
University of Groningen, Department of Pharmacokinetics, Toxicology and Targeting, Groningen, Netherlands
- MP-95 From niche application to essential research tool: why SFC-MS is the must have technique**  
*G. J. Langley, J. M. Herniman*  
University of Southampton, Chemistry, Southampton, United Kingdom
- MP-96 Conventional-flow liquid chromatography–mass spectrometry for exploratory proteomic analyses**  
*J. Lenčo*  
Charles University, Faculty of Pharmacy in Hradec Kralove, Department of Analytical Chemistry, Hradec Králové, Czech Republic
- MP-97 Modern mobile mass spectrometry for on-site analysis of VOCs**  
*A. Marcillo, A. Widdig, C. Birkemeyer*  
University of Leipzig, Institute of Analytical Chemistry, Research Group of Mass Spectrometry, Leipzig, Germany
- MP-98 Determination of multi-residue antibiotics in surface water by SPE and UHPLC-MS/MS**  
*D. J. Mattern, Y. Li, Z. Gan, R. Liao, X. Li, X. Zhou, C. Cai, Y. Xie, F. Qin, J. Wu*  
PerkinElmer, Chromatography Support, Rodgau, Germany
- MP-99 Evaluation of capillary electrophoresis and ion mobility for cyclic lipopeptides analysis**  
*A. Mc Cann, J. Far, C. Delvaux, J. Liigand, L. Quinton, E. De Pauw*  
MSlab, Université de Liège, Liège, Belgium
- MP-100 Tandem Ionisation for GC(xGC)-MS: Complementary soft electron ionisation for increased confidence in compound identification**  
*N. Bukowski, L. Mcgregor, J. Blanch, P. Grosshans*  
SepSolve Analytical, SepSolve Analytical, Peterborough, United Kingdom
- MP-101 Fluorous modification of peptides for mass spectrometric applications**  
*A. Molnár, M. Berta, A. Steckel, K. Uray, J. Rábai, G. Schlosser*  
ELTE Eötvös Loránd University, Department of Analytical Chemistry, Budapest, Hungary
- MP-102 Evaluating the capability of different non-targeted MS-based approaches for the comprehensive characterization of olive tree-derived matrices**  
*L. Olmo-García, N. Kessler, A. Bajoub, C. M. Sánchez-Arévalo, A. Muñoz de la Peña, H. Neuweger, C. Baessmann, A. Carrasco-Pancorbo, A. Fernández-Gutiérrez*  
University of Extremadura, Department of Analytical Chemistry, Badajoz, Spain

- MP-103 An energy-resolved tandem mass spectrometry approach towards identification of small isomeric metabolites**  
*T. Nakamura, T. Hama, M. Sekimoto, F. Sato*  
RIKEN CSRS, Molecular Structure Characterization, Wako, Saitama, Japan
- MP-104 Highly efficient on-line protein digestion and peptide analysis: exploiting new short-bed trypsin-reactors**  
*M. Naldi, U. Cernigoj, A. Strancar, M. Bartolini*  
Alma Mater Studiorum University of Bologna, Department of Pharmacy and Biotechnology, Bologna, Italy
- MP-105 A comparison of the results obtained for the analysis of South African pinotage wines using GCxGC-ToFMS with hydrogen and helium as carrier gases**  
*Y. Naudé, P. C. Gorst-Allman*  
University of Pretoria, Pretoria, South Africa
- MP-106 Analysis of an antiparasitic fraction against gastrointestinal nematodes of sheep from leaves of *Maytenus ilicifolia* by LC-ESI-IT-MS<sup>n</sup>**  
*M. Escobal, G. De Souza, A. Mederos, C. Olivaro*  
Universidad de la República, Espacio de Ciencia y Tecnología Química, Tacuarembó, Uruguay
- MP-107 First report about the structure of an immunoadjuvant saponin fraction from *Quillaja brasiliensis* leaves by LC-ESI-IT-MS<sup>n</sup>**  
*F. Wallace, Z. Bennadji, F. Ferreira, C. Olivaro*  
Universidad de la República, Espacio de Ciencia y Tecnología Química, Tacuarembó, Uruguay
- MP-108 A versatile semi-preparative HPLC platform, including HRMS and NMR, to support process development in industrial biotechnology**  
*B. Ozalp*  
DSM, R&D, Delft, Netherlands
- MP-109 Various chromatography approaches hyphenated with mass spectrometry for the determination of flavonoids and their metabolites**  
*V. Pilarová, J. Pavlík, T. Lacmanová, E. Espinola, L. Nováková*  
Charles University, Faculty of Pharmacy in Hradec Králové, Department of Analytical Chemistry, Hradec Králové, Czech Republic
- MP-110 Multidimensional gas chromatography coupled to isotope ratio mass spectrometry in sports drug testing**  
*T. Piper, M. Putz, M. Thevis*  
German Sport University Cologne, Institute of Biochemistry - Center for Preventive Doping Research, Cologne, Germany
- MP-111 MEMS Time-of-Flight mass spectrometer for in situ gas mixture analysis**  
*F. Progent, A. Sonnette, J. Tupinier, P. Buthier, J. Lictévout, S. Vigne, T. Alava*  
CEA, DAM, DIF, Arpajon, France
- MP-112 Atmospheric pressure chemical ionization – constructing ionization efficiency scale and derivatization reagent suitability**  
*R. Rebane, P. Liigand, J. Liigand, M. Oldekop, K. Herodes, I. Leito*  
University of Tartu, Institute of Chemistry, Tartu, Estonia
- MP-113 Microfluidic CE-MS for newborn screening: a single system for monitoring small molecule and protein biomarkers**  
*E. Redman, J. Mellors*  
908 Devices Inc., Life Sciences, Boston, USA
- MP-114 Development of rapid screening apparatus with DIP and PI/MS for additives in polymer materials**  
*Y. Mishima, T. Tsugoshi*  
NMIJ, AIST, Tsukuba, Japan
- MP-115 Comparison of the displacement mode versus gradient mode for proteomics using an online 2D-LC-MS/MS system**  
*H. Schlueter*  
University Medical Center Hamburg-Eppendorf, Mass Spectrometric Proteomics, Hamburg, Germany

- MP-116 Low-flow atmospheric pressure chemical ionization based on a gas dynamic virtual nozzle nebulizer**  
*T. Strmen, V. Vrkoslav, O. Paces, J. Cvacka*  
 Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Department of Analytical Chemistry, Faculty of Science, Charles University in Prague, Prague, Czech Republic
- MP-117 Analysis of enzymes in laundry detergent using SDS-PAGE and MALDI-ToF-MS**  
*Z. Talebpour, G. Abedi, A. Ghassempour*  
 Alzahra University, Department of Chemistry, Tehran, Iran
- MP-118 Mechanistic reaction insights by in-situ monitoring of an AACVD reaction using GC-MS: studying the ZnFe<sub>2</sub>O<sub>4</sub> thin film growth process**  
*I. C. Usen, U. Wijayantha-Kahagala-Gamage, J. C. Reynolds*  
 Loughborough University, Department of Chemistry, Loughborough, United Kingdom
- MP-119 Pulsed extraction mode for off-axis time of flight mass spectrometer**  
*W. Guanyi, L. Zhiming, Z. Lihua, Y. Xianglong, D. Hu, S. Xiaopan, W. Wenliang*  
 Northwest Institute of Nuclear Technology, Xi'an, China
- MP-120 Probing the limits of on-line reaction monitoring by small footprint ESI-MS and NMR**  
*C. Whitmore, A. Kenwright, A. Ray, S. Coombes, J. Mosely*  
 Durham University, Department of Chemistry, Durham, United Kingdom
- MP-121 Improvement of electrostatic quadrupole zoom lens for fixed multi-collector system in LRI-MS**  
*X. Yuan, Z. Li, L. Zhai, J. Xu, X. Shen, H. Deng, W. Wang*  
 Northwest Institute of Nuclear Technology, Xi'an, China

### **MPS-S05 - Volatile Molecules & Nose-Space Analysis**

- MP-122 Overview of the volatile components of the Corsican liverwort *Scapania undulata***  
*A. Pannequin, A. Tintaru, J.-M. Desjobert, J. Costa, A. Muselli*  
 Université de Corse, Laboratoire de Chimie des Produits Naturels, Corte, France
- MP-123 Effect of germination time, roasting level and altitude in the aroma released by coffee powder monitored by proton transfer reaction mass spectrometry and gas chromatography mass spectrometry**  
*M. Bodner, K. Morozova, P. Kruathongsri, P. Thakeow, S. Angeli, M. Scampicchio*  
 Free University of Bolzano-Bozen, Faculty of Science and Technology, Bolzano, Italy
- MP-124 Feasibility of selected ion flow tube mass spectrometry (SIFT-MS) to real-time monitoring of exhaled breath volatile organic compounds (VOCs) in cancer patients**  
*G. Corona, G. Miolo, A. Carretta, A. Steffan*  
 IRCCS National Cancer Institute, Immunopathology and Cancer Biomarkers, Aviano(PN), Italy
- MP-125 *Clostridium tetani* (C. tetani) cultivation process monitoring by Headspace solid-phase microextraction (HS-SPME) combined with GC-MS**  
*A. Es-Haghi, M. Ghader, N. Shokoufi, K. Kargosha*  
 Razi Vaccine & Serum Research Institute, Department of Physico Chemistry, Karaj, Iran
- MP-126 SPME-GC/MOX sensor system: a new method for the evaluation of human semen quality**  
*V. Longo, A. Forleo, P. S. Pinto, D. D. Montagna, L. Coppola, V. Zara, A. Ferramosca, P. Siciliano, S. Capone*  
 National Research Council, Institute for Microelectronics and Microsystems, Lecce, Italy
- MP-127 The volatile faecal metabolome in Cushing's syndrome mouse model of type 2 diabetes**  
*C. Lourenço, M. Cauchi, L. Bentley, R. D. Cox, C. Turner*  
 Cranfield University, School of Aerospace, Transport and Manufacturing, Cranfield, Bedfordshire, United Kingdom
- MP-128 Investigations of VOCs present in breath using PTR-MS: preliminary studies of ketones and anaesthetics**  
*M. Malásková, D. Olivenza-León, F. Piel, P. Mochalski, M. Klieber, C. Mayhew*  
 University of Innsbruck, Institute for Breath Research, Innsbruck, Austria

- MP-129** An innovative analysis method for fragrance of sake using an introducing device for volatile compounds combined with DART-MS  
*C. Takei, Y. Otake, K. Yoshizawa, H. Nishimoto, T. Akashi*  
 BioChromato, Fujisawa, Japan
- MP-130** Exploring inter-individual differences in In-vivo flavour release by SIFT-MS  
*M. Pedrotti, L. Menghi, I. Khomenko, A. Caretta, E. Aprea, A. Cavazzana, T. Hummel, F. Gasperi, F. Biasoli*  
 Foundation Edmund Mach, Wageningen University FQD, Wageningen, Netherlands

### **MPS-S06 - Clinical Chemistry**

- MP-131** Impact of CYP2D6 genetic polymorphism on the pharmacokinetics of tramadol and its three main metabolites in Koreans  
*J. Bae, S. Lee, K. Chun, M. Je Choi, S. Hong*  
 Keimyung University, College of Pharmacy, DAEGU, Republic of Korea
- MP-132** Individual and cyclic estrogenic profile in woman: structure and variability of the data  
*C. Bozzolino, S. Vaglio, E. Amante, E. Alladio, E. Gerace, M. Vincenti*  
 Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", University of Turin, Department of Chemistry, Turin, Italy
- MP-133** Pharmacokinetic of Myriocin in rabbit's eyes  
*M. Dei Cas, F. M. Rubino, J. Rizzo, S. Paola, E. Strettoi, C. Platania, C. Bucolo, R. Pignatello, R. Ghidoni, R. Paroni*  
 University of Milan, Department of Health Sciences, Milan, Italy
- MP-134** Comparison of ESI, APCI and APPI ionization techniques for testosterone (T), dihydrotestosterone (DHT) and estradiol (E2) LC-MS/MS assay  
*R. Desai, P. Keski-Rahkonen, T. Harwood, D. Handelsman*  
 Anzac research institute, Andrology, Concord, Sydney, Australia
- MP-135** Highly selective and fast identification of Brucella by immunoaffinity- MALDI-ToF mass spectrometry  
*H. Hamidi, M. Zarrineh, I. Soleimani, N. R. Bagheri, A. Es-Haghi, A. Ghassempour*  
 Medicinal Plants and Drugs Research Institute, Shahid Beheshti University, Tehran, Iran
- MP-136** Analysis of protein biomarkers from low sample volumes  
*T. G. Halvorsen, C. Rosting, M. C. S. Levernæs, L. Reubsæet*  
 University of Oslo, School of Pharmacy, Oslo, Norway
- MP-137** Early and non-invasive mass spectrometry tool for diagnosing aspergillosis  
*R. Dobias, A. Skriba, T. Pluhacek, M. Petrik, P. Lyskova, V. Havlicek*  
 Institute of Microbiology, Academy of Sciences of the Czech Republic, Prague, Czech Republic
- MP-138** Analysis of underivatized amino acids in exhaled breath condensate samples as monitoring therapy for children with type 1 diabetes  
*M. Pyszka, L. Konieczna, M. Okońska, Ł. Szmygel, M. Myśliwiec, T. Bączek*  
 Medical University of Gdańsk, Department of Pharmaceutical Chemistry, Gdańsk, Poland
- MP-139** Development and validation of a high sensitivity assay of estrogens in human plasma by UHPLC-MS/MS without derivatization  
*M. Levi, H. Kobayashi, J. Watanabe*  
 Shimadzu Corporation, MS BU, Kyoto, Japan
- MP-140** ICP-MS immunoassay using metal-doped nanoparticles for multiplex detection of HIV-1 p24 and HBsAg  
*H. B. Lim, C. Kim*  
 Dankook University, Chemistry, Chunan, Republic of Korea
- MP-141** Solid phase microextraction coupled to mass spectrometry via microfluidic open interface for point-of-care testing of tranexamic acid in plasma of cardiac surgical patients  
*N. Looby, M. Tascon, J. Acquaro, N. Reyes-Garcés, T. Vasiljevic, G. A. Gómez-Ríos, M. Wasowicz, J. Pawliszyn*  
 University of Waterloo, Department of Chemistry, Waterloo, Canada

- MP-142 Study of non-covalent interaction between ALS-linked mutant PFN1 protein and natural compound by mass spectrometry**  
*M. Nekouei, P. Ghezellou, M. Kiaei, A. Ghassempour*  
Shahid Beheshti University, Medicinal Plants and Drugs Research Institute, Tehran, Iran
- MP-143 Detection and quantification of carbohydrate deficient transferrin by MALDI-compatible protein chips prepared by ambient ion soft landing**  
*P. Novak, P. Darebna, M. Volny, V. Ruzicka, J. Spicka, R. Kucera, P. Pompach*  
Institute of Microbiology, Laboratory of Structural Biology, Prague, Czech Republic
- MP-144 Acetylcholine and acetylcholinesterase in a non-neuronal tissue (Corneal epithelium)**  
*I. Oulie, L. Reubsæet, T. G. Halvorsen, A. Ringvold*  
University of Oslo, School of Pharmacy, Dept. of Pharmaceutical Chemistry, Pharmaceutical analysis, Oslo, Norway
- MP-145 Development and validation of a sensitive LC-linear ion trap method for the determination of trace di-iodothyronines in human blood serum**  
*K. Richards, J. Köhrle, D. Rathmann, R. Monk*  
Charite Universitätsmedizin Berlin, Institute for Experimental Endocrinology, Berlin, Germany
- MP-146 Using data dependent acquisition to produce specific and reliable MRM transitions for suspects on a Qtrap instrument**  
*S. K. Steffensen, I. Fomsgaard*  
Aarhus University, Department of Agroecology/Flakkebjerg, Denmark
- MP-147 Evaluation of UDP-glucuronosyltransferase 1A1 activity towards bilirubin**  
*A. Takeuchi*  
Instrumental Analysis Center, Kobe Pharmaceutical University, Kobe, Japan
- MP-148 A Biomphalaria glabrata peptide that stimulates extreme behaviour modifications in aquatic free-living Schistosoma mansoni miracidia**  
*T. Wang, R. Wyeth, D. Liang, U. Bose, G. Ni, D. Mcmanus, S. Cummins*  
University of the Sunshine Coast, School of Science and Engineering, Sippy Downs, Australia
- MP-149 Analysis of sweeteners in urine using novel stationary phase and selective LC-MS/MS method**  
*B. Cervinkova, R. Kay, A. Koulman*  
NIHR BRC Nutritional Biomarker Laboratory, University of Cambridge, Cambridge, United Kingdom
- MP-150 Pharmacokinetics and bioavailability of different acetylsalicylic acid formulations assessed by liquid chromatography-tandem mass spectrometry in healthy subjects**  
*J. Rizzo, M. Dei Cas, F. M. Rubino, R. C. Paroni*  
University of Milan, Department of Health Sciences, Milan, Italy
- MP-151 Which LC-MS/MS platform is most appropriate for the quantitative analysis of Steroids in urine, serum and oral fluid for Clinical Research**  
*S. Indelicato, R. M Doyle, D. McDowell*  
Thermo Fisher, CMD, Paris, France
- MP-152 GC-MS and LC-MS profiling of exhaled breath condensate: investigation of sampling considerations**  
*A. K. C. Laserna, H. F. Lim, N. S. Tan, E. Horiyanto, B. H. Ng, R. Verma, N. Paton, S. F. Y. Li*  
National University of Singapore, Department of Chemistry, Singapore
- MP-153 Set up of a simple, fast and flexible LC-MS/MS ID method for the simultaneous determination of steroids in different biological samples.**  
*G. Bartolucci, M. Pallecchi, S. Gozzo, G. Danza*  
University of Florence, department of experimental biomedical and clinical science, Firenze, Italy
- MP-154 Chemometric optimization of UPLC-MS/MS assay for clinical diagnosis and pharmacotherapy monitoring of patients with APRT deficiency**  
*M. Thorsteinsdóttir, U. A. Thorsteinsdóttir, F. F. Eiriksson, H. L. Runolfsdóttir, V. O. Edvardsson, R. Palsson*  
University of Iceland, Faculty of Pharmaceutical Sciences, Reykjavik, Iceland

**MPS-S07 - Quantitative Proteomics**

- MP-155 Optimization of biotin enrichment protocol and its application for the analysis of organelle-enriched proteins by LC-MS/MS**  
*S. Ahmadi, D. Winter*  
University of Bonn, Institute of Biochemistry and Molecular Biology, Bonn, Germany
- MP-156 Sample multiplexing by isoelectric focusing (pI-Coding) for isobaric labeling and label-free quantification**  
*J. Astorga-Wells, C. Beusch, T. Lavold, R. A. Zubarev*  
Karolinska Institutet, Medical Biochemistry and Biophysics, Stockholm, Sweden
- MP-157 Differential proteomic analysis of actinic keratosis, bowen's disease and cutaneous squamous cell carcinoma by Sequential Window Acquisition of All Theoretical Mass Spectra (SWATH-MS)**  
*A. Azimi, M. Ali, K. Kaufman, P. Yang, G. Mann, P. Fernandez-Penas*  
The University of Sydney, Centre for Translational Skin Research, Westmead, Australia
- MP-158 Tape stripped stratum corneum samples prove to be suitable for comprehensive proteomic investigation of actinic keratosis**  
*A. Azimi, M. Ali, K. Kaufman, G. Mann, P. Fernandez-Penas*  
The University of Sydney, Centre for Translational Skin Research, Westmead, Australia
- MP-159 A high-resolution organellar proteomics approach to study protein subcellular distribution and dynamics in cells**  
*C. Steinbrueck, J. Jordan, M. Kocylowski, A. Kollwe, W. Bildl, A. Haupt, B. Fakler, U. Schulte*  
University of Freiburg, Institute of Physiology, Faculty of Medicine, Freiburg, Germany
- MP-160 Evaluation of proteomics quantitative methods on a reconstructed skin model**  
*S. Bourassa, C. Gotti, M. Scott-Boyer, J. Marcoux, I. Kelly, A. Droit*  
CHU de Quebec proteomics Platform, Laval University, Quebec, Canada
- MP-161 New pharmacological targets for cystic fibrosis treatment from extensive proteomic profiling of  $\Delta F508$ -CFTR expressing cells**  
*C. Braccia, V. Tomati, N. Pedemonte, A. Armirotti*  
Istituto Italiano di Tecnologia, Università degli Studi di Genova, Genova, Italy
- MP-162 Straight forward phosphoproteomic analysis pipeline in CHO cells as mammalian non-model organism**  
*L. Brachtvogel, A. Pries, S. Walter, T. Noll, R. Hoffrogge*  
Cell Culture Technology, Bielefeld University, Bielefeld, Germany
- MP-163 Comparative proteomics study for elucidation of potential mechanisms underlying yeast resistance to alcohols**  
*J. Bubs, V. Gorshkov, F. Kjeldsen, M. Gorshkov, I. Tarasova, D. Spasskaya, D. Karpov*  
Talrose Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation
- MP-164 Quantitative label-free proteomics in a novel cellular knock out model of methylmalonic acidemia**  
*M. Costanzo, M. Caterino, A. Cevenini, I. C. Guerrero, M. Ruoppolo*  
University of Naples "Federico II", Department of Molecular Medicine and Medical Biotechnology, Naples, Italy
- MP-165 Inactivated Poliovirus vaccine antigen determination: a proteomics approach**  
*M. Creskey, D. Viel, T. Wu, T. Cyr*  
Health Canada, Biologics and Genetic Therapies Directorate, Ottawa, Canada
- MP-166 TMT-based quantitative approach discloses Monacolin K-induced proteome alterations in triple negative breast cancer cells**  
*F. del Gaudio, M. C. Monti, S. Rontogianni, K. Stecker, I. C. Guerrero, R. Riccio, A. J. R. Heck, M. A. F. Altelaar*  
Department of Pharmacy, University of Salerno, Salerno, Italy
- MP-167 High throughput signaling pathway monitoring based on fast LC-PRM analyses**  
*S. Gallien, A. Gajadhar, B. Patel, T. Arrey, D. Sarracino, Y. Xuan, E. Chen*  
Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, USA

- MP-168 Quantitation of amylase/trypsin-inhibitors in various wheat species**  
*S. Geisslitz, K. Scherf, P. Koehler*  
 Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Freising, Germany
- MP-169 Peptide migration profiles: a tool to trace proteolytic processes - Factor XII contact system activation**  
*L. Heikaus, H. Schlüter*  
 University Medical Center Hamburg-Eppendorf, Mass Spectrometric Proteomics, Hamburg, Germany
- MP-170 Myelin proteomics 2.0: application to mouse models for myelin-related diseases**  
*O. Jahn, S. Siems, D. Hesse, S. Tenzer, H. Werner*  
 Max-Planck-Institute of Experimental Medicine, Proteomics Group, Göttingen, Germany
- MP-171 Simplifying the use of ion libraries during data processing of data independent acquisition proteomics data**  
*M. Huebsch, D. Waidelich, A. Lau, K. Lewis, N. Morrice, J. Dojahn, D. Merkel, R. Sayers, Z. Demianova, S. Ahadi, C. Hunter, J. Jasak*  
 Sciex, Darmstadt, Germany
- MP-172 The improvement in cognitive functions in 5XFAD Alzheimer's transgenic mouse model via natural compound administration**  
*M. Karayel Başar, I. Kiris, B. Gürel, T. Mroczek, K. Skalicka-Wozniak, A. T. Baykal, M. Y. Günal*  
 Acibadem Mehmet Ali Aydınlar University, Medical Biochemistry, İstanbul, Turkey
- MP-173 Simultaneous dual proteome analysis towards understanding neutrophil interaction with the human-pathogenic fungus *Aspergillus fumigatus***  
*T. Krüger, I. A. Shopova, T. Müller, M. Dittrich, D. J. Mattern, T. Conrad, O. Kniemeyer, A. A. Brakhage*  
 Leibniz Institute for Natural Product Research and Infection Biology (Hans Knöll Institute), Department of Molecular and Applied Microbiology, Jena, Germany
- MP-174 Biomarker discovery of atherosclerotic stroke in individual serum sample**  
*J. Lee, S. Mun, A. Park, Y. Lee, A. Seok, H. Kim, Y. Lee, H. Kang*  
 Eulji University, Department of Biomedical Laboratory Science, College of Health Sciences, Seongnam-si, Gyeonggi-do, Republic of Korea
- MP-175 Development of a simple and efficient quantification method of human follicular fluid (hFF) proteome**  
*A. Lewandowska, A. Fel, K. Macur, P. Czaplewska, J. Liss, K. Lukaszuk, S. Oldziej*  
 Intercollegiate Faculty of Biotechnology UG-MUG, University of Gdansk, Gdansk, Poland
- MP-176 A target fishing and shotgun proteomics approaches to study the effect of a new drug against *M. tuberculosis***  
*M. Manfredi, L. Chiarelli, A. Buzzi, M. Pasca, F. Gosetti, E. Barberis, E. Robotti, E. Marengo*  
 University of Piemonte Orientale, Department of Sciences and Technological Innovation, Alessandria, Italy
- MP-177 A cost-effective approach to produce <sup>15</sup>N-labelled amino acids employing *Chlamydomonas Reinhardtii* CC503**  
*J. M. Marchante-Gayón, C. J. Nicolás, G. P. Rodríguez, G. L. Valledor, V. M. J. Cañal, A. J. I. García*  
 University of Oviedo, Department of Physical and Analytical Chemistry, Oviedo, Spain
- MP-178 Characterization of protein extracts from yeast cells exposed to fermented *Spirulina (Arthrospira platensis)* using high resolution Orbitrap mass spectrometry**  
*J. Masten, B. Cillero-Pastor, R. Mohren, N. Ogrinc, P. Jamnik*  
 Jožef Stefan Institute, Jožef Stefan International Postgraduate School, Department of Environmental Sciences, Ljubljana, Slovenia
- MP-179 QConCat-based absolute quantification of the lysosomal proteome by multiple reaction monitoring**  
*P. Mosen, R. Sakson, T. Ruppert, V. Giesemann, D. Winter*  
 Institute of Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany
- MP-180 Validation strategies for the purity assessment of peptide standards by isotope dilution mass spectrometry**  
*J. Nicolas-Carcelen, A. Gonzalez-Gago, A. Suarez-Fernandez, J. M. Marchante-Gayon, P. Rodriguez-Gonzalez, J. I. Garcia-Alonso*  
 University of Oviedo, Analytical and Physical Chemistry, Oviedo, Spain



- MP-181 Quantitative microproteomics for the characterization of central and peripheral nervous system of the Twitcher mouse**  
*D. Pellegrini, G. Ambra Del, L. Angella, N. Giordano, I. Tonazzini, M. Caleo, M. Cecchini, L. McDonnell*  
 NEST, Scuola Normale Superiore, Pisa, Italy
- MP-182 Quantitative study of metabolic pathways in *C. Elegans* using MS Western**  
*B. K. Raghuraman, A. Shevchenko*  
 Max Planck Institute of Molecular Cell Biology and Genetics, Biological Mass Spectrometry, Dresden, Germany
- MP-183 Application of manual chromatography device for fractionation of complex peptide samples prior nanoESI-MS/MS**  
*P. Rehulka, H. Rehulkova, V. Franc, M. Sebel, R. Kupcik, Z. Bilkova, J. Stulik*  
 University of Defence, Faculty of Military Health Sciences, Hradec Králové, Czech Republic
- MP-184 Discussion of the pros and cons of isobaric labelling compared to single shot data-independent acquisition**  
*J. Muntel, R. Bruderer, J. M. Kirkpatrick, O. M. Bernhardt, L. Verbeke, T. Gandhi, T. Huang, O. Vitek, A. Ori, L. Reiter*  
 Biognosys, R&D, Schlieren, Switzerland
- MP-185 High speed, high sensitivity and highly reproducible and accurate label free quantification using the PASEF method on a TIMS QToF**  
*G. Kruppa, M. Lubeck, H. Koch, V. Tellström, P. Shan, C. Cox, S. Koch*  
 Bruker France, Proteomics, Wissembourg, France
- MP-186 FAIMS reduces interference and improves quantitative accuracy in multiplexed proteomics**  
*D. Schweppe, S. Prasad, R. Huguet, P. J. Navarrete, J. Paulo, M. Jedrychowski, G. Mcalister, S. Abbatiello, M. Belford, V. Zabrouskov, S. Gygi*  
 Harvard Medical School, Boston, USA
- MP-187 A targeted multiple reaction monitoring method for quantifying Nav1.6 protein in HEK239 cells and mouse hippocampus**  
*M. Tung, R. Kwan, C. Xi, J. Li, C. Dang, L. E. Sojo*  
 Xenon Pharmaceuticals Inc., Compound Properties Group, Burnaby, Canada
- MP-188 Comparative proteogenomic analysis of colistin-dependence in *Acinetobacter baumannii***  
*S. Chamoun, J. Welander, C. Claesson, E. Vikström, M. Turkina*  
 Linköping University, Department of Clinical and Experimental Medicine, Linköping, Sweden
- MP-189 TMT quantification using spectral libraries in SpectroMine**  
*L. Verbeke, T. Gandhi, O. M. Bernhardt, L. Reiter*  
 Biognosys AG, Bioinformatics, Schlieren, Switzerland
- MP-190 Multiplex quantitative assay of inflammation protein markers in feces samples**  
*V. Vidova, V. Thon, J. Klanova, Z. Spacil*  
 Research Centre (RECETOX), Masaryk University, Faculty of Science, Brno, Czech Republic
- MP-191 Development of a quality control standard for Tandem Mass Tags (TMT) workflows**  
*J. Choi, A. Robitaille, T. N. Arrey, R. Viner, A. Huhmer, J. C. Rogers*  
 Thermo Fisher Scientific, San Jose, USA
- MP-192 Solving the yellow mystery of *Papaver nudicaule* with an integrated -omics approach**  
*B. Dudek, N. Wielsch, R. C. Menezes, A. Warskulat, Y. Hupfer, S. Lorenz, H. Vogel, C. Paetz, B. Schneider, A. Svatos*  
 Max Planck Institute for Chemical Ecology, Mass Spectrometry / Proteomics Group, Jena, Germany
- MP-193 A streamlined workflow for high-throughput, precise, and comprehensive large-scale quantitative proteomics analysis**  
*Y. Xuan, Y. Zhou, S. Gallien, O. Boychenko, J. J. Nicklay, J. Ho, S. Peterman, P. Navarro, E. I. Chen, K. Miller*  
 Thermo Fisher Scientific, Chromatography and Mass Spectrometry Division (CMD), Bremen, Germany

- MP-194 Advancing mass spectrometry-based large-cohort proteomics for precision medicine – An international Cancer Moonshot multi-site study**  
Y. Xuan, N. W. Bateman, Y. Chen, A. Sickmann, B. Wollscheid, C. R. Jimenez, M. R. Larsen, H. Zhou, S. Liu, Z. Chen, T. Kislinger, B. Crossett, S. Gallien, Y. Zhou, P. Navarro, R. Birhanu Kitata, C. Lorenz, S. Goetze, S. Piersma, D. Chiasserini, M. Tahir, H. Zhu, G. Hou, X. Sun, A. Macklin, A. Khoo, B. L. Parker, S. J. Cordwell, T. P. Conrads  
 Thermo Fisher Scientific, Chromatography and Mass Spectrometry Division (CMD), Bremen, Germany
- MP-195 Global analysis of protein complexes in *Trypanosoma brucei* using cross-linking mass spectrometry**  
F. Almeida, M. Tinti, M. Ferguson  
 The University of Dundee, Biological Chemistry and Drug Discovery, Dundee, United Kingdom
- MP-196 Abundant protein depletion of human plasma samples – Sample preparation approaches for quantitative comparison studies**  
R. Bomgardien, S. Snovida, K. Herting, R. Ganapathy, B. Kaboord, J. Rogers  
 Thermo Fisher Scientific, R&D, Rockford, USA
- MP-197 Quantification of human insulin and its analogues by immunopurification and LC-MS/MS**  
 J. Kooistra, J. Grzetic-Martens, Y. Lamkadam, T. Noij  
 Charles River Laboratories, Bioanalysis, Den Bosch, Netherlands
- MP-198 Parallel evaluation of MALDI-ToF and tandem LC-ESI mass spectrometry for rapid quantification of abrin toxin in complex matrices**  
S. Livet, S. Worbs, E. Hansbauer, H. Volland, S. Simon, C. Junot, F. Fenaille, B. G. Dorner, F. Becher  
 CEA Saclay, DRF - Institut des sciences et du vivant Frédéric Joliot - Service de Pharmacologie et d'Immunoanalyse (SPI), Gif-su- Yvette, France
- MP-199 Proteomic analysis of unconventional protein secretion**  
C. Mayrhofer, K. Nöbauer, G. Brem  
 University of Veterinary Medicine Vienna, Institute of Animal Breeding and Genetics, Institute of Biotechnology in Animal Production, IFA Tulln, Wien, Austria
- MP-200 Proteome of avian pathogenic *E. coli* during infection: methods and results.**  
A. Nawrocki, A. E. Johansen, J. Møller-Jensen, J. E. Olsen, M. R. Larsen  
 University of Southern Denmark, Biochemistry and Molecular Biology, Odense, Denmark
- MP-201 Comparative study of three MS-based approaches for quantitative proteomics analysis**  
D. Taverna, M. Gaspari, M. Catracchia  
 Proteomics-UMG lab, Department of Experimental and Clinical Medicine, Magna Graecia University of Catanzaro, Italy
- MP-202 Proteomic and metabolomic alterations in the rat brain after ischemic stroke**  
J. Teppo, A. Vaikkinen, K. Mätlik, T. Kotiaho, M. Airavaara, R. Kostainen  
 University of Helsinki, Faculty of Pharmacy, Helsinki, Finland
- MP-203 Determination of peptide purity by UV-MS and quantitative NMR**  
F. A. Torma, M. Quaglia, J. Warren  
 LGC LTD, Chemical Measurement and Calibration, Teddinton, United Kingdom
- MP-204 Universal S-Trap sample processing: standardized reproducible sample workup from <math>\mu\text{g}</math> to > mg scales for all sample types**  
J. Wilson, D. J. Pappin  
 Cold Spring Harbor Laboratory, Cold Spring Harbor, USA

### **MPS-S08 - Chiral Discrimination**

- MP-205 Self-assembled binuclear  $\text{Cu(II)}$ -histidine complex for absolute configuration and enantiomeric excess determination of naproxen by tandem mass spectrometry**  
 X. Yu, M. Chau, W. Kit Tang, C. Siu, Z. Yao  
 City University of Hong Kong, Department of Chemistry, Kowloon Tong, Hong Kong
- MP-206 Spectroscopic discrimination of diastereomeric complexes involving an axially chiral receptor**  
 A. Filippi, C. Fraschetti, L. Guarcini, C. Zazza, T. Ema, M. Speranza  
 Sapienza, University of Rome, Chemistry and Technology of Drugs Department, Rome, Italy

- MP-207 **Acid-based recognition of diastereoisomeric peptides using ion mobility mass spectrometry**  
M. Zimnicka  
 Polish Academy of Sciences, Institute of Organic Chemistry, Warsaw, Poland

### **MPS-S09 - Ambient MS and New Ionization Methods**

- MP-208 **A versatile integrated Ambient Ionization Source (iAmIS) platform and its applications**  
Y. Bai, W. Ai, S. Xu, H. Liu  
 Peking University, College of Chemistry, Beijing, China
- MP-209 **The role of new materials as sampling substrates for the DESI-HRMS determination of new psychoactive substances in saliva**  
F. Bianchi, S. Agazzi, N. Riboni, M. Hakkarainen, L. Ilag, R. Cecchi, L. Anzillotti, M. Careri  
 University of Parma, Department of Chemistry, Life Sciences and Environmental Sustainability/CIPACK, Parma, Italy
- MP-210 **Matrix effects in Low Temperature Plasma Ionization (LTPI) mass spectrometry**  
 A. Kiontke, B. Scholz, W. Honscha, C. Birkemeyer  
 Universität Leipzig, Leipzig, Germany
- MP-211 **Application of LDTD/TQMS-HRMS methods for quantification of psychoactive compounds in tissue microsamples**  
A. Borik, A. Vojs Stanova, K. Grabicova, T. Randak, R. Grabic  
 University of South Bohemia in Ceske Budejovice, Faculty of Fisheries and Protection of Waters, Laboratory of Environmental Chemistry and Biochemistry, Vodnany, Czech Republic
- MP-212 **Breath analysis with Secondary Ionization High-Resolution Mass Spectrometry (SESI-HRMS) in the clinical environment with a focus on disease specific biomarkers in children with cystic fibrosis**  
T. Bruderer, N. Haas-Baumann, R. Weber, A. Baghdasaryan, S. J. Micic, S. Mueller, F. Singer, R. Zenobi, A. Moeller  
 University Children's Hospital Zurich, Division of Respiratory Medicine, Zurich, Switzerland
- MP-213 **One size does not fit all: DART and complementary ambient ionization methods**  
R. Cody  
 JEOL USA, Inc., Mass Spectrometry, Peabody, USA
- MP-214 **Enhanced coupling of Acoustic Levitation SAIL mass spectrometry for direct ionization and reaction monitoring**  
E. A. Crawford, D. Dietrich, C. Esen, D. A. Volmer  
 Saarland University, Institute of Bioanalytical Chemistry, Saarbruecken, Germany
- MP-215 **Direct Infusion Resonance-Enhanced Multiphoton Ionization Mass Spectrometry of liquid samples under vacuum conditions**  
H. Czech, C. Kruth, M. Sklorz, J. Passig, S. Ehlert, A. Cappiello, R. Zimmermann  
 University of Rostock, Chair of Analytical Chemistry, Rostock, Germany
- MP-216 **Ion chemistry fundamentals of secondary electrospray ionization mass spectrometry (SESI-MS) for VOC analyses**  
K. Dryahina  
 J. Heyrovský Institute of Physical Chemistry, Department of Chemistry of Ions in Gaseous Phase, Prague, Czech Republic
- MP-217 **SpiderMass a novel tool to tackle in-vivo mass spectrometry**  
 P. Saudemont, A. Baud, E. Bouchaert, Q. Pascal, M. Ziskind, D. Tierny, M. Salzet, J. Fournier  
 PRISM Inserm U1192, University of Lille, Lille, France
- MP-218 **Molecular Surgery Navigation by the combination of mass spectrometry with molecular resonance probe desorption**  
V. Frankevich, V. Chagovets, A. Kononikhin, G. Sukhikh  
 Federal State Budget Institution "Research Center for Obstetrics, Gynecology and Perinatology" Ministry of Healthcare and Social Development of the R, Systems Biology, Moscow, Russian Federation

- MP-219 A comparison between diathermic knife and CO<sub>2</sub>-laser coupled to REIMS-ToF for instantaneous tissue classification**  
*M. Genangeli, R. M.A. Heeren, T. Porta*  
 M4I, Maastricht University, Maastricht, Netherlands
- MP-220 Multi-scheme chemical ionization inlet for atmospheric pressure mass spectrometry applications**  
*M. P. Rissanen, J. Mikkilä, J. Hakala*  
 Karsa Ltd, Karsa Ltd, Helsinki, Finland
- MP-221 Observable charge states in native MS: differences between ESI and LILBID**  
*J. Hoffmann, K. Karimi, N. Morgner*  
 University, Goethe University Frankfurt, Institute of Physical and Theoretical Chemistry, Frankfurt, Germany
- MP-222 Performance enhancement using He buffer gas in a small-scale LIT for in-the-filed mass spectrometry**  
*A. Janulyte, Y. Zerega, J. Andre*  
 Aix-Marseille University, CNRS, Laboratoires PIIM (UMR 7345), Madirel (UMR 7246), Marseille, France
- MP-223 Charaterization of cold electron ionization for portable mass spectrometers**  
*S. Y. Kim, W. Jeong, B. Yi, Y. Eo Jae, B. Kang, H. S. Kim, M. Yang*  
 Korea Basic Science Institute, Mass Spectrometry & Advanced Instrumentation, Cheongju, Republic of Korea
- MP-224 Graphene layer substrate assisted laser desorption at atmospheric pressure for high spatial resolution mass spectrometry imaging**  
*J. Y. Kim, S. Y. Lee, H. . Lim, J. Park, D. Lim, D. W. Moon*  
 Mass Spectrometry & Advanced Instrumentation Group, Korea Basic Science Institute, Cheongju Republic of Korea
- MP-225 Portable Time-of-flight mass spectrometer using a cold electron beam pulse**  
*W. Jeong, S. Y. Kim, B. Yi, J. Y. Eo, B. Kang, H. S. Kim, M. Yang*  
 Div. of Scientific Instrumentation, Korea Basic Science Institute, Cheongju, Republic of Korea
- MP-226 Soft and hard ionization of volatile organic compounds by EI followed by MS/MS analysis**  
*A. Kornilova, L. Cousins, R. Javahery*  
 PerkinElmer Inc., RND, Woodbridge, Canada
- MP-227 Ion source multiplexing on a single mass spectrometer**  
*Y. Kostyukevich, A. Zhrebker, E. Nikolaev*  
 Skoltech, Skoltech, Moscow, Russian Federation
- MP-228 Identification of chemicals in different objects by direct analysis in real time mass spectrometry**  
*Á. Kuki, B. Antal, L. Nagy, T. Nagy, G. Zelei, M. Zsuga, S. Kéki*  
 University of Debrecen, Department of Applied Chemistry, Debrecen, Hungary
- MP-229 Explosives detection with a mobile Thermal Desorption Direct Analysis in Real Time Mass Spectrometry system (TD- DART-MS)**  
*F. Lj, B. Laramee, P. Liang, B. Musselman*  
 IonSense, Inc., Chemistry, Saugus, USA
- MP-230 Predicting aAgents that "supercharge"**  
*R. O. Loo, R. O'brien-Johnson, M. Nshanian, J. Loo*  
 UCLA, DOE Laboratory for Genomics & Proteomics, Los Angeles, USA
- MP-231 Substrate modification for the analysis of highly volatile chemical warfare agents by paper spray mass spectrometry**  
*P. Mach, E. Dhummakupt, P. Demond, D. Carmany, M. Busch, T. Tovar, A. Ploskonka, J. Decoste, T. Glaros*  
 Excet, Inc., Research & Technology Directorate, Springfield, USA
- MP-232 Laser-Ablation Rapid Evaporative Ionization Mass Spectrometry (LA-REIMS) for lipidomics analysis of living CHO cells directly from the cell culture**  
*S. Maneta-Stavarakaki, S. J. Cameron, J. Abda, A. Perdones-Montero, J. Maldutyte, Y. Chim, P. Diaz-Fernandez, Z. Takáts*  
 Department of Surgery and Cancer, Sir Alexander Fleming Building, Imperial College, London, United Kingdom

- MP-233** **Optical characteristics of matrix materials for matrix-assisted laser desorption/ionization**  
*N. Masaki, S. Okazaki*  
Department of Medical Spectroscopy, Hamamatsu University School of Medicine, Hamamatsu, Japan
- MP-234** **Extending the polarity range for direct SPME-MS analyses by using novel capillary DBDI and APPI sources**  
*M. F. Mirabelli, A. K Huba, R. Zenobi*  
ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland
- MP-235** **Combined Infrared and Ultraviolet Laser Ablation Electrospray Ionization Mass Spectrometry**  
*K. K. Murray, R. Lawal, F. Donnarumma*  
Louisiana State University, Department of Chemistry, Baton Rouge, USA
- MP-236** **Rapid qualitative analysis of two flavonoids, rutin and silybin, in medical pills by direct analysis in real time mass spectrometry (DART-MS) combined with in situ derivatization**  
*L. Nagy, T. Nagy, Á. Kuki, M. Zsuga, S. Kéki*  
University of Debrecen, Department of Applied Chemistry, Debrecen, Hungary
- MP-237** **A novel modular and versatile ToF platform combinable with various ion sources**  
*A. Jordan, E. Piel, S. Feil, E. Hartungen, G. Hanel, J. Herbig, K. Winkler, R. Gutmann, L. Märk, P. Sulzer*  
Ionicon Analytik GmbH, University of Innsbruck, Institute for Ion Physics and Applied Physics, Innsbruck, Austria
- MP-238** **Ionization products of terpene species in LTP FT-ICR-MS measurements**  
*B. Raupers, J. Grottemeyer*  
Institute of Physical Chemistry, University of Kiel, Kiel, Germany
- MP-239** **Development and application of a novel plasma ion source with GC-MS/MS**  
*M. Sarrafzadeh, R. Javahery, C. Jolliffe*  
PerkinElmer, Woodbridge, Canada
- MP-240** **A novel voltage-assisted paper spray-APPI-HRMS method for the screening and quantification of semi-volatile fluorinated compounds**  
*L. R. Seró, C. J. F. Ayala, V. F. J. Santos, M. E. Moyano*  
University of Barcelona, Chemical Engineering and Analytical Chemistry, Barcelona, Spain
- MP-241** **Advances in Selected Ion Flow-Drift Tube Mass Spectrometry, SIFDT-MS, for ambient quantification of trace volatile compounds in air**  
*P. Španel, A. Spesyvyi, D. Smith, K. Sovová*  
Czech Academy of Sciences, J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic
- MP-242** **A triple reagent ion source for trace VOCs quantification by Selected Ion Flow-Drift Tube Mass Spectrometry**  
*A. Spesyvyi, P. Španel*  
J. Heyrovský Institute of Physical Chemistry of the CAS, v. v. i., Department of Chemistry of Ions in Gaseous Phase, Prague, Czech Republic
- MP-243** **Airborne laser-spark ion source for direct microfluidic coupling**  
*S. van Wasen, A. Bierstedt, J. Riedel, D. Volmer*  
Humboldt-Universität zu Berlin, Department of Chemistry, Berlin, Germany
- MP-244** **Development and the application of a 96 high throughput solid phase microextraction (SPME) transmission mode (TM) system for direct analysis in real time (DART) mass spectrometry (MS)**  
*T. Vasiljevic, G. A. Gómez-Ríos, J. Pawliszyn*  
University of Waterloo, Waterloo, Canada
- MP-245** **Single-use poly(etheretherketone) solid-phase microextraction-transmission mode devices for rapid screening and quantitation of drugs of abuse in oral fluid and urine via direct analysis in real-time**  
*T. Vasiljevic, G. A. Gómez-Ríos, J. Pawliszyn*  
University of Waterloo, Waterloo, Canada
- MP-246** **Improvements in small molecule detection via MALDI-MS using binary mixtures of novel ionless matrices**  
*J. Weissflog, A. Svatoš*  
Max-Planck-Institute for Chemical Ecology, Research Group Mass Spectrometry/Proteomics, Jena, Germany

- MP-247 Matrix-Assisted-Ionization-In-Vacuum coupled to high-resolution Fourier transform mass spectrometry (MAI-FTMS) in characterizing lipids in cooking oil and bacteria**  
*R. Liyanage, J. Gidden, J. O. Lay Jr., C. Wilkins*  
University of Arkansas, Chemistry and Biochemistry, Fayetteville, USA
- MP-248 3D-printed low-temperature plasma (3D-LTP) probe for imaging and in vivo studies**  
*S. Martínez-Jarquín, A. Moreno-Pedraza, H. Guillén-Alonso, H. Herrera-Ubaldo, I. Rosas-Román, C. Ovando-Vázquez, S. De Folter, R. Winkler*  
CINVESTAV Unidad Irapuato, Biotechnology and Biochemistry, Irapuato, Mexico
- MP-249 Identification of medulloblastoma subgroups on intrasurgical timescales with picosecond infrared laser desorption mass spectrometry**  
*M. Woolman, C. Kuzan-Fischer, I. Ferry, T. Kiyota, B. Luu, M. Wu, D. Munoz, S. Das, A. Aman, M. Taylor, J. Rutka, H. Ginsberg, A. Zarrine-Afsar*  
University of Toronto, Department of Medical Biophysics, Toronto, Canada
- MP-250 Improvement of nanoelectrospray and desorption nanoelectrospray signal by regulation of pressure in an inlet of triple quadrupole mass spectrometer**  
*L. Borovcová, P. Frycák, D. Mosler, Š. Dostál, V. Havlíček, K. Lemr*  
Department of Analytical Chemistry, Faculty of Science, Palacký University, Olomouc, Czech Republic
- MP-251 Acoustic mist ionisation platform for high-throughput ms-based drug discovery**  
*P. Deland, I. Sinclair, G. Davies, D. Murray, E. Mouchet, M. Bachman, M. Rohman, J. Wingfield*  
Labcyte Inc., Mass Spectrometry Product Management, San Jose, USA
- MP-252 Study on the ionization mechanism of polymers under cluster ion irradiation**  
*M. Fujii, J. Matsuo*  
Yokohama National University, Graduate School of Environment and Information Sciences, Yokohama, Japan
- MP-253 A unique approach to charging ions for LC-MS**  
*C. Jolliffe, L. Cousins, R. Javahery, A. Kornilova, H. Gamble, M. Sarrafzadeh*  
PerkinElmer Inc., RND, Woodbridge, Canada
- MP-254 Development of mass spectrometry-based explosives trace detectors for secure city**  
*S. Kumano, M. Sugiyama, Y. Takada, H. Nagano, H. Mizuno, T. Ito, T. Nojiri, M. Iida, H. Maruyama*  
Hitachi, Ltd., Research & Development Group, Tokyo, Japan
- MP-255 Using automated low volume pipetting to enable high throughput DART-MS detection of drugs directly from biological matrices**  
*F. Li, P. Liang, B. Laramée, B. Musselman*  
IonSense, Inc., Chemistry, Saugus, USA
- MP-256 Toward high throughput screening of cell-material response using liquid extraction surface analysis-mass spectrometry (LESA-MS)**  
*J. Meurs, J. Bunch, M. Alexander, D. Barrett, D. Kim*  
Advanced Materials & Healthcare Technologies Division, University of Nottingham, Nottingham, United Kingdom
- MP-257 Development of a multimodal imaging platform based on photoinduced thermal desorption and analysis by atmospheric pressure chemical ionization mass spectrometry**  
*M. Lorenz, M. Viani, A. Labuda, S. Jesse, R. Proksch, O. Ovchinnikova*  
Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, Oak Ridge, USA
- MP-258 What determines the postionisation efficiency in MALDI-2: A combined soft-/hardware-based set-up to semi-automatically characterize the role of five relevant input parameters**  
*A. Potthoff, K. Dreisewerd, J. Soltwisch*  
University of Münster, Institute of Hygiene, Münster, Germany

### **MPS-S10 – Polymers**

- MP-259 A combination of FAIMS separation with synchrotron UV-photo activation for the tandem MS analysis of synthetic polymers**  
*V. Legros, I. Aloui, A. Giuliani, W. Buchmann*  
LAMBE (CNRS-UEVE-CEA-UCP, UMR8587), Université Paris-Saclay (Univ Evry), Evry, France

- MP-260**    **"Advanced Kendrick mass defect analysis": a toolkit**  
*T. Fouquet, R. B. Cody, T. Satoh, H. Sato*  
 National Institute of Advanced Industrial Science and Technology (AIST), Research Institute for Sustainable Chemistry (ISC), Tsukuba, Japan
- MP-261**    **Potential of liquid extraction surface analysis for mass spectrometric evaluation of safety and functionalization of polymer food packing materials**  
*A. Issart, S. Godin, H. Preud'homme, A. Allal, J. Szpunar*  
 IPREM, UMR 5254 CNRS- UPPA, Pau, France
- MP-262**    **Study on the synthesis and characterization of surface activities of hydrophilic derivatives of  $\beta$ -sitosterol**  
*J. C. Lim*  
 Dongguk University-Seoul, Department of Chemical and Biochemical Engineering, Seoul, Republic of Korea
- MP-263**    **Mass-Remainder Analysis (MARA): to understand mass spectra of copolymers**  
*T. Nagy, Á. Kuki, G. Deák, L. Nagy, M. Zsuga, S. Kéki*  
 University of Debrecen, Department of Applied Chemistry, Debrecen, Hungary
- MP-264**    **Compositional analysis of high molecular weight biodegradable polymers by high-resolution MALDI-ToFMS combining on-plate degradation with resolution-enhanced KMD analysis**  
*S. Nakamura, T. Fouquet, H. Sato*  
 National Institute of Advanced Industrial Science and Technology, Research Institute for Sustainable Chemistry, Tsukuba, Japan
- MP-265**    **Cold plasma treatment of polymer substrates for SALD ICP MS**  
*J. Preisler, M. Stiborek, M. Shekargoftar, V. Kanicky, J. Kelar*  
 Masaryk University, Department of Chemistry, Brno, Czech Republic
- MP-266**    **Remainders of Kendrick mass: keeping the best of a Kendrick mass defect analysis for low-accuracy mass spectra of polymers**  
*H. Sato, T. Fouquet*  
 National Institute of Advanced Industrial Science and Technology (AIST), Research Institute for Sustainable Chemistry, Tsukuba, Japan
- MP-267**    **Analysis of degraded polybutyleneterephthalate (PBT) products by Thermal Desorption and Pyrolysis combined with DART-MS (TDP/DART-MS)**  
*C. Takei, K. Yoshizawa*  
 BioChromato, Inc., Application support, Fujisawa, Japan
- MP-268**    **Evaluation of thermal history of thermoplastic resins by Thermal Desorption and Pyrolysis Combined with DART-MS (TDP/DART-MS)**  
*C. Takei, K. Yoshizawa*  
 BioChromato, Inc., Application support, Fujisawa, Japan
- MP-269**    **MALDI-LID-ToF/ToF analysis of statistical and diblock polyacrylate copolymers**  
*J. Town, G. Jones, D. Haddleton*  
 University of Warwick, Chemistry, Coventry, United Kingdom

## TUESDAY, August 28<sup>th</sup>, 2018

### TPS-S01 - Therapeutic Drug Monitoring and Drug Discovery

- TP-1**        **Phosphoproteomics of non-small-cell lung cancer cells treated with erlotinib reveals drug-resistant signatures and potential targets**  
*J. Adachi, Y. Abe, M. Nagano, J. Isoyama, M. Kishida, T. Tomonaga*  
 National Institutes of Biomedical Innovation, Health and Nutrition, Laboratory of Proteomics for Drug Discovery, Osaka, Japan

- TP-2 **Comparison of methionine oxidation profiles of biosimilar TUR01 monoclonal antibody to its reference under oxidative stress**  
A. E. Atik, Z. Z. Yildirim Keles, G. Güven, I. E. Gülser, Y. Erdemgil, D. Bayçin, Ö. Can, R. S. Alpan  
 Turgut Pharmaceuticals, Biotechnology Group, İstanbul, Turkey
- TP-3 **Quantitative evaluation of adenosine 5'-tetrphosphate and other five analytes related to nicotinamide phosphoribosyltransferase by LC-MS in Melanoma cells and mouse plasma**  
M. Bianchi, A. Grolla, C. Travelli, S. Garavaglia, A. Genazzani, G. Orsomando, E. Del Grosso  
 University of Piemonte Orientale, Department of Pharmaceutical Sciences, Novara, Italy
- TP-4 **Analytical aspects of sunitinib and its geometric isomerism towards therapeutic drug monitoring in clinical routine**  
M. Buzzo, B. Posocco, E. Marangon, G. Toffoli  
 National Cancer Institute of Aviano, University of Trieste, Aviano, Italy
- TP-5 **A LC-MS-based assay for the determination of activity and inhibition of Anopheles gambiae 3-hydroxykynurenine transaminase enzyme**  
R. Canavesi, U. Galli, R. Miggiano, F. Rossi, E. Del Grosso  
 Università del Piemonte Orientale, Department of Pharmaceutical Sciences, Novara, Italy
- TP-6 **Rapid, sensitive fentanyl detection by thermal desorption PTR-MS and collision induced dissociation**  
L. Cappellin, F. Lopez  
 TOFWERK AG, R&D, Thun, Switzerland
- TP-7 **A validated and robust analytical method for pesticides measurement in cannabis by liquid chromatography tandem mass spectrometry**  
C. Clarysse  
 Perkin Elmer, Chrom and Mass Spec. Division, Villebon Sur Yvette, France
- TP-8 **Data independent acquisition modes for identification, quantification and monitoring of low-abundance host cell proteins during monoclonal antibody bioprocessing**  
C. Doneanu, A. Xenopoulos, R. Skudas, Q. Yu Ying, A. Chakraborty, W. Chen  
 Waters, Biopharmaceutical Sciences, Milford, USA
- TP-9 **Clinical validation of a UPLC/MS/MS-based assay to concurrently monitor four direct oral anticoagulants in dried blood spots**  
K. I. Foerster, A. Huppertz, A. D. Meid, O. J. Müller, L. Tilemann, T. Rizos, W. E. Haefeli, J. Burhenne  
 Heidelberg University Hospital, Department of Clinical Pharmacology and Pharmacoepidemiology, Heidelberg, Germany
- TP-10 **Development of a SPME tool for the determination of a small molecule-drug conjugate against carbonic anhydrase in cancer chemotherapy**  
S. Ghiasikhou, J. Scheuermann, S. Cazzamalli, D. Neri, R. Zenobi  
 ETH Zurich, Switzerland
- TP-11 **In vivo assessment of the contribution of surfactant replacement therapy in rabbits by stable isotopes natural abundance approach**  
S. Giambelluca, F. Ricci, M. Simonato, L. Vedovelli, A. Correani, C. Casiraghi, M. Storti, P. Cogo, F. Salomone, V. P. Carnielli  
 Padova University Hospital, Department of Women's and Children's Health, Padova, Italy
- TP-12 **BiopharmaView™ for fast and efficient monitoring of pH induced deamidation**  
 F. Sanchez, L. Ji, K. Pohl, J. Dojahn, A. Uppal, S. Heidelberger  
 Sciex, Biologics, Warrington, United Kingdom
- TP-13 **Unrevealing phase I metabolism of combretastatin A4 by a multi-tool MS-based approach**  
K. Jaroch, P. Z. Goryńska, K. Goryński, T. Stefański, B. Bojko  
 Nicolaus Copernicus University in Torun, Collegium Medicum in Bydgoszcz, Department of Pharmacodynamics and Molecular Pharmacology, Faculty of Pharmacy, Bydgoszcz, Poland
- TP-14 **Application of triple quadrupole MS for drug-to-antibody ratio and molecular weight determination of antibody-drug conjugates**  
M. Källsten, R. Hartmann, M. Pijnappel, L. S. Bergström, J. Bergquist, F. Lehmann  
 Uppsala university, Department of Chemistry-BMC, Uppsala, Sweden



- TP-15 **Drawing the activity of auranofin by an electrochemical reaction cell coupled to an ESI MS/MS**  
*P. Katarzyna, M. Kupiec, R. Ziolkowski*  
Warsaw University of Technology, Faculty of Chemistry, Chair of Analytical Chemistry, Warsaw, Poland
- TP-16 **Therapeutic effect of a natural alkaloid observed in 5xFAD transgenic Alzheimer's transmodel: a proteomics study**  
*I. Kirs, M. Karayel Başar, B. Gürel, T. Mroczek, K. Skalicka-Wozniak, A. T. Baykal*  
Acibadem Mehmet Ali Aydınlar University, Medical Biochemistry, İstanbul, Turkey
- TP-17 **Simultaneous determination of aripiprazole, dehydro-aripiprazole, olanzapine, risperidone, paliperidone, quetiapine and clozapine in human plasma by LC-MS/MS**  
*D. Koller, A. Wojnicz, F. Abad-Santos*  
Hospital Universitario de la Princesa, Clinical Pharmacology, Madrid, Spain
- TP-18 **LC-MS identification and quantification of bleomycin in serum and tumor tissue**  
*T. Kosjek, T. Gornik, D. Zigon, M. Bosnjak, S. Kranjc, M. Krzan, A. Grosej, M. Cemazar, G. Sersa*  
Jozef Stefan Institute, Dept. Envir. Sci., Ljubljana, Slovenia
- TP-19 **Solid phase microextraction for the quantification of doxorubicin and untargeted metabolic profiling of lung tissue during in vivo lung perfusion**  
*N. Looby, B. Bojko, G. A. Gómez-Ríos, M. Tascon, A. Roszkowska, K. Gorynski, J. Pawliszyn*  
University of Waterloo, University of Waterloo, Department of Chemistry, Waterloo, Canada
- TP-20 **Assessment of antibody-derived therapeutics at the intact and middle-up level by CESI-MS**  
*E. Domínguez-Vega, R. Haselberg, G. W. Somsen, J. Thorn, C. Löbner, S. Lock*  
Sciex, CE and Biopharma, Darmstadt, Germany
- TP-21 **Detection and characterization of stable iminium ion reactive metabolite using high resolution mass spectrometry.**  
*T. Miraval*  
Idorsia LTD, DMPK, Allschwil, Switzerland
- TP-22 **Phytochemical composition of extracts from wood and leaves of Lebanese Cedar (*Cedrus libani*) using GC/MS**  
*S. Mokh, M. Al Iskandarani, M. Locatelli, S. Carradori, C. Celia, J. Farouk*  
Lebanese atomic energy commission, Laboratory of analysis of organic compound, Beirut, Lebanon
- TP-23 **A combination of chemical proteomics and DARST-based approaches to disclose natural products biological targets**  
*F. Del Gaudio, S. Ceccacci F. Pollastro, M. Mozzicafreddo, A. Minassi, R. Riccio, M. C. Monti*  
Dept. of Pharmacy, University of Salerno, Fisciano (Salerno), Italy
- TP-24 **Focal adhesion kinase binding partner study in human colon cancer cell HCT-116 using immunoprecipitation method coupled with nano-LC/MSMS technique**  
*B. T. Nguyen, M.-J. Kang*  
Korea Institute of Science and Technology, Korea University of Science and Technology, Seoul, Republic of Korea
- TP-25 **Comprehensive N-glycan structure catalogue of therapeutic antibodies**  
*M. J. Oh, N. Seo, J. An Hyun*  
AGRS, Chungnam National University, Daejeon, Republic of Korea
- TP-26 **Monitoring of sequence variants by MAM using high resolution mass spectrometry**  
*K. Pohl, Y. Li, C. Nortcliffe, A. Uppal, F. Sanchez, J. Dojahn, S. Heidelberger*  
Sciex, Biologics, Darmstadt, Germany
- TP-27 **Epitope peptides identified by online biosensor-MS neutralize pathophysiological antibodies and open new clinical therapy approaches for lysosomal diseases**  
*M. Przybylski, L. Lupu, P. Wiegand, Z. Kukacka, S. Maeser, Y. Baschung, F. Völklein, A. Lazarev, A. Maria Papini, J. Hennermann, K. Schmitz*  
Steinbeis Centre for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany
- TP-28 **Chromatography coupled to mass spectrometry for stability studies in drug discovery**  
*L. Queguiner, D. Speybrouck, S. Thomas*  
Janssen Resarch & Development, Discovery Sciences, Val de Reuil, France

- TP-29 **ABCs of mABs and ADCs**  
*S. Reeksting, T. Chapman, B. Alkhwaja, A. Watts, A. Lubben*  
 University of Bath, Faculty of Science, Chemical Characterisation and Analysis Facility (CCAF), Bath, United Kingdom
- TP-30 **Development of a hybrid LC-MS/MS method for the quantification of antibody-conjugated payload in in-vivo and in-vitro ADC samples**  
*F. Riccardi Sirtori, E. Bertotti, A. Ariaudo, F. Molinaro, I. De Salve, L. Barbero, S. Kumar, S. Riva, T. Goletz*  
 RBM-Merck group, NBE Drug Disposition, QPD, Colletterto Giacosa (TO), Italy
- TP-31 **Epitope and affinity determination of recombinant Mycobacterium tuberculosis Ag85B antigen towards anti-Ag85 antibodies using proteolytic-affinity mass spectrometry and biosensor analysis**  
*F. Rinaldi, L. Lupu, H. Rusche, Z. Kukacka, S. Tengattini, R. Bernardini, L. Piubelli, T. Bavaro, S. Maeser, L. Pollegioni, E. Calleri, M. Przybylski, C. Temporini*  
 University of Pavia, Department of Drug Sciences, Pavia, Italy
- TP-32 **Monitoring of therapeutic doses of antipsychotic drugs in saliva and serum samples with the use of solid-phase microextraction technique**  
*A. Roszkowska, L. Konieczna, W. Zukowicz, M. Galewska, W. Cubala, T. Baczek*  
 University of Waterloo, Department of Chemistry, Waterloo, Canada
- TP-33 **Multi-attribute monitoring (MAM) to identify differences in Trastuzumab from 2 manufacturers.**  
*F. Sanchez, C. Nortcliffe, K. Pohl, J. Dojahn, S. Heidelberg*  
 Sciex, Biologics, Barcelona, Spain
- TP-34 **LC-MS/MS analysis and rat pharmacokinetics of the novel cyclin-dependent kinase inhibitors BP-14 and BP-20**  
*J. Široká, M. Čečková, L. Urbánek, V. Kryštof, T. Gucký, J. Hofman, M. Štrnad, F. Štaud*  
 Palacký University, Laboratory of Growth Regulators, Olomouc, Czech Republic
- TP-35 **Identification of 5-fluorocytosine and its metabolites in complex samples by liquid chromatography coupled with mass spectrometry**  
*P. Škvára, M. Matúšková, E. Duriniková, S. Andrea Vojs*  
 Comenius University in Bratislava, Department of Analytical Chemistry, Faculty of Natural Sciences, Bratislava, Slovak Republic
- TP-36 **Efficient dereplication with high resolution high accuracy mass spectrometry for the discovery of novel bioactive natural products**  
*L. Song*  
 Dept Chemistry, University of Warwick, Coventry, United Kingdom
- TP-37 **Collision-induced dissociation study of antimicrobial peptide dendrimers**  
*A. Tintaru, L. Charles*  
 Aix-Marseille Université - CNRS, Institut de Chimie Radicalaire UMR7273, Marseille, France
- TP-38 **Mass spectrometry characterization of an NMS proprietary drug conjugated antibody (ADC)**  
*S. Troianj, R. Perego, U. Cucchi, P. Orsini, M. Salsa, M. Caruso, B. Valsasina*  
 Nerviano Medical Sciences srl, Oncology/Biotechnology, Nerviano (MI), Italy
- TP-39 **Assessing the drugability of PTP1B non-catalytic sites with mass spectrometry**  
*G. A. Villar, C. Buning, J. Czech, M. Dreyer, G. Hessler, S. Matthias Petry, N. Tennagels, S. Welte*  
 Sanofi-Aventis Deutschland GmbH, Integrated Drug Discovery, Frankfurt am Main, Germany
- TP-40 **Ultrafast detection of drugs and metabolites in urine by Flow Injection Analysis (FIA) coupled to Magnetic Resonance Mass Spectrometry (MRMS)**  
*M. Witt, M. Godejohann, A. Barsch*  
 Bruker Daltonik GmbH, MRMS Solutions, Bremen, Germany
- TP-41 **Efficient phospholipids removing clean-up SPE-LC-MS/MS method for simultaneous plasma quantification of 11 tyrosine kinase inhibitors and caffeine. Application to therapeutic drug monitoring**  
*A. Wojnicz, D. Koller, V. Vaitsekhovich, O. J. L. Steegmann, F. Abad-Santos*  
 Hospital Universitario de la Princesa, Clinical Pharmacology Department, Madrid, Spain
- TP-42 **Quantification of major peanut protein allergen isoform groups from peanut protein extracts**  
*K. Alving, P. DeMontigny, B. Wang*  
 Sanofi, Analytical Research and Development, Waltham, USA

- TP-43 Validation of breath biopsy platform for longitudinal measurement of VOCs in breath using TD-GC-MS**  
*J. Boschmans, R. Smith, M. van der Schee, S. Kitchen, B. Boyle, M. Allsworth*  
 Owlstone Medical Ltd., Chemistry, Cambridge, United Kingdom
- TP-44 Elimination profile of betamethasone and metabolites in urine after different administration routes**  
*S. Coll, X. Matabosch, N. Monfort, E. Alechaga, C. Pérez-Mañá, J. A Mateus, J. Monfort, J. Llorente-Onaindia, R. Ventura*  
 Institut del Mar d'Investigacions Mèdiques, Catalanian anti-doping laboratory, Barcelona, Spain
- TP-45 Variability and values in glycosylation analyses of monoclonal antibodies: an interlaboratory study**  
*M. L. A. De Leoz, D. L. Duewer, S. E. Stein*  
 National Institute of Standards and Technology (NIST), Material Measurement Laboratory, Gaithersburg, USA
- TP-46 Application of Acoustic Mist Ionization Mass Spectrometry (AMI-MS) for the development of kinase assays**  
*D. Srivastava, P. Deland, J. Wingfield, J. Tart, P. Clarkson, M. Tonge*  
 Labcyte inc., Mass Spectrometry Product Management, San Jose, USA
- TP-47 A mass spectrometry toolbox for the optimization of K-RAS G12C covalent inhibitors**  
*S. Raibaud, A. Buzy, S. Hamon, P. Paul, J.-C. Guillemot, V. Lalleman, P. Didier, R. Arrebola, F. Duffieux, A. Parent, A. Rak, G. McCort, L. Debussche, F. Fassy*  
 Sanofi, Research Platform & Oncology, Chilly-Mazarin & Vitry sur Seine, France
- TP-48 LC-MS/MS method for analysis of therapeutic peptide Axon Peptide 108 in AADVac1 drug product**  
*J. Galba, J. Piestansky, P. Barath, B. Kovacech, A. Kovac*  
 Axon Neuroscience SE R&D, Proteomics & Metabolomics, Bratislava, Slovakia
- TP-49 Analysis of host cell proteins in antibody preparations using PASEF**  
*M. Greig, S. Pengelley, G. Tremintin, D. Suckau, W. Evers*  
 Bruker Daltonics, San Jose, USA
- TP-50 Simultaneous determination of tramadol, O-desmethyltramadol, and N-desmethyltramadol in human plasma by liquid chromatography-tandem mass spectrometry and its application to a pharmacokinetic study**  
*C.-M. Lee, Y. Kim, W. Chae, E. Hyun Jung, S. Lee*  
 Sungkyunkwan University, School of Pharmacy, Suwon, Republic of Korea
- TP-51 A rapid and highly sensitive liquid chromatography-tandem mass spectrometry method for simultaneous determination of meloxicam and 5'-carboxymeloxicam in human plasma and its application to a pharmaco**  
*C.-M. Lee, E. Hyun Jung, J. Lee Yun, H. Lee, J. Lee, S. Lee*  
 Sungkyunkwan University, School of Pharmacy, Suwon, Republic of Korea
- TP-52 Investigation of amyloid-beta 1-42 reactivity and stable adduct(s) formation by mass spectrometry-based approach**  
*M. Naldi, A. De Simone, D. Tedesco, M. Bartolini, V. Andrisano*  
 Alma Mater Studiorum University of Bologna, Department of Pharmacy and Biotechnology, Bologna, Italy
- TP-53 Dose- and time-dependent effects of hepatotoxicants on ADME proteins in 3D human liver spheroids by PRM**  
*N. Selevsek, W. E. Wolski, L. Kunz, H. Cordes, V. Baier, L. Kuepfer, O. Clayton, A. Roth, R. Schlapbach*  
 Functional Genomics Center Zurich, ETH Zurich, Zurich, Switzerland

### **TPS-S02 - Single Cell**

- TP-54 Function of PIWIL3 in mammalian oocytes**  
*M. Tan, H. Van Tol, M. Damen, T. Stout, W. Wu, B. Roelen*  
 Utrecht University, Biomolecular Mass Spectrometry & Proteomics, Utrecht, Netherlands

- TP-55 **Picoliter pressure-probe-electrospray-ionization mass spectrometry for in situ monitoring single plant cell metabolite changes under stress conditions**  
*R. Erra-Balsells, K. Nakata, H. Wada, H. Nonami*  
 Departamento de Química Organica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, Argentina
- TP-56 **Drug uptake and metabolism in single liver cells**  
*L. Pedro, P. Rudewicz*  
 Novartis Institutes for BioMedical Research, GDC, Emeryville, USA

### **TPS-S03 - Noncovalent Interactions**

- TP-57 **The assembly of islet amyloid polypeptide (IAPP) and the role of the disulfide bond**  
*M. Bowers, A. Ilitchev, D. Bishop, S. Buratto*  
 UCSB, Chemistry and Biochemistry, Santa Barbara, USA
- TP-58 **Gas-phase complexation of  $\alpha$ -/ $\beta$ -cyclodextrin with amino acids studied by ion mobility-mass spectrometry and molecular dynamics simulations**  
*Y. Chen, Z. Zuo, W. Wang, C. Ding*  
 Fudan University, Chemistry Department, Shanghai, China
- TP-59 **Investigating the interlocked nature of catenanes and knots with mass spectrometry and ion mobility spectrometry**  
*A. Krüve, C.A. Schalley*  
 Freie Universität Berlin, Institut für Chemie und Biochemie, Berlin, Germany
- TP-60 **Collision induced dissociation of multiply charged peptide aggregates**  
*M. Al-Majidi, A. Magyar, G. Schlosser*  
 ELTE Eötvös Loránd University, Department of Analytical Chemistry, Budapest, Hungary
- TP-61 **Novel, bilateral fluorine alkoxide-based clusters discovered by ambient ionization mass spectrometry**  
*M. Berta, T. Nagy, S. Kéki, J. Rábai, G. Schlosser*  
 ELTE Eötvös Loránd University, Department of Analytical Chemistry, Budapest, Hungary
- TP-62 **Noncovalent complexes in natural extracts**  
*P. Traldi, S. D'Aronco, S. Crotti, M. Agostini, L. Mattoli, M. Burico, S. Tamimi*  
 Fondazione Istituto di Ricerca Pediatrica Città della Speranza, Città della Speranza, Padova, Italy
- TP-63 **Steric structure and stability of the gas-phase complexes of macrocyclic receptors with anions**  
*M. Zimnicka, A. Wasilewska, K. Dabrowa, W. Danikiewicz*  
 Polish Academy of Sciences, Institute of Organic Chemistry, Warsaw, Poland

### **TPS-S04 - High Resolution MS: Instrumentation, Methods & Applications**

- TP-64 **Towards routine intact level quantification of monoclonal antibody in plasma by HRMS**  
*Y. Alelyunas, M. Wrona, H. Shion, C. Dunning, J. Kirk*  
 Waters Corp, Scientific Operations, Milford, USA
- TP-65 **Progress towards implementing accurate mass ms for routine biotherapeutic analysis**  
*H. Shion, W. Alley, J. Pugh, R. Lewis, Q. Yu Ying, W. Chen*  
 Waters Corp, Milford, USA
- TP-66 **Multiplexed analysis of environmental samples by GCxGC-HRMS with multi-ionization capabilities**  
*V. Artaev, G. Tikhonov, A. Lebedev*  
 LECO Corporation, St. Joseph, USA
- TP-67 **Gas chromatography-atmospheric pressure photoionization-high resolution mass spectrometry for the determination of semi-volatile fluorinated compounds**  
*J. F. Ayala-Cabrera, E. Moyano, F. J. Santos*  
 University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain

- TP-68 **Determination of quantitative amounts and ratio between enzyme variants in a sample, by spiking with stable isotope labelled peptide**  
T. Janne Bech  
DuPont Nutrition Biosciences ApS, Advanced Analysis, Brabrand, Denmark
- TP-69 **Think positive: finding the best matrix in MALDI-ToF MS for croconaine dyes investigation**  
C. D. Calvano, M. Capozzi, A. Punzi, G. Farinola, F. Palmisano, T. Cataldi  
University of Bari, Chemistry, Bari, Italy
- TP-70 **Efficient preparation of organoimido derivatives of Lindqvist hexamolybdate in leidenfrost droplets**  
J. Cao, Q. Wang  
Beijing Institute of Technology, School of Chemistry and Chemical Engineering, Beijing, China
- TP-71 **A novel PTR-ToF reaction cell superposing DC and RF fields leads to ten-fold improvements in sensitivities and LODs**  
L. Cappellin, F. Lopez, M. Hutterli, J. E. Krechmer, S. Klee, B. Plet  
ToFWERK AG, R&D, Thun, Switzerland
- TP-72 **Determining acetylcholinesterase activity using paper spray mass spectrometry**  
D. Carmany, G. Boyd, P. Mach, E. Dhummakupt, P. Demond, M. Busch, T. Glaros  
Excet Inc, ECBC, Gunpowder, USA
- TP-73 **LC-HRMS by means of untargeted data-dependent acquisition for the characterization of 'superfoods'**  
F. Di Ottavio, J. Gauglitz, L. Felix Nothias, M. Panitchpakdi, P. Dorrestein, D. Compagnone, M. Sergi  
University of Teramo, Faculty of Bioscience, Teramo, Italy
- TP-74 **High-resolution mass spectrometry in combination with in silico prediction models to improve accuracy for compound identification**  
E. Dossin, P. Diana, A. Glabasnia, M. Bentley, P. A. Guy  
Philip Morris Product S.A., R&D Chemical Research, Neuchatel, Switzerland
- TP-75 **High-throughput quan/qual LC-MS analysis: where is the sweet spot?**  
A.-C. Dubbelman, F. Cuyckens, L. Dillen, R. J. Vreeken, T. Hankemeier  
Leiden University, Leiden Academic Centre for Drug Research, Systems Biomedicine and Pharmacology, Leiden, Netherlands
- TP-76 **UHPLC-HRMS method for targeted analysis of cyanotoxins in freshwater**  
D. Filatova, M. Picardo, O. Núñez, M. Farré  
Institute of Environmental Assessment and Water Research, Spanish National Research Council, University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain
- TP-77 **Direct gas analysis using a multi-turn high-resolution mass spectrometer**  
M. Hashimoto, M. J. van der Schans, J. A. Van der Meer, B. Van der Meer  
JEOL(EUROPE)SAS, European Application Group, Croissy-sur-Seine, France
- TP-78 **Development of an LC-HRMS method to aid in identification and confirmation of chlorinated and brominated contaminants**  
A. Jonas, A. Miralles-Marco, G. Codling, S. Vojta, L. Melymuk, J. Klánová  
Research Centre for Toxic Compounds in the Environment (RECETOX) Brno, Czech Republic
- TP-79 **Combination of different ionization sources expands the analysis of complex mixtures**  
A. Kondylj, W. Schrader  
Max Planck Institut für Kohlenforschung, Mass Spectrometry, Mülheim an der Ruhr, Germany
- TP-80 **Aberration-based numerical optimization of ion mirrors**  
I. Kopaev, D. Grinfield, M. Monastyrskiy, M. Alexander  
General Physics Institute/T8, Optoelectronics Department, Moscow, Russian Federation
- TP-81 **Application of ETHCD for leucine/isoleucine discrimination in peptides**  
S. Kovalev, M. Tolpina, S. Zhokhov, T. Samguina, A. Lebedev  
Moscow State University, Chemistry Department, Moscow, Russian Federation
- TP-82 **A new LC-MS/MS method for determination of Apixaban in tablets**  
M. Kozanli, Ö. Can Nafiz  
Anadolu University, Faculty of Pharmacy, Department of Analytical Chemistry, Eskisehir, Turkey

- TP-83 **Multiplexed operation of high resolution orthogonal multi-reflecting time-of-flight mass spectrometer**  
*B. Kozlov, J. Brown, V. Artaev*  
Waters Corporation, Wilmslow, United Kingdom
- TP-84 **Screening for anthraquinones in chilean mushrooms by HPTLC - negative ion DESI high-resolution mass spectrometry**  
*A. Laub, A. Sendatzki, G. Palfner, N. Arnold, L. Wessjohann, J. Schmidt*  
Leibniz Institute of Plant Biochemistry, Bioorganic Chemistry, Halle, Germany
- TP-85 **The advantages of using an MRMHR acquisition for increased sensitivity for targeted analysis using a QToF instrument**  
*D. Mcmillan, P. Taylor, K. Hyland, C. Borton*  
Sciex, Business Development, Warrington, United Kingdom
- TP-86 **Contextualization of dark matter in MS1 FT-ICR MS<sup>1</sup> data**  
*F. Moritz, M. Kaling, J. Schnitzler, P. Schmitt-Kopplin*  
Helmholtz Zentrum Muenchen, Research Unit Analytical BioGeoChemistry, Neuherberg, Germany
- TP-87 **Simultaneous determination of nine water-soluble synthetic colorants in cosmetics by LC-Q-ToF/MS and LC-MS/MS**  
*S. Park, H. Kim Jun, G. Kang, A. Min, H. Lee Ji, H. Park, T. Hwang, S. Heo, Y. Eom Kwon, D. Woo Shin, S. Park, H. Kang*  
National Institute of Food and Drug Safety Evaluation, Division of Advanced Analysis, Chungcheongbuk-do, Republic of Korea
- TP-88 **SFC-ESI-QToF-MS: ddeveloping an innovative one-run method for chocolate quality and authenticity control**  
*M. Rektorisova, V. Hrbek, M. Tomaniova, J. Hajslova*  
University of Chemistry and Technology, Department of Food Analysis and Nutrition, Prague, Czech Republic
- TP-89 **Using Atomic Layer Deposition (ALD) to enhance MCPs for mass spectrometry**  
*M. Breuer, P. Holmes, J. Harper*  
Photonis, Research and Development, Sturbridge, USA
- TP-90 **The combination of hydrophilic interaction liquid chromatography and ion mobility mass spectrometry for diesel fuel analysis**  
*E. Smit, S. De Goede, E. Rohwer*  
University of Pretoria, Lynnwood Rd, Pretoria, South Africa
- TP-91 **Applying high-resolution mass spectrometry to elucidate the formation and fate of ozonation TPs in wastewater treatment**  
*J. Schollee, R. Gulde, M. Bourgin, M. Rutsch, J. Fleiner, M. Boehler, J. Hollender, U. Von Gunten, C. Mcardell*  
Eawag, Environmental Chemistry, Duebendorf, Switzerland
- TP-92 **Analysis of cationic polar pesticides in baby food using ion chromatography and MS/MS or high resolution accurate mass spectrometry**  
*F. Schoutsen, J. E Madden, J. S Rohrer, J. Beck*  
TFS, Breda, Netherlands
- TP-93 **An automated workflow for high-throughput nicotine quantitation using high performance liquid chromatography coupled to high resolution accurate mass spectrometry for prototype testing**  
*S. Sendyk, Q. Dutertre, A. Knorr, J. Hoeng, M. Bentley*  
Philip Morris, Science & Innovation, Neuchatel, Switzerland
- TP-94 **Characterization of stress degradation products of fosamprenavir calcium using Q Exactive™ Plus Orbitrap and LTQ XL™ mass spectrometers, and prediction of their toxicity using ADMET Predictor™**  
*D. K. Singh, M. K. Ladumor, C. N. Kotimoole, K. B. Batkulwar, A. Y. Deshpande, S. Giri, S. Singh*  
Department of Pharmaceutical Analysis, National Institute of Pharmaceutical Education and Research (NIPER), S.A.S. NAGAR, India

- TP-95 **Quadrupole-resolved all ions MS/MS for reliable quantitation of pesticides in complex matrices using untargeted acquisition**  
*L. Tölgyesi, A. Mielcarek, C. Klein, T. Knotts, D. Yang, B. Frazer, T. Anumol, J. Lee, W. E. Barry*  
Agilent Technologies Sales & Services GmbH & Co. KG, Global Laboratory Solution Sales (LSS) Marketing, Waldbronn, Germany
- TP-96 **Identification of electrochemical degradation products of selected pharmaceuticals by high resolution mass spectrometry**  
*A. Vojs Stanova, E. Medvecká, A. Borik, R. Grabic, P. Skvara, T. Mackulak, M. Marton, M. Vojs*  
Comenius University in Bratislava, Department of Analytical Chemistry, Faculty of Natural Sciences, Bratislava, Slovak Republic
- TP-97 **Removal of isobaric interferences by laser resonance ionization mass spectrometry for determination of  $^{126}\text{Sn}/^{121}\text{Sn}$  ratio**  
*W. Wang, X. Shen, L. Zhai, H. Deng, Z. Li*  
Northwest Institute of Nuclear Technology, Applied Physics and Chemistry Department, Xi'an, China
- TP-98 **Improving coverage in transmembrane domains of integral membrane proteins with ultra-violet photodissociation**  
*J. Whitelegge*  
University of California Los Angeles, The Pasarow Mass spectrometry Laboratory, Los Angeles, USA
- TP-99 **Study for mass resolution of quadrupole mass spectrometers according to the rod electrode alignment**  
*K. Yoshinari, Y. Terui*  
Hitachi, Ltd. Research & Development Group, Center for Technology Innovation, Hitachi-shi, Ibaraki-ken, Japan
- TP-100 **SweEt HRMS workflow strategy for screening unhealthy substances in food**  
*S. Ekroth, M. Johansson*  
National Food Agency, Chemistry Department, Uppsala, Sweden
- TP-101 **Simple workflow for proteoform separation and analysis using 2D gel electrophoresis-high resolution mass spectrometry**  
*M. Gaikwad, B. Dreyer, H. Schlüter*  
University Medical Center Hamburg Eppendorf, Mass Spectrometric Proteomics Institute for Clinical Chemistry and Laboratory Medicine, Hamburg, Germany
- TP-102 **Rapid and effective multi-class analysis of antibiotics in feedingstuffs at carry-over level by LC-MS/MS techniques**  
*I. Di Marco Pisciotto, L. Giannetti, B. Neri, M. Fiori, C. Civitareale, P. Stacchini, P. Gallo*  
Istituto Zooprofilattico Sperimentale del Mezzogiorno, Department of Chemistry, Portici (NA), Italy
- TP-103 **Determination of organic arsenic compounds by means of high resolution molecular MS/MS**  
*R. Glabonjat, K. Jensen, N. Guttenberger, K. Francesconi*  
University of Graz, Analytical Chemistry, Graz, Austria
- TP-104 **Linear dynamic range improvement in ToF-MS/MS mode on X500 QToF system**  
*F. Zhong, S. Liu, W. Jin, D. Simmons, N. Bloomfield, R. Haufler*  
Sciex, Research, Concord, Canada
- TP-105 **Applying a novel component detection algorithm to help accelerate metabolomics discovery workflows**  
*C. Hinz, E. G. Armitage, K. Hobby, N. Loftus, N. Gray, M. Y Schar, J. P. E. Spencer*  
Shimadzu UK Limited, LCMS technical department, Milton Keynes, United Kingdom
- TP-106 **Comprehensive analysis of flame retardants and other halogenated contaminants in dust from an e-waste recycling centre**  
*A. Jonas, K. Jobst, L. Melymuk, D. Bowman, M. Diamond, V. Arrandale, M. Venier, L. Jantunen, E. Reiner, J. Klánová*  
Masaryk University, RECETOX, Brno, Czech Republic
- TP-107 **Metabolomic and N-glycan characterization of skin fibroblasts from aged and young donors**  
*A. K. C. Laserna, B. H. Ng, J. Masilamani, T. T. Phan, S. F. Y. Li*  
National University of Singapore, Department of Chemistry, Singapore

- TP-108 Lean approach of automated sample preparation for LC-MS of intact proteins on a liquid handling robot**  
*K. List, D. Wetzel, M. Pauers*  
 Boehringer Ingelheim GmbH & Co. KG, Biologicals Development, Biberach, Germany
- TP-109 Combination of chemical ionization (CI) and low-energy electron ionization with high-resolution GC/Q-ToFMS**  
*V. Lopez-Avila, S. Nieto, H. Prest, J. Kernan, G. Yefchak, R. Clark, N. Eno, J. Oppenheimer, B. Russ, N. Cimino*  
 Agilent Technologies, Mass Spectrometry, Santa Clara, USA
- TP-110 Liquid chromatography coupled to quadrupole-Orbitrap high resolution mass spectrometry based method for target analysis and suspect screening of non-ionic surfactants in textiles**  
*X. Luo, Z. Niu, X. Ye, Z. Tang, L. Zhang*  
 Qingdao Customs, Inspection and Quarantine Technical Center, Qingdao, China
- TP-111 Comprehensive analysis of multi-class hazardous chemicals in plastic products using high resolution mass spectrometry**  
*Z. Niu, X. Luo, X. Ye, Z. Tang, L. Zhang*  
 Qingdao Customs, Inspection and Quarantine Technical Center, Qingdao, China
- TP-112 High resolution mass spectrometry based method for screening and identification of 48 prohibited dyes in textiles using data-dependent acquisition mode**  
*Z. Niu, X. Luo, Z. Tang, X. Ye, L. Qu*  
 Qingdao Customs, Inspection and Quarantine Technical Center, Qingdao, China
- TP-113 Quantitation of serum creatinine in mice using Hydrophilic Interaction Liquid Chromatography (HILIC) coupled with high-resolution accurate-mass (HRMS) Orbitrap mass spectrometer**  
*H. Takada, Y. Ube, M. Sakai, Y. Hasegawa, T. Kitayama, Y. Yamazaki, T. Uchimura*  
 Kyowa Hakko Kirin Co., Ltd, Translational Research Unit, R&D Division, Sunto-gun, Japan
- TP-114 Ultrasensitive detection of protein biomarkers by signal amplification mass spectrometry**  
*Y. Wang, R. Du, L. Qiao, B. Liu*  
 Department of Chemistry, Fudan University, Shanghai, China

### **TPS-S05 - MS Imaging: Instrumentation**

- TP-115 Development of optics of a stigmatic imaging mass spectrometer with high spatial resolution**  
*J. Aoki*  
 Osaka University, Graduate School of Science, Toyonaka, Japan
- TP-116 Developing MS Imaging in the context of chemical ecology - laser ablation electrospray ionization on three-dimensional samples**  
*B. Bartels, D. Hölscher, P. Kulkarni, A. Svatoš*  
 Research Group Mass Spectrometry/Proteomics, Max Planck Institute for Chemical Ecology, Jena, Germany
- TP-117 Improved sensitivity and speed of acquisition using quadrupole based mass spectrometer for DESI-MSI**  
*E. Claude, P. Harapanahalli, E. Jones*  
 Waters Corporation, Scientific Operations, Wilmslow, United Kingdom
- TP-118 Atmospheric pressure MALDI imaging Orbitrap MS using a Masstech APMALDI UHR ion source**  
*G. Frache, D. El Assad*  
 Luxembourg Institute of Science and Technology, Materials research and technology, Belvaux, Luxembourg
- TP-119 Hybrid SIMS: A new SIMS instrument for high resolution organic imaging with highest mass-resolving power and MS/MS**  
*S. Kayser, A. Pirkl, R. Moellers, D. Scurr, N. Starr, E. Niehuis*  
 IONTOF GmbH, Sales, Muenster, Germany



- TP-120 **Desorption electrospray ionization triple quadrupole mass spectrometry: Targeted drug and metabolite imaging in bioanalytical research**  
*L. Lamont, G. Eijkel, E. Jones, B. Flinders, S. Ellis, T. Porta, R. Vreeken, R. Heeren*  
Maastricht University, Maastricht Multimodal Molecular Imaging (M4I) Institute, Maastricht, Netherlands
- TP-121 **Open development kit for building an ambient mass imaging robot with micrometric resolution**  
*A. Moreno-Pedraza, C. Ovando-Vázquez, H. Guillén-Alonso, I. Rosas-Román, S. Gibb, R. Winkler*  
CINVESTAV, Biotechnology and Biochemistry, Irapuato, Mexico
- TP-122 **Big data post-processing for higher throughput MALDI/DESI FTMS imaging**  
*K. O. Nagornov, A. N. Kozhinov, P. C. Kooijman, E. Nicol, P. A. D. Kilgour, S. R. Ellis, R. M. A. Heeren, Y. O. Tsybin*  
Spectroswiss, Biomolecular Mass Spectrometry, Lausanne, Switzerland
- TP-123 **Paternò-Büchi photo-derivatization protocol for MALDI-MS imaging of carbon-carbon double bond positional isomers of phospho- and glycolipids in biological tissues**  
*A. Bednarik, S. Bölsker, J. Soltwisch, K. Dreisewerd*  
University of Münster, Institute for Hygiene, Biomedical Mass Spectrometry, Münster, Germany
- TP-124 **Heat-assisted laser ablation electrospray ionization (HA-LAESI) for MS imaging of animal tissue**  
*J. Hietä, R. Räsänen, J. Kopra, H. Rääkkönen, R. Kostiaainen, T. Kauppila*  
University of Helsinki, Faculty of Pharmacy, Helsinki, Finland
- TP-125 **Performance-enhanced data acquisition utilizing real-time DSP**  
*U. Lindblad, C. Watolla*  
Teledyne Signal Processing Devices Sweden AB, N/A, Linköping, Sweden
- TP-126 **Electrospray ionization/atmospheric pressure interfaces: comprehensive simulation of gas flow, space charge and electric fields**  
*P. Krah, L. Bernier, S. Rauschenbach, J. Reiss*  
Technical University Berlin, ISTA, Berlin, Germany

### **TPS-S06 - Post Translational Modifications**

- TP-127 **Improvement of proteomic analysis targeting multiple post-translational modifications using immunoprecipitation with pan-PTM antibodies**  
*Y. Abe, A. Tada, J. Isoyama, T. Tomonaga, J. Adachi*  
National Institute of Biomedical Innovation, Health, and Nutrition, Proteome Research Project, Osaka, Japan
- TP-128 **The role of thiols in redox biology: HPLC-MS characterization of cysteine derivatives generated by interaction with cold plasma jets, powerful sources of nitrogen and oxygen species**  
*G. Bruno, J. Lackmann, S. Wenske, S. Bekeschus, K. Weltmann, T. Von Woedtke, K. Wende*  
Leibniz Institute for Plasma Science and Technology (INP Greifswald), ZIK plasmatis, Greifswald, Germany
- TP-129 **A rapid, multiplexed kinase activity assay using iTRAQ labeling and MALDI-ToF/ToF MS**  
*C. Chen, Y. Liu*  
China Medical University, Taichung, Taiwan, Province of China
- TP-130 **Using sub-ranked database matching scores for improving the peptide and protein identification performance**  
*Y.-R. Chen, Y.-L. Chen, W.-H. Chang*  
Academia Sinica, Agricultural Biotechnology Research Center, Taipei, Taiwan, Province of China
- TP-131 **Separation of combinatorial PTMs on histone H3 tail with an advanced data analysis and ion mobility**  
*Y. Chikaoka, H. Ueda, R. Kajita, K. Yamamoto, L. Sujin, T. Tanaka, T. Kawamura*  
Isotope Science Center, The University of Tokyo, Tokyo, Japan
- TP-132 **Quantitative phosphoproteomics identifies alterations of doublecortin-like kinase 1 (DCLK1) in neural progenitor cell differentiation**  
*A. Dehghani, M. Goedderz, V. Giesemann, D. Winter*  
University of Bonn, Institute of Biochemistry and Molecular Biology, Bonn, Germany

- TP-133 Analysis of protein-phenolic compound modifications using electrochemistry coupled to mass spectrometry**  
*C. Kallinich, S. Schefer, S. Rohn*  
 Hamburg School of Food Science, University of Hamburg, Department Food Chemistry, Hamburg, Germany
- TP-134 A new phosphoproteome enrichment strategy in small-scale using phospho-specific antibodies with online mHFER-nanoLC-ESI-MS/MS**  
*Y. L. Sun, K. Kim, D. Kang*  
 Korea Research Institute of Standards and Science, Division of Chemical and Medical Metrology, Daejeon, Republic of Korea
- TP-135 Histone middle-down analysis using by multiple dissociation methods**  
*T. Kawamura, H. Ueda, D. Higo, Y. Chikaoka, K. Yamamoto, L. Sujin*  
 Isotope Science Center, The University of Tokyo, Tokyo, Japan
- TP-136 Influence of digestion conditions on post-translational modifications in monoclonal antibodies**  
*M. Khalikova, A. Ortiz, K. Sandra*  
 Charles University, Faculty of Pharmacy, Hradec Kralov , Czech Republic
- TP-137 Identification and characterization of O-Xylosylation and O-Glycosylation of recombinant protein therapeutics by mass spectrometry**  
*V. Larraillet*  
 Roche Pharmaceutical Research and Early Development, Biochemical and Analytical Research, Roche Innovation Center, Munich, Germany
- TP-138 Specific mass tag of methylated amino acid validates the SUMOylation sites by HCD on Orbitrap mass spectrometer**  
*F. Li, Y. Cheng*  
 Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan, Province of China
- TP-139 How does CE-MS compare with LC-MS in PTM analysis?**  
*K. Faserl, B. Sarg, H. Lindner, J. Thorn, C. L bner, S. Lock*  
 Sciex, CE and Biopharma, Darmstadt, Germany
- TP-140 Characterization of NIST monoclonal antibody on Intact, Subunit, and Peptide level with Monitoring of CQA's on the 6600**  
*C. Nortcliffe, K. Pohl, J. Dojahn, F. Sanchez*  
 Sciex, Phoenix House, Warrington, United Kingdom
- TP-141 The PASEF method on a TIMS-QToF mass spectrometer for High Sensitivity Phosphoproteomics**  
*P.-O. Schmit, H. Koch, T. Kosinsky, M. Willets, M. Lubeck, S. Koch, O. Raether, G. Kruppa, A. Alving*  
 Bruker France, Proteomics, Wissembourg, France
- TP-142 The citrulline effect in the dissociation of deiminated peptides**  
*A. Steckel, K. Uray, D. Papp, G. Schlosser*  
 ELTE E tv s Lor nd University, Doctoral School of Chemistry, Department of Organic Chemistry, Budapest, Hungary
- TP-143 Chemical acetylation of histone lysine residues at the protein level using acetic anhydride**  
*A. van Pijkeren, M. D. Kwiatkowski, R. P. H. Bischoff*  
 Rijksuniversiteit Groningen, Analytical Biochemistry, Groningen, the Netherlands
- TP-144 High resolution mass spectrometry based approach for the characterization of plasma proteins oxidative modifications by ROS**  
*A. Vasilyeva, L. Yurina, M. Indeykina, A. Bugrova, A. Kononikhin, M. Rosenfeld, E. Nikolaev*  
 N.M. Emanuel Institute of Biochemical Physics, RAS, Laboratory of Thermodynamics of Biosystems, Moscow, Russian Federation
- TP-145 Mass spectrometry-based investigations of cold physical plasma-induced PTM's in peptides**  
*S. Wenske, J. Lackmann, G. Bruno, S. Bekeschus, K. Weltmann, T. Von Woedtke, K. Wende*  
 INP Greifswald e.V., ZIK plasmatis, Greifswald, Germany
- TP-146 Next-generation proteomics insights into Bacillus cereus virulome highlights the key role of methionine oxidation of exoproteins**  
*B. Alpha-Bazin, J. P. Madeira, H. Omer, J. Armengaud, C. Duport*  
 CEA, DRF/JOLIOT/DMTS, Bagnols-sur-Ceze, France

- TP-147** **Identifying the disulfide bond pattern and ECM interaction site of TGFBIp**  
*M. V. Lukassen, C. Scavenius, I. B. Thøgersen, J. J. Enghild*  
 Aarhus University, Interdisciplinary Nanoscience Center (iNANO), Aarhus, Denmark
- TP-148** **Increasing variants in hydrophobic interaction chromatography during stability study of humanised monoclonal antibody identified by LC-MS ESI Q-ToF top down, middle down and bottom up analyses**  
*M. Pauers, K. List, D. Wetzel*  
 Boehringer Ingelheim Pharma GmbH & Co KG, Pharmaceutical Development Biologicals, Biberach an der Riss, Germany
- TP-149** **High resolution mass spectrometry characterization of the oxidation pattern of methionine and cysteine residues in human mitochondria voltage-dependent anion selective channel isoforms**  
*R. Saletti, M. G. G. Pittalà, P. Risiglione, V. Cunsolo, V. De Pinto, S. Foti*  
 Department of Chemical Sciences, University of Catania, Catania, Italy
- TP-150** **Understanding epigenetic control of histone modifications during drought acclimation in sorghum using top-down mass spectrometry**  
*M. Zhou, N. Malhan, A. Ahkami, K. Engbrecht, G. Myers, J. Dahlberg, J. Hollingsworth, J. Sievert, R. Hutmacher, M. Madera, P. Lemaux, K. Hixson, C. Jansson, L. Paša-Tolić*  
 Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, Richland, USA

### **TPS-S07 - Mass Spectrometric Analysis of Forensic Science Evidence**

- TP-151** **Human salivary glycomics for saliva-specific signatures by nanoPGC-LC/MS**  
*J. B. Kim, J. Y. Park, H. J. An*  
 Graduate School of Analytical Science and Technology & Asia-Pacific Glycomics Reference Site, Chungnam National University, Daejeon, Republic of Korea
- TP-152** **Single-injection screening of 664 Forensic Toxicology Compounds using an Innovative Benchtop High Resolution Mass Spectrometer**  
*J. Anichina, O. G. Cabrices, X. He, H. McCall, L. Baker, A. Wang, A. Taylor*  
 Sciex, Product Applications Laboratory, Concord, Canada
- TP-153** **Ultra-sensitive forensic analysis workflow of cocaine and metabolites in hair samples using LC-MS/MS**  
*J. Anichina, O. G. Cabrices*  
 Sciex, Product Applications Laboratory, Concord, Canada
- TP-154** **FT-ICR fingerprinting of human fingerprints**  
*A. C. Assis, M. H. Florêncio, C. Cordeiro*  
 Laboratório de Polícia Científica da Polícia Judiciária, University of Lisbon, Laboratório de FTICR e Espectrometria de Massa Estrutural, FCUL, Lisbon, Portugal
- TP-155** **A qualitative/quantitative LC-QToF-MS assay for forensic drug screening in urine – Feasibility study and basic method validation**  
*L. Huppertz, R. Peter, M. Schmidt, Z. Czentnar, V. Auwärter*  
 Bruker Daltonik GmbH, Application/Applied, Bremen, Germany
- TP-156** **Analysis of substances relevant to § 24a (2) of the German road traffic act using LC-MS<sup>n</sup> – A method development as a first step to avoid immunoassay pre-screening**  
*J. Kempf, V. Auwärter, F. Ehrhardt, Z. Czentnar*  
 Bruker Daltonik GmbH, Application/Applied, Bremen, Germany
- TP-157** **Isolation and identification of thick skin microbiota using MALDI-ToF Biotyper**  
*G. De Oliveira Dias, A. M. Araújo Martins, R. Persighini Del Sarto*  
 Polícia Civil do Distrito Federal, Universidade de Brasília, Brasília, Brasil
- TP-158** **Application of ToF-SIMS technique to detection and imaging of fingerprints contaminated by cannabis**  
*E. Mackiewicz, J. Rogowski, A. Parczewski, M. I. Szyrkowska*  
 Lodz University of Technology, Faculty of Chemistry, Lodz, Poland

- TP-159 **Validation of blood proteomic signatures for the forensic determination of blood and its provenance**  
*C. Heaton, L. Deininger, E. Patel, M. R. Clench, V. Sears, C. Sammon, L. Cole, S. Francese*  
 Sheffield Hallam University, Biomolecular Research Centre, Sheffield, United Kingdom
- TP-160 **Development and validation of a gas-chromatography mass spectrometry method for the analysis of testosterone esters in biological matrices**  
*M. Iannone, C. Lattanzi, F. Botrè, X. De La Torre*  
 Laboratorio Antidoping FMSI Rome, Dipartimento di Chimica e Tecnologia del Farmaco, Sapienza University of Rome, Rome, Italy
- TP-161 **Elemental analysis of ink by laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS)**  
*A. Pawlaczyk, K. Zalecka, M. I. Szykowska*  
 Lodz University of Technology, Faculty of Chemistry, Institute of General and Ecological Chemistry, Lodz, Poland
- TP-162 **Detection of ricin and abrin toxins in complex matrices by two novel galactose enrichment methods and high resolution LC-MS/MS**  
*A. Puustinen, M. Rapinoja, M. Karjalainen, P. Vanninen*  
 Verifin, Dept of Chemistry, University of Helsinki, Helsinki, Finland
- TP-163 **LC-HRMS vs NMR for the identification of Ketocaine in seized material**  
*A. M. Caputo, S. Detti, S. Napoletano, G. De Sangro, R. Sacrpone, F. Sciubba, F. Vincenti, M. Sergi, D. Compagnone*  
 University of Teramo, Faculty of Bioscience, Teramo, Italy
- TP-164 **Targeted and untargeted analyses by means of LC-MS to characterize the illicit substances on seized material of vegetal origin.**  
*A. M. Caputo, S. Detti, S. Napoletano, V. Fraioli, A. Possi, A. Zompanti, R. Scarpone, F. Di Ottavio, M. Sergi, F. Vincenti, L. Felix Nothias, P. Dorrestein*  
 University of Teramo, Faculty of Bioscience, Teramo, Italy
- TP-165 **Modafinidz metabolites identification by means of LC-HRMS: from in silico prediction to in vitro confirmation with rat hepatocytes**  
*F. Vincenti, F. Fanti, A. Gregori, A. Rita Togna, D. Compagnone, M. Sergi*  
 Sapienza, University of Rome, Department of Chemistry, Roma, Italy
- TP-166 **Identification of Fine plastic materials by Thermal Desorption and Pyrolysis combined with DART-MS (TDP/DART-MS)**  
*C. Takei, K. Yoshizawa*  
 BioChromato, Inc., Application support, Fujisawa, Japan
- TP-167 **ToF-SIMS determination of detection limit of amphetamine in 'street drugs' and polluted fingerprints**  
*M. Gajek, E. Mackiewicz, J. Rogowski, A. Parczewski, M. I. Szykowska*  
 Lodz University of Technology, Faculty of Chemistry, Lodz, Poland

### **TPS-S08 - Ion Activation and Dissociations**

- TP-168 **Tandem mass spectrometry to assist the design of information-containing synthetic polymers: an efficient approach to facilitate their sequencing and increase their storage density**  
*J. Amalian, G. Cavallo, S. Poyer, J. Lutz, L. Charles*  
 Institut de Chimie Radicalaire, Aix-Marseille Université, Marseille, France
- TP-169 **Facile electron capture dissociation on Q-ToFs and Orbitraps for top- and middle-down proteomics at chromatographic time scales**  
*J. Beckman, V. Voinov*  
 e-MSion, Oregon State University, Corvallis, USA
- TP-170 **The role of H<sub>2</sub>O in the dissociation chemistry of [W<sub>6</sub>O<sub>19</sub>]<sup>2-</sup>: a combinational study by mass spectrometry and DFT calculation**  
*J. Cao, C. Ci*  
 Beijing Institute of Technology, School of Chemistry and Chemical Engineering, Beijing, China

- TP-171 **Controlled collision induced dissociation of large aromatic ions in a LQIT**  
*M. Carlos, H. Sabbah, C. Joblin*  
Institut de Recherche en Astrophysique et Planétologie, Université de Toulouse, CNRS, CNES, Toulouse, France
- TP-172 **Ultraviolet photodissociation of peptides and proteins, generated by electrospray and matrix-assisted laser desorption/ionization, on the same Q-Exactive mass spectrometer**  
*M. Dillillo, E. De Graaf, A. Yadav, M. Belov, L. McDonnell*  
Fondazione Pisana per la Scienza - ONLUS, Proteomics Laboratory, San Giuliano Terme, Italy
- TP-173 **Gas phase reactions of Indocyanine green using femtosecond-laser-pulse induced photodissociation and collision-induced dissociation**  
*E. Mitrofanov, T. Muskat, J. Grottemeyer*  
University of Kiel, Institute of Physical Chemistry, Kiel, Germany
- TP-174 **Lost in phase space: fragmentation energetics in quadrupole ion traps**  
*T. Neugebauer, T. Drewello*  
Friedrich-Alexander-University Erlangen-Nuremberg, Chair of Physical Chemistry I, Erlangen, Germany
- TP-175 **Collision induced dissociation of hydrogen deficient radical ions on the Omnitrap platform**  
*D. Papanastasiou, R. Zubarev*  
Fasmatech Science & Technology, Patriarchou Gregoriou, Agia Paraskevi, Athens, Greece
- TP-176 **Comprehensive glycomics study by nanoLC-EED-MS/MS**  
*Y. Tang, J. Wei, C. Costello, C. Lin*  
Boston University, Boston University, Department of Chemistry, Boston, USA
- TP-177 **ESI(-)MS/MS of 2-oxocarboxylate hydrazones: carboxyl group participation in two fragmentation pathways**  
*R. L. White, B. W. Firth, L. M. LeBlanc, J. S. Grossert*  
Dalhousie University, Chemistry, Halifax, Canada
- TP-178 **Assessing binding affinity with LILBID-MS**  
*P. Young, G. Hense, N. Morgner*  
Institute of Physical and Theoretical Chemistry, Goethe Universität Frankfurt, Frankfurt am Main, Germany
- TP-179 **Tuning mass spectrometric proteomics experiments: Collision energy dependence of Mascot score**  
*A. Revesz, T. A. Rokob, D. Jeanne Dit Fouque, L. Turiak, A. Memboeuf, K. Vekey, L. Drahos*  
Research Centre for Natural Sciences, Hungarian Academy of Sciences, MS Proteomics Research Group, Budapest, Hungary
- TP-180 **Structural characterization of complex lipids by ozone-induced dissociation and ultraviolet photodissociation on high-resolution mass spectrometers**  
*A. Criscuolo, D. L. Marshall, M. Zeller, B. L. J. Poad, J. Hauschild, T. W. Mitchell, G. E. Reid, S. J. Blanksby*  
Thermo Fisher Scientific GmbH, Life Science Mass Spectrometry, Bremen, Germany

### **TPS-S09 - Astrochemistry**

- TP-181 **PIRENEA 2: a new setup to study cosmic dust in the laboratory**  
*A. Bonnamy, P. Jusko, M.-C. Ji, P. Moretto-Capelle, S. Zamith, J.-M. L'Hermite, M. Pellarin, C. Joblin*  
Institut de Recherche en Astrophysique et Planétologie, Université de Toulouse, CNRS, CNES, Toulouse, France
- TP-182 **Mass spectrometry a new approach to study thunderstorms**  
*L. F. C. Oliveira, D. U. Tega, F. Galembek, M. N. Eberlin*  
UNICAMP, Chemistry Institute, Campinas, Brazil
- TP-183 **Reaction dynamics of substituted PAH ions**  
*P. Mayer, B. West, L. Lesniak, J. Burner*  
University of Ottawa, Dept. of Chemistry and Biomolecular Sciences, Ottawa, Canada

- TP-184 **A multi-vendor applicable target system for (MA)LDI instruments with distinct performance characteristics for the analysis of small organic molecules related to C chondrites**  
*E. Rados, E. Pittenauer, J. Frank, K. Varmuza, G. Allmaier*  
 TU Wien, Institute of Chemical Technologies and Analytics, Vienna, Austria
- TPS-S10 - Metabolomics**
- TP-185 **Measuring trehalose 6-phosphate (Tre6P) in different plant materials – the technical challenge of working at the femtomole scale**  
*R. Feil, M. G. Annunziata, J. E. Lunn*  
 Max Planck Institute of Molecular Plant Physiology, Dept. Metabolic Networks, Potsdam, Germany
- TP-186 **Identification of novel long chain N-acylhomoserine lactones of chain length C20 from the marine phototrophic bacterium *Rhodovulum sulfidophilum***  
*N. Arashida, K. Shimbo, T. Terada, T. Okimi, Y. Kikuchi, S. Hashiro, S. Umekage, H. Yasueda*  
 Ajinomoto Co., Inc., Institute for Innovation, Kawasaki, Japan
- TP-187 **Fatty acid  $\beta$ -oxidation fuels tricarboxylic acid cycle to sustain cell proliferation**  
*M. Audano, S. Pedretti, D. Caruso, N. Mitro, E. De Fabiani*  
 Università degli Studi di Milano, Milano, Italy
- TP-188 **Diagnostic performance of methylmalonic acid testing by LC-MS/MS compared to Holotranscobalamin by Immunoassay for vitamin B12 deficiency**  
*F. Bahadory, P. Stanford, A. R. Horvath*  
 NSW Health Pathology, Prince of Wales Hospital, Sydney, NSW, Australia
- TP-189 **Pycmetrix a framework for gas chromatography - mass spectrometry for clinical data pre-processing, analysis and feature extraction**  
*A. Barcaru, R. Heiner-Fokkema, P. Horvatovich*  
 University Medical Center of Groningen, Laboratory of medicine, Groningen, Netherlands
- TP-190 **The utilization of tandem mass spectrometry techniques in diagnosis of patients with homocystinurias**  
*J. Bártl, J. Krijt, P. Chrastina, J. Hodik, M. Paulová, R. Pinkasová, J. Sokolová, V. Kožich, K. Peškova*  
 General University Hospital in Prague and 1st Faculty of Medicine, Charles University in Prague, Clinic of Pediatrics and Adolescent Medicine, Prague, Czech Republic
- TP-191 **CESI-MS - A sensitive and versatile approach for metabolomics**  
*W. Belloni*  
 Sciex Spa, Separations CE, Milano, Italy
- TP-192 **Assessment of kidney graft quality by SPME-(LC)-HRMS: going beyond clinical routine**  
*I. Stryjak, M. Hamar, M. Selzner, B. Bojko*  
 Nicolaus Copernicus University in Torun, Department of Pharmacodynamics and Molecular Pharmacology, Faculty of Pharmacy, Collegium Medicum in Bydgoszcz, Bydgoszcz, Poland
- TP-193 **Multilayer omics strategy for tracing the metabolic routes exploited by KRAS oncogenetic mutation in NSCLC**  
*L. Brunelli, E. Caiola, F. Falcetta, S. Giordano, M. Marabese, M. Broggin, R. Pastorelli*  
 IRCCS-Istituto di Ricerche Farmacologiche Mario Negri, Environmental Health Sciences, Milano, Italy
- TP-194 **Conversion of coenzyme A thioesters by native chemical ligation – a new approach for characterizing an important class of biomolecules**  
*N. Cakic, H. Wilkes*  
 Institute for Chemistry and Biology of the Marine Environment (ICBM), University of Oldenburg, Oldenburg, Germany
- TP-195 **Enhanced metabolite identification using an Orbitrap Tribrid mass spectrometer**  
*K. Comstock, S. Ma, S. Sharma, H. Cardasis, Y. Chen*  
 Thermo Fisher Scientific, 1, San Jose, USA

- TP-196 **Targeted approach for determination of metabolites of flavonoids and isoflavonoids in biological samples**  
*L. Chrenková, V. Pilarová, L. Applová, I. Najmanová, P. Mladenka, L. Nováková*  
 Charles University, Faculty of Pharmacy, Department of Analytical Chemistry, Hradec Králové, Czech Republic
- TP-197 **Exploring serum targeted metabolomics mass spectrometry profile analysis to implement risk criteria for first-degree relatives (FDR) of gastric cancer (GC) patients**  
*G. Corona, R. Cannizzaro, G. Miolo, A. Steffan, V. De Re*  
 IRCCS National Cancer Institute, Immunopathology and Cancer Biomarkers, Aviano(PN), Italy
- TP-198 **Phytochemical screening of fagioli bianchi di Rotonda beans DOP (Phaseolus Vulgaris L.) and evaluation of their biological activity for functional food properties**  
*D. Coviello, A. Onzo, G. Bianco, R. Pascale, P. Schmitt-Kopplin, P. Iannece, C. Gaeta*  
 Università degli Studi della Basilicata, Dipartimento di Scienze, Potenza, Italia
- TP-199 **Two-dimensional gas chromatography as a powerful tool for discriminating VOCs in monovarietal and commercial extra virgin olive oil**  
*A. Da Ros, S. Carlin, D. Masuero, S. Riccadonna, F. Mattivi, N. Mulinacci, U. Vrhovsek*  
 Fondazione Edmund Mach, Food quality and Nutrition, San Michele all'Adige, Italy
- TP-200 **A targeted metabolomics assay to investigate steroid hormones in women during pregnancy and early postpartum period**  
*S. Di Palma, E. Laczko*  
 Functional Genomics Center Zurich, University of Zurich/ETH, Zurich, Switzerland
- TP-201 **EcoMetabolomics of root exudates in german grassland communities**  
*S. Dietz, S. Döll, K. Gorzolka, D. Scheel*  
 Leibniz Institute of Plant Biochemistry, Stress and Developmental Biology, Halle-Saale, Germany
- TP-202 **A novel labeled metabolomics workflow applying Isotope Ratio Outlier Analysis (IROA) and SWATH® acquisition for unambiguous compound identification**  
*P. Cyrus, C. Beecher, F. A. De Jong, B. Ubhi, J. Dojahn*  
 Sciex, Darmstadt, Germany
- TP-203 **Untargeted metabolomics in plant biochemistry**  
*S. Döll, H. Treutler, S. Neumann, D. Scheel*  
 Leibniz Institute of Plant Biochemistry, Stress and Developmental Biology, Halle, Germany
- TP-204 **An investigation of biomarkers in the serum of developmental disorders using an intellectual disability model mouse, which show impaired social behaviours**  
*K. Gamoh, M. Nishimura, T. Akashi, Y. Nishiwaki, T. Kashio, S. Mitsui*  
 Kochi University and Gunma University Graduate School of Health Sciences, Kochi, Japan
- TP-205 **Electrochemical oxidation of primary bile acids: Simulation of endogenous metabolism**  
*L. Navarro Suarez, L. Brückner, S. Rohn*  
 Hamburg School of Food Science, University of Hamburg, Hamburg, Germany
- TP-206 **Low invasive metabolomic phenotyping: a potential alternative for genotyping of gliomas**  
*P. Z. Gorynska, K. Gorynski, K. Chmara, J. Furtak, D. Paczkowski, M. Harat, B. Bojko*  
 Faculty of Pharmacy Collegium Medicum, Department of Pharmacodynamics and Molecular Pharmacology, Nicolaus Copernicus University in Toruń, Bydgoszcz, Poland
- TP-207 **<sup>13</sup>CO<sub>2</sub> Isotope labelling of Arabidopsis thaliana: Tracking labelled carbon in metabolites from leaves to roots to exudates**  
*K. Gorzolka, G. Balcke, H. Treutler, S. Neumann, D. Scheel*  
 Leibniz Institute of Plant Biochemistry, Stress and Developmental Biology, Halle, Saale, Germany
- TP-208 **Metabolomic approach to investigate metabolite alterations attributed to a 25-hydroxyvitamin D in healthy Korean adults**  
*M.-R. Gwon, B. K. Kim, B. Ohk, S. Cho, S. J. Seong, Y.-R. Yoon*  
 Cell and Matrix Research Institute, Department of Biomedical Science, School of Medicine, Kyungpook National University, DAEGU, Republic of Korea
- TP-209 **An analytical framework for the exploration of endogenous peptides integrating peptide structure prediction and tandem mass spectrometry**  
*C. Kawano, E. Hayakawa, H. Watanabe*  
 Okinawa Institute of Science and Technology, Okinawa, Japan

- TP-210 **Towards the deciphering of the mechanism of action of an experimental drug against Chagas disease, using multi-omics platform**  
*K. Hennig, J. Abi-Ghanem, A. Bunescu, X. Meniche, E. Biliaut, F. Bequet, M. Lewis, J. Kelly, S. Braillard, G. Courtemanche, E. Chatelain*  
 BIOASTER, Metabolomics and proteomics unit, Lyon, France
- TP-211 **Metabolomic approach for the estimation of age of bloodstain**  
*H.-G. Kang, Y. Lee, A. Seok, Y. Lee, A. Park, S. Mun, H. Kim*  
 Eulji University, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Daejeon, Republic of Korea
- TP-212 **Metabolomic analysis of human plasma to characterize metabolite changes associated with exposure to persistent organic pollutants**  
*B. K. Kim, M.-R. Gwon, B. Ohk, S. Cho, S. J. Seong, D. Lee, Y.-R. Yoon*  
 Kyungpook National University, Department of Biomedical Science, School of Medicine, Daegu, Republic of Korea
- TP-213 **A Rapid Microbore Metabolic Profiling (RAMMP) analytical platform for discovery metabolomics and lipidomics**  
*A. King, L. Mullin, I. Wilson, P. Rainville, R. Plumb, L. Gethings, D. Heywood, G. Maker, R. Trengove*  
 Waters Corporation, Scientific Operations, Wilmslow, United Kingdom
- TP-214 **Rapid and simultaneous determination of 23 amino acids in non-invasive and invasive biological samples from obesity patients by liquid chromatography-tandem mass spectrometry after derivatization**  
*L. Konieczna, A. Krawczyńska, J. Siebert, P. Gutknecht, M. Skrzypkowska, Ł. Kaska, J. Bigda, M. Proczko-Stepaniak, T. Bączek*  
 Medical University of Gdańsk, Department of Pharmaceutical Chemistry, Gdańsk, Poland
- TP-215 **Identification of internal standard metabolites for standardization bloodstains**  
*J. Lee, H. Kim, Y. Lee, A. Eun Seok, A. Park, S. Mun, Y. Lee, H. Kang*  
 Eulji University, Department of Biomedical Laboratory Science, College of Health Sciences, Seongnam-si, Gyeonggi-do, Republic of Korea
- TP-216 **An infusion "shotgun" approach for high-throughput untargeted metabolomics**  
*M. Maldini, C. Papan, Z. Demianova, J. Dojahn, B. K. Ubhi*  
 Sciex, Darmstadt, Germany
- TP-217 **SWATH® acquisition improves metabolite coverage over traditional data dependent techniques for untargeted metabolomics**  
*M. Maldini, Z. Demianova, C. Papan, J. Dojahn, B. K. Ubhi*  
 Sciex, Darmstadt, Germany
- TP-218 **Analytical ion spectroscopy - a new route to metabolite identification**  
*J. Martens, G. Berden, R. Van Outersterp, L. Kluijtmans, R. Wevers, J. Oomens*  
 FELIX Laboratory, Radboud University, Nijmegen, Netherlands
- TP-219 **Microflow metabolomics differentiates pre-classified healthy and cancer samples**  
*D. Merkel, C. Papan, Z. Demianova, J. Dojahn, M. Maldini, K. Motamedchaboki, B. K. Ubhi, E. Lin*  
 SCIEX Germany, Application Support, Darmstadt, Germany
- TP-220 **High-throughput LC-MS/MS-based chiral metabolic profiling focusing on amino acids and related metabolites**  
*Y. Nakano, M. Taniguchi, E. Fukusaki*  
 Osaka university, Advance Science and Biotechnology, Osaka, Japan
- TP-221 **Study of auxin biosynthesis using in vivo labelling**  
*A. Pencik, P. Vonka, M. Kubes, K. Ljung, O. Novak*  
 Institute of Experimental Botany AS CR & Palacky University, Laboratory of Growth Regulators, Olomouc, Czech Republic
- TP-222 **Can obstructive sleep apnoea be diagnosed by real-time analysis of exhaled breath using secondary electrospray ionization mass spectrometry - a validation study**  
*N. Nowak, A. Engler, D. Schneeberger, S. Thiel, T. Gaisl, M. T. Gaugg, S. P. Martinez-Lozano, A.-S. Stöberl, M. Kohler, R. Zenobi*  
 ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland



- TP-223 **A dual separation/high resolution accurate mass spectrometry system for improved metabolome coverage and increased throughput**  
*I. Ntaj, M. Samonig, A. Paulus, R. Tautenhahn, A. Souza, A. Huhmer*  
Thermo Fisher Scientific, San Jose, USA
- TP-224 **Intelligent MS<sup>n</sup> workflow for improved metabolome coverage and increased confidence in unknown identification**  
*I. Ntaj, I. Mohtashemi, R. Tautenhahn, G. Mcalister, S. Sharma, V. Zabrouskov, A. Souza, A. Huhmer*  
Thermo Fisher Scientific, San Jose, USA
- TP-225 **Non-target metabolomic analysis of peperoni di Senise peppers IGP (*Capsicum Annuum* L.) and evaluation of their nutraceutical properties**  
*A. Onzo, D. Coviello, G. Bianco, R. Pascale, P. Schmitt-Kopplin, P. Iannece, C. Gaeta*  
Università degli Studi della Basilicata, Dipartimento di Scienze, Potenza, Italy
- TP-226 **Determination of metabolization of new fluorescently labeled auxin-like compounds in plant material using UHPLC-MS/MS**  
*B. Parížková, A. Žukauskaite, T. Vain, P. Gronos, M. Kubeš, M. Kieffer, K. Doležal, S. Kepinski, M. Strnad, S. Robert, O. Novák*  
Centre of the Region Haná for Biotechnological and Agricultural Research, Department of Chemical Biology and Genetics, Faculty of Science, Palacký University, Olomouc, Czech Republic
- TP-227 **Metabolomic approaches to investigate the role of the mitochondrial regulator Zc3h10 in adipocytes**  
*S. Pedretti, M. Audano, E. De Fabiani, D. Caruso, N. Mitro*  
Università degli Studi di Milano, Department of Pharmacological and Biomolecular Sciences, Milan, Italy
- TP-228 **LC-MS/MS quantification of thiol-containing metabolites within the de novo glutathione synthesis pathway over the lifespan of *Caenorhabditis elegans***  
*G. Ferguson, R. Pickford, W. Bridge*  
University of New South Wales, Bioanalytical Mass Spectrometry Facility, Kensington, Australia
- TP-229 **Integration of tandem mass spectrometry molecular networking and gas-phase fragmentation reactions for structural analysis of flavonoid glycoconjugates**  
*A. C. Pilon, N. F. Carnevale, H. Gu, D. Raftery, V. Da Silva Bolzani, N. Peprine Lopes, G. Ian Castro*  
University of São Paulo, Faculty of Pharmaceutical Sciences, Ribeirão Preto, Brazil
- TP-230 **Typical LC-MS metabolomics workflow for profiling urine samples of patients with colorectal cancer**  
*I. Plyushchenko, T. Bolotnik, D. Shakhmatov, S. Achkasov, O. Sushkov, O. Shpigun, I. Rodin*  
Lomonosov Moscow State University, Chemistry Department, Moscow, Russian Federation
- TP-231 **Metabolomics analysis of urine in mice with prostate cancer**  
*L. C. Rodas Sánchez, P. Rodriguez-González, A. J. I. García, P. González-Menéndez, J. C. Mayo Barrallo, R. Sainz Menéndez, A. López- González, C. Barbas*  
University of Oviedo, Department of Physical and Analytical Chemistry, Faculty of Chemistry, Oviedo, Spain
- TP-232 **A novel integrative strategy to prevent colorectal cancer within the diet-host-microbiota TRIANGLE: from organoids to human in vivo reality**  
*J. Rubert, F. Mattivi, A. Lunardi*  
Centre for Integrative Biology (CIBIO), University of Trento, Trento, Italy
- TP-233 **Indolome analysis for nutraceutical and physiological studies**  
*F. M. Rubino, M. Dei Cas, A. Penoni, M. Iriti, R. Clara Paroni, J. Rizzo*  
Università degli Studi di Milano, Dipartimento di Scienze della Salute, Milano, Italy
- TP-234 **Rapid analysis of NCI60 panel metabolic and lipid profiles with an automatic well plate reader using laser assisted REIMS**  
*R. Schäffer, J. Balog, D. Simon, N. Kucsma, A. Lovrics, G. Szakacs, S. Pringle, Z. Takats*  
Waters Research Center, R&D, Budapest, Hungary
- TP-235 **A wellness study using microflow targeted metabolomics to investigate the effects of diet and exercise on the metabolome**  
*Z. Demianova, K. Motamedchaboki, B. Ubhi, D. Schleuder*  
Sciex, Darmstadt, Germany

- TP-236 **Fecal metabolomics of a mouse model of autism**  
*E. Sekera, T. Wood, H. Rudolph, S. Carro*  
 University at Buffalo, Department of Chemistry, Buffalo, USA
- TP-237 **Liquid extraction surface analysis and direct ESI/nanoESI mass spectrometry for high throughput urinary metabolomics applied to malaria**  
*S. Abdelrazig, C. Ortori, D. Barrett*  
 University of Nottingham, School of Pharmacy, Nottingham, United Kingdom
- TP-238 **Urinary metabolic profile of newborns with transposition of great arteries undergoing cardiac surgery with cardiopulmonary bypass**  
*M. Simonato, L. Vedovelli, M. Padalino, G. Stellin, S. Carollo, A. Bandini, V. Carnielli, P. Cogo*  
 Istituto di Ricerca Pediatrica "Città della Speranza", Padova, Italy
- TP-239 **Volatilome analysis for Parkinson's disease diagnostics**  
*E. Sinclair, D. Trivedi, Y. Xu, C. Liscio, P. Banks, J. Milne, M. Silverdale, T. Kunath, R. Goodacre, P. Barran*  
 University of Manchester, Chemistry, Manchester, United Kingdom
- TP-240 **Detection of metabolic signatures of Crohn's disease using an intelligent MS<sup>n</sup>-based discovery workflow**  
*I. Ntai, A. Souza, R. Tautenhahn, G. Tan, A. Huhmer*  
 Thermo Fisher Scientific, Metabolomics Program, San Jose, USA
- TP-241 **Monoamine mapping by mass spectrometry identified brain nuclei regulating anxiety in a serotonin deficiency model**  
*Y. Sugiura, E. Sugiyama*  
 Keio University, School of Medicine, Tokyo, Japan
- TP-242 **Construction and application of a high-resolution MS/MS library including retention time information for rapid identification of endogenous metabolites**  
*M. Szesny, S. Zhao, X. Luo, W. Chan, U. Schweiger-Hufnagel, A. Barsch, L. Li*  
 Bruker Daltonik GmbH, Metabolomics, Bremen, Germany
- TP-243 **Developing a robust LC-MS panel for assessing residual platelets and other sample quality issues in plasma**  
*W. Tan, C. Drum*  
 National University of Singapore, NUS Graduate School for Integrative Sciences and Engineering, Singapore, Singapore
- TP-244 **Revealing the hidden part of bacterial metabolism**  
*E. Dairij, P. L. Saaidi, A. Perret, M. Salanoubat*  
 CEA - Genoscope, Evry, France
- TP-245 **Assessment of the THS exposition in animal models by multiplatform metabolomics analysis**  
*S. Torres, S. Samino, P. Rafols, N. Adhami, M. Martins-Greens, X. Correig, N. Ramirez*  
 Rovira y Virgili University, Department of Electronic, Electrical and Automatic Control Engineering, Tarragona, Spain
- TP-246 **Simultaneous quantitative analysis method for hydroxyproline and 4-hydroxyglutamic acid using isotopologue-SRM to clarify hydroxyproline metabolism**  
*M. Tsuji*  
 Daiichisankyo RD Novare Co., Ltd., Pharmaceutical and Biomedical Analysis, Tokyo, Japan
- TP-247 **An untargeted metabolomics approach to go beyond Aspirin canonical effect**  
*L. Turnu, C. M. Manega, B. Porro, A. Di Minno, F. Veglia, D. Caruso, E. Tremoli, V. Cavalca*  
 Centro Cardiologico Monzino IRCCS, Unit of metabolomics and cellular biochemistry of atherotrombosis, Milano, Italy
- TP-248 **Evaluation of high speed, high resolution data independent acquisition for the analysis of metabolomic flux, kinetics and pathway mapping**  
*Z. Demianova, B. K Ubhi, L. Olson, J.-B. Vincendet*  
 Sciex, France
- TP-249 **Utilizing a standardized and targeted quantitative assay coupled to HRAM MS for the analysis of serum metabolites obtained from diabetic study subjects**  
*A. Kalli, S. Webb, M. Kratzke, M. Langsdorf, S. Dearth, H. Tuan Pham, T. Koal, A. Huhmer*  
 Thermo Fisher Scientific, San Jose, USA

- TP-250 **Development of a simultaneous analysis of the fat-soluble vitamin using the lithium ion**  
*N. Yamada, T. Matsui, H. Kuno*  
 Japan Tobacco Inc., Toxicology Research Laboratories, Hadano, Japan
- TP-251 **Human metabolite identification by searching a high quality and comprehensive tandem mass spectral library**  
*X. Yang, P. Neta, S. Stein*  
 NIST, Mass Spectrometry Data Center, Gaithersburg, USA
- TP-252 **TiO<sub>2</sub> assisted laser desorption/ionization mass spectrometry for rapid profiling of candidate metabolite biomarkers from antimicrobial resistant bacteria**  
*R. Zhang, Q. Qin, B. Liu, L. Qiao*  
 Fudan University, Shanghai, China
- TP-253 **Metabolic characterization of THP-1 macrophages polarization using LC-MS-based metabolite profiling**  
*A. Abuawad, D. Barrett, A. Ghaemmaghami, D. Kim*  
 University of Nottingham, University of Nottingham, Advanced Materials and Healthcare Technologies, Nottingham, United Kingdom
- TP-254 **Investigating the differences in the molecular effects of free and nanoparticle loaded methotrexate on proliferative and nonproliferative cancer cells using advance cell based metabolomics**  
*M. Al-Natour, A. Alazzo, A. Ghaemmaghami, D.-H. Kim, A. Cameron*  
 University of Nottingham, School of pharmacy, Division of Molecular Therapeutics and Formulation, Nottingham, United Kingdom
- TP-255 **Characterization of phenolic compounds and determination of anti-inflammatory and anti-cholinesterase activity in 2 Colombian fruits: Borojoa Patinoi and Bactris Gasipaes**  
*D. Arias Ramirez*  
 Universidad de los Andes, Chemistry Department, Bogotá D.C., Colombia
- TP-256 **Phenolic, alkaloids and lipids of Ochroma pyramidale, Tapirira guianensis and Inga edulis, host plants of the caterpillar Lonomia descimoni**  
*F. Benavides, C. Carazzone*  
 Universidad de los Andes, Chemistry Department, Bogotá D.C., Colombia
- TP-257 **Multi-omics profiling of pancreatic cancer stem-like cells**  
*C. Di Carlo*  
 Università degli Studi di Verona, Biotechnology, Verona, Italy
- TP-258 **Informed unTargeted Metabolomics using LC-MS/MS**  
*J. Folberth, O. Jöhren, M. Schwaninger, A. Othman*  
 University of Luebeck, Institute for Experimental and Clinical Pharmacology and Toxicology, Luebeck, Germany
- TP-259 **LC-MS analysis of nonribosomal peptidome from a Brazilian cyanobacterium Nostoc sp. CENA543**  
*J. Jokela, L. Heinilä, T. Keiko Shishido, M. Wahlsten, D.P. Fewer, M. Fátima Fiore, E. Haapaniemi, P. Permi, K. Sivonen*  
 University of Helsinki, Department of Microbiology, Helsinki, Finland
- TP-260 **Comparative evaluation of different ginseng berry species based on UPLC-QToF/MS and HR-MAS NMR metabolite profiles**  
*D. Y. Lee, J. W. Lee, B. Choi, D. Yoon, Y. C. Kim, S. Kim*  
 National Institute of Horticultural and Herbal Science, Department of Herbal Crop Research, Eumseong, Republic of Korea
- TP-261 **Untargeted metabolomics with parallel accumulation – serial fragmentation (PASEF) on a novel trapped ion mobility mass spectrometer**  
*F. Meier, C. Vasilopoulou, K. Sulek, A. Brunner, U. Schweiger-Hufnagel, S. Meyer, A. Barsch, M. Mann*  
 Max Planck Institute of Biochemistry, Proteomics and Signal Transduction, Martinsried, Germany
- TP-262 **Automated parallel derivatization strategy with broad metabolite coverage coupled to SWATH/MS data acquisition for qualitative and quantitative analysis**  
*D. Ruskic, M. F. C. Girard, R. Piconi, M. F. Mirabelli, G. Böhm, G. Hopfgartner*  
 CTC Analytics AG, Zwingen, Switzerland

- TP-263 **Targeted metabolomics applied to heart failure patients – a pilot study**  
*R. Nilsson, L. Löfgren, F. Michopoulos, M. Ryaboshapkina, P. Davidsson, C. Linde, B. Persson*  
 AstraZeneca, Translational science, Mölndal, Sweden
- TP-264 **Phospholipid removal by solid phase extraction for untargeted metabolomics: improved sensitivity for polar metabolites in brain**  
*P. Pöhö, A. Vaikkinen, E. Scurti, M. Airavaara, T. Kotiaho, R. Kostainen*  
 University of Helsinki, Division of Pharmaceutical Chemistry and Technology, Helsinki, Finland
- TP-265 **Coffee metabolomics by LC-HRMS and molecular networking**  
*C. M. Rezende, N. M. D. Sá, R. G. Costa*  
 Federal University of Rio de Janeiro, Chemistry Institute, Rio de Janeiro, Brazil
- TP-266 **Untargeted metabolomics of native tasmanian plants: comparison with their medicinally-known relatives**  
*K. Skraskova, R. Wilson, J. Smith*  
 University of Tasmania, School of Chemistry, Hobart, Australia
- TP-267 **Hydrophilic interaction liquid chromatography – field asymmetric waveform ion mobility spectrometry – mass spectrometry as a platform for untargeted metabolomic studies**  
*K. Szykula, M. Turner, C. Creaser, J. Reynolds*  
 Loughborough University, Department of Chemistry, Centre for Analytical Science, Loughborough, United Kingdom

## WEDNESDAY, August 29<sup>th</sup>, 2018

### WPS-S01 - Native MS and Structural Proteomics

- WP-01 **Acidic XPLex: a multiplex alternative to NHS esters for faster cross-linking reactions at lower temperatures**  
*B. C. Amaral, F. C. Gozzo, D. B. Lima, P. C. Carvalho*  
 University of Campinas, Dalton Mass Spectrometry Laboratory, Institute of Chemistry, Campinas, Brazil
- WP-02 **Intact mass analysis of macromolecular PEG-Fab conjugate using multi-mode native LC coupled to ultra-high mass range native MS**  
*A. Bailey, G. Han, J. Josephs, W. Sandoval, E. Damoc*  
 Thermo Fisher Scientific, San Jose, USA
- WP-03 **Native mass spectrometry analysis of recombinant antibodies directly from the growth medium**  
*G. Ben-Nissan, S. Vimer, A. Katz, S. Warszawsky, R. Diskin, S. Fleishman, M. Sharon*  
 Weizmann Institute of Science, Department of Biomolecular Sciences, Rehovot, Israel
- WP-04 **Coupling online separations to native MS for the characterization of designed protein complexes**  
*F. Busch, M. Jia, Z. Vanaernum, A. Sahasrabudde, Z. Chen, S. Boyken, D. Baker, V. Wysocki*  
 The Ohio State University, Department of Chemistry and Biochemistry, Columbus, USA
- WP-05 **Structural characterisation of wild-type and  $\Delta N6$   $\beta 2$ -microglobulin comparing HDX and FPOP chemical labelling**  
*O. Cornwell, J. Ault, S. Radford, A. Ashcroft*  
 University of Leeds, Faculty of Biological Sciences, Leeds, United Kingdom
- WP-06 **Double mutant cycles in the gas phase: measuring inter-protein pairwise interaction energies from crude cell lysates by native MS**  
*J. Cveticanin, R. Netzer, G. Arkind, S. Fleishman, A. Horovitz, M. Sharon*  
 Weizmann Institute of Science, Department of Biomolecular Sciences, Rehovot, Israel
- WP-07 **Advances in Orbitrap™ instrumentation for native top-down analysis of non-covalent protein complexes**  
*E. Damoc, R. Viner, A. Konijnenberg, K. Fort, M. Reinhardt-Szyba, M. Belov, A. Makarov*  
 Thermo Fisher Scientific, Bremen, Germany

- WP-08 Architecture of eukaryotic mRNA 3'-end processing machinery - The role of cross-linking and mass spectrometry**  
*G. Degliesposti, M. Skehel, A. Casanal, A. Kumar, C. Hill, A. Easter, P. Emsley, Y. Gordiyenko, B. Santhanam, J. Wolf, K. Wiederhold, G. Dornan, C. V. Robinson, L. A. Passmore*  
 Laboratory of Molecular Biology (MRC LMB), Cambridge, United Kingdom
- WP-09 The influence of substrates and nucleotides on complex formation in ABC transporters – insights from mass spectrometry**  
*F. Fiorentino, J. R. Bolla, S. Mehmood, C. V. Robinson*  
 University of Oxford, Department of Chemistry, Oxford, United Kingdom
- WP-10 Chemico-structural and functional characterization of filgrastim originator and three of its biosimilar drugs**  
*A. Gianoncelli, M. Bertuzzi, M. Guarienti, M. Memo*  
 University of Study of Brescia, Molecular and Translational Medicine, Brescia, Italy
- WP-11 Characterization of calcium-mediated alpha-synuclein aggregation pathway at the molecular level**  
*J. Y. Han, H. I. Kim*  
 Korea University, Department of Chemistry, Seoul, Republic of Korea
- WP-12 Characterization of intact monoclonal antibodies under native and reverse phase conditions using high resolution mass spectrometry**  
*C. Nortcliffe, R. Yokoyama, S. Heidelberger, K. Pohl, J. Dojahn, F. Sanchez, A. Uppal*  
 Sciex, Biologics, Warrington, United Kingdom
- WP-13 Native mass spectrometry of biomolecules: a comparison of nESI-MS and LILBID-MS**  
*N. Hellwig, O. Peetz, N. Morgner*  
 Goethe-University, Institute of Physical and Theoretical Chemistry, Frankfurt, Germany
- WP-14 Evaluation of an Isotope-Labeled MS/MS-Cleavable Cross-Linker for Protein Structure Analysis**  
*C. Ihling, P. Springorum, M. Götze, C. Hage, M. Schäfer, A. Sinz*  
 Martin Luther University Halle-Wittenberg, Institute for Pharmacy, Halle, Germany
- WP-15 Deep biosimilarity assessment by monitoring multiple critical quality attributes of an intact monoclonal antibody drug using native IEC and SEC coupled to native Orbitrap MS**  
*J. Josephts, A. Bailey, T. Zhang, S. Houel, S. Lin, G. Han, B. Gamez, K. Southwick, W. Sandoval, J. Josephts*  
 Thermo Fisher Scientific, Chromatography and Mass Spectrometry, San Jose, USA
- WP-16 Structural comparison and epitope mapping of innovator and biosimilar therapeutic antibodies**  
*C. Lento, K. Brown, D. Wilson*  
 York University, Chemistry, Toronto, Canada
- WP-17 LILBID-MS reveals influences of ThT and Coomassie on aggregation kinetics of amyloid- $\beta$  (1-42) and  $\alpha$ -synuclein**  
*J. Martin, R. Zangl, T. Lieblein, N. Morgner*  
 Goethe University, Institute of Physical and Theoretical Chemistry, Frankfurt, Germany
- WP-18 Quantification of substrate and inhibitor binding to wild type and mutant isocitrate dehydrogenase (IDH1) by non-denaturing mass spectrometry**  
*V. Mikhailov, S. Liu, C. Schofield, J. McCullagh*  
 University of Oxford, Department of Chemistry, Oxford, United Kingdom
- WP-19 An optimized enrichment strategy for improved mass spectrometry analysis of chemically cross-linked peptides**  
*R. Viner, L. Foster, E. Raja, C. Etienne, R. Bomgardner, M. Oppermann*  
 Thermo Fisher Scientific, Europe, Stockholm, Sweden
- WP-20 Towards defining of the molecular maturation pathway of the mitochondrial sulfhydryl oxidase Erv1**  
*K. Pacholarz, X. Tang, H. Lu, P. Barran*  
 Manchester Institute of Biotechnology, The University of Manchester, Manchester, United Kingdom
- WP-21 Enrichment of electrochemically cleaved peptides for middle-down proteomics applications**  
*H. Permentier, T. Zhang, X. Tian, R. Bischoff*  
 University of Groningen, Analytical Biochemistry, Groningen, Netherlands

- WP-22 Heterogeneous protein complexes in synaptic vesicles mediate signal transduction in neurons**  
*S. Wittig, C. Haupt, M. Ganzella, S. Kostmann, R. Jahn, C. Schmidt*  
 HALOmem, Charles Tanford Protein Center, Institute for Biochemistry and Biotechnology, Martin Luther University, Halle, Germany
- WP-23 Hydroxyl radical footprinting study for structural characterization of aluminum hydroxide-adsorbed calmodulin by mass spectrometry**  
*A. Vadi*  
 GSK Vaccines S.r.l., Analytical Research and Development, Siena, Italy
- WP-24 Rapid characterization of overproduced proteins using native mass spectrometry**  
*S. Vimer, G. Ben-Nissan, H. Cohen-Dvashi, E. Morag, Y. Peleg, T. Unger, M. Yona, R. Diskin, M. Sharon*  
 Weizmann Institute of Science, Department of Biomolecular Sciences, Rehovot, Israel
- WP-25 Integrative structural proteomics analysis of the 20s proteasome complex**  
*R. Viner, D. M. Horn, E. Damoc, A. Konijnenberg*  
 Thermo Fisher Scientific, San Jose, USA
- WP-26 Assembly studies of *Acetobacterium woodii* F1FO-ATP synthase and analyzing conformational changes of TmrABby nESI**  
*K. Vu Huu, S. Brüchert, R. Tampé, V. Müller, N. Morgner*  
 Goethe-University, Institute of Physical and Theoretical Chemistry, Frankfurt am Main, Germany
- WP-27 Gas-phase electrophoresis (nES GEMMA) of virus-like particles: relating particle surface-dry size and molecular weight**  
*V. U. Weiss, R. Pogan, S. Zoratto, C. Uetrecht, G. Allmaier*  
 TU Wien, Inst. Chem. Technologies and Analytics, Vienna, Austria
- WP-28 Native mass spectrometry to identify stoichiometries and stability of CRISPR-cascade complexes**  
*S. Wittig, M. Rutkauskas, R. Seidel, C. Schmidt*  
 HALOmem, Charles Tanford Protein Center, Institute for Biochemistry and Biotechnology, Martin Luther University, Halle, Germany
- WP-29 Characterization of deuterated alpha-crystalline using bench-top MALDI-ToFMS**  
*Y. Yamazaki, K. Morishima, N. Sato, R. Inoue, M. Sugiyama*  
 Shimadzu Corp., Global application development center, Kyoto, Japan
- WP-30 Development of a cryo-stage for LESA mass spectrometry-towards truly native surface sampling of proteins**  
*B. Yan, A. Taylor, J. Bunch*  
 National Physical Laboratory, National Centre of Excellence in Mass Spectrometry Imaging, Teddington, United Kingdom
- WP-31 Native mass spectrometry analysis of norovirus glycan interaction**  
*H. Yan, J. Lockhauserbäumer, K. Bücher, R. Creutzmacher, A. Mallagaray, T. Peters, L. Hartmann, C. Uetrecht*  
 Leibniz Institute for Experimental Virology, Heinrich-Pette-Institut, Hamburg, Germany
- WP-32 Top-down and middle down sequencing of immunoglobulin using electron capture dissociation – Time of Flight mass spectrometer combined with online disulfide bond reduction**  
*T. Baba, L. C. Y. Leblanc, P. Ryumin, B. Loyd*  
 Sciex, Research, Concord, Canada
- WP-33 Cation exchange chromatography in displacement mode for online analysis of intact proteins by mass spectrometry**  
*S. N. Hidayah, D. Kroesser, B. Dreyer, H. Schluter*  
 University Medical Center Hamburg Eppendorf, Institute for Clinical Chemistry and Laboratory Medicine, Mass Spectrometric Proteomics, Hamburg, Germany
- WP-34 High affinity epitopes of aptamer complexes of the multi-domain protein C-Met revealed by proteolytic affinity mass spectrometry**  
*L. Lupu, F. Rinaldi, Y. Baschung, M. V. Berezovski, M. Przybylski*  
 Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, University of Rostock, Proteome Center, Rüsselsheim, Germany

## **WPS-S02 - Reaction Mechanisms and Elusive Intermediates**

- WP-35 **Analysis for reforming processes for gasoline surrogate fuel-air pre-mixtures by non-thermal plasmas using ion attachment mass spectrometry**  
*D. Asakawa, E. Takahashi, N. Saito*  
AIST, Research Institute for Measurement and Analytical Instrumentation, Tsukuba, Japan
- WP-36 **Elusive monofunctional adducts of cisplatin with natural aminoacids revealed by IRMPD spectroscopy and photofragmentation kinetics**  
*D. Corinti, R. Paciotti, C. Coletti, N. Re, S. Piccirillo, P. Maitre, B. Bellina, P. Barran, B. Chiavarino, M. Elisa Crestoni, S. Fornarini*  
Sapienza, University of Rome, Dipartimento di Chimica e Tecnologie del Farmaco, Roma, Italy
- WP-37 **Characterization of a nitrogen-operated dielectric barrier discharge ionization source**  
*L. Gyr, F. David Klute, J. Franzke, R. Zenobi*  
ETH Zurich, Zurich, Switzerland
- WP-38 **A targeted metabolomics approach for diagnosis of Inborn Errors of Metabolism**  
*M. Jacob, A. Malkawi, N. Albast, S. Al Bougha, A. Lopata, M. Dasouki, A. Abdelrahman*  
King Faisal Hospital and Research Center, Genetics, Riyadh, Saudi Arabia
- WP-39 **Steroid bisconjugates: unearthing hidden treasures of steroid metabolism**  
*M. Mcleod, C. Fitzgerald*  
Research School of Chemistry, Australian National University, Canberra, Australia
- WP-40 **Investigating the reaction mechanism of the oxidation of heptafulvenes into tropones by a microreactor coupled online to mass spectrometry and density functional theory calculations**  
*S. M. E. Nilsson, H. Henschel, G. Scotti, M. Haapala, A. Kiriazis, G. Boije af Gennäs, T. Kotiaho, J. Yli-Kauhaluoma*  
University of Helsinki, Drug Research Program, Division of Pharmaceutical Chemistry and Technology, Helsinki, Finland
- WP-41 **How to modify the acidity of charged droplets?**  
*M. Ojakivi, J. Liigand, A. Kruve*  
The University of Tartu, Institute of Chemistry, Tartu, Estonia
- WP-42 **Studies of a L-proline catalyzed inverse electron demand Diels-Alder reaction by ESI-MS**  
*A. Schnell, J. A. Willms, M. Engeser*  
University of Bonn, Research group Engeser, Bonn, Germany
- WP-43 **Fragmentation of arsenic-containing chemical warfare agents in GC-EI/MS and LC-ESI/MS**  
*M. Söderström, P. Vanninen*  
VERIFIN, University of Helsinki, Helsinki, Finland
- WP-44 **Identification and interconversion of isomeric 4,5-functionalized 1,2,3-thiadiazoles and 1,2,3-triazoles in conditions of electrospray ionization**  
*M. Zimens, D. Mazur, V. Bakulev, A. Lebedev*  
Lomonosov Moscow State University, Organic Chemistry Department, Moscow, Russian Federation

## **WPS-S03 - Pharmaceuticals**

- WP-45 **Ultrasound assisted extraction parameters optimization by experimental design for steroidal saponins from plant material and cell cultures of *Dioscorea deltoidea***  
*B. Sarvin, T. Baygildiev, D. Kochkin, A. Stavrianidi, I. Rodin*  
Lomonosov Moscow State University, Department of Chemistry, Moscow, Russian Federation
- WP-46 **Analysis of pesticide residues in cannabis regulated by California and Oregon state using LC/MS/MS with Dual Electrospray and APCI source**  
*T. Becker, A. Dalmia, E. Cudjoe, T. Ruthenberg, J. Ye, M. Murphy, F. Qin, D. Welkie*  
PerkinElmer (LAS) Germany GmbH, BLL/FAS-Group, Rodgau-Jügesheim, Germany
- WP-47 **Identification of a novel metabolite originating from JWH-015 using LCMS-IT-ToF**  
*O. D. Can, U. D. Ozkay, S. Levent, Y. N. Turan, T. F. Alyu, Y. Ozturk*  
Anadolu University, Faculty of Pharmacy, Department of Pharmacology, Eskisehir, Turkey

- WP-48 **Synthesis and antifungal activity evaluation of new benzimidazole-triazole derivatives as potential ergosterol biosynthesis inhibitors using LC-MS/MS**  
*N. Oncu Can, C. Ulviye Acar, B. Nurpelin Saglik, S. Levent, Y. Ozkay, Z. A. Kaplancikli*  
Anadolu University, Faculty of Pharmacy, Department of Analytical Chemistry, Eskisehir, Turkey
- WP-49 **Optimized MS<sup>n</sup> workflow for improved structure elucidation of pharmaceutically relevant extractables and leachables**  
*S. Sharma, K. Comstock, D. E Kiehl, G. Mcalister, R. Komatsuzaki, C. Ding, R. Tautenhalm, D. J Bailey, L. Lin, T. Stratton, S. Eliuk, I. Mohtashemi, H. Cardasis, J. J. Josephs, V. Zabrouskov*  
Thermo Fisher Scientific, San Jose, USA
- WP-50 **Comprehensive metabolite identification of DM4, a maytansinoid anti-tumor agent, in S100 fractions of Human Liver microsomes, by UPLC-QToF Mass Spectrometry**  
*E. Ciuti, F. Tavani, V. Chirulli, C. Carboni, A. Triolo*  
Menarini Ricerche SpA, Laboratory of Analytical Chemistry for Development, Firenze, Italy
- WP-51 **Investigation of monoamine oxidase inhibitory activities of new chalcone derivatives: Comparison of LC-MS/MS and fluorometric methods**  
*Ü. Özkay, N. Öncü Can, S. Levent, Y. Özkay, Ö. D. Can*  
Anadolu University, Faculty of Pharmacy, Department of Pharmacology, Eskisehir, Turkey
- WP-52 **Long term stability of Candesartan cilexetil after micronization**  
*A. M. A. P. Fernandes, M. Menezes, P. H. Amaral, M. N Eberlin, N. F. Höehr*  
State University of Campinas, Institute of Chemistry, Labmass Laboratory, Campinas, Brazil
- WP-53 **Mass spectrometric characterization of a polymeric degradation product formed from the antibiotic Cefazidime**  
*A. M. A. P. Fernandes, N. S. Camilo, E. P. Tessaro, M. N. Eberlin*  
State University of Campinas, Institute of Chemistry, Labmass Laboratory, Campinas, Brazil
- WP-54 **Full validation of Metformin in human bloods using volumetric absorptive microsampling**  
*N. Ha, K. Jang, S. Han, S. Eui Lee, M. Kim*  
Center for Clinical Pharmacology and Biomedical Research Institute, Chonbuk National University Hospital, Jeonju, Republic of Korea
- WP-55 **Determination of an isonicotinohydrazone derivative, a novel positive inotropic compound, in mouse plasma by LC-MS/MS and its application to a pharmacokinetics study**  
*R. Hui, J. Liu, B. Feng*  
Jiangnan University, School of Pharmaceutical Science, Wuxi, China
- WP-56 **LC-MS/MS chiral method for simultaneous determination of R,S-ketamine and its metabolites in rat plasma and brain samples from pharmacokinetic studies**  
*M. Janicka, M. Matłoka, M. Mach, R. Moszczyński-Pętkowski, E. Tratkiewicz, J. Pieczykolan, M. Wieczorek*  
Celon Pharma S.A., R&D, Łomianki, Poland
- WP-57 **Characterization of a novel Zetamicin impurity by LC-MS and NMR: an orthogonal techniques approach for the structural elucidation of low-level byproducts**  
*E. Libralesso, E. Ciuti, A. Triolo, F. Lamonaca, M. Gentili*  
Menarini Ricerche spa, Preclinical Development, Firenze, Italy
- WP-58 **Prediction of ionisation efficiencies in complicated biological matrices**  
*P. Liigand, J. Liigand, F. Cuyckens, R. J. Vreeken, A. Kruve*  
University of Tartu, Institute of Chemistry, Tartu, Estonia
- WP-59 **A Novel GC-MS Method for Simultaneous Determination of Seven Paraben Derivatives in Pharmaceutical and Cosmetic Products Consumed in Turkey**  
*S. Ozcan, S. Levent, A. Geven, N. O. Can*  
Anadolu University, Faculty of Pharmacy, Department of Analytical Chemistry, Doping and Narcotic Compounds Analysis Laboratory, Eskisehir, Turkey
- WP-60 **Anticancer activity evaluation of new Phortress analogues and identification of bioactive metabolism products using LCMS-IT-ToF**  
*Y. Özkay, D. Osmaniye, B. N. Saglik, S. Levent, S. Ilgin, Z. A. Kaplancikli*  
Anadolu University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Eskisehir, Turkey



- WP-61 Investigation of isomeric metabolite structures using a combination of IMS, MS/MS and chemometrics: application to biotransformation**  
*C. Palaric, S. Rigaud, D. Mathiron, R. Molinié, J. Beaumal, T. Renaud, S. Pilard*  
University of Picardie Jules Verne (UPJV), Analytical Platform (PFA), Amiens, France
- WP-62 Complex approach for isolation and HPLC-MS determination of steroidal glycosides from plant material and suspension cell culture**  
*I. Rodin, B. Sarvin, A. Stavrianidi, T. Baygildiev*  
Lomonosov Moscow State University, Department of Chemistry, Moscow, Russian Federation
- WP-63 Use of high resolution mass spectrometry for tropane alkaloids determination and untargeted analysis in drugs and homeopathic products from *Atropa Belladonna* seed extracts**  
*R. Romero González, J. Marin Sáez, A. Garrido Frenich*  
University of Almería, Dept. Chemistry and Physics, Almería, Spain
- WP-64 All-in-one method for profiling and quantification of Polysorbate, by combined Data-Independent and Data-Dependent tandem MS**  
*S. Staccioli, A. Triolo, E. Ciuti*  
Menarini Ricerche, Laboratory of Analytical Chemistry for Development, Firenze, Italy
- WP-65 Rapid HPLC-MS/MS evaluation of the batch-to-batch consistency of the payloads substitution of a lysine antibody-drug-conjugates (ADCs)**  
*F. Tavanj, A. Triolo*  
Menarini Ricerche SpA, Analytical Chemistry for the Development, Florence, Italy
- WP-66 MALDI ToF mass spectrometry for the characterization of antitumour ruthenium(ii) polypyridyl complexes**  
*R. Masnikosa, F. Veljkovic, B. Rajcic, A. Rilak, S. Velickovic*  
University of Belgrade, Vinča Institute of Nuclear Sciences, Belgrade, Serbia
- WP-67 Energy resolved tandem mass spectrometry experiments for resolution of isobaric compounds: a case of cis/trans isomerism**  
*L. Braconi, M. Menicatti, S. Dei, E. Teodori, G. Bartolucci*  
University of Florence, NEUROFARBA Dept., Sesto Fiorentino, Italy
- WP-68 Stability study in plasma of novel ester-linked NSAID - carbonic anhydrase inhibitor hybrids**  
*S. Bua, M. Menicatti, P. Gratteri, A. Nocentini, C.T. Supuran, G. Bartolucci*  
University of Florence, NEUROFARBA Dept., Pharmaceutical and Nutraceutical section, Sesto Fiorentino, Italy
- WP-69 Identification of dipropylaminopretadafilil using high resolution mass spectrometry under multi-stage fragmentation pathways**  
*A. Chin, C. L. Kee*  
Health Sciences Authority, Pharmaceutical Laboratory, Singapore, Singapore
- WP-70 Evaluation of small molecule drugs retention in fluorinated silica nanoparticle stabilized pickering emulsion using ESI\_Mine(TM) platform**  
*X. Li, J. Francis, C. Pilkington, A. Clay, C. Smith*  
Sphere Fluidics Limited, R&D, Cambridge, United Kingdom
- WP-71 Generic method for parallel artificial liquid membrane extraction of nonpolar basic drugs from human plasma**  
*M. Lid, A. Gjelstad, S. Pedersen-Bjergaard*  
University of Oslo, Pharmaceutical Institute, Oslo, Norway
- WP-72 Application of linear equations deconvolution analysis (LEDA) algorithm in ion trap mass spectrometry: resolution of isomeric pairs of carbonic anhydrase and cyclooxygenase hybrids inhibitors**  
*D. Squillaci, M. Menicatti, S. Bua, C. Supuran, G. Bartolucci*  
University of Florence, NEUROFARBA Dept., Sezione di Scienze Farmaceutiche, Sesto Fiorentino, Italy

## **WPS-S04 - Food integrity, Authenticity & Traceability**

- WP-73**      **Pigment profiling in olive oils by ultra-high performance liquid chromatography – atmospheric pressure chemical ionization–high resolution mass spectrometry**  
*A. Arrizabalaga-Larrañaga, P. Rodriguez, M. Medina, F. J. Santos, E. Moyano*  
University of Barcelona, Chemical Engineering and Analytical Chemistry, Barcelona, Spain
- WP-74**      **Isotopic mapping of milk and groundwater in the production area of Parmigiano Reggiano for food traceability**  
*M. Boito, P. Iacumin, N. Ogrinc*  
Università degli Studi di Parma, Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Parma, Italy
- WP-75**      **Wine traceability: "Vigneto Italia" project**  
*C. Brilli, B. Bronzi*  
Ruffino srl, Laboratory, Pontassieve, Italy
- WP-76**      **UHPLC-ESI-MS/MS for the determination of polyphenols in Spanish paprika (*Capsicum annum* L.). Application to protected designation of origin (PDO) classification by chemometrics.**  
*G. Campmajó, S. Barbosa, O. Núñez, J. Saurina, L. Puignou*  
University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain
- WP-77**      **A novel multi-platform high resolution mass spectrometry non-targeted approach facing extra virgin olive oil adulteration**  
*D. Cavanna, K. Hurkova, Z. Dzuman, A. Serani, C. Dall'asta, J. Hajslova, M. Suman*  
Barilla G. & R. Fratelli S.p.A., University of Parma - Department of Food and Drug, Parma, Italy
- WP-78**      **Shrimp fraud: evaluating characteristic metabolomic features for authentication by high and unit mass resolution spectrometry**  
*O. Chevallier, N. Chatterjee, E. Wielogorska, C. Black, C. Elliott*  
Queens University Belfast, Mass Spectrometry Core Unit, Belfast, United Kingdom
- WP-79**      **Optimization, validation and application of GC-FID and GC-IRMS methods for the determination of fatty acids without derivatisation**  
*A. Ciric, J. Masten, L. Strojnik, N. Ogrinc*  
Jozef Stefan Institute, Department of Environmental Science, Ljubljana, Slovenia
- WP-80**      **Multi-class LC-MS and GC-MS methodologies to discriminate extra virgin olive oils from different Protected Designations of Origin**  
*L. Olmo-García, K. Wendt, A. Bajoub, C. M. Sánchez-Arévalo, A. Muñoz de la Peña, C. Baessmann, A. Carrasco-Pancorbo, A. Fernández-Gutiérrez*  
University of Granada, Department of Analytical Chemistry, Granada, Spain
- WP-81**      **Determination of melatonin and related compounds in beverages using liquid chromatography coupled to low and high resolution mass spectrometry**  
*M. L. Jiménez Medina, L. Manzano Sánchez, J. Marín Sáez, R. Romero González, A. Garrido Frenich*  
University of Almería, Dept. Chemistry and Physics, Almería, Spain
- WP-82**      **UHPLC-ESI-HRMS characterization of turmeric and curry samples based on profiling and fingerprinting approaches**  
*N. Núñez, O. Núñez, S. Sentellas, J. Saurina*  
University of Barcelona, Department of Chemical Engineering and Analytical Chemistry, Barcelona, Spain
- WP-83**      **Monoterpenes characterization in grape spirits using fast gas chromatography tandem mass spectrometry**  
*M. Paolini, S. Poli, L. Tonidandel, S. Moser, R. Larcher*  
Fondazione Edmund Mach, Technology Transfer Centre, San Michele all'Adige, Italy
- WP-84**      **Elucidation of oligosaccharides in milk reference materials by HILIC-MS/MS and the NIST tandem MS libraries**  
*C. Remoroza, S. Stein*  
National Institute of Standards and Technology, Mass Spectrometry Data Center, Gaithersburg, USA

- WP-85** **Ikknife, a novel ambient mass spectrometry approach for the real-time identification of food samples**  
*F. Rigano, D. Mangraviti, L. Mondello*  
Chromaleont Srl, c/o Dipartimento ChiBioFarAm, University of Messina, Messina, Italy
- WP-86** **Determination of crocin isomers and isoforms by means UHPLC-MS/MS as quality marker for saffron**  
*R. Rocchi, M. Mascini, M. Sergi, D. Compagnone, P. Pittia*  
University of Teramo, Faculty of Bioscience and Technology for Food, Agriculture and Environment, Teramo, Italy
- WP-87** **Real-time authentication of food and beverages Using DART-QDa LiveID analysis**  
*S. Stead, J. Kirk, K. Organtini*  
Waters Corporation, Scientific Operations, Manchester, United Kingdom
- WP-88** **Evaluation of solid-phase microextraction for the isotopic analysis of volatile compounds in apple**  
*L. Strojnik, F. Camin, L. Ziller, N. Ogrinc*  
Jožef Stefan Institute, Department of Environmental Sciences, Ljubljana, Slovenia
- WP-89** **Aromatic compounds profile of DOC Piedmontese wines by GC-MS with HS-SPME**  
*E. Bonometti, R. Rabezzana, G. Cerrato, L. Operti, E. Diana, F. Turco, E. Priola, A. Giordana*  
University of Turin, Department of Chemistry-CrisDi Interdepartmental Centre for Crystallography, Turin, Italy
- WP-90** **Proteomics approach for the differentiation of Tuna species**  
*I. Brümmer, J. Brockmeyer*  
University of Stuttgart, Food Chemistry, Stuttgart, Germany
- WP-91** **Identification and quantification of polyphenol in cocoa extract, study of the effects of fermentation**  
*G. Cazals, F. Guéhi Gbogbri, S. Munier, R. Boulanger, A. Michel, C. Enjalbal, P. Poucheret*  
LMP, Université de Montpellier, Montpellier, France
- WP-92** **Investigation into the cis isomers of dichlorogenic acids in coffee**  
*S. Colomban, E. Guercia, E. De Angelis, L. Navarini*  
illycaffè spa, Aromalab, Trieste, Italy
- WP-93** **Comparative proteomic analysis of the metabolic fractions composition in modern and old wheat genotypes**  
*A. Di Francesco, R. Saletti, V. Cunsolo, V. Muccilli, P. De Vita, S. Foti*  
University of Catania, Department of Chemical Sciences, Catania, Italy
- WP-94** **Proteomics going nuts? Proteome profiling of walnut kernels**  
*B. Dreyer, D. Kroesser, H. Schlueter*  
University Medical Center Hamburg-Eppendorf, Mass spectrometric proteomics, Hamburg, Germany
- WP-95** **Untargeted high resolution mass spectrometry methods to assess salmon authenticity**  
*G. Maria Fiorino, M. Fresch, I. Brümmer, J. Brockmeyer, I. Losito, L. Monaci*  
National Research Council of Italy (CNR), Institute of Sciences of Food Production (ISPA), Bari, Italy
- WP-96** **Characterization and quantitation of water-soluble vitamins in wine by liquid chromatography-high resolution and tandem mass spectrometry**  
*G. Inzalaco, F. Borghini, A. Cavaglioni, G. Giorgi*  
Università degli Studi di Siena, Dipartimento Biotecnologie, Chimica e Farmacia, Siena, Italy
- WP-97** **Sample Profiler – A cloud-based application for confirming food authenticity**  
*S. Kailasam, R. Tautenhahn, T. Stratton*  
ThermoFisher Scientific, LSMS, Bangalore, India
- WP-98** **Rapid and direct analysis of coffee beans (green and roasted) and online monitoring of coffee roasting by SIFT-MS: focus on volatile aldehydes**  
*I. Khomenko, A. Caretta, V. Lonzarich, F. Biasioli, L. Navarini*  
Edmund Mach Foundation, Food quality and nutrition, San Michele all'Adige, Italy

- WP-99**     **Differential proteomic profiling of truffles**  
*D. Kroesser, B. Dreyer, H. Schlueter*  
 University Medical Center Hamburg-Eppendorf, Mass Spectrometric Proteomics, Hamburg, Germany
- WP-100**    **A novel robust probe for the rapid, on-line characterisation of food samples using rapid evaporative ionisation mass spectrometry**  
*A. Marton, J. Balog, R. Schäffer, S. Pringle, Z. Takáts*  
 Waters Research Center, R&D, Budapest, Hungary
- WP-101**    **Correlating consumer sensory experience of apple aroma with VOC profiles acquired by automated TD-GC-MS**  
*G. Roberts, D. Barden, N. Bukowski, L. Mcgregor, M. Santoro, N. D. Spadafora*  
 SepSolve Analytical, SepSolve Analytical, Peterborough, United Kingdom
- WP-102**    **Food proteomics: a novel approach to food authentication using global protein signatures and species specific marker peptides**  
*L. Viet, P. Krimm, J. Brockmeyer*  
 University of Stuttgart, Food Chemistry, Stuttgart, Germany
- WPS-S05 - MS Tools in Doping & Toxicology**
- WP-103**    **Development and validation of multi-target analytical procedures for the identification of potential doping agents in 'over the counter' products**  
*F. Comunità, F. Botrè, M. Capozzi, X. De La Torre, M. Mazzarino*  
 Laboratorio Antidoping Federazione Medico Sportiva Italiana, Rome, Italy
- WP-104**    **Large volume injection: improving the detection capacity of endogenous anabolic steroids by GC-C-IRMS**  
*L. Iannella, C. Colamonici, D. Curcio, F. Botrè, X. De La Torre*  
 Laboratorio Antidoping Federazione Medico Sportiva Italiana, Rome, Italy
- WP-105**    **Is GC-MS analysis sufficient for identification of illicit drugs from festive gatherings?**  
*S. Magréault, C. Grondin, C. Lamoureux, E. Bourgogne*  
 AP-HP-hopital Lariboisière/Université Paris Descartes, Laboratoire de toxicologie, Paris, France
- WP-106**    **Evaluation of the metabolic profile of 2-methiopropamine by LC-MS/MS in mice and in human liver microsomes**  
*C. Camuto, S. Pellegrini, M. Mazzarino, X. De La Torre, F. Botrè, M. Marti, F. De Giorgio*  
 FMSI Antidoping, University La Sapienza-Department of Chemistry, Rome, Italy
- WP-107**    **Quantitation of five barbiturates in human urine by liquid chromatography-tandem mass-spectrometry**  
*A. Chulovskaya, D. Rakov, E. Mochalova*  
 National Anti-Doping Laboratory (MSU, Moscow), Moscow, Russian Federation
- WP-108**    **A systems biology approach for discovering biomarkers indicative of exposure to Carfentanil**  
*E. Dhummakupt, B. Tran, D. Carmany, G. Boyd, P. Mach, M. Feasel, J. Sekowski, T. Glaros*  
 Edgewood Chemical Biological Center, Research & Technology Directorate, Aberdeen Proving Grounds, USA
- WP-109**    **Co-exposure to silver nanoparticles and cadmium ions induces metabolic adaptation in HepG2 cells**  
*R. Miranda, V. Gorshkov, B. Korzeniowska, S. Kempf, F. Neto, F. Kjeldsen*  
 University of Southern Denmark, Dept. of Biochemistry and Molecular Biology, Odense, Denmark
- WP-110**    **Application of dispersive liquid-liquid microextraction (DLLME) for identification of synthetic cannabinoids in plasma by LC-MS/MS**  
*T. Lino, I. L. Barbosa, D. O. K. Diniz, M. N. Eberlin, J. L. Costa*  
 UNICAMP, School of Medical Sciences, Campinas, Brazil
- WP-111**    **Development and validation of an LC-MS/MS method for the determination of maternal and fetal tissue distribution of permethrin and its metabolites in pregnant rats**  
*S. Personne, A. Corona, C. Brochot, K. Chardon, S. Baltora, S. Pilard, V. Bach, F. Zeman, P. Marcelo*  
 Université de Picardie Jules Verne, Plateforme ICAP, Amiens, France

- WP-112 Proton transfer reaction – mass spectrometry and its applications to homeland security: detection of illicit drugs**  
*D. Olivenza-León, P. Watts, F. Reich, C. Mayhew*  
 University of Birmingham, School of Physics and Astronomy, Birmingham, United Kingdom
- WP-113 Assessment of chemical trace elements in cosmetics' eyeshadows**  
*A. Pawlaczyk, M. Balcerek, M. I. Szykowska*  
 Lodz University of Technology, Faculty of Chemistry, Institute of General and Ecological Chemistry, Lodz, Poland
- WP-114 Generic extraction method for screening of 8 narcotic drugs in saliva with a quick turnaround analysis by LDTD-MS/MS**  
*P. Picard, J. Lacoursiere, S. Auger*  
 Phytrolix Technologies Inc, Quebec City, Canada
- WP-115 Improvement of the Athlete Biological Passport by blood steroid profiling: challenges of a steroidomic approach**  
*F. Ponzetto, J. Boccard, R. Nicoli, T. Kuuranne, S. Rudaz, M. Saugy*  
 Swiss Laboratory for Doping Analysis, CHUV - University of Lausanne, Lausanne, Switzerland
- WP-116 Analysis of removal of pesticides and drugs in waste water by plants using Flow Injection Analysis (FIA) Magnetic Resonance Mass Spectrometry (MRMS)**  
*M. Witt, A. Barsch, C. Villette, D. Heintz*  
 IBMP-CNRS, University of Strasbourg, Strasbourg, France
- WP-117 Improvement for high sensitivity of the drug screening by thermal desorption and pyrolysis combined with DART-MS (TDP/DART-MS)**  
*H. Abe, C. Takeji, K. Yoshizawa, M. Sakakura, T. Shiota, D. Yajima, H. Iwase*  
 BioChromato, Inc., Application support, Fujisawa, Japan
- WP-118 Detection of IGF-1 in serum as a biomarker of growth hormone abuse by athletes**  
*M. Yunin, I. Zvereva, D. Rakov, E. Mochalova*  
 National Anti-Doping Laboratory (MSU, Moscow)
- WP-119 Development of a LC-HRMS based strategy for the screening of conjugated steroids in equine urine**  
*X. Zuo, Z. Kaabia, F. Bagilet, B. Georges, M. Collard, Y. Moulard, P. Garcia, M. Popot, L. Bailly-Chouriberry*  
 Laboratoire des Courses Hippiques (LCH), Anabolic agents anti-doping department, Paris, France
- WP-120 Fast GC-MS/MS for high throughput androgenic anabolic steroids analysis in equine urine**  
*K. Histel, M. Collard, B. Georges, F. Bagilet, M. Popot, Z. Kaabia, L. Bailly-Chouriberry*  
 Laboratoire des Courses Hippiques (LCH), Anabolic agents anti-doping department, Paris, France
- WP-121 In-vitro/vivo study of Andarine metabolism, a selective androgen receptor modulator (SARM), in the context of horse doping control**  
*S. Trevisiol, Y. Moulard, S. Boyer, M. Jaubert, B. Loup, P. Garcia, M. Popot, L. Bailly-Chouriberry*  
 Laboratoire des courses hippiques, LCH, Verrière-le-Buisson, France

### **WPS-S06 - MS Imaging: Applications**

- WP-122 Microbial MALDI-(2)-MS imaging of steam-inactivated co-cultured bacterial colonies at high mass resolution**  
*E. U. Brockmann, D. Steil, J. Soltwisch, K. Dreisewerd*  
 University of Muenster, Institute for Hygiene; Interdisciplinary Center for Clinical Research (IZKF), Münster, Germany
- WP-123 Bioimaging of rat kidneys after single administration of iodinated contrast agents (ICAs)**  
*C. Brungs, M. Viehoff, R. Schmid, M. Sperling, U. Karst*  
 University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany
- WP-124 Reversing the polarity – Targeted mass-spectrometry imaging analysis of fatty acids in positive detection mode**  
*A. Dannhorn, E. Kazanc, P. Inglese, J. Mckenzie, N. Strittmatter, R. J. A. Goodwin, Z. Takats*  
 Imperial College London, Department of Surgery and Cancer, London, United Kingdom

- WP-125** **Mass spectrometry imaging breaks the silence**  
*Y. Dong, P. Sonawane, G. Polturak, L. Feldberg, I. Rogachev, A. Aharoni*  
 Weizmann Institute of Science, Rehovot, Israel
- WP-126** **Mass spectrometry imaging in skin with AP-MALDI and ToF-SIMS**  
*D. El Assad, G. Frache*  
 Luxembourg Institute of Science and Technology, Materials research and technology, Belvaux, Luxembourg
- WP-127** **Elucidation of natural product biosynthesis in Amazon wood *Sextonia rubra* by in situ tandem MS identification with 100 nm-scale imaging**  
*G. L. Fisher, T. Fu, D. Touboul, S. Della-Negra, E. Houel, N. Amusant, C. Duplais, A. Brunelle*  
 Physical Electronics, Marketing & Applications, Chanhassen, USA
- WP-128** **DESI mass spectrometry imaging of the distribution of a fluorescence marker in malignant glioblastoma brain tumours**  
*M. Gentry, E. Jones, D. Coope, A. McMahon*  
 University of Manchester, Division of Informatics, Imaging and Data Sciences, Manchester, United Kingdom
- WP-129** **Maleic anhydride proton sponge and its derivatives toward MALDI-MSI based brain tumor diagnosis**  
*M. Giampà, A. Zurowietz, T. Lammert, J. Fuchser, V. H. Hans, O. Gembruch, U. Kellner, T. W. Nattkemper, H. Bednarz, K. Niehaus*  
 Bielefeld University/Proteome and metabolome research, Bielefeld, Germany
- WP-130** **The effect of protein binding of drug substances in Desorption Electrospray Ionization Mass Spectrometry Imaging**  
*A. Handler, K. Troensegaard Nielsen, C. Janfelt*  
 University of Copenhagen, LEO Pharma A/S, Copenhagen, Denmark
- WP-131** **MS for MS; a mass spectrometry-based study into multiple sclerosis**  
*B. Heijs, F. De Graaff, E. Steenvoorden, M. Giera, G. Kooij*  
 Leiden University Medical Center, Center for Proteomics & Metabolomics, Leiden, Netherlands
- WP-132** **Gold-coated Black Silicon: An Efficient Substrate for Laser Desorption Ionization Mass Spectrometry**  
*S. A. Iakab, P. Rafols, O. Yanes, X. Correig*  
 Universitat Rovira i Virgili, Department of Electrical Electronic Engineering and Automation, Tarragona, Spain
- WP-133** **Application of isotope-labeling in whole-body DESI-MSI studies for intra-animal comparison of drug administration routes**  
*L. Morineau, S. C. Jacobsen, K. Kleberg, H. S. Hansen, C. Janfelt*  
 University of Copenhagen, Department of Pharmacy, Copenhagen, Denmark
- WP-134** **Single cell LiveScan mass spectrometry profiling and imaging**  
*F. Kaftan, M. Vallet, T. Baumeister, G. Pohnert, A. Svatoš*  
 Max Planck Institute for Chemical Ecology, Research Group Mass Spectrometry/Proteomics, Jena, Germany
- WP-135** **Evaluation of embedding strategies for fragile and small specimen in MSI analysis**  
*E. Kazanc, A. Danhorn, P. Inglese, J. Mckenzie, Z. Takats*  
 Imperial College of London, Surgery and Cancer, London, United Kingdom
- WP-136** **Visualizing molecular distributions across/under the human skin by 2D-DESI MS imaging of tape-stripped stratum corneum**  
*K. Kihara, A. Motoyama*  
 Shiseido, Global Innovation Center, Yokohama, Japan
- WP-137** **Distribution of lipids and anti-TB drugs in mouse lung tissue**  
*J. Kokesch-Himmelreich, A. Treu, K. Walter, C. Hölscher, A. Römpp*  
 University of Bayreuth, Bioanalytical Sciences and Food Analysis, Bayreuth, Germany

- WP-138**     **Calcium and lipid imaging of regenerated bony rays of Zebrafish caudal fin using Time-of-Flight Secondary Ion Mass Spectrometry**  
*S. Y. Lee, J. Y. Kim, D. W. Moon*  
 Daegu Gyeongbuk Institute of Science and Technology (DGIST), Department of New Biology, Daegu, Republic of Korea
- WP-139**     **ToF-SIMS imaging of rat and Drosophila brain tissue sections prepared by using the new sampling method**  
*T. G. Lee, H. K. Shon, U. T. Le Minh, J. G. Son, S. Yoon, J. H. Moon, C. Y. Shin, S. B. Lee*  
 KRIS, Center for Nano-Bio Measurement, Daejeon, Republic of Korea
- WP-140**     **MALDI MSI and immunohistochemistry analysis of colorectal carcinoma spheroids**  
*M. Machálová, J. Navrátilová, B. Pavlatovská, K. A. Radaszkiewicz, A. Pruška, J. Preisler*  
 Masaryk University, Department of Chemistry, Brno, Czech Republic
- WP-141**     **Multimodal imaging of undecalcified tissue sections by MALDI MS and  $\mu$ XRF**  
*A. Svirikova, A. Turyanskaya, C. Strel, M. Marchetti-Deschmann*  
 TU Wien, Institute of Chemical Technologies and Analytics, Wien, Austria
- WP-142**     **Mass spectrometry imaging in liver cancer: LA-ICP and DESI analysis of cirrhosis and hepatocellular carcinoma**  
*P. H Vendramini, G. S Pessoa, R. M Oliveira, A. L Rennó, J. H P Garcia, M. A Arruda, M. N Eberlin, A. Sussulini, A. M A Martins*  
 UnB / UniCeub, Medicine / Surgery, Brasilia, Brazil
- WP-143**     **Complementary bioimaging to determine nanoparticle and phospholipid distribution in lung tissue**  
*A. Niehoff, D. Dietrich, M. Sperling, U. Karst*  
 Shimadzu Europa GmbH, Innovation Center, Duisburg, Germany
- WP-144**     **Distinguishing the core and penumbra by lipid profiles using Mass Spectrometry imaging in mice after experimental infarct induction**  
*N. Ogrinc Potocnik, I. Mulder, L. Broos, A. Prop, A. Maagdenberg, R. Heeren*  
 Maastricht University, Maastricht MultiModal Molecular Imaging Institute (M4I), Maastricht, Netherlands
- WP-145**     **The management of haemoglobin interference for the MALDI-MSI analysis of in-vivo thyroid biopsies**  
*I. Piga, G. Capitoli, V. Denti, S. Tettamanti, S. Galimberti, F. Magni, F. Pagni*  
 University of Milano-Bicocca, Department of Medicine and Surgery - Clinical Proteomics and Metabolomics Unit, Vedano al Lambro, Italy
- WP-146**     **High spatial resolution imaging of aged human retina tissue**  
*K. Schey, D. Anderson, J. Messinger, N. Heath Patterson, C. Curcio*  
 Vanderbilt University, Biochemistry, Nashville, USA
- WP-147**     **Ambient mass spectrometry imaging on whole body skin for biomolecules**  
*J. Shiea*  
 National Sun Yat-Sen University, Department of Chemistry, Kaohsiung, Taiwan, Province of China
- WP-148**     **Aldosterone specific visualization in primary aldosteronism using imaging mass spectrometry**  
*S. Shimma, E. Takeo, K. Nishimoto, Y. Sugiura*  
 Osaka University, Graduate School of Engineering, Osaka, Japan
- WP-149**     **MALDI-MS imaging in the search for proteomic indicators of response to therapy in membranous nephropathy**  
*A. Smith, V. L'imperio, M. Mazza, E. Ajello, F. Pagni, F. Magni*  
 University of Milano Bicocca, Department of Medicine and Surgery, Clinical Proteomics and Metabolomics Unit, Vedano al Lambro, Italy
- WP-150**     **Precision medicine for diabetic nephropathy and hypertensive nephrosclerosis: a MALDI-MSI pilot study**  
*A. Smith, V. Iablokov, M. Stella, M. Mazza, B. Heijs, P. Van Veelen, D. Muruve, F. Magni*  
 University of Milano Bicocca, Department of Medicine and Surgery, Clinical Proteomics and Metabolomics Unit, Vedano al Lambro, Italy

- WP-151 High-resolution AP-SMALDI MS imaging of parasites**  
*B. Spengler, P. Kadesch, T. Hollubarsch, A. Taubert, C. Hermosilla, C. Grevelding, T. Quack, S. Gerbig, K. Strupat, M. Kompauer, M. Müller, S. Heiles*  
Justus Liebig University, Institute of Inorganic and Analytical Chemistry, Giessen, Germany
- WP-152 A molecular snapshot of clear cell renal cell carcinoma: multimodal MALDI-MSI and nLC-MS/MS of N-glycans and proteins**  
*M. Stella, F. Boyaval, A. Smith, M. Grasso, G. Bovo, B. Heijs, F. Magni*  
University of Milano Bicocca, Department of Medicine and Surgery, Clinical Proteomics and Metabolomics Unit, Veduggio al Lambro, Italy
- WP-153 Exploring metabolic deregulation in mouse models of breast cancer with multimodal mass spectrometry imaging**  
*A. Taylor, T. Fu, B. Yan, A. Dexter, T. Murta, S. Thomas, Y. Panina, A. Al-Afeef, E. Elia, C. Nikula, R. Phillip, R. Steven, S. Barry, K. Brindle, I. Gilmore, R. Goodwin, J. Marshall, G. Poulogiannis, O. Sansom, Z. Takats, M. Yuneva, J. Bunch*  
National Physical Laboratory, National Centre of Excellence in Mass Spectrometry Imaging, Teddington, United Kingdom
- WP-154 New Frontiers of MALDI-IMS and Lipidomics: An Untargeted Approach to Skin Lipids Mapping**  
*S. Tortorella, F. Xie, P. Tiberi, G. Cruciani, S. Castellino*  
Molecular Horizon, R&D, Bettona, PG, Italy
- WP-155 MALDI-mass spectrometric imaging for the investigation of metabolites in *Linum usitatissimum* L. roots inoculated with *Fusarium oxysporum***  
*G. Vladimirov, N. Melnikova, A. Dmitriev, N. Bolsheva, R. Novakovskiy, A. Zhrebker, A. Yablokov, E. Nikolaev*  
Skolkovo Institute of Science and Technology, Skoltech Center for Translational Biomedicine, Moscow, Russian Federation
- WP-156 Identification of asbestos fibres in a malignant mesothelioma model**  
*O. Voloaca, L. Cole, M. Clench, A. Managh, C. Greenhalgh, S. Haywood-Small*  
Sheffield Hallam University, Biomolecular Science Research Centre, Sheffield, United Kingdom
- WP-157 Two dimensional metabolic profile of bile acids and lipids in fibrosis of NASH-model liver using MALDI Imaging at 20 µm spatial resolution**  
*Y. Yamazaki, S. Yamaguchi, T. Oshikawa, D. Miura, M. Yamazaki*  
Shimadzu Corp., Global application development center, Kyoto, Japan
- WP-158 Matrix-assisted laser desorption/ionization-mass spectrometry imaging for direct visualization of plant wound stress phytohormones in situ**  
*C. Zhang, K. Doležal, O. Novák*  
Palacký University Olomouc, Laboratory of Growth Regulators, Olomouc, Czech Republic
- WP-159 A ToF-SIMS study of lipid changes in *E. coli* mutants with impaired plasmid transfer capability**  
*K. Dimovska Nilsson, M. Palm, A. Farewell, J. S. Fletcher*  
University of Gothenburg, Department of Chemistry and Molecular Biology, Gothenburg, Sweden
- WP-160 Chemical imaging of aggressive basal cell carcinoma using time-of-flight secondary ion mass spectrometry**  
*K. Dimovska Nilsson, M. Munem, O. Zaar, N. Neittaanmäki, J. S. Fletcher, J. Paoli*  
University of Gothenburg, Department of Chemistry and Molecular Biology, Gothenburg, Sweden
- WP-161 An untargeted approach to elucidate the metabolism and tissue distribution of phosphorothioate linked oligonucleotides by high resolution mass spectrometry**  
*B. Steinhuber, C. Husser, A. Brink*  
F. Hoffmann-La Roche AG, PS, Basel, Switzerland
- WP-162 A case study for demonstrating the usefulness of imaging mass spectrometry in toxicity assessment using an amiodarone-induced phospholipidosis model**  
*K. Tanaka, A. Kashimura, H. Sato*  
Mitsubishi Tanabe Pharma Corporation, DMPK Research Laboratories, Toda, Japan



## WPS-S07 - Gas Phase Ion Chemistry & Thermochemistry

- WP-163 **A quantum chemical tool for the prediction of mass spectra and the identification of fragmentation pathways**  
*J. Cautereels, F. Blockhuys*  
University of Antwerp, Department of Chemistry, Antwerp, Belgium
- WP-164 **Isomerization and dissociation of alpha-centered and pi-centered glycyglycyltryptophan radical cations: structural, energetic, mechanistic, and spectroscopic investigations**  
*A. C. K. Siu, J. Martens, A. Sze, J. Oomens, I. K. Chu*  
The University of Hong Kong, Department of Chemistry, Hong Kong, China
- WP-165 **Nitrogen oxides binding to cobalamin: ion chemistry by FT-ICR mass spectrometry**  
*M. E. Crestoni, A. Maccelli, S. Fornarini*  
Sapienza Università di Roma, Dipartimento di Chimica e Tecnologie del Farmaco, Roma, Italy
- WP-166 **Tandem mass spectrometry as a tool to evaluate ligand electronic effect on Au(I) complexes**  
*D. Gatineau, D. Lesage, H. Dossmann, H. Clavier, A. Millet, Y. Gimbert*  
DCM UMR 5250, CNRS-Université Grenoble Alpes, Grenoble, France
- WP-167 **Energy-resolved collision-induced dissociation study of proton-bound heterodimers of guanine and cytosine**  
*S. Yun Han, J. Ju Park, C. Sik Lee*  
Gachon University, Department of Nanochemistry, Seongnam, Republic of Korea
- WP-168 **Correlation between structure and stability of gas phase oligonucleotides probed by tuned collision- and VUV-MS/MS**  
*S. Ickert, J. Riedel, S. Beck, M. W. Linscheid*  
Humboldt Universität zu Berlin, Federal Institute for Materials Research and Testing, Berlin, Germany
- WP-169 **Measurement of protonated water clusters using High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS)**  
*A. T. Kirk, M. Allers, S. Zimmermann*  
Leibniz Universität Hannover, Department of Sensors and Measurement Technology, Hannover, Germany
- WP-170 **Challenges of soft chemical ionization mass spectrometry: ion chemistry of glyoxal**  
*M. Lacko, F. Piel, A. Mauracher, A. Knížek, P. Španel*  
J. Heyrovský Institute of Physical Chemistry of the CAS, Prague, Czech Republic
- WP-171 **Walk-on-sphere rearrangement and retro-Bingel reaction of gas-phase fullerene malonate ions**  
*J. Oschwald, M. B. Minameyer, K. L. Maxouti, A. Hirsch, T. Drewello*  
Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Chemie und Pharmazie, Erlangen, Germany
- WP-172 **Gas phase structures and thermochemical parameters of protonated 5-HMF isomers**  
*F. Pepi, S. Garzoli, P. Giacomello, G. De Petris, A. Troiani, R. Ragno, A. Patsilnakos, L. Antonini, A. Ricci, C. Salvitti*  
"Sapienza" University of Rome, Department of Chemistry and Drugs Technologies, Rome, Italy
- WP-173 **Selective conversion of protonated D-fructose to 5-HMF and 2-FA: a nitrogen-base assisted dehydration process in the gas-phase**  
*A. Troiani, G. De Petris, F. Pepi, S. Garzoli, M. Rosi, A. Ricci, C. Salvitti*  
Università della Campania "L. Vanvitelli", Dip. di Matematica e Fisica, Caserta, Italy
- WP-174 **Sulfur dioxide uptake by sodium carbonate cluster anions in the gas-phase**  
*C. Salvitti, A. Troiani, G. De Petris*  
"Sapienza" University of Rome, Department of Chemistry and Technology of Drugs, Rome, Italy
- WP-175 **Development of tuner integrated microwave driven radical beam sources for radical induced dissociation molecular structural analysis**  
*Y. Shimabukuro, H. Takahashi, S. Iwamoto, K. Tanaka, M. Wada*  
Doshisha University, Plasma Physics Laboratory, Kyotanabe, Japan

- WP-176 **Controlled reactions of methyl cation with oxygen compounds and hydrocarbons**  
*R. Thissen, C. Romanzin, C. Alcaraz*  
 Université Paris Saclay, Laboratoire Chimie Physique, Orsay, France
- WP-177 **Two molecules are better than one: cooperative effects of two sulfur dioxide and sulfur dioxide/water in bond forming and hydrolysis reactions of polyvanadate dianions in the gas phase**  
*A. Troiani, M. Rosi, S. Garzoli, C. Salvitti, G. De Petris*  
 "Sapienza" University of Rome, Dipartimento di Chimica e Tecnologie del Farmaco, Rome, Italy
- WP-178 **Gas-phase fragmentation mechanisms studies of doubly-protonated peptide ions containing basic amino acid residues by mass spectrometry**  
*T. Yalcin, A. Emin Atik*  
 Izmir Institute of Technology, Faculty of Science, Dept. of Chemistry, Urla-Izmir, Turkey

### **WPS-S08 - FTMS and Innovative Methods for (Bio)Analyses**

- WP-179 **Top-down analysis of endogenous tau fragments in human cerebrospinal fluid using immunoprecipitation and Fourier Transform Mass Spectrometry**  
*G. Brinkmalm, C. Cicognola, J. Gobom, E. Portelius, H. Zetterberg, K. Blennow, K. Höglund*  
 University of Gothenburg, Sahlgrenska Academy, Mölndal, Sweden
- WP-180 **Extreme resolution FT-ICR-MS top-down analysis of glycated proteins**  
*C. Cordeiro*  
 Universidade de Lisboa, Laboratório de FT-ICR e Espectrometria de Massa Estrutural, Faculdade de Ciências, Lisboa, Portugal
- WP-181 **Identification of new ligand-protein complex for Mycobacterium Tuberculosis using Fourier Transform Mass Spectrometry**  
*A. Di Capua, P. Myler, R. Quinn*  
 Griffith Institute for Drug Discovery, Nathan, Australia
- WP-182 **Coupling gas-phase fractionation and proton-transfer reaction for improved top-down proteomics**  
*L. Fornelli, R. Huguet, C. Mullen, R. Fellers, R. Melani, J. Syka, N. Kelleher*  
 Northwestern University, Molecular biosciences/Chemistry, Evanston, USA
- WP-183 **Detailed analysis of temporal ion cloud distributions undergoing Coulomb interactions in FT-ICR mass spectrometry: a many-particle simulation**  
*M. Fujiwara, H. Takahashi, N. Happo, K. Tanaka*  
 Hiroshima City University, Grad School of Information Sciences, Hiroshima, Japan
- WP-184 **FT-ICR MS with absorption-mode data acquisition: method development and high-resolution applications**  
*A. N. Kozhinov, K. O. Nagornov, Y. O. Tsybin*  
 Spectroswiss Sàrl, EPFL Innovation Park, Lausanne, Switzerland
- WP-185 **Factor Xa anticoagulant bioactive proteins derived from scorpion venom**  
*M. Li, Y. P. Y. Lam, P. Chen, R. Gavard, C. K. C. Chiu, C. A. Wootton, Q. Wu, M. P. Barrow, H. Fu, P. B. O'connor*  
 University of Warwick, Department of Chemistry, Coventry, United Kingdom
- WP-186 **Microchip capillary electrophoresis-ESI-MS for rapid, multi-level analysis of complex proteins**  
*J. Scott Mellors, E. Redman*  
 908 Devices Inc., Life Sciences, Boston, USA
- WP-187 **Flavonoid annotation using a product ion-dependent MS<sup>n</sup> data acquisition method on a Tribrid Orbitrap mass spectrometer**  
*R. Kiyonami, I. Sakane, S. Sharma, G. Mcalister, A. Souza, C. Ding, A. Huhmer*  
 Thermo Fisher Scientific, Metabolomics Program, San Jose, USA
- WP-188 **Fundamentals of FT-ICR MS at the cyclotron frequency**  
*O. Tsybin, K. Nagornov, A. Kozhinov, Y. Tsybin*  
 Peter the Great Saint-Petersburg State Polytechnic University, Ion Physics Laboratory, Saint-Petersburg, Russian Federation

- WP-189** Use of SIFT-MS in the analysis of volatile compounds arising from the addition of sodium hypochlorite as an irrigant in infected root canal treatment  
*K. Ioannidis, S. Niazi, S. Deb, F. Mannocci, D. Smith, C. Turner*  
The Open University, School of Life, Health & Chemical Sciences, Milton Keynes, United Kingdom
- WP-190** Optimal signal-to-noise and peak assignment for two-dimensional mass spectrometry  
*A. Maria Van, R. Gavard, A. Lynch, T. Morgan, C. Wootton, L. Chiron, M. Delsuc, M. Barrow, P. O'Connor*  
University of Warwick, Department of Chemistry, Coventry, United Kingdom
- WP-191** Signal amplification mass spectrometry bioassay for attomolar detection of genes  
*S. Xu, Y. Bai, H. Liu*  
Peking University, College of chemistry, Beijing, China
- WP-192** Two-dimensional (2D) FT-ICR MS at high resolution on precursor ions  
*C. Rolando, F. Bray, J. Bouclon, P. Pelupessy, M. Delsuc*  
CNRS, University of Lille, Villeneuve d'Ascq, France

### **WPS-S09- Food Additives and Contaminants**

- WP-193** Determination of undesired substances in edible oils by UHPLC-MS/MS  
*A. Baldi Talini, Y. Gao, Z. Zhen, M. Zhu, F. Qin, J. Ye*  
PerkinElmer Inc, Mass Spectrometry, Shelton, USA
- WP-194** Development and validation of an LC-MS/MS method to quantify fumonisins and hydrolysed fumonisins in porcine serum  
*G. Bichl, T. Czabany, H. Schwartz-Zimmermann, D. Schatzmayr, I. Dohnal*  
Biomim, Research Center, Tulln, Austria
- WP-195** Identification of synthetic food dyes by nanoelectrospray ionization  
*L. Borovcová, E. Mácalová, K. Lemr*  
Palacký University, Department of Analytical Chemistry, Faculty of Science, Olomouc, Czech Republic
- WP-196** Acrylamide determination in potato and/or cereals based food by LC-MS/MS method: one year of monitoring in North-West Italy  
*V. Ciccotelli, L. A. Masiello, V. Savio, B. Vivaldi, C. Ercolini*  
Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle D'Aosta (sezione di Genova), N.R.L. for pesticides in cereals and feed, Genova, Italy
- WP-197** Determination of pesticides in fruit, vegetables and feed by multiresidue methods: one year of monitoring in North-West Italy  
*V. Ciccotelli, R. Nappi, B. Rutigliano, A. Galleggiante Crisafulli, E. Poma Genin, E. Alesso, B. Vivaldi*  
Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle D'Aosta (sezione di Genova), N.R.L. for pesticides in cereals and feed, Genova, Italy
- WP-198** Robust multiresidue pesticide analysis in baby food with enhanced sensitivity GC-MS/MS technology  
*E. Ciceri, R. Law, T. Anderson, C. I. Cojocariu*  
Thermo Fisher Scientific, CMD, Milan, Italy
- WP-199** Sensitive and robust determination of phthalates in cooking oil using advanced electron ionization single quadrupole GC-MS technology  
*E. Ciceri, A. Lamb, C. I. Cojocariu*  
Thermo Fisher Scientific, CMD, Milan, Italy
- WP-200** Bee pollen and pyrrolizidine alkaloids: a contamination profile analysis using LC-MS/MS  
*L. De Jesus Inacio, L. Lucatello, V. Bisutti, A. Sartorato, R. Merlanti, F. Capolongo*  
University of Padua, Department of Comparative Biomedicine and Food Science, Legnaro - PD, Italy
- WP-201** Towards untargeted chemical food safety assessment  
*G. Delaporte, M. Cladière, V. Camel*  
Ingénierie Procédés Aliments, AgroParisTech, INRA, Université Paris-Saclay, Massy, France

- WP-202 **Characterisation and quantification of known/unknown migrating substances in food using LC & GC high resolution mass spectrometry**  
*Y. Hammel, B. Bodet, S. Koster*  
Nestle Research Center, Institute Food Safety & Analytical Science, Lausanne, Switzerland
- WP-203 **Mercaptomic: towards the profiling of reactive metabolites in toxicology**  
*E. Jamin, R. Costantino, J. Martin, L. Debrauwer, F. Guéraud*  
INRA, MetaboHUB-MetaToul-AXIOM platform, Toulouse, France
- WP-204 **Fast and automatic data processing for targeted and non-targeted pesticide analysis**  
*J. Jasak, J. Meltretter, J. Stahl-Zeng, V. Raguvaran, D. Cox*  
Sciex, Darmstadt, Germany
- WP-205 **Simultaneous determination of propoxycarbazone and its metabolite in food by UHPLC-MS/MS, applying a QuEChERS extraction based method**  
*M. Vargas-Pérez, J. Marín-Sáez, M. L. Jiménez Medina, F. J. Egea González, A. Garrido Frenich*  
University of Almería, Dept. Chemistry and Physics, Almería, Spain
- WP-206 **Sensitive determination of 44 toxic pyrrolizidine alkaloids in spices and culinary herbs using liquid chromatography tandem-mass spectrometry**  
*F. Kaltner, M. Rychlik, M. Gareis, C. Gottschalk*  
Ludwig Maximilian University of Munich, Chair of Food Safety, Oberschleissheim, Germany
- WP-207 **Analytical method development of multi residue pesticides in Livestock Products by Gas chromatography-mass spectrometry(GC-MS/MS)**  
*H. S. Kang, E. J. Kim, M. Lim, E. J. Chang, K. No, D. M. Choi, H. Choi*  
Gyeongin Regional Office of Food and Drug Safety, Division of Hazardous Substances Analysis, Incheon, Republic of Korea
- WP-208 **Limitations of gas chromatography–single quadropole mass spectrometry in the identification of compounds migrating from food contact materials**  
*C. Kirckeszner, Z. Eke, Z. Nyiri, N. Petrovics*  
Joint Research and Training Laboratory on Separation Techniques, Eötvös Loránd University, Budapest, Hungary
- WP-209 **Multi-analyte method based on liquid chromatography coupled with single quadrupole mass analyzer for fast and effective control of food additives**  
*A. Krmela, V. Schulzova, J. Pulkrabova, J. Hajslova*  
UCT Prague, Department of Food analysis and nutrition, Prague, Czech Republic
- WP-210 **Aflatoxin M1 residues detection in milk, infant food and cheese by LC-MS/MS**  
*G. L. Ferro, S. Massafra, P. Stella, E. Pennazio, M. Leporati, D. Marchis, M. Gili*  
Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta, S.S. Igiene dei Mangimi, Torino, Italy
- WP-211 **Analytical method based on UHPLC-ESI-MS/MS for quantification of plant toxins in herbal food supplements**  
*S. Malysheva, J. Picron, B. Huybrechts*  
Sciensano, Organic contaminants and additives, Brussels, Belgium
- WP-212 **Comparison between HPLC-ESI-Qq-MS/MS and SPME-GC-MS technique for acrylamide determination in potatoes chips**  
*S. Marzocchi, S. Marziali, M. Fiorenza Caboni*  
University of Bologna, Department of Agro-Food Science, Cesena, Italy
- WP-213 **A multi-residue confirmatory method for the determination of sedatives by HPLC-MS/MS**  
*P. Metalnikov, I. Batov, R. Selimov, A. Komarov, V. Nikulin*  
VGNKI, Food Safety, Moscow, Russian Federation
- WP-214 **Determination of Fenpyroximate from four types of honey by LC/MS/MS**  
*S. Myung, J. Kim, S. Lee*  
Kyonggi University, Chemistry, Suwon, Republic of Korea
- WP-215 **Supercritical fluid chromatography – mass spectrometry as a new tool for determination of synthetic food dyes**  
*V. Pauk, M. Uhrová, K. Lemr*  
RCPTM, Department of Analytical Chemistry, Palacky University in Olomouc, Olomouc, Czech Republic

- WP-216 Simultaneous screening of 6 different antibiotic families in meat using LDTD-MS/MS quantitation at 9 seconds per sample**  
*P. Picard, J. Lacoursiere, S. Auger*  
 Phytronix Technologies Inc, Quebec, Canada
- WP-217 NDL-PCBs, PBDEs, HBCDs levels and temporal trends in mussels (*Mytilus galloprovincialis*) from Middle Adriatic Sea**  
*A. Piersanti, T. Tavoloni, T. Stecconi, A. Stramenga, R. Galarini*  
 Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Sezione di Ancona, Ancona, Italy
- WP-218 Automated Solid Phase Microextraction (SPME) with UHPLC-MS/MS to determine veterinary drugs in chicken meat**  
*J. Wu, A. Khaled, F. Qin, J. Pawliszyn*  
 PerkinElmer, Woodbridge, Canada
- WP-219 Simultaneous quantitation of fat soluble vitamins in infant milk formulae using 5500 QTRAP LC-MS/MS system**  
*A. Sage, J. Stahl-Zeng, A. Verma, A. Kumar, M. Pillai*  
 Sciex, Market Development, Warrington, United Kingdom
- WP-220 Multiclass method for the quantitative analysis of 108 veterinary drugs in meat and milk by liquid-chromatography quadrupole-orbitrap mass spectrometry**  
*G. Saluti, I. Diamanti, R. Rossi, C. Barola, D. Giusepponi, S. Moretti, R. Galarini*  
 Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Centre for Development and Validation of Methods, Perugia, Italy
- WP-221 Fungicides in red wines produced in South America**  
*T. Vargas, N. Salustriano, B. Klein, S. Da Silva, W. Romão, R. Wagner, R. Scherer*  
 University of Vila Velha, Vila Velha, Brazil
- WP-222 A robust and sensitive method for the direct analysis of polar pesticides in food and environmental samples**  
*D. Schleuder, U. Chiuminatto, W. Broer*  
 AB SCIEX Germany GmbH, Support, Darmstadt, Germany
- WP-223 Non-targeted fast screening of hundreds residual pesticides on fruits, eggs and soil using ambient mass spectrometry**  
*J. Shiea*  
 National Sun Yat-Sen University, Department of Chemistry, Kaohsiung, Taiwan, Province Of China
- WP-224 The time trend of PBDE in breast milk from Beijing within the first six months postpartum**  
*S. Song*  
 National Research Center for Geoanalysis, Department of Organic Analysis, Beijing, China
- WP-225 Screening and quantitation for food matrices using scanning SWATH acquisition**  
*J. Stahl-Zeng, D. M. Cox, J. Rivera, H. Lee, V. Raguvaran*  
 Sciex, MDM, Darmstadt, Germany
- WP-226 LC-MS/MS versus GC-MS/MS for hexabromocyclododecanes (HBCDs) analysis in food**  
*A. Stramenga, T. Tavoloni, T. Stecconi, A. Piersanti*  
 Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Sezione di Ancona, Ancona, Italy
- WP-227 GC-MS/MS and LC-MS/MS applied to the analysis of brominated flame retardants (PBDEs and HBCDs) in fish species from Italian market**  
*T. Tamara, A. Stramenga, G. Scortichini, T. Stecconi, A. Piersanti*  
 Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Sezione di Ancona, Ancona, Italy
- WP-228 Organic (PBDEs,NDL-PCBs) and inorganic (Pb, Cd, Hg, As, Ni, Mn) contaminants assessment in wild boar (*Sus scrofa*) by GC-MS/MS and ICP-MS**  
*T. Tavoloni, A. Stramenga, V. Castro, M. Ciriaci, M. Conquista, F. Griffoni, P. Palombo, G. Scortichini, T. Stecconi, A. Piersanti*  
 Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Sezione di Ancona, Ancona, Italy

- WP-229** Screening and quantitative analysis of non intentionally added substances eluted from polyethylene terephthalate bottle by high-resolution mass spectrometry  
*A. Yamamoto, T. Murakami, M. Shizuma, E. Kishi, A. Ozaki*  
Tottori University of Environmental Studies, Faculty of Environment, Tottori, Japan
- WP-230** Development of a rapid method for analysis of heterocyclic aromatic amines by QuEChERS extraction and UHPLC-APCI-MS/MS assay  
*S. Chevolleau, J. François, A. Bouville, L. Debrauwer*  
INRA /Toxalim, Metatoul-AXIOM Platform, Toulouse, France
- WP-231** In vivo efficacy of a YCW-based product in reducing oral bioavailability of zearalenone in pigs  
*V. D'Ascanio, A. Catteuw, E. Santovito, V. Marquis, S. Croubels, D. Greco, A. Logrieco, G. Avantaggiato*  
Institute of Sciences of Food Production (ISPA), National Research Council (CNR), Bari, Italy
- WP-232** Exploiting the potential of HRMS for deciphering mycotoxin modification in micropropagated wheat: the case of deoxynivalenol  
*T. Damiani, L. Righetti, E. Rolli, M. Suman, R. Bruni, C. Dall'Asta*  
University of Parma, Department of Food and Durg, Parma, Italy
- WP-233** Sensitive mass spectrometric method for the detection of palytoxins in shellfish using lithium cationization  
*A. Gerssen, M. D. Klijnstra*  
RIKILT, Wageningen University and Research, Wageningen, Netherlands
- WP-234** Development of a simple multi-residue determination method of 80 veterinary drugs in fish tissues by liquid chromatography coupled to quadrupole Orbitrap mass spectrometry  
*X. Luo, Z. Tang, Z. Niu, X. Ye, F. Zhao*  
Qingdao Customs, Inspection and Quarantine Technical Center, Qingdao, China
- WP-235** Comparison of different strategies for the determination of veterinary drug residues in food by UPLC-MS/MS using Orbitrap Elite  
*P. Metalnikov, R. Selimov, A. Efimov, I. Batov, A. Dzhathdueva, A. Komarov*  
VGNKI, Food Safety, Moscow, Russian Federation
- WP-236** UHPLC-HRMS analysis of theobromine in Costa Rican Theobroma cacao  
*K. Mladenovic, Y. Root, D. Ramanathan*  
Kean University, STEM, Union, USA
- WP-237** LC-MS/MS method to evaluate the presence of exogenous glycerol in wines  
*L. Tonidandel, S. Moser, D. Trainotti, R. Larcher*  
Edmund Mach foundation, CTT, San Michele all'Adige, Italy
- WP-238** Approaches to minimize and control external contamination during sample handling and analysis of ubiquitous environmental phenolic compounds in food samples  
*M. A. Zuberovic Muratovic, U. Rybinska, K. Hellenäs*  
National Food Agency, Department of Chemistry / Division of Science, Uppsala, Sweden
- WP-239** A study on migration of heavy metals from ceramics and glassware using inductively coupled plasma mass spectrometry (ICP-MS)  
*K. C. Cho, Y. E. Cho, Y. C. Park, D. M. Choi*  
Gyeongin Regional Food and Drug Administration, Center for Food and Drug Analysis, Incheon, Republic of Korea

### **WPS-S10 - Atomic Mass Spectrometry: Metallomics and Isotope Ratio Mass Spectrometry**

- WP-240** Isotopic niche space of songbirds migrating through the Southern Alps  
*A. Franzoi, F. Camin, P. Pedrini, L. Bontempo*  
Fondazione Edmund Mach, Department of Food Quality and Nutrition, Research and Innovation Centre, San Michele all'Adige, Italy
- WP-241** Experimental evaluation of TIMS-based detection methods for isotopic analysis of uranium at ultra-trace level  
*J. Park, K. Jeong*  
Korea Atomic Energy Research Institute, Nuclear Chemistry Research Division, Daejeon, Republic of Korea

- WP-242 **C and H stable isotope ratio analysis using GC-IRMS for vanillin authentication**  
*M. Perini, S. Pianezze, F. Camin*  
 Fondazione Edmund Mach, Technology Transfer Centre, San Michele all'Adige, Italy
- WP-243 **Stable isotope ratio analysis for authentication of chitosan**  
*M. Perini, T. Nardin, M. Venturelli, S. Pianezze, R. Larcher*  
 Fondazione Edmund Mach, Technology Transfer Centre, San Michele all'Adige, Italy
- WP-244 **Development of novel compact carbon dating instrument based on Collinear Resonance Ionisation Spectroscopy (CRIS)**  
*G. Edwards, K. Flanagan, B. Cooper, S. Alsufyani, C. Ricketts, C. Binnersley*  
 The University of Manchester, School of Physics & Astronomy, Manchester, United Kingdom

THURSDAY, August 30<sup>th</sup>, 2018

Wednesday

**ThPS-S01 - Glycomics, Saccharides and Glycoconjugates**

- ThP-1 **Reductive alkaline release of N-glycans generates a variety of unexpected, useful products**  
*R. Figl, F. Altmann*  
 University of Natural Resources and Life Sciences, Chemistry, Glycobiology, Vienna, Austria
- ThP-2 **Analysis of mouse brain N-glycans by (PGC-)LC-ESI-MS using isotopically labeled standards**  
*C. Grünwald-Gruber, A. Thader, J. Urteil, D. Maresch, F. Altmann*  
 University of Natural Resources and Life Sciences, Department of chemistry, Vienna, Austria
- ThP-3 **Assignment of linkage, anomeric configuration, and branch location of oligosaccharides via a logically derived MS<sup>n</sup> approach**  
*H. C. Hsu, C. Y. Liew, S. Huang, S. Tsai, C. Ni*  
 Institute of Atomic and Molecular Sciences, Academia Sinica, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, Province of China
- ThP-4 **Fragmentation of oligosaccharides and suppression of metal-salt induced adducts using electrospray ionization**  
*V. Iwan, J. Grotemeyer*  
 Christian-Albrechts-University Kiel, Institute of Physical Chemistry, Kiel, Germany
- ThP-5 **MALDI-MS analysis of sucrose using a charcoal matrix**  
*J. Kim*  
 Chungnam National University, Yuseong-Gu, Daejeon, Republic of Korea
- ThP-6 **Multiplexed isotope labeled standards for isomeric analysis of N-glycans**  
*D. Maresch, C. Grünwald-Gruber, A. Thader, F. Altmann*  
 University of Natural Resources and Life Sciences, Department of Chemistry, Vienna, Austria
- ThP-7 **N-glycan analysis of various Chlorella strains by MALDI-ToF and LC-ESI-MS**  
*R. T. Mocsaj, R. Figl, E. Svehla, F. Altmann*  
 University of Natural Resources and Life Sciences, Department of Chemistry, Vienna, Austria
- ThP-8 **Semi-targeted analysis of metabolites in Saponaria officinalis by LC-MS**  
*K. Pawlak, K. Lech, K. Wojciechowski, I. Goral, P. Bartosz, P. Kosior, T. Kiehl, A. Ornoch, K. Kaczmarczyk*  
 Warsaw University of Technology, Faculty of Chemistry, Chair of Analytical Chemistry, Warsaw, Poland
- ThP-9 **Semi-automatic site specific quantitative analysis of high mannose and hybrid type glycosylation in liver tissue associated with HCC and cirrhosis**  
*M. Sanda, J. Benicky, Z. Brnakova, L. Zhang, R. Goldman*  
 Georgetown University, Department of Oncology, Washington, USA

- ThP-10 Integrating ion spectroscopy with mass spectrometry for the structural analysis of carbohydrates**  
*B. Schindler, G. Renois-Predelus, I. Compagnon*  
Institut Lumière Matière, Université de Lyon, Lyon, France
- ThP-11 Isomer-specific MRM profiling of serum N-glycome for Behcet disease monitoring**  
*N. Seo, K. H. Kim, J. K. Ahn, H. S. Cha, J. Kim, J. An Hyun*  
Chungnam National University, Graduate School of Analytical Science and Technology,  
Daejeon, Republic of Korea
- ThP-12 Glycosaminoglycan analysis of prostate cancer tissue microarrays**  
*G. Tóth, O. Ozohanics, A. Ács, Á. Révész, K. Vékey, L. Drahos, L. Turiák*  
MS Proteomics Group, Research Center for Natural Sciences, Hungarian Academy of Sciences,  
Budapest, Hungary
- ThP-13 Thin-layer chromatography coupled with nano-matrix based MALDI-ToF mass spectrometry for structural elucidation of glycans**  
*E. Gizaw, M. Tseng, Y. Chen*  
Academia Sinica, Institute of Chemistry, Taipei, Taiwan, Province Of China
- ThP-14 Glycolipidomics of human brain by combined modern mass spectrometry methods: chip nano ESI MS and ESI IMS MS<sup>n</sup>**  
*M. Sarbu, Z. Vukelic, D. Clemmer, A. D. Zamfir*  
National Institute for Research and Development in Electrochemistry and Condensed Matter,  
Department of Condensed Matter, Timisoara, Romania
- ThP-15 Top down proteomics of human  $\alpha$ -acid-glycoprotein: fast and unambiguous glycan analysis**  
*M. Bärenfänger, B. Meyer*  
University of Hamburg, Department of Organic Chemistry, Hamburg, Germany
- ThP-16 Development of a new method for the identification of Follicle Stimulating Hormone (FSH) glycoforms involved human fertility**  
*C. Melchiorre, CA. Illiano, G. Pinto, A. Carpentieri, A. Amoresano*  
University of Naples Federico II, Department of Chemical Science, Napoli, Italy

### **ThPS-S02 - Probing Protein Structure and Dynamics**

- ThP-17 Structural diversity of nucleosomes characterized by nanoESI-MS and structural calculation**  
*K. Saikusa, A. Osakabe, D. Kato, S. Fuchigami, A. Nagadoi, Y. Nishimura, H. Kurumizaka, S. Akashi*  
Yokohama City University, Grad. Sch. of Med Life Science, Yokohama, Japan
- ThP-18 Native state organization of outer membrane porins unraveled by HDX-MS**  
*D. Donnarumma, C. Maestri, P.I. Giammarinaro, L. Capriotti, E. Bartolini, D. Veggi, R. Petracca, M. Scarselli, N. Norais*  
GSK Vaccines, Siena, Italy
- ThP-19 Effects of oxidative stress on the conformational stability of hemoglobin measured by variable temperature nESI-IMS-MS**  
*D. Woodall, T. El-Baba, C. Brown, D. Fuller, S. Raab, D. Clemmer*  
Indiana University, Bloomington, USA

### **ThPS-S03 - Natural Substances and Their Complexes**

- ThP-20 Development of LC-MS/MS analytical protocol for artemisinin and its derivative compounds quantification in the *Artemisia annua* L. extracts for cosmetic applications**  
*R. M. Alberici, E. C. Cabral, G. C. Nogueira, R. Vardanega, M. A. A. Meireles, M. N. Eberlin*  
University of Campinas, Thomson Mass Spectrometry Laboratory, Campinas, Brazil
- ThP-21 Metabolomic UHPLC-qToF method to analyze tannins in natural complex products using All-Ions fragmentation acquisition**  
*M. Burico, L. Mattoli, P. Traldi*  
Aboca Spa Società Agricola, Sansepolcro, Italy
- ThP-22 Characterization of beta amino acid esters in *Ononis* species**  
*N. Gampe, A. Darcsi, L. Ladocsi, L. Kursinszki, S. Béni*  
Semmelweis University, Department of Pharmacognosy, Budapest, Hungary



- ThP-23 Investigation of plant extracts for medical research**  
*M. Gronbach, C. Oppermann, J. M. Modenbach, M. Sendler, M. Lerch, U. Kragl*  
 University of Rostock, Department of Chemistry, Rostock, Germany
- ThP-24 MS analysis of protein interactions relevant for the biosynthesis of APE**  
*K. Karimi, G. L. C. Grammbitter, H. B. Bode, N. Morgner*  
 Goethe University Frankfurt am Main, Institute of physical and theoretical chemistry, Frankfurt am Main, Germany
- ThP-25 Analytical authentication of *Ophiogopon japonicus* samples: an essential step to secure its supply and its use for the development of a safe and effective dermo-cosmetic ingredient**  
*S. Richer, D. Laporte, L. Verzeaux, D. Boudier, I. Fourasté, M. Howes, M. Simmonds, B. Closs*  
 SILAB, R&D Department, Brive la Gaillarde, France
- ThP-26 LC-ESI-MS/MS analysis of short-chain peptides with anti-aging properties**  
*M. Shamshiddinova, Y.-M. Lee*  
 Chungbuk National University, College of Pharmacy, Cheongju, Republic of Korea
- ThP-27 From massive chicken death to insect poison diet through the mass spectrometry prism**  
*E. Stashenko, J. R. Martinez, F. Prada, J. Lozano, Y. Bautista, J. Zambrano, N. Nãñez*  
 Universidad Industrial de Santander, School of Chemistry, Bucaramanga, Colombia
- ThP-28 Characterization of environmental microorganisms by proteins and lipids MALDI-ToF fingerprints**  
*V. Guérineau, M. Barthélemie, V. Eparvier, D. Touboul*  
 CNRS-ICSN, Université Paris Saclay, Gif sur Yvette, France
- ThP-29 Mass spectrometry technique for studying the peptides cyclisation by native chemical ligation**  
*M. Wierzbicka, O. Skwara, S. D. Ozan, P. Stefanowicz*  
 University of Wrocław, Faculty of Chemistry, Wrocław, Poland
- ThP-30 An unusual TMS artifact in EI mass spectrometry - Perrhenic acid TMS**  
*W. G. Mallard, Y. Zheng, S. P. Markey, J. L. Little*  
 NIST, MSDC, Gaithersburg, USA
- ThP-31 Comparing the profiles of yellow-legged hornet venom (*Vespa velutina nigrithorax*) to evaluate the influences of seasonal variations**  
*T. N. Le, D. Da Silva, C. Colas, E. Darrouzet, P. Baril, L. Petit Leseurre, B. Maunit*  
 Institut de Chimie Organique et Analytique (ICOA), UMR 7311, Université d'Orléans-CNRS, Orléans, France
- ThP-32 GC-MS/MS determination of cis and trans- $\Delta^9$ -THC isomers in *Cannabis sativa* L**  
*S. Valera, G. Allegrone, F. Pollastro*  
 Università Piemonte Orientale, Dipartimento di Scienze del Farmaco, Novara, Italy

### **ThPS-S04 - Environmental Mass Spectrometry**

- ThP-33 Strategy to identify industrial peak emissions based on long-term HRMS data time series**  
*S. Anliker, M. Loos, M. Ruff, R. Comte, K. Fenner, H. Singer*  
 Eawag, Environmental Chemistry, Dübendorf, Switzerland
- ThP-34 Transformation product formation in drinking water treatment**  
*A. M. Brunner, D. Vughs, W. Siegers, C. Bertelkamp, A. Kolkman, T. Ter Laak*  
 KWR Watercycle Research Institute, Chemical Water Quality and Health, Nieuwegein, Netherlands
- ThP-35 Molecular level investigation of oil contaminated soils generated during the Gulf War with two-dimensional gas chromatography (GCxGC) and ultra-high resolution mass spectrometry**  
*E. Cho, M. Park, Y. H. Kim, G. Kang, Y. Cho, S. Kim*  
 Kyungpook National University, Department of Chemistry, Daegu, Republic of Korea
- ThP-36 Occurrence of organophosphate flame retardants in swimming pools and their endocrine disrupting potential**  
*P. Chou, W. Shih*  
 National Cheng Kung University, Department of Environmental Engineering, Tainan City, Taiwan

- ThP-37 Assessment of BPA and DEHP metabolites in urine samples from mother-child pairs of LIFE PERSUADED project**  
*V. Della Latta, F. Carli, E. Buzzigoli, D. Ciociaro, M. Gaggini, A. Paola Pala, A. Raffaelli, R. Conte, L. Busani, F. Maranghi, S. Tait, S. Cianfarani, C. La Rocca, A. Gastaldelli*  
 CNR, Consiglio Nazionale delle Ricerche, Institute of Clinical Physiology, IFC, Pisa, Italy
- ThP-38 Duloxetine: degradation processes, transformation products elucidation by mass spectrometry and in silico analysis**  
*R. Osawa, M. Conceição, O. Monteiro, M. H. Florêncio*  
 Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal
- ThP-39 Multi-mode ionization techniques for efficient MS/MS analysis of pesticides**  
*H. Gamble, C. Jolliffe, A. Dalmia*  
 Perkin Elmer, R&D, Woodbridge, Canada
- ThP-40 Multiclass analysis of antibiotics in sediments by LC-Q-Orbitrap HRMS. Application to the Nera River**  
*D. Giusepponi, F. Scoppetta, M. Sargenti, G. Saluti, S. Moretti, R. Rossi, M. Capuccella, R. Galarini*  
 Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Centre for Development and Validation of Methods, Perugia, Italy
- ThP-41 Determination of 16 polycyclic aromatic hydrocarbons by core-shell molecularly imprinted polymers prepared by reversible addition fragmentation chain transfer polymerization with APGC-MS/MS**  
*A. Golbabanezhad-Azizi, F. Shahhoseini, C. Bottaro*  
 Memorial University of Newfoundland, Department of Chemistry, St. John's, Canada
- ThP-42 Fate and behavior of oil sands naphthenic acids in a pilot-scale treatment wetland as characterized by negative-ion electrospray ionization Orbitrap mass spectrometry**  
*C. Ajaero, K. Peru, M. Simair, V. Friesen, S. Hughes, D. McMartin, G. O'sullivan, J. Headley*  
 Watershed Hydrology & Ecology Research Division, Water Science & Technology Directorate, Environment & Climate Change Canada, Saskatoon, Canada
- ThP-43 Photocatalytic activity of titanium dioxide films under visible light evaluated by ESI(-)-MS**  
*D. Holanda Pereira de Souza, T. Carita Correra, V. de Moraes Zamarion*  
 Universidade de São Paulo, Institute of Chemistry, São Paulo, Brazil
- ThP-44 Study on the degradation mechanism of atrazine in sewage by UHPLC-MS/MS**  
*J. Li, J. Yan, B. Lai, X. Lia, K. Kahen, J. Wu*  
 PerkinElmer, Woodbridge, Canada
- ThP-45 Comparison of organic mixtures from particulate matters collected in Korea and China by using GCxGC/High resolution mass spectrometry**  
*M. Park, G. Bang, K. Jang, K. Park, S. Kim, Y. Hwan Kim*  
 Korea Basic Science Institute, Biomedical Omics Group, Cheongju, Republic of Korea
- ThP-46 Biocide spray product exposure: measured gas, particle and surface concentrations compared with spray model predictions**  
*V. Kofoed-Sørensen, A. Nørgaard, M. Frederiksen, P. Wolkoff, P. A. Clausen*  
 National Research Center for the Working Environment, Chemical working environment, Copenhagen, Denmark
- ThP-47 Occurrence and human exposure to brominated and organophosphate flame retardants from Finnish household dust**  
*E. Kumar, P. Rantakokko, J. Braber, J. Koponen, T. Huang, H. Kiviranta*  
 National Institute for Health and Welfare (THL), Health Security, Kuopio, Finland
- ThP-48 Novel drinking water disinfection by-products**  
*A. Lebedev, D. Kosyakov, N. Ul'yanovskii, M. Popov, T. Latkin*  
 Lomonosov Moscow State University, Chemistry Department, Moscow, Russian Federation
- ThP-49 A comparative study of ultra-trace-level uranium by thermal ionization mass spectrometry with continuous heating: static and peak-jumping modes**  
*C. G. Lee, J. Park, S. H. Lim, S. H. Han*  
 Korea Atomic Energy Research Institute, Nuclear Chemistry Research Division, Daejeon, Republic of Korea

- ThP-50**      **Analysis of natural radionuclides concentrations in monazite using acid digestion by quadrupole ICP-MS**  
*J. Lee, S. Yi*  
 Korea Institute of Nuclear Safety, Department of Natural Radiation Safety, Daejeon, Republic of Korea
- ThP-51**      **Determination of global DNA methylation and oxidation of DNA and Lipid biomarkers in metal oxide nanomaterial-handling workers by liquid chromatography-tandem mass spectrometry**  
*H. Lee, S. Liou*  
 Fu Jen Catholic University, Chemistry, New Taipei City, Taiwan, Province Of China
- ThP-52**      **Mass spectrometry identification of halogenated peptides in treated drinking water**  
*P. Jiang, G. Huang, L. Blackstock, X.-Fang Li*  
 University of Alberta, Faculty of Medicine and Dentistry, Edmonton, Canada
- ThP-53**      **Iodine distribution and bioavailability in soil from Fenyang, Shanxi province, China**  
*W. Liu, J. Hu*  
 Chinese Academy of Geological Sciences, National Research Center for Geoanalysis, Beijing, China
- ThP-54**      **Determination of Ag nanoparticles in Vltava river (Prague, Czech Republic) by single particle ICP-MS**  
*M. Loula, A. Kana, O. Mestek*  
 University of Chemistry and Technology Prague, Department of Analytical Chemistry, Prague, Czech Republic
- ThP-55**      **Antibiotics in waters along the Grand Canal, China**  
*G. Lu, H. Piao, S. Chen, X. Jiao, Y. Yang*  
 Chinese Academy of Geological Sciences, National Research center for Geoanalysis, Beijing, China
- ThP-56**      **GC×GC-MS in environmental analysis: from efficient separation to introduction of retention index data base**  
*D. Mazur, I. Zenkevich, V. Artaev, O. Polyakova, A. Lebedev*  
 Lomonosov Moscow State University, Organic Chemistry Department; Lomonosov Northern (Arctic) Federal University, Core Facility Center "Arktika", Moscow, Arkhangelsk, Russian Federation
- ThP-57**      **The analysis of environmental samples using high resolution mass spectrometry to identify novel PFAS compounds**  
*D. Mcmillan, S. Roberts, C. Butt, C. Borton*  
 Sciex, Business Development, Warrington, United Kingdom
- ThP-58**      **Characterization of organic compounds in aquatic sediment by ion profiles obtained using GC-MS system**  
*Z. Moldovan*  
 National Institute of Research and Development for Isotopic and Molecular Technology, Mass Spectrometry, Cluj-Napoca, Romania
- ThP-59**      **Study of pharmaceuticals removal rates in wastewater treatment plant using GC-MS analytical technique**  
*Z. Moldovan, O. Marincas, I. Feher*  
 National Institute of Research and Development for Isotopic and Molecular Technology, Mass Spectrometry, Cluj-Napoca, Romania
- ThP-60**      **Citalopram photodegradation: Identification of transformation products by mass spectrometry**  
*R. Osawa, M. Conceição, O. Monteiro, M. H. Florêncio*  
 Universidade de Lisboa, Faculdade de Ciências, Lisboa, Portugal
- ThP-61**      **A novel analytical integrated approach based on mass spectrometry for the evaluation of imidacloprid exposure during CNS development**  
*A. Passoni, R. Bagnati, M. De Paola, E. Davoli, A. Mariani*  
 IRCCS - Istituto di Ricerche Farmacologiche Mario Negri, Environmental Health Sciences Department, Milan, Italy
- ThP-62**      **Non-targeted approach for the study of labile dissolved organic matter**  
*C. Patriarca, P. J.R. Sjöberg, J. Bergquist, L. J. Tranvik, J. A. Hawkes*  
 Uppsala University, Department of Chemistry, Uppsala, Sweden

- ThP-63 Screening of pharmaceutical and their metabolites in fish by HRMS using data-base support**  
*J. M. Peña-Herrera, N. Montemurro, S. Pérez, D. Barceló*  
 IDAEA-CSIC, Environmental Chemistry, Barcelona, Spain
- ThP-64 Suspected screening of natural toxins in surface water by liquid chromatography high resolution mass spectrometry**  
*M. Picardo, D. Filatova, O. Nuñez, M. Farré*  
 Spanish Council for Scientific Research (CSIC), University of Barcelona, Analytical Chemistry, Barcelona, Spain
- ThP-65 Airbone measurement of organic gases and particles in the atmosphere with PTR-MS**  
*F. Piel, T. Mikoviny, M. Müller, S. A. Schiller, S. Feil, G. Hanel, P. Mutschlechner, A. Jordan, L. Märk, P. Sulzer, A. Wisthaler*  
 Ionicon Analytik GmbH, University of Innsbruck, Institute for Ion Physics and Applied Physics, Innsbruck, Austria
- ThP-66 Dissipation studies of dimethachlor and metabolites in soil and water by UHPLC-Orbitrap-MS**  
*R. López Ruiz, R. Romero González, J. L. Martínez Vidal, A. Garrido Frenich*  
 University of Almería, Dept. Chemistry and Physics, Almería, Spain
- ThP-67 Paving the way for the analysis of trace compounds in metallurgical gases by proton-transfer-reaction time-of-flight mass spectrometry. Importance of background**  
*J. I. Salazar Gómez, C. Klucken, M. Sojka, H. Ruland, K. Kähler, L. Masliuk, T. Lunkenbein, R. Schlögl*  
 Max-Planck Institute for Chemical Energy Conversion, Department of Heterogeneous Reactions, Mülheim a.d. Ruhr, Germany
- ThP-68 Novel application of molecularly imprinted polymers with gas chromatography-atmospheric pressure ionization-mass spectrometry for high through-put determination of 16 PAHs**  
*F. Shahhoseini, A. Golbabanezhad-Azizi, S. Egli, C. Bottaro*  
 Memorial university of Newfoundland, Department of Chemistry, St. John's, Canada
- ThP-69 New analysis method for organotin compounds by Tandem-LC/MS without the derivatization step**  
*J. E. An, Y. C. Song, Y. S. Kim, K. C. Yi*  
 Korea Apparel Testing and Research Institute, Environment analysis center, Anyang city, Republic of Korea
- ThP-70 Continuous-introduction aerosol-to-liquid sampler and its coupled use with ICP-MS for on-line sensitive analysis of atmospheric aerosol**  
*Y. Su, Z. Li, W. Wang, S. Fang*  
 Northwest Institute of Nuclear Technology, Xi'an, China
- ThP-71 Acetone degradation in a plasma reactor studied in real-time by PTR-MS**  
*S. Thomas, M. Heninger, N. Blin-Simian, L. Magne, H. Mestdagh, S. Pasquier, E. Louarn*  
 Univ. Paris Sud, CNRS, Univ. Paris Saclay, Laboratoire de Chimie Physique, Orsay, France
- ThP-72 Uptake of dioctyl phthalate by *Populus alba* Villafranca**  
*F. Vannucchi, E. C. Pierattini, A. Raffaelli, A. Francini, L. Sebastiani*  
 Biolabs, Institute of Life Science, Scuola Superiore Sant'Anna, Pisa, Italy
- ThP-73 Identification of degradation products of selected pharmaceuticals in soils by high resolution mass spectrometry**  
*A. Vojs Stanova, K. Grabicova, A. Borik, R. Kodesova, A. Klement, R. Grabic*  
 University of South Bohemia in České Budějovice, Faculty of Fisheries and Protection of Waters, South Bohemian Research Center of Aquaculture and Biodiversity of Hydrocenoses, Vodňany, Czech Republic
- ThP-74 The study of sampling pipeline effect for gases partial pressure measure with mass spectrometer**  
*R. Yan*  
 Beijing Institute of Spacecraft Environment Engineering, CAST, Beijing, China
- ThP-75 Direct analysis of 17 perfluorinated compounds in water at low parts-per-trillion levels by LC-MS/MS workflow**  
*J. Ye Sha, J. Wu, F. Qing, F. Kero, L. Piatti, S. Edler, D. Mattern, M. Gori*  
 Perkin Elmer, Woodbridge, Canada

- ThP-76**      **Molecular composition of dissolved organic matter in the TALDICE ice core**  
R. Zangrando, V. Zanella, O. Karroca, E. Barbaro, N. M. Kehrwald, D. Battistel, A. Gambaro, C. Barbante  
 Consiglio Nazionale delle Ricerche, Institute for the Dynamics of Environmental Processes, Mestre-Venezia, Italy
- ThP-77**      **Investigations on the adsorption of REEs by GO with different sizes: mechanism and application**  
W. Zhao  
 Chinese Academy of Geological Sciences, National Research Center for Geoanalysis, Beijing, China
- ThP-78**      **HILIC-MS (non-)target screening, monitoring and toxicological evaluation of highly polar compounds in drinking water and sources**  
A. Kolkman, R. Sjerps, P. Kooij, K. Baken, P. De Voogt  
 KWR Watercycle Research Institute, Laboratory for Materials Research and Chemical Analysis, Nieuwegein, Netherlands
- ThP-79**      **Direct analysis of phenolic compounds in cork wastewater by HPLC-QToF**  
C. F. J. Yuste, C. B. Godoy  
 Cicytex, ICMC, Mérida, Spain

### **ThPS-S05 - Safe & Valuable Food**

- ThP-80**      **A new analytical method for the quantification of three lignans in espresso coffee by using HPLC-MS/MS triple quadrupole**  
S. Angeloni, G. Caprioli, G. Khamitova, L. Navarini, G. Sagratini, S. Vittori  
 University of Camerino, School of Pharmacy, Camerino, Italy
- ThP-81**      **Catabolic markers 24,25-dihydroxyvitamin D2/D3 in bovine and porcine sera show inter-species differences between vitamin D2 and vitamin D3 metabolism**  
K. G. Dowling, G. L. J. Hull, A. Hayes, S. K. Duffy, A. K. Kelly, J. V. O'Doherty, K. D. Cashman  
 University College Cork, Cork Centre for Vitamin D and Nutrition Research, School of Food and Nutritional Sciences, Cork, Ireland
- ThP-82**      **Evaluation of oxidative stress markers in human biological matrices by means of UHPLC-MS/MS**  
F. Fantì, F. Vincenti, N. Bernabò, M. Serafini, D. Compagnone, M. Sergi  
 University of Teramo, Faculty of Bioscience and Technology for Food, Agriculture and Environment, Teramo, Italy
- ThP-83**      **Comprehensive characterization of Minimas, a natural complex food supplement, by different mass spectrometry techniques**  
E. Flamini, G. Fodaroni, S. Tamimi, S. Bedont, D. Decarli, M. Burico, A. Gaetano, L. Mattoli, P. Traldi  
 Aboca Spa Società Agricola, Area Ricerca Fitochimica, Sansepolcro, Italy
- ThP-84**      **The synergism of MALDI LIFT-ToF/ToF MS and ESI-Q-ToF MS instruments to discover new isoforms of allergens from hazelnut oleosin extract**  
 S. Nebbia, C. Lamberti, M. Manfredi, E. Marengo, L. Cavallarin, M. G. Giuffrida  
 CNR, ISPA, Colletterto Giacosa, Italy
- ThP-85**      **Determination of pyrrolizidine alkaloids in plant material using on-line SPE coupled to UHPLC-MS/MS**  
A. Grüning, J. Sander, S. Vedder  
 Shimadzu Europa, CIPS, Duisburg, Germany
- ThP-86**      **Free fatty acids and hexanal as shelf life markers in cheese: evaluation of food packaging efficiency through a quantitative HS-SPME-GC-MS method**  
A. F. Kamgang Nzekoue, E. Vittori, S. Vittori, G. Caprioli, G. Sagratini  
 University of Camerino, Camerino, Italy
- ThP-87**      **Bioactive compounds of brazilian green coffee beans collected in different levels of maturation by ESI-LTQ-ORBITRAP**  
M. Lemos, C. Perez, D. Ifa, R. Scherer  
 Universidade Vila Velha, Natural Products, Vila Velha, Brazil

- ThP-88 Development of a LC-MS/MS method for the detection of species-specific muscle peptides in PAPs**  
*D. Marchis, M. Leporati, A. Altomare, G. Aldini, C. Casalone*  
 Istituto Zooprofilattico Sperimentale del Piemonte, Liguria e Valle d'Aosta, S.S. Igiene dei Mangimi, Torino, Italy
- ThP-89 Metabolic survey of Italian vegetables: FTICR-MS and NMR-based untargeted analyses**  
*A. Maccelli, A. P. Sobolev, D. Capitani, B. Chiavarino, S. Fornarini, L. Mannina, M. Elisa Crestoni*  
 Sapienza Università di Roma, Dipartimento di Chimica e Tecnologie del Farmaco, Roma, Italy
- ThP-90 GC-MS monitoring of volatiles in grappa during aging in two different wood barrels**  
*M. De Rosso, C. M. Mayr, R. Castagner, R. Sonogo, R. Flamini*  
 Council for Agricultural Research and Economics - Research Center for Viticulture & Enology CREA, Conegliano, Italy
- ThP-91 Sensitive and specific allergen screening analysis using LC-MS/MS**  
*A. Sage, J. Stahl-Zeng, C. Borton, L. New*  
 Sciex, Market Development, Warrington, United Kingdom
- ThP-92 LC-MS/MS: a useful tool to investigate marine lipophilic toxins in mussels**  
*M. Siracusa, S. Bacchiocchi, S. Evangelista, A. Piersanti*  
 Centro Referenza Nazionale controllo microbiologico e chimico molluschi bivalvi, Istituto Zooprofilattico Sperimentale Umbria e Marche "Togo Rosati", Perugia, Italy
- ThP-93 Advances in mass spectrometry for food safety and authenticity**  
*D. Tsjpi, H. Botitsi*  
 General Chemical State Laboratory, Food Safety & Quality Laboratories, Athens, Greece
- ThP-94 Development of infant formula certified reference material for nutrient element analysis**  
*K. Lee, J. Ki Suh, S. W. Heo, S. H. Kim, Y. Lim, M. S. Han, M. C. Lim, H. S. Min, E. Hwang, Y. Yim*  
 KRISS, Center for Analytical Chemistry, Daejeon, Republic of Korea
- ThP-95 Analysis of penta-O-galloyl- $\beta$ -D-glucose in functional foods by LC-MS/MS**  
*S. Yong-Woon*  
 Ministry of Food and Drug Safety, Nutrition and Functional Research Team, Cheongju-si, Republic of Korea
- ThP-96 Lipid fingerprint to determine *Fusarium* contamination in melon**  
*D. Zampieri, R. Dantas, K. R. Belaz, M. N. Eberlin, A. H. Oster, E. D. O. Silva, G. J. Zocolo*  
 Federal University of Ceara, Organic and Inorganic Department, Fortaleza, Brazil
- ThP-97 Investigation of the gliadin fraction composition in old and modern wheat genotypes**  
*V. Cunsolo, M. A. De Santis, A. Di Francesco, R. Saletti, M. M. Giuliani, Z. Flagella, S. Foti*  
 University of Catania, Department of Chemical Sciences, Catania, Italy
- ThP-98 Non-targeted characterization of the degradation products of soybean oil after frying process by HS-SPME-GC-MS and LLE-LC-HRMS**  
*M. Lee, C. Chen, Y. Tsai*  
 National Chung Hsing University, Chemistry, Taichung, Taiwan, Province Of China
- ThP-99 Metabolites from cafestol - a coffee diterpene- by Zebrafish tank model and LC-MS/MS**  
*C. M. Rezende, C. V. Andriolo, H. M. G. Pereira, V. F. Sardela, F. J. M. Novaes*  
 Federal University of Rio De Janeiro, Chemistry Institute, Rio De Janeiro, Brazil

### **ThPS-S06 – Lipidomics**

- ThP-100 Novel skin lipid biomarkers associated with atopic dermatitis**  
*E. Berdyshev, E. Goleva, I. Bronova, J. Jung, M. A Seibold, D. Ym Leung*  
 National Jewish Health, Department of Medicine, Denver, USA
- ThP-101 Quantum chemical mass spectrometry as a tool for the prediction of mass spectra and the identification of fragmentation pathways - Peptides and lipids**  
*F. Blockhuys, J. Cautereels*  
 University of Antwerp, Department of Chemistry, Antwerp, Belgium

- ThP-102** **A new UHPLC/MS-QToF method to evaluate effects of environmental metabolic disruptors on hepatic lipidomic profile**  
*F. Carli, M. Gaggini, V. Della Latta, S. Tait, F. Maranghi, R. Tassinari, C. La Rocca, A. Gastaldelli*  
 CNR, Institute of Clinical Physiology, Pisa, Italy
- ThP-103** **A quantum chemical tool for the identification of fragmentation pathways: additional insight into lipid-specific fragmentation mechanisms**  
*J. Cautereels, F. Blockhuys*  
 University of Antwerp, Department of Chemistry, Antwerp, Belgium
- ThP-104** **Robust and sensitive LC-MS/MS based plasma lipid profiling on a Thermo Scientific™ Q Exactive™ HF-X mass spectrometer**  
*T. N. Array, E. Sokol, A. Criscuolo, C. Dauly, A. Harder*  
 Thermo Fisher Scientific, CMD, Villebon sur Yvette, France
- ThP-105** **Verified HILIC LC-MS/MS assay for high-throughput targeted lipidomics analysis**  
*C. Papan, K. K. S. Gorti, L. Fu, B. Ubhi, M. J Pearson, L. Xiong, P. Baker, J. Dojahn*  
 Sciex, Darmstadt, Germany
- ThP-106** **Structure elucidation of Gram-negative microbial glycolipids by energy-resolved tandem mass spectrometry**  
*A. Dornyei, V. Sandor, A. Kilar, N. Eros, B. Kocsis, F. Kilar*  
 University of Pecs, Department of Analytical and Environmental Chemistry and Szentágothai Research Center, Pecs, Hungary
- ThP-107** **Development of a comprehensive panel of eicosanoids and related fatty acid metabolites for high-sensitivity and quantitative LC-MS/MS analysis**  
*Y. Fujito, M. Yamada, H. Lin, S. Fujita*  
 Shimadzu Corporation, Global Application Development Center, Kyoto, Japan
- ThP-108** **Rapid targeted LC-MS/MS assay for ESKAPE pathogen identification direct from biological fluids**  
*D. Goodlett, T. Liang, B. Oyler, C. Chandler, S. Hwan Yoon, R. Ernst*  
 UMB, Pharmacy, Baltimore, USA
- ThP-109** **Biomarker research and short time chromatography: a utopia?**  
*L. Hahnefeld, G. Geisslinger, N. Ferreirós*  
 Goethe University Frankfurt, Institute of Clinical Pharmacology, Frankfurt, Germany
- ThP-110** **Investigation into the bleaching of vegetable oils using high resolution mass spectrometry**  
*A. Hambly, J. Van Duijneveldt, P. Gates*  
 University of Bristol, School of Chemistry, Cantock's Cl, Bristol, United Kingdom
- ThP-111** **Analysis of a complex lipid profile in human sebum by using GCxGC-HRToFMS**  
*M. Hashimoto, K. Okuda, A. J. Dane, R. B. Cody, B. van der Meer*  
 JEOL(EUROPE)SAS, European Application Group, Croissy-sur-Seine, France
- ThP-112** **Applicability of MALDI-Orbitrap-MS for the early diagnosis of renal cell carcinoma based on the lipidomic analysis of blood and urine samples**  
*R. Jirásko, D. Wolrab, I. Brabcová, M. Holcapek, D. Vrána, V. Študent, B. Melichar*  
 University of Pardubice, Department of Analytical Chemistry, Pardubice, Czech Republic
- ThP-113** **Changes of specific sphingomyelins depending on the severity of nonalcoholic fatty liver disease**  
*Y. Jung, J. Seo, G. Hwang*  
 KBSI, Seodaemun-gu, Seoul, Republic of Korea
- ThP-114** **A comprehensive method for total lipid analysis in biological matrices by hydrophilic interaction liquid chromatography electrospray ionization mass spectrometry HILIC/ESI-MS**  
*S. Houry, S. Cabaret, E. A. Y. Masson, O. Berdeaux*  
 UMR CSGA - INRA - CNRS, University of Bourgogne Franche-Comté, Dijon, France
- ThP-115** **Graphical identification of lipids using three-dimensional Kendrick mass plots**  
*A. Korf, C. Vosse, H. Hayen*  
 University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany
- ThP-116** **Analysis of polyglycerophospholipids using isotope-labeled methylation by nUPLC-ESI-MS/MS**  
*J. Lee, M. Moon*  
 Yonsei University, Chemistry, Seoul, Republic of Korea

- ThP-117 Plasma lipidomic profiling of five different types of cancer by nUPLC-ESI-MS/MS**  
*G. Lee, J. Lee, M. Moon*  
 Yonsei Univ., Chemistry, Seoul, Republic of Korea
- ThP-118 MALDI-ToF/MS analyses determined urinary phospholipids as a potential biomarker for prostate cancer**  
*X. Li, K. Nakayama, T. Goto, S. Akamatsu, K. Shimizu, O. Ogawa, T. Inoue*  
 Kyoto University, Department of Urology, Kyoto, Japan
- ThP-119 Investigation of one novel oxidized 1-palmitoyl-2-arachidonoyl-sn-glycero-3-phosphocholine molecule on human aortic endothelial cells by LC-MS/MS**  
*Y. Chen, H. Tsou, Y. Shieh, M. Liu*  
 National Changhua University of Education, Department of Chemistry, Changhua, Taiwan
- ThP-120 A translational pilot study of global lipid profile as risk marker in coronary plaque: mass spectrometry approach on asymptomatic patients**  
*M. U. B. Paiva, D. V. N. Paiva, L. J. S. R. Alves, H. L. Machado, H. J. B. De Souza, F. N. dos Santos, M. N. Eberlin, R. M. De Oliveira, M. M. Martins, F. A. Atik, A. M. A. Martins*  
 UnB / UniCeub, Medicine / Surgery, Brasilia, Brazil
- ThP-121 Lipid profiling of non-steroidal anti-inflammatory drugs (NSAIDs) on prostate cancer cell lines with ToF-SIMS and DESI-MS**  
*D. J. McDougall, E. Jones, C. Hart, M. Brown, A. McMahon, N. Lockyer*  
 University of Manchester, Department of Chemistry, Manchester, United Kingdom
- ThP-122 Defining structural differences in cardiolipins from an actinomycete marine sponge symbiont and *S. aureus***  
*B. Oylar, C. Chandler, F. Zhang, R. Ernst, R. Hill, D. Goodlett*  
 University of Maryland, Baltimore, School of Medicine, Baltimore, USA
- ThP-123 Untargeted lipidomics for the assessment of arsenic exposure in rice (*Oryza sativa japonica*)**  
*M. C. Pérez Cova, F. R. Tauler, S. J. Jaumot*  
 CSIC-IDAEA, Química Ambiental. Quimiometría, Barcelona, Spain
- ThP-124 High-resolution multiple reaction monitoring method development for quantification of steroidal hormones in plasma**  
*A. P. F. Peti, G. A. Locachevic, M. K. B. Prado, L. A. B. De Moraes, L. H. Faccioli*  
 Universidade de São Paulo - USP, DACTB, Ribeirão Preto, Brazil
- ThP-125 Micro-UPLC-MS high-throughput screening assay for sphingolipids pathway analysis**  
*K. Randall, H. Klodnitsky, D. Tietz, C. Phaneuf, M. Olszewski, E. Makino, K. Murphy, A. Belenky*  
 Sanofi, Pre-development sciences, Waltham, USA
- ThP-126 Ceramidome plasticity through iso-energetic precursor and neutral loss discovery scans**  
*F. M. Rubino, M. Dei Cas, P. Signorelli, R. C. Paroni, R. Ghidoni, J. Rizzo*  
 Università degli Studi di Milano, Dipartimento di Scienze della Salute, Milano, Italy
- ThP-127 Serum lipidomic changes in Zika and Dengue virus infection reveals potential targets for assertive clinical diagnosis**  
*F. Santos, A. Martins, K. Magalhães, M. Eberlin*  
 University of Campinas, Analytical Chemistry, Campinas, Brazil
- ThP-128 Fishing for lactones: method development for selective identification of lactone-containing lipids**  
*E. Slutsky Smith, S. Khatib, A. Szuchman-Sapir*  
 Migal--Galilee Research Institute, Laboratory of Vascular Signaling Research, Kiryat Shmona, Israel
- ThP-129 Challenges of lipid isomers and isobars in mass spectrometry-based biomarker research**  
*U. Sommer, H. Pham-Tuan, T. Koal*  
 Biocrates Life Sciences AG, R&D, Innsbruck, Austria
- ThP-130 Applying Trapped Ion Mobility Separation (TIMS) in combination with Parallel Accumulation Serial Fragmentation (PASEF) for analysis of lipidomics samples**  
*M. Szesny, S. Götz, S. Meyer, U. Schweiger-Hufnagel, A. Barsch, N. S. Meitei*  
 Bruker Daltonik GmbH, Metabolomics, Bremen, Germany
- ThP-131 How to ensure quality in the analysis of endogenous compounds in biological samples**  
*D. Thomas, S. C. Fleck, R. Gurke, G. Geisslinger, N. Ferreirós*  
 Goethe University, Institute of Clinical Pharmacology, Frankfurt, Germany



- ThP-132 Study of acetogenins in a natural extract using SFC-HRMS/MS and post-column metal cationisation**  
*L. Laboureur, P. Champy, D. Touboul*  
CNRS, ICSN, Gif-sur-Yvette, France
- ThP-133 Improved lipid annotation utilizing positive and negative ion MS<sup>2</sup> / MS<sup>3</sup> HCD and CID spectra**  
*D. Peake, R. Kiyonami, D. Gachotte, Y. Yokoi, S. Webb, A. Huhmer*  
Thermo Fisher Scientific, San Jose, USA
- ThP-134 A Simple and Rapid Extraction of Lipids in Plasma Using Spin Column with Superabsorbent Polymer Beads**  
*G. Bang, J. H. Choi, Y. J. H. Park, J. A. Kim, Y. H. Kim*  
Korea Basic Science Institute, Biomedical Omics Group, Cheong-ju, Republic of Korea
- ThP-135 Lipidomic approach for algal oil characterization by FTICR mass spectrometry**  
*S. Chiaberge, R. Miglio, D. Deriu, S. Perucchini, A. Siviero*  
eni s.p.a., Renewable Energy & Environmental R&D, Novara, Italy
- ThP-136 Dual mass spectrometry as a tool to improve annotation and quantification in targeted plasma lipidomics**  
*L. Gao, A. Cazenave-Gassiot, B. Burla, M. Wenk, F. Torta*  
National University of Singapore, Life Sciences Institute, Singapore, Singapore
- ThP-137 New peak alignment software: MetaboAlign improving issues of LC-MS/MS lipidomics enables highthroughput data analysis for thousands of lipids in biological materials**  
*A. Hayashi, T. Matsuzaka, H. Shimano*  
ONO Pharmaceutical Co.,LTD., Minase Research Institute, Mishima-gun, Japan
- ThP-138 Structural analysis of lipids from cells of Bacteria of the Good, the Bad and of the Ugly**  
*F. Hsu, C. Frankfater, W. Henson, A. Haas, J. Turk, G. Purdy, R. Tatituri*  
Washington University School of Medicine, St. Louis, USA
- ThP-139 Joint application of ESI and MALDI lipidomic profiles for classification of brain tumors**  
*D. Ivanov, A. Sorokin, E. Zhvansky, V. Shurkhay, S. Pekov, I. Popov, E. Nikolaev*  
Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russian Federation
- ThP-140 Development and application of an enhanced lipidomic profiling method using LC-MS**  
*M. Jaber, D. Barrett, D. Kim*  
University of Nottingham, Advanced Materials and Healthcare Technologies, Nottingham, United Kingdom
- ThP-141 UPLC-QqQ/MS-based lipidomics analysis of high glucose induced HepG2 cells treated with herbal medicine extracts**  
*J. Lee, D. Choi, B. Choi, Y. Lee, G. Kim, D. Lee*  
National Institute of Horticultural and Herbal Science, Department of Herbal Crop Research, Eumseong, Republic of Korea
- ThP-142 Construction of novel lipidomics platform combined of targeted and non-targeted analysis**  
*Y. Yokoi, H. Kuwabara, T. Hoshino, A. Hayashi*  
Mitsui Knowledge Industry Co., Ltd., Bioscience Department, Tokyo, Japan

### **ThPS-S07 - Developments and Applications In Ion Mobility MS**

- ThP-143 A high-resolution ion mobility spectrometer coupled to a time-of-flight mass spectrometer**  
*M. Allers, L. Timoumi, A. T. Kirk, F. Schlottmann, S. Zimmermann*  
Leibniz Universität Hannover, Institute of Electrical Engineering and Measurement Technology, Department of Sensors and Measurement Technology, Hannover, Germany
- ThP-144 Application of PASEF MS/MS scans to monoclonal antibody peptide mapping**  
*A. Alving, S. Pengelley, G. Trementin, D. Sukau*  
Bruker Daltonics, Biopharma, Billerica, USA
- ThP-145 A clip on ion mobility device. Enabling gas phase ions separation and collision cross section measurements to any mass spectrometers**  
*B. Bellina, J. Commandeur, P. Barran*  
University of Manchester, Manchester Institute of Biotechnology, Manchester, United Kingdom

- ThP-146 Exploring the chemical coverage and structural assignment of natural products by ion mobility spectrometry combined with ultra-performance liquid chromatography/mass spectrometry**  
*F. Carnevale Neto, J. M. Egan, L. V. Costa-Lotufo, N. P. Lopes, R. G. Linington*  
Faculdade de Ciências Farmacêuticas da Universidade de São Paulo, Ribeirão Preto, São Paulo, Brazil
- ThP-147 Influence of protomers on dissociation of sequence-defined oligo(alkoxyamine amide)s**  
*C. Chendo, S. Poyer, D. Siri, J. Lutz, L. Charles*  
Fédération des Sciences Chimiques, Aix Marseille Université, Marseille, France
- ThP-148 Trapped ion mobility spectrometry as novel separation technique for the investigation on isomer formation during the simulation of Phase I Metabolism by means of Electrochemistry/Mass Spectrometry**  
*J. Fangmeyer, S. Gereon Scheeren, R. Schmid, U. Karst*  
University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany
- ThP-149 Prion protein conformational landscape studied by mass spectrometry and ion mobility**  
*F. Halgand, G. Van der Rest, H. Rezaei*  
CNRS, Chemistry, Orsay, France
- ThP-150 Secondary structure of ionized peptoids by ion mobility mass spectrometry**  
*E. Halin, S. Hoyas, J. De Winter, V. Lemaur, J. Cornil, S. Laurent, P. Gerbaux*  
UMONS, Université de Mons, Mons, Belgium
- ThP-151 Collision cross section (CCS) as a complementary parameter to characterize human and veterinary drugs: creation of a database**  
*C. Tejada-Casado, M. Hernández-Mesa, F. Monteau, F. J. Lara, M. del Olmo-Iruela, A. M. García-Campaña, B. Le Bizec, G. Dervilly-Pinel*  
École nationale vétérinaire, agroalimentaire et de l'alimentation de Nantes-Atlantique (Oniris), Laboratoire d'Etudes des Résidus et Contaminants dans les Aliments (LABERCA), INRA UMR 1329, Nantes, France
- ThP-152 Collision cross section as a novel parameter for the characterization of steroids**  
*M. Hernández-Mesa, B. Le Bizec, F. Monteau, A. M. García-Campaña, G. Dervilly-Pinel*  
École nationale vétérinaire, agroalimentaire et de l'alimentation de Nantes-Atlantique (Oniris), Laboratoire d'Etudes des Résidus et Contaminants dans les Aliments (LABERCA), INRA UMR 1329, Nantes, France
- ThP-153 Application of CO<sub>2</sub> drift gas in travelling wave ion mobility mass spectrometry for the structural elucidation of environmentally relevant isobaric isomer compounds**  
*Y. Iinuma, E. Hayakawa, S. Inomata, K. Sato, H. Ren, S. Yue, P. Fu*  
Okinawa Institute of Science and Technology, Onna, Japan
- ThP-154 Profiles of arrival time distributions in different drift gases as a tool for identification of isomers**  
*L. Borovcová, J. Ondruchová, V. Havlíček, K. Lemr*  
Palacký University, Regional Centre of Advanced Technologies and Materials, Department of Analytical Chemistry, Faculty of Science, Olomouc, Czech Republic
- ThP-155 Analysing disease triggering amyloids: combining ESI-IMS and LILBID-MS**  
*T. Lieblein, R. Zangl, J. Martin, N. Morgner*  
Goethe-University, Institute for Physical and Theoretical Chemistry, Frankfurt/Main, Germany
- ThP-156 Differential Mobility Separation (DMS)-based separation of bile acid isomers**  
*D. Merkel, C. Papan, V. Kaefer, H. Bähre, J. Dojahn*  
SCIEX Germany, Application Support, Darmstadt, Germany
- ThP-157 Addition of collision cross sections to searchable libraries: a robust approach to enhance cumulative specificity in screening assays**  
*R. Mortishire-Smith, M. McCullagh, M. Herman, E. van Hoeck, S. Gosciny*  
Waters, Wilmslow, United Kingdom
- ThP-158 The use of CCS-enabled libraries for drug metabolism applications**  
*R. Mortishire-Smith, D. Veyel, B. Krawczyk, J. Vissers*  
Waters, Wilmslow, United Kingdom
- ThP-159 Separation of intact protein isoforms with differential mobility**  
*K. Pohj, C. Nortcliffe, F. Sanchez, J. Dojahn, A. Uppal, S. Heidelberg, J. Yves Leblanc*  
Sciex, Biologics, Darmstadt, Germany

- ThP-160 Ion guide with very strong axial transporting fields**  
*S. Poteshin, A. Burykina*  
 NRNU MEPhI, Molecular Physics, Moscow, Russian Federation
- ThP-161 Thermal denaturation of proteins by variable-temperature electrospray ionization paired with ion mobility spectrometry-mass spectrometry**  
*S. Raab, T. El-Baba, D. Woodall, D. Clemmer*  
 Indiana University, Department of Chemistry, Bloomington, USA
- ThP-162 Separation of Isomers with ultra-high-resolution ion mobility spectrometry**  
*C.-R. Raddatz, A. T. Kirk, S. Zimmermann*  
 Leibniz Universität Hannover, Institute of Electrical Engineering and Measurement Technology, Sensors and Measurement Technology, Hannover, Germany
- ThP-163 Deconvolution of direct infusion TIMS-MS analyses**  
*P. Sander, S. Meyer*  
 Bruker Daltonics, R&D, Bremen, Germany
- ThP-164 Ion mobility mass spectrometry for profiling and structural characterization of human hippocampus gangliosides**  
*M. Sarbu, Z. Vukelic, D. Clemmer, A. D. Zamfir*  
 National Institute for Research and Development in Electrochemistry and Condensed Matter, Department of Condensed Matter, Timisoara, Romania
- ThP-165 A computer code for optimization of Hadamard transform and Fourier transform ion mobility spectrometry experimental conditions**  
*A. Sarycheva, A. Adamov, S. Poteshin, A. Sysoev*  
 National Research Nuclear University MEPhI, National Research Nuclear University MEPhI, Molecular Physics Department, Moscow, Russian Federation
- ThP-166 FAIMS-MS-IR spectroscopy workflow: a multidimensional platform for the analysis of molecular isoforms**  
*B. Schindler, I. Compagnon, F. Lépine*  
 Institut Lumière Matière, Université de Lyon, Lyon, France
- ThP-167 Protomer separation, characterization and ion-molecule reactions using differential ion mobility**  
*P. Schorr, D. Volmer*  
 Humboldt University of Berlin, Institute of Chemistry, Berlin, Germany
- ThP-168 Protein analysis using ion mobility MS and in-source ion activation combined with ECD ion fragmentation**  
*R. Kurulugama, V. Voinov, K. Newton, C. Klein, N. Lopez, G. Stafford, J. Beckman, J. Fjeldsted*  
 Agilent Technologies, R&D, Santa Clara, CA, USA
- ThP-169 Analysis of insulin and insulin analogues from dried blood spots by means of LC-IM-HRMS**  
*A. Thomas, M. Thevis*  
 German Sport University Cologne, Biochemistry, Cologne, Germany
- ThP-170 5 Hour single shot human proteome analysis using LC-FAIMS-MS/MS**  
*A. Hebert, S. Prasad, M. Belford, D. Bailey, S. Abbatiello, R. Huguet, G. Mcalister, E. Wouters, J. Dunyach, M. Westphal, J. Coon*  
 University of Wisconsin-Madison, Biotechnology Center, Madison, USA
- ThP-171 Differentiation of Panax ginseng, Panax quinquefolius, and Ginseng products by using differential ion mobility spectrometry coupled with tandem mass spectrometry**  
*R. Wu, T. W. D. Chan*  
 The Chinese University of Hong Kong, Faculty of Science, Department of Chemistry, Hong Kong
- ThP-172 Ultra-high throughput screening for engineered synthetic biology libraries based on sample chips combined with DESI MS Imaging**  
*C. Yan, E. Garcia-Ruiz, M. Dunston, K. Hollywood, N. Swainston, A. Jervis, E. Jones, A. Lejeune-Dodge, E. Kempa, Y. Cai, E. Takano, N. Scrutton, S. Flitsch, P. Barran*  
 Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom
- ThP-173 Structural insights into potentially toxic conformations of  $\beta$ -Amyloid (1-42) oligomers**  
*R. Zangl, J. Martin, T. Lieblein, N. Morgner*  
 Goethe University, Institute of Physical and Theoretical Chemistry, Frankfurt, Germany

- ThP-174 **timsToF Pro and PASEF multiplying sequencing speed and sensitivity in mass spectrometry-based proteomics**  
*A. Brunner, F. Meier, S. Beck, H. Koch, M. Lubeck, N. Goedecke, M. Krause, N. Drechsler, J. Cox, O. Raether, M. Mann*  
 Max Planck Institute of Biochemistry, Department for Proteomics and Signal Transduction, Planegg, Germany
- ThP-175 **Cross section of selected extractable and leachable compounds: influence of mobile phase composition**  
*V. Hanot, R. Feliciano, P. Hu, C. Jones*  
 Baxter, Mass Spectrometry, Braine L'alleud, Belgium
- ThP-176 **Lipid and fatty acid isomer analysis using a travelling wave cyclic ion mobility separator**  
*M. Mccullagh, M. Palmer, G. Isaac, R. Mortishire-Smith, J. Langridge, J. Vissers*  
 Waters Corporation, Wilmslow, United Kingdom

### **ThPS-S08 - Petroleomics, Hydrocarbons and Biofuels**

- ThP-177 **Detailed look in SARA fractionation: saturates, not only saturated compounds!**  
*Z. Farmani, W. Schrader*  
 Max-Planck-Institut für Kohlenforschung, Mass Spectrometry dept., Mülheim a.d. Ruhr, Germany
- ThP-178 **Evaluation of degradation degree of lubricating oil by thermal desorption and pyrolysis combined with DART-MS (TDP/DART-MS)**  
*C. Takei, Y. Otake, K. Yoshizawa*  
 BioChromato, Inc., Application support, Fujisawa, Japan

### **ThPS-S09 - Materials & Nanomaterials**

- ThP-179 **Radicals generated by nanoparticles in contact with liquid water using spin trapping and mass spectrometry**  
*P. A. Clausen, V. Kofoed-Sørensen, A. W. Nørgaard, N. R. Jacobsen, K. A. Jensen*  
 National Research Centre for the Working Environment, New Technologies, Copenhagen Ø, Denmark
- ThP-180 **A novel nanocomposite coating based on sol-gel Titania/Hydroxyapatite for solid-phase microextraction coupled to GC-MS**  
*F. Rahmani, A. Es-Haghi, H. Mohammad-Reza Milani, A. Mollahosseini*  
 Razi Vaccine & Serum Research Institute, Department of Physico Chemistry, Karaj, Iran
- ThP-181 **Mass analysis of surface immobilizations of phenol-containing molecules through chemical modifications**  
*H. Hwang, I. Choi, Y. Kim, W. Yeo*  
 Konkuk University, Department of Bioscience and Biotechnology, Seoul, Republic of Korea
- ThP-182 **New binding properties of Pyridine[4]arene capsules studied by IM-MS and IRMPD**  
*A. Kiesilä, A. Kruve-Viil, C. Schalley, P. Barran, J. Moilanen, E. Kalenius*  
 University of Jyväskylä, Department of Chemistry, Jyväskylä, Finland
- ThP-183 **Mass spectrometric analysis of vicinal diol-containing flavonoid molecules via enrichment with boronic acid-functionalized particles**  
*E. Kim, J. Song, H. Mok, W. Yeo*  
 Konkuk University, Department of bioscience and biotechnology, Seoul, Republic of Korea
- ThP-184 **Spectral interferences affecting the nanoparticles determination using sp-ICP-MS**  
*M. Loula, A. Kana, O. Mestek*  
 University of Chemistry and Technology Prague, Department of Analytical Chemistry, Prague, Czech Republic
- ThP-185 **Influence of silica nanoparticles surface charge in MALDI-MS analysis of peptides**  
*S. Maghari, P. Ghezellou, A. Ghassempour*  
 Shahid Beheshti University, Medicinal Plants and Drugs Research Institute Department: Phytochemistry, Tehran, Iran

- ThP-186 **Using LDI-ToF MS for the characterization of covalently functionalized graphene**  
*M. B. Minameyer, D. Dasler, R. A. Schäfer, J. F. Hitzenberger, F. Hauke, T. Drewello, A. Hirsch*  
 Friedrich-Alexander University (FAU), Physical Chemistry I, Erlangen-Nürnberg, Germany
- ThP-187 **The measurement of the oxidation reaction of ferrocenes using LC-MS with ESI**  
*Y. Okada, M. Tsuchida*  
 Ritsumeikan University, Department of Applied Chemistry, Kusatsu, Japan
- ThP-188 **Mass spectrometry-based methods as a tool for monitoring the micro scale chemoenzymatic peptide syntheses on solid support**  
*H. Plóciennik, P. Stefanowicz*  
 University of Wrocław, Faculty of Chemistry, Wrocław, Poland
- ThP-189 **LC-MS characterization of dynamic combinatorial libraries of TASP molecules with novel scaffold**  
*G. Wolczanski, M. Modzel, P. Stefanowicz, M. Lisowski*  
 University of Wrocław, Faculty of Chemistry, Wrocław, Poland
- ThP-190 **Elemental analysis by Au-nanoparticles enhanced LA-ICP-MS**  
*F. Mastroiocco, L. C. Giannossa, A. Mangone*  
 Università di Bari, Department of Chemistry, Bari, Italy

### **ThPS-S10 - Novel food; Nanoparticles in Food and Beverage; Future Applications**

- ThP-191 **A new by-product enriched in phenolic compounds, evaluated by UHPLC-HRMS, from olive mill wastewater**  
*G. Avellone, V. Di Stefano, M. E. Novara, R. Pitonzo*  
 University of Palermo, STEBICEF, Palermo, Italy
- ThP-192 **Optimization of espresso coffee extraction with different particle size distribution and analysis through GC-MS and HPLC-VWD**  
*G. Khamitova, S. Angeloni, G. Caprioli, G. Sagratini, S. Vittori*  
 University of Camerino, Department of Chemistry and Pharmacy, Camerino, Italy
- ThP-193 **Studying of phenotypic and physiological influences of abiotic stressors (TiO<sub>2</sub> and excess irradiation) on tomato plants**  
*J. A. Ko*  
 Korea Institute of Toxicology, Future Environment Research Center, Jinju, Republic of Korea

### **ThPS-S11 - Informatics Tools and Data Analysis**

- ThP-194 **TAMI Software for the provision of elemental formula from your single quadrupole GC-MS or LC-MS data**  
*A. Amirav, A. Fialkov, T. Alon*  
 Tel Aviv University, School of Chemistry, Tel Aviv, Israel
- ThP-195 **The database for cross-platform mining biomarkers in the brain tumor tissue**  
*K. Bocharov, A. Sorokin, V. Shurkhay, I. Popov, E. Zhvansky, A. Potapov, E. Nikolaev*  
 Moscow Institute of Physics and Technology, Laboratory of Ionic and Molecular Physics, Dolgoprudny, Russian Federation
- ThP-196 **Combining GC-MS with machine learning for non-invasive cancer and disease diagnostics**  
*M. Cauchi*  
 University of Limerick, Mathematics & Statistics, Limerick, Ireland
- ThP-197 **One small step for Influenza – New mass-based bioinformatics and phylogenetics approach reveals insights into the evolution of the virus**  
*K. Downard, E. Akand*  
 University of New South Wales, Medicine, Sydney, Australia
- ThP-198 **Interoperable and scalable metabolomics data analysis with microservices**  
*P. Emami Khoonsari, S. Herman, M. Capuccini, M. Carone, A. Larsson, J. Burman, S. Neumann, C. Steinbeck, K. Kultima, O. Spjuth*  
 Uppsala University, Department of Medical Sciences, Clinical Chemistry, Uppsala, Sweden

- ThP-199 **Validation of analytical methods for the determination of residues in food: the stumbling block of data processing**  
R. Galarini  
Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Center for Method Development and Validation, Perugia, Italy
- ThP-200 **Interfacing third party software applications to mass spectrometry data systems**  
J. Goshawk, M. Mccullagh, R. Mortishire-Smith  
Waters, Scientific Operations, Wilmslow, United Kingdom
- ThP-201 **Metabolomic analysis of high density MS data**  
A. Luterova, T. Furst, M. Strnad, J. Gruz  
Palacky University, LGR, Olomouc, Czech Republic
- ThP-202 **A strategy to analyze the spectral datasets of unknown compounds using mass spectral similarity network**  
E. Hayakawa  
Okinawa Institute of Science and Technology, Okinawa, Japan
- ThP-203 **A low pulse current measurement circuit for current monitor system at mass spectrometer**  
Z. H. He  
Xi'an Jiaotong University, Xi'an, China
- ThP-204 **DART imaging for molecular accumulations on the mud surface**  
Y. Hongo, M. Sakakura, T. Shiota, K. Yoshiya  
Tokyo Institute of Technology, Earth-Life Science Institute, Tokyo, Japan
- ThP-205 **High resolution tandem mass spectrometric analysis of natural products**  
E. S. Ji, K. H. Kim, G. W. Park, J. S. Yoo, J. Y. Kim  
Korea Basic Science Institute, Biomedical Omics Group, Cheongju-si, Republic of Korea
- ThP-206 **Characterising the catabolism of peptides using ion mobility enabled high resolution mass spectrometry with Mass-MetaSite integration for data processing**  
J. Kirk, I. Zamora, A. Riera, T. Radchenko, A. Escola, R. Mortishire-Smith, Y. Alelyunas, M. Wrona  
Waters Corporation, Scientific Operations, Wilmslow, United Kingdom
- ThP-207 **Semi-quantitative LC/ESI/MS analysis using predictive models of ESI ionization efficiencies**  
J. Liigand, P. Liigand, M. Ojakivi, K. Kaupmees, A. Kruve  
University of Tartu, Institute of Chemistry, Tartu, Estonia
- ThP-208 **MSIML – An Open-Source program for the visualisation and pixel-by-pixel classification of mass spectrometry imaging datasets**  
L. Migas, E. Jones, R. Chapman, S. Pringle, P. Barran  
Manchester Institute of Biotechnology, University of Manchester, Manchester, United Kingdom
- ThP-209 **Bayesian approach to automatic mass spectrum peak identification in atom probe tomography**  
A. Mikhalychyev, N. Lappo, A. Ulyanenko  
Atomicus OOO, Minsk, Republic of Belarus
- ThP-210 **Demystifying match factors in library searching**  
A. Moorthy, A. Kearsley, W. Wallace  
National Institute of Standards and Technology, Mass Spectrometry Data Center, Gaithersburg, USA
- ThP-211 **Towards automated reporting and review of metabolic pathways for large multimodal MSI studies**  
T. Murta, A. Dexter, S. A. Thomas, R. T. Steven, C. J. Nikula, E. Elia, A. J. Taylor, T. Fu, A. Al-Afeef, B. Yan, R. Philip, K. N. Robinson, J. Bunch  
National Physical Laboratory, NiCE-MSI, London, United Kingdom
- ThP-212 **MODplus: towards searching for hundreds of post-transnational modifications in shotgun proteomics**  
S. Na, J. Kim, E. Paek  
Hanyang University, Dept. of Computer Science, Seoul, Republic of Korea

- ThP-213**    **Development and validation of semi-automatic MALDI-HDX sample preparation and data analysis tools**  
*S. Macintyre, I. Nebl*  
 CSIRO, Biomolecular Interactions, Parkville, Australia
- ThP-214**    **<http://ms.cheminfo.org>: the ultimate tool for mass spectra processing on-line**  
*D. Ortiz, L. Menin, L. Patiny*  
 EPFL, ISIC/SSMI, Lausanne, Switzerland
- ThP-215**    **Comparison of high- and low-resolution MS data for direct tissue profiling: moving from a laboratory into the clinical practice**  
*I. Popov, A. Sorokin, E. Zhvansky, V. Eliferov, A. Vorobyev, S. Pekov, V. Shurkhay, A. Potapov, E. Nikolaev*  
 Moscow Institute of Physics and Technology, Moscow Institute of Physics and Technology, Dolgoprudnyj, Russian Federation
- ThP-216**    **Integration of high mass accuracy GC-ToFMS results using EI and FI ionization methods**  
*Y. Ueda, A. Kubo, K. Nagatomo, M. Ubukata, T. Satoh*  
 JEOL Ltd., MS business unit, Tokyo, Japan
- ThP-217**    **Beyond the acquisition of FTMS spectra - Data interpretation and visualization of accurate data from complex samples**  
*A. Vetere, W. Schrader*  
 Max-Planck-Institut für Kohlenforschung, Department for Mass Spectrometry, Mülheim an der Ruhr, Germany
- ThP-218**    **Automatic identification of metal-bound biomolecules using SNAP-LC, imaging, and 2D-MS**  
*C. Wootton, M. Willetts, Y. Lam, M. van Agthoven, M. Barrow, P. Sadler, P. O'Connor*  
 University of Warwick, Chemistry, Coventry, United Kingdom
- ThP-219**    **Bacterial whole cell typing by mass spectra pattern matching with bootstrapping assessment**  
*Y. Yang, Y. Lin, Z. Chen, T. Gong, P. Yang, H. Girault, B. Liu, L. Qiao*  
 Fudan University, Department of Chemistry, Shanghai, China
- ThP-220**    **Decoy methods for false discovery rate estimation in high mass accuracy peptide spectral library searches**  
*Z. Zhang, M. Burke, Y. Mirokhin, D. Tchekhovskoi, S. Markey, S. Stein*  
 National Institute of Standards and Technology, Mass Spectrometry Data Center, Gaithersburg, USA
- ThP-221**    **TiSane denoising algorithm for large dense spectra**  
*L. Chiron, M. Delsuc*  
 Casc4de, Data analysis, Strasbourg, France
- ThP-222**    **Validation data processing by Adverse 2.0 free software package: assessment of the analytical requirements of GC-MS method for the determination of 16 PAHs in smoked fish**  
*A. Piersanti, T. Tavoloni, L. Scrucca, R. Galarini*  
 Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche "Togo Rosati", Center for Method Development and Validation, Perugia, Italy
- ThP-223**    **Unambiguous precursor mass assignment enables accurate and sensitive peptide identification of data-independent acquisition mass spectrometry data**  
*D. Mun, S. Lee*  
 Korea University, Seoul, Republic of Korea
- ThP-224**    **CycloBranch: an open tool for annotation of isotopic fine structures of natural products**  
*J. Novak, A. Skriba, J. Zapal, M. Kuzma, V. Havlicek*  
 Czech Academy of Sciences, Institute of Microbiology, Prague, Czech Republic

### **ThPS-S12 - Nutraceuticals Directions**

- ThP-225**    **Microwave-assisted extraction of olive leaves to obtain phenolic compounds with modulating activity of AMPK**  
*B. Martin-Garcia, S. Pimentel-Moral, A. M. Gomez-Caravaca, D. Arraez-Roman, A. Muñoz-de-la-peña, A. Segura-Carretero, A. Fernandez-Gutierrez*  
 University of Granada, Dept. of Analytical Chemistry, Granada, Spain

- ThP-226 **Development of isotope dilution-liquid chromatography/tandem mass spectrometry for the accurate determination of trans- and cis-vitamin K1 isomers in food**  
*B. Kim, H. Lee, H. Hee Lee*  
Korea Research Institute of Standards and Science, Center for Analytical Chemistry, Daejeon, Republic of Korea

### **ThPS-S13 - Cultural Heritage and Archaeology**

- ThP-227 **Mass spectrometry analysis of medieval archaeological jewels**  
*M. Cechová, L. Kucera, P. Bednár*  
RCPTM, Palacký University, Olomouc, Czech Republic
- ThP-228 **Determination of the wine and food traces from archaeological materials by GC/MS methods**  
*I. Farcas, Z. Moldovan, N. Pop*  
University of Agricultural Sciences and Veterinary Medicine, Doctoral School of Agricultural Engineering Sciences, Cluj-Napoca, Romania
- ThP-229 **Stable isotope composition of the modern and fossil freshwater gastropods: implications for paleoclimate reconstructions**  
*A. Macri, P. Iacumin, D. Usai, V. Linseele, S. Salvatori*  
University of Parma, Department of Chemistry, Life Sciences and Environmental Sustainability, Parma, Italy
- ThP-230 **Mass spectrometry studies of Theriac from "Spezieria di Santa Maria della Scala" (Rome): modern technologies to learn from the past**  
*L. Mattoli, E. Flamini, M. Burico, V. Mercati, R. Pagiotti, P. M. L. Vázquez de Ágredos, P. Traldi*  
Aboca Spa Società Agricola, Sansepolcro, Italy
- ThP-231 **Molecular characterization of the preparative layers of XXII<sup>nd</sup> Sarcophagus, a mass spectrometry approach**  
*C. Melchiorre, G. Ntasi, L. Birolo, P. Cennamo, G. Trojsi, G. Fatigati, A. Amoresano, A. Carpentieri*  
University of Naples Federico II, Department of Chemical Science, Napoli, Italy