IMSC 2014

20th International Mass Spectrometry Conference

August 24-29, 2014 Geneva, Switzerland

Detailed Programme

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International Mass Spectrometry Conference Geneva, Switzerland August 24–29, 2014







Monday, August 25 th		
09h00 11h00	MOSO1 - Fourier-Transform MS Chairs: Yury Tsybin, Julia Chamot-Rooke	Room 1
M0S01-1	<u>Keynote</u> : 40 Years of Fourier Transform Mass Spectrometry: progress and prospects Alan Marshall - Florida State University, USA	
M0S01-2	Novel mass analyzers for rapid high-performance FTMS Yury O. Tsybin - Ecole Polytechnique Federale de Lausanne, Switzerland	
MOS01-3	2D FT-ICR MS using non-uniform sampling (NUS) and advanced data processing. Application to human plasma triglyacylglycerols (TAG) analyzed by nano ESI/IRMPD Christian Rolando - Université Lille 1, France	1
M0S01-4	New developments in speeding up Orbitrap mass spectrometry Alexander Makarov - ThermoFisher Scientific (Bremen) GmbH, Germany	
M0S01-5	Non orbital electrostatic traps and MR-TOF Anatoly Verenchikov - Mass Spectrometry Consulting, MSC-CG, Montenegro	
09h00 11h00	MOSO2 - Synthetic Macromolecules Chairs: Anna Crecelius, Ulrich Schubert, Gérard Hopfgartner	Room 2
M0S02-1	<u>Keynote</u> : MALDI-TOF Mass Spectrometry as a powerful tool for the structure elucidation of complex ploymers Harald Pasch - University of Stellenbosch, South Africa	
M0S02-2	CID versus activated EPD for the characterization of PAMAM dendrimers Aura Tintaru - Aix-Marseille University & CNRS, UMR 7273: Institut de Chimie Radicalaire, France	
M0S02-3	Atmospheric pressure solid analysis probe with ion mobility-mass spectrometry as a new powerful tool for the characterization of complex industrial mixtures Caroline Barrère - Normandie University, France	e
M0S02-4	MS/MS of incompletely and fully condensed POSS with different substituents – folding and unfolding routes. Thierrey Fouquet - Public Research Centre Henri Tudor, Luxembourg	
M0S02-5	Segregation in dried droplet polymer sample spots examined by MALDI Imaging MS Steffen Michael Weidner - Federal Institute for Materials Research and Testing (BAM), Germany	
09h00 11h00	MOSO3 - Mass Spectrometry Instrumentation Chairs: Matthias Frank, Günter Allmaier	Room 3
M0S03-1	<u>Keynote</u> : Analysis of viruses, VLP-antibody complexes and vaccines by means of nano ESI combined with different mobility analyzer and bionanoparticles collection Günter Allmaier - Vienna University of Technology, Austria	erential
M0S03-2	Precision mass spectrometry on short-lived nuclides: new methods and results Lutz Schweikhard - University of Greifswald, Germany	
M0S03-3	A new primary ion beam source for secondary ion mass spectrometry using vacuum electrospray of ionic liquid Yukio Fujiwara - National Institute of Advanced Industrial Science and Technology (AIST), Japan	ids
M0S03-4	Gas flow in electrospray ionization/athmopheric pressure interfaces: simulation and experiment Julius Reiss - TU Berlin, Germany	
M0S03-5	Development of high mass resolution tandem time-of-flight (TOF) mass spectrometer applicable to High Energ Electron Transfer Dissociation (HE-ETD) Shigeo Hayakawa - Osaka Prefecture University, Japan	у
09h00 11h00	MOSO4 - Aerosol MS and Atmospheric Science Chairs: Urs Baltensperger, Renato Zenobi	Room 4
M0S04-1	<u>Keynote</u> : Molecular characterization of atmospheric aerosols by High-Resolution Mass Spectrometry Alexander Laskin - Pacific Northwest National Laboratory, USA	
M0S04-2	Simultaneous gas- and particle- phase measurements using a chemical ionization high-resolution time-of-flig spectrometer Claudia Mohr - University of Washington, USA	yht mass
M0S04-3	Characterization of organic trace species in gaseous and particulate emissions of a ship diesel engine fueled of diesel and heavy fuel oil Thorsten Streibel - University of Rostock, Germany	with

M0S04-4	Molecular characterization of secondary organic aerosol from the green leaf volatile 3-Z-hexenal and related	
	precursors Mohammad Safi Shalamzari - University of Antwerp (Campus Drie Eiken), Belgium	
M0S04-5	New soft ionisation ultra-high resolution mass spectrometry methods for characterizing the organic fraction of atmospheric particles Markus Kalberer - University of Cambridge, UK	f
09h00 11h00	MOSO5 - Nucleic Acids Chairs: Daniele Fabris, Eric Forest	Room 6
M0S05-1	<u>Keynote</u> : Mass spectrometry for nucleic acids biophysics Valérie Gabelica - Inserm/Univ. Bordeaux (U869), France	
M0S05-2	Ligand binding to DNA G-quadruplexes studied by ESI-MS from potassium solutions Adrien Marchand - Inserm / Univ. Bordeaux, France	
M0S05-3	Formation and dissociation of the tetramolecular DNA i-motif by the sequences d(XnC4Ym) in the gas- and sol phase Xinhua Guo - Jilin University, China	ution-
M0S05-4	Non-standard gas-phase fragmentation of short, highly charged oligonucleotides Rahel Eberle - University of Bern, Switzerland	
M0S05-5	MS-based elucidation of RNA structures Matteo Scalabrin - The RNA Institute, University at Albany, USA	
15h00 17h00	MOS06 - Clinical Applications and Screening Chairs: Yoshi Wada, Ruedi Aebersold	Room 1
M0S06-1	<u>Keynote</u> : Direct mass spectrometric analysis of mucosal membranes – experimental approaches and application <i>Zoltan Takats - Imperial College London, UK</i>	ons
M0S06-2	Individualized tissue analysis for EGFR-dependent phosphoproteomic signature in non-small-cell lung cancer Yi Ting Wang - Chemical Biology and Molecular Biophysics Program, Taiwan International Graduate Program, Institute of Chemistry, Academia Sinica, Taipei, Taiwan and Institute of Biochemical Sciences, National Taiwan University, Taipei, Taiwan University, Taiwan University	
M0S06-3	Screening of biological samples by SWATH acquisition and processing by high resolution reference spectra Stefan König - IRM Bern, Switzerland	
M0S06-4	Ultrasensitive detection and quantitation of neuroactive steroids using a post-activation ion-molecule reaction mediated by lithium Scott A. Shaffer - University of Massachusetts Medical School, USA	
M0S06-5	New approaches to multiplex newborn screening of lysosomal storage disorders by tandem mass spectrometr Frantisek Turecek - University of Washington, USA	у
15h00 17h00	MOSO7 - Imaging MS – Instrumentation Chairs: Ron Heeren, Markus Stöckli	Room 2
M0S07-1	<u>Keynote</u> : Expanding the usefulness of secondary ion mass spectrometry for biologically relevant measurement <i>Christopher Anderton - PNNL, USA</i>	ts
M0S07-2	A comparison of DESI and MALDI ionisation on an oa-TOF MS for tissue imaging experiments Emmanuelle Claude - Waters Corporation	
M0S07-3	MALDI-MS Imaging with a Synapt G2-S Mass Spectrometer: improving the lateral resolution to ~7 µm and the sensitivity for lipid analysis by use of novel matrices Hans Kettling - University of Münster, Germany	
M0S07-4	Low temperature plasma mass imaging (LTP-MSI): do-it-yourself instrumentation and applications in biology. Robert Winkler - CINVESTAV Unidad Irapuato, Mexico	
M0S07-5	High performance platform for atmospheric pressure high resolution MALDI mass spectrometry imaging Bernhard Spengler - Justus Liebig University Giessen, Germany	
15h00 17h00	MOSO8 - Carbohydrates Chairs: Catherine Costello, Leopoldo Ceraulo	Room 3
M0S08-1	<u>Keynote</u> : Automated, detailed glycan analysis by LC/MS for biotherapeutics and integrated biology Pauline Rudd - National Institute for Bioprocessing Research and Training, Fosters Avenue, Blackrock, Dublin, Ireland	
M0S08-2	CE-ESI-MS/MS as a tool in protein glycosylation analysis Guinevere Kammeijer - Leiden University Medical Center (LUMC), The Netherlands	

M0S08-3	Xylan oligosaccharide mass profiling method for identification of arabidopsis thaliana with altered 0-acetylation in glucuronoxylans Sun-Li Chong - Department of Food and Environmental Sciences, University of Helsinki, Finland
MOS08-4	Meaning and consequence of the competitive presence of the hydrogen bond and salt interactions on the dissociation orientation of deprotonated adducts in ESI Ekaterina Dariy - CEA-Genoscope/UMR8030, France
M0S08-5	Rational identification of glycan structure from MALDI spectra based on informatics and quantum chemical calculation Hiromitsu Takaba - Kogakuin University, Japan
15h00 17h00	MOSO9 - Environment - Biological Systems Interactions Chairs: Kristin Schirmer, Thomas Hofstetter
M0S09-1	<u>Keynote</u> : Deciphering the chemical language of insects by Mass Spectrometry <i>Joanne Yew - Temasek Life Sciences Laboratory, Singapore</i>
M0S09-2	Characterization of plant glycated proteome and its changes during ageing and under environmental stress conditions Andrej Frolov - Universität Leipzig, Germany
M0S09-3	Metabolomic approaches to assess neurotoxic effects of Imidacloprid on the freshwater snail Lymnaea stagnalis Sara Tufi - VU Amsterdam, The Netherlands
M0S09-4	Distribution and characteristics of methyl mercury in the tissues of shark and whale Hyun-Mee Park - Korea Institute of Science and Technology, South Korea
M0S09-5	Cocktail approach for microsomal CYP450 phenotyping using UHPLC-QTOF Dany Spaggiari - Université de Genève, Switzerland
15h00 17h00	MOS10 - Microbes and Viruses Chairs: Günter Allmaier, Robert Hettich
MOS10-1	<u>Keynote</u> : Rapid characterization of microorganisms by Mass Spectrometry: what can be learned and how Catherine Fenselau - Univ of Maryland, USA
M0S10-2	Top-down Mass Spectrometry probes immune evasion by pathogenic neisseria meningitidis Julia Chamot-Rooke - Institut Pasteur, France
MOS10-3	Improvement in bacterial strain differentiation by MALDI-TOF MS profiling by using microwave-assisted enzymatic digestion Zbynek Zdrahal - Masaryk University, Czech Republic
MOS10-4	Discrimination of cyanobacterium microcystis aeruginosa by MALDI-MS and analysis of Its genetic diversity Liwei Sun - Southeast University, China
MOS10-5	Deep quantitative proteomics to reveal regulatory mechanisms that govern carbon metabolism in mycobacteria. Marc Moniatte - EPFL, Switzerland

Tuesday, August 26 th		
09h00 11h00	TOS11 - Targeted and Quantitative Proteomics Chairs: Paola Picotti, Markus Stöckli	Room 1
T0S11-1	Keynote: Dynamic signaling interactomes in health and disease Anne-Claude Gingras - Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital / Department of Molecular Gountersity of Toronto, Canada	enetics,
T0S11-2	The impact of biochemical background on quantification ranges of data-dependent, directed and targeted pro strategies Alexander Schmidt - Biozentrum, University of Basel, CH-4056 Basel, Switzerland	teomics
T0S11-3	Quantitative proteomic analysis by variable SWATH acquisition of differentially expressed proteins in monocyt dendritic cells Ying Zhang - University of Geneva, Switzerland	e-derived
T0S11-4	Comprehensive proteomic analysis of 3D human liver and cardiac spheroids for drug toxicity investigation Nathalie Selevsek - Functional Genomics Center Zurich (FGCZ), Zurich, Switzerland	
T0S11-5	Multiplex quantification of microbial and plant protein toxins in complex matrices by immuno-extraction and resolution targeted mass spectrometry Mathieu Dupre - CEA, France	high
09h00 11h00	TOS12 - Lipidomics Chairs: Andrej Shevchenko, Eric Forest	Room 2
T0S12-1	<u>Keynote</u> : Natural variation of a signalling lipid Markus Wenk - National University of Singapore, Singapore	
T0S12-2	Novel oxysterols in mouse and man William Griffiths - Swansea University, UK	
T0S12-3	Lipidomic characterization of tumor tissues using LC/MS, SFC/MS, MALDI-MS and multivariate data analysis Michal Holčapek - University of Pardubice, Czech Republic	
T0S12-4	Malarial parasite development: lipidomic analysis of the P. falciparum life cycle in human erythrocytes Todd W Mitchell - University of Wollongong, Australia	
T0S12-5	Identification and immunomodulatory functions of novel galactosylceramides from gut commensal microbe Bacteroides fragilis Sungwhan Oh - Harvard Medical School, USA	
09h00 11h00	TOS13 - Gas-Phase Ion Spectroscopy Chairs: Jos Oomens, Julia Chamot-Rooke	Room 3
T0S13-1	<u>Keynote</u> : Spectroscopy of ions in aqueous nanodrops Evan Williams - University of California, Berkeley, USA	
T0S13-2	Two-dimensional photofragmentation mass-spectrometry of cold ions. Oleg Boyarkine - EPFL, Switzerland	
T0S13-3	Gas phase reactions of seleniranium ions results in Pi-ligand exchange in competition with electron transfer George N. Khairallah - School of Chemistry - University of Melbourne, Australia	
T0S13-4	Conformational equilibrium of single and double protonated 1,4-diamine-2-butenes by IRMPD spectroscopy Thiago C. Correra - Institute of Chemistry - University of São Paulo, Brazil	
T0S13-5	Laser Spectroscopic Investigations of Dichlorofluorobenzenes by REMPI and MATI Spectroscopy Sascha Krüger - Kiel University, Department of Physical Chemistry, Germany	
09h00 11h00	TOS14 - Detectors and High-Mass MS Chairs: Renato Zenobi, Günter Allmaier	Room 4
T0S14-1	<u>Keynote</u> : High mass detection in imaging mass spectrometry Ron M.A. Heeren - FOM-AMOLF, The Netherlands	
T0S14-2	Development of a time and position sensitive ion detector for a stigmatic imaging mass spectrometer Yosuke Kawai - Osaka University, Japan	
T0S14-3	Factors that affect transmission of high mass MALDI ions in a multi-quadrupoles rectilinear ion trap mass spe Wen-Ping Peng - National Dong Hwa University, Taiwan	ectrometer
T0S14-4	A novel freestanding ultra-nanocrystalline diamond membrane for protein mass detection using MALDI-TOF-M Diana Hildebrand - Center for Hybrid Nanostructures (CHYN) & Institute of Applied Physics, University of Hamburg, Ger	

T0S14-5	Heavy ion mass spectrometry using STJ cryodetectors from Ferritin to the +1 charge state of bacteriophag capsid at 13MTh Mark Bier - Carnegie Mellon University, USA	е НК97
09h00 11h00	TOS15 - Effect-Directed Analytical MS Chairs: Marc Suter, Olivier Laprévote	Room 5
T0S15-1	<u>Keynote</u> : Towards higher throughput in effect-directed analysis Marja Lamoree, Institute for Environmental Studies, VU University, Amsterdam, The Netherlands	
T0S15-2	Identification of emerging pharmaceutical pollutants and human metabolites in urban wastewater treatment using Effect Directed Analysis Caroline Gardia-Parège - EPOC-LPTC, France	plant
T0S15-3	Online LCxLC-ToF MS for effect-directed analysis in effluent and surface water Xiyu Ouyang - Institute for Environmental Studies (IVM), VU University Amsterdam, The Netherlands	
T0S15-4	Exploring the performance of a nontarget screening workflow on known environmental contaminants Meng Hu - Department Effect-Directed Analysis, Helmholtz Centre for Environmental Research - UFZ, Germany; RWTi University, Department of Ecosystem Analyses, Institute for Environmental Research, Germany	H Aachen
T0S15-5	Direct mass spectrometry-to-bioassay correlation for rapid identification of toxic pollutants in water using hithroughput effect directed analysis Jeroen Kool - VU University, the Netherlands	gh-
15h00 17h00	TOS16 - Labelling Strategies and Quantitative Biomolecule Analysis Chairs: Paola Picotti, Marc Suter	Room 1
T0S16-1	<u>Keynote</u> : Measuring protein synthesis and breakdown using stable isotopes and mass spectrometry Dwight Matthews - University of Vermont, USA	
T0S16-2	Using Selective Reaction Monitoring (SRM) mass spectrometry to unmask regulatory feedback loops controll adipogenesis Robert Ahrends - ISAS, Germany	ing
T0S16-3	Assessing the variability of ¹⁵ N metabolic labeling-based proteomics in mouse brain and plasma Giuseppina Maccarrone - Max Planck Institute of Psychiatry, Germany	
T0S16-4	A novel SWATH-MS platform for comprehensive characterization of the epigenetic histone modifications Joerg Dojahn - AB Sciex, Germany	
T0S16-5	MeCAT - New possibilities of protein analysis and quantification David Benda - Humboldt-Universität zu Berlin, Germany	
15h00 17h00	TOS17 - Protein Phosphorylation and other Post-translational Modifications <i>Chairs: Jesper Olsen, Ruedi Aebersold</i>	Room 2
T0S17-1	<u>Keynote</u> : Mapping high resolution kinase-substrate network Andy Tao - Purdue University, USA	
T0S17-2	Characterization of N-linked glycans from vaccine antigens: The CYD tetravalent Dengue vaccine Jean Dubayle - Sanofi Pasteur, France	
T0S17-3	Characterization of N-terminal acetylated proteins in Pseudomonas aeruginosa PA14 strain Julie Hardouin - University of Rouen, France	
T0S17-4	Monitoring dynamic protein phosphorylation on intact proteins by native MS on an orbitrap EMR Violette Gautier - Utrecht University, Utrecht, The Netherlands	
T0S17-5	Characterization of unusual post-transitional modifications in antibodies and related molecules Patrick Schindler - NOVARTIS, Switzerland	
15h00 17h00	TOS18 - Ion-Molecule and Ion-Ion Reactions in the Gas-Phase Chairs: Peter Armentrout, Gianluca Giorgi	Room 3
T0S18-1	<u>Keynote</u> : Non-covalent molecular recognition as probed by tandem mass spectrometry Mary Rodgers - Department of Chemistry, Wayne State University, Detroit, Michigan, USA	
T0S18-2	Using a charge-tagged proline-based organocatalyst for mass spectrometric mechanistic studies Johann Alexander Willms - Rheinische Friedrich-Wilhelms-Universität, Germany	
T0S18-3	Electrospray mass spectrometric study of the metal triflates used as catalysts in their interaction with organisomer recognition Claudio lacobucci - Université Nice Sophia Antipolis, France	c ligands:

TOS14-5 Heavy ion mass spectrometry using STJ cryodetectors -- from Ferritin to the +1 charge state of bacteriophage HK97

T0S18-4 Selective decomposition of formic acid into H _a and CO _c eatalyzed by coinage metal hydride cluster ions Athanasios Zavras - The University of Melbourne - Australia T0S18-5 Ion/ion reactions: new chemistries for metal ion removal, oxidation of peptides, and esterification in the Gas Phase Scott McLuckey - Purdue University, USA 15h00 T0S19 - Microfluidic Devices and Nanotechnology Room T0S19-1 Keynote: Recombinant protein QC and disease diagnostics using chip integrated affinity MALDI strategies Thomas Laurell - Dongguk University, Evoul, South Korea T0S19-2 When ambient ionization meets miniature ion trap mass apectrometer: chemistry, instruments and applications Zheng Ouyang - Purdue University, USA T0S19-3 Microfluidics lipidomics using a novel integrated mass spectrometry technology Gluseppe Astarita - Waters Corp T0S19-4 Membrane-assisted isoelectric focusing device as a micro-preparative fractionator for two dimensional shotgun proteomics Mohammad Pirmoradian - Karolinska Institute, Sweden T0S19-5 Ultrafast peptide decomposition by superheating Matthias O. Altmeyer - Twente University, Germany 15h00 T0S20-1 Imaging MS - Applications Chairs: Olivier Laprivote, Markus Stöckii T0S20-1 Keynote: MALDI molecular imaging of proteins, metabolites and drugs for preclinical and clinical research Axel Walch - Helinholtz-Zentrum München, Germany T0S20-3 High spatial and high mass resolution of metabolite analysis using AP-MALDI MSI Dhaka Bhandari - Justus-Liebeig-Universitä Glessen, Germany T0S20-4 Towards quantification based MS imaging: filling the gap between MALDI MS Imaging and tissue microproteomics Isabelle Fournier - Université Lille 1, France T0S20-5 TLC-MALDI-FT-ICR-MS coupled to imaging mass spectrometry — A unique approach to first identify then subsequently map parasite specific lipid markers in vivo. Berin Boughton - Metabolomics Australia, University of Melbourne, Australia			
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	T0S20-5	map parasite specific lipid markers in vivo.	tly

Wedne	Wednesday, August 27 th		
09h00 11h00	WOS21 - New Ionization Techniques Chairs: Frantisek Turecek, Silvia Catinella	Room 1	
W0S21-1	<u>Keynote</u> : The development and future of spray ionization techniques Brian Chait - Rockefeller University, USA		
W0S21-2	Development of surface acoustic wave nebulization David Goodlett - University of Maryland, USA		
W0S21-3	Charged droplet beam source for secondary ion mass spectrometry using nano electrospray in vacuum Satoshi Ninomiya - University of Yamanashi, Japan		
W0S21-4	Matrix-free desorption/ionization induced by neutral cluster impact for soft analysis of complex (bio-)sample Michael Durr - Justus Liebig University Giessen, Germany	s	
W0S21-5	UV-LDI- and MALDI-mass spectrometry augmented by UV-LaserPostionization: coupling a wavelength-tunabl laser (213-400 nm) to a synapt G2-S mass spectrometer Jens Soltwisch - University of Münster, Germany	e 0P0-	
09h00 11h00	WOS22 - Cell Biology and Cellular Pathways Chairs: Anne-Claude Gingras, Gérard Hopfgartner	Room 2	
W0S22-1	<u>Keynote</u> : Quantitative interaction proteomics for epigenetics Michiel Vermeulen - Radboud University Nijmegen, The Netherlands		
W0S22-2	Characterisation of human cell lines using rapid evaporative ionization mass spectrometry Nicole Strittmatter - Imperial College London, UK		
W0S22-3	The production pipeline of the MHC peptidome Arie Admon - Technion - Israel Institute of Technology, Israel		
W0S22-4	A sentinel protein assay for the quantification of cellular process activities using PRM and DIA Paul J. Boersema - Insitute of Biochemistry, ETH Zürich, Switzerland		
W0S22-5	Quantifying 14-3-3 protein interaction and phosphorylation dynamics with SWATH mass spectrometry Ben C. Collins - ETH Zurich, Switzerland		
09h00 11h00	W0S23 - Top-down Proteomics Chairs: Julia Chamot-Rooke, Yury Tsybin	Room 3	
W0S23-1	<u>Keynote</u> : A Version of the human proteome project that embraces quantitative top down MS Neil Kelleher - Northwestern University, USA		
W0S23-2	Sequencing of native protein complexes Mikhail Belov - Thermo Fisher Scientific, Germany		
W0S23-3	Top-down native ETD yields conformationally selective fragment patterns Albert Konijnenberg - Universiteit Antwerpen, Belgium		
W0S23-4	Combining low- and high-resolution top-down mass spectrometry for hemoglobin disorder diagnosis Didia Coelho Graça - Geneva University, Geneva, Switzerland		
W0S23-5	Extreme ultraviolet activation and fragmentation of peptide and protein ions Alexandre Giuliani - Synchrotron SOLEIL / INRA, France		
09h00 11h00	WOS24 - Trace Gas Analysis of Breath and Food Flavours Chairs: Patrik Spanel, Gianluca Giorgi	Room 4	
W0S24-1	<u>Keynote</u> : Clinical breath (VOC) analysis - pearls and pitfalls Wolfram Miekisch - University Medicine of Rostock, Germany		
W0S24-2	Breath acetone to monitor life style interventions in field conditions: an exploratory study using proton transfermass spectrometry (PTR-MS) Devasena Samudrala - Radboud University, The Netherlands	er reaction	
W0S24-3	In vivo exhaled breath analysis: adding to lung disease diagnosis and drug monitoring Pablo M-L Sinues - ETH Zurich, Switzerland		
W0S24-4	PTR-TOF-MS characterization of roasted coffees (C. arabica) from different geographic origins Sine Yener - Fondazione Edmund Mach, Italy		
W0S24-5	Evolved gas analysis by single photon ionization—Mass Spectrometry: a tool to distinguish different types of of Michael Fischer - Helmholtz Zentrum München, Germany	coffee	

09h00 11h00	WOS25 - Nanomaterials in MS, Nanomaterials Characterization Chairs: Hui-Fen Wu, Laurent Fay	Room 5
W0S25-1	<u>Keynote</u> : Nanomaterial-based affinity mass spectrometry for the analysis of biomolecules Yu-Chie Chen - National Chiao Tung University, Taiwan	
W0S25-2	Novel metal oxide nanomaterials for global phosphoproteome Yu Bai - Peking University, College of Chemistry, China	
W0S25-3	Characterization of nobel metal nanoclusters and nanocages on atomic scale by ESI-Q-TOF mass spectrometry Elina Kalenius - University of Jyväskylä, Finland	
W0S25-4	Analysis of organic surface modifications of manufactured nanomaterials by thermogravimetry coupled to MS (MS) Per Axel Clausen - National Research Centre for the Working Environment, Denmark	(TGA-
W0S25-5	A new ICP-TOF-MS and new capabilities for the analysis of micro- and nanosamples Olga Borovinskaya - ETH Zürich, Switzerland	
15h00 17h00	WOS26 - Metabolomics Chairs: Oliver Fiehn, Olivier Laprévote	Room 1
W0S26-1	<u>Keynote</u> : From MS data to systems biology applications in medicine – with specific emphasis on metabolic disc and their co-morbidities <i>Matej Oresic - Steno Diabetes Center, Denmark</i>	orders
W0S26-2	Advanced LC-HRMS and GC-MS based methods for metabolomics of Fusarium head blight on wheat Rainer Schuhmacher - University of Natural Resources and Life Sciences Vienna (BOKU), Austria	
W0S26-3	Combination of double isotopic labeling and high resolution mass spectrometry: a novel method for untargeted metabolic profiling Emilien Jamin - INRA, ToxAlim UMR1331, Platform MetaToul-AXIOM, France	fungal
W0S26-4	Deciphering de novo induction of novel biomarkers in mycobiome interactions by MS-based metabolomics and microNMR Jean-Luc Wolfender - School of Pharmaceutical Sciences, Switzerland	
W0S26-5	GC-MS based metabolite profiling as a means to hybrid performance prediction in winter wheat Andrea Matros - IPK-Gatersleben, Germany	
15h00 17h00	WOS27 - Small Molecules – Data Acquisition and Analysis Chairs: Thomas Hankemeier, Silvia Catinella	Room 2
W0S27-1	<u>Keynote</u> : Beyond the elemental composition: computer-assisted identification methods in a high resolution era Robert Mistrik - HighChem, Slovakia	
W0S27-2	Data-independent vs data-dependent fragmentation analysis for comprehensive screening of polar organic sub in environmental samples using LC-ESI-Orbitrap Matthias Ruff - Eawag - Aquatic Research, Switzerland	stances
W0S27-3	Application of MALDI imaging to analyze glycosyl flavonoids from plant tissue, a method to localize and difference isomeric compounds by MS/MS data. Norberto Lopes - Univeristy of São Paulo, Brazil	ntiate
W0S27-4	Supersonic gas jet shift with respect to the radio-frequency quadrupole axis for increasing efficiency of environ chemical analysis by mass spectrometry Valerii Raznikov - The Branch of Talrose Institute for Energy Problems of Chemical Physics of Russian Academy of Scient Russia	
W0S27-5	Comparison of the qTOF and Orbitrap configurations for the global metabolomic profiling on the example of the Pseudomonas Aeruginosa endometabolome. Victor Nesatyy - NUS, Singapore	
15h00 17h00	WOS28 - Biomolecular Conformation in the Gas-Phase and in Solution Chairs: Lars Konermann, Julia Chamot-Rooke	Room 3
W0S28-1	<u>Keynote</u> : Protein structure and folding in the Gas Phase Kathrin Breuker - CCB - Centrum für Chemie und Biomedizin, University of Innsbruck, Austria	
W0S28-2	Discovering a new subunit for an old complex by native mass spectrometry Sharon Michal - Weizmann Institute of Science, Israel	

WOS28	3 Stability of the B2B3-beta crystallin heterodimer to increased oxidation by radical probe and ion mobility mass spectrometry Kevin Downard - University of Sydney, Australia
W0S28-	Investigating the effects of ligands on nucleic acid structure and dynamics by IMS-based approaches Dan Fabris - The RNA Institute, University at Albany, USA
W0S28-	Conformational dynamics of cellobiose dehydrogenase probed by structural mass spectrometry Alan Kadek - Institute of Microbiology ASCR, Prague, Czech Republic
15h00 17h00	
W0S29	1 <u>Keynote</u> : Ambient MS in motion: 3D robotic sampling, dynamic ionization, and microplasmas Facundo Fernandez - Georgia Institute of Technology, USA
W0S29	Reactions in DART source and analysis examples - mechanism study Shuying Liu - Changchun Institute of Applied Chemistry, China
W0S29	3 Sub-mm linear ion trap mass spectrometer made using lithographically patterned ceramic plates Daniel Austin - Brigham Young University, USA
W0S29	Progress on pocket Mass Spectrometer development Mo Yang - Korea Basic Science Institute, South Korea
W0S29	Miniaturised laser-based mass spectrometer for in situ investigation of planetary bodies Peter Wurz - University of Bern, Switzerland
15h00 17h00	
W0S30-	Keynote: High precision mass spectrometry in a cometary coma: first results from the Churyumov Gerasimenko comet nucleus exploration Kathrin Altwegg - University of Bern, Switzerland
W0S30-	Formation of negative ions from "water group" positive ions at high collision energies: implications for the ionosphere of Titan. Miroslav Polasek - J. Heyrovský Institute of Physical Chemistry of the ASCR, Czech Republic
W0S30-	In situ exploration of solar system bodies: the potentiality of an Orbitrap Based Mass Analyser Christelle Briois - LPC2E, France
W0S30	The study of leak detection for spacecraft with quadrupole mass spectrometer Yan Rongxin - Beijing Institute of Spacecraft Environment Engineering, China
W0S30-	5

Th0S31-1 Biomarkers and Diagnostics Chairs: Silvia Catinella, Gérard Hopfgartner Th0S31-1 Keynote: Mass spectrometric profiling strategies for population phenotyping Matthew Lewis - MRC-NIHR National Phenome Centre, Department of Surgery and Cancer, Imperial College London, Lo Th0S31-2 Automated dried blood spot instrumentation coupled to HPLC-QqQ mass spectrometry – A vitamin D and E cas Götz Schlotterbeck - FHNW, Switzerland Th0S31-3 Biomarker MS assays for small cell lung cancer: exploring Molecular Imprinted Polymer potential in clinical pro Cecilia Rossetti - University of Oslo, Norway Th0S31-4 Ovarian cancer: hunting biomarkers by Mass Spectrometry Imaging and tissue proteomic	e study
Matthew Lewis - MRC-NIHR National Phenome Centre, Department of Surgery and Cancer, Imperial College London, Lo Th0S31-2 Automated dried blood spot instrumentation coupled to HPLC-QqQ mass spectrometry – A vitamin D and E cas Götz Schlotterbeck - FHNW, Switzerland Th0S31-3 Biomarker MS assays for small cell lung cancer: exploring Molecular Imprinted Polymer potential in clinical pro Cecilia Rossetti - University of Oslo, Norway	e study
Götz Schlotterbeck - FHNW, Switzerland Th0S31-3 Biomarker MS assays for small cell lung cancer: exploring Molecular Imprinted Polymer potential in clinical proceeding Rossetti - University of Oslo, Norway	
Cecilia Rossetti - University of Oslo, Norway	oteomics.
ThOS31-4 Ovarian cancer: hunting biomarkers by Mass Spectrometry Imaging and tissue proteomic	
Michel Salzet - Université Lille 1, France	
Th0S31-5 Discrimination of metastasis from breast and pancreatic cancer by MALDI imaging Soeren Deininger - Bruker Daltonik GmbH, Germany	
09h00 11h00 Th0S32 - Ion Mobility MS Chairs: Dave Clemmer, Günter Allmaier	Room 2
Th0S32-1 Keynote: An (Ion Mobility) Mass Spectrometry based framework to understand protein structure Perdita Barran - The University of Manchester, UK	
Th0S32-2 Structural and energetics studies of iron porphyrine complexes by Ion Mobility Mass Spectrometry and collision induced dissociation Ameneh Gholami - University of Ottawa, Canada	n
Th0S32-3 Choosing the right buffer gas in ion mobility spectrometry: the effect of ion-neutral interactions Thomas Wyttenbach - UCSB, USA	
Th0S32-4 FAIMS-HRMS as a novel tool for in-depth analysis of crude oil Alessandro Vetere - Max-Planck-Institut für Kohlenforschung, Germany	
Th0S32-5 Ion mobility separation of star- and linear-shaped poly- and oligothiophenes – limits and possibilities to determ structures Martina Marchetti-Deschmann - Vienna University of Technology, Austria	nine 3D
09h00 11h00 Th0S33 - Data Analysis - General Chairs: Pietro Franceschi, Yury Tsybin	Room 3
Th0S33-1 Keynote: Central dogma of proteomics provides identification of protein targets, action mechanisms and cellula pathways of small molecule drugs **Roman Zubarev - Karolinska Institutet, Sweden**	ır death
Th0S33-2 New approaches for optimizing the FTMS resolution in proteomics Marc-André Delsuc - Université de Strasbourg, France	
Th0S33-3 Dynamically harmonized FT-ICR cell. Further characterization and new potential applications Evgeny Nikolaev - Institut of Energy Problems of Chemical Physics Russian Academy of Sciences, Russia	
Th0S33-4 Evaluation of spectral accuracy in triple quadrupole instruments Jose Ignacio Garcia Alonso - University of Oviedo, Spain	
Th0S33-5 Predicting concentrations of small molecules without standard substances in LC/ESI/MS via ionization efficien Anneli Kruve - University of Tartu, Estonia	cy scales
09h00 11h00 Th0S34 - JMS Award Symposium Chair: Michael Linscheid	Room 4
Th0S34-1 A novel, ultrasensitive approach for quantitative carbohydrate composition and linkage analysis using LC-ESI i tandem mass spectrometry Kathirvel Alagesan - Max Planck Institute of Colloids and Interfaces, Germany	on trap
Th0S34-2 Method of duty cycle enhancement for orthogonal accelerator T0F MS with axial symmetric mass analyser, corwith drift tube IMS Denis Mikhailovich Chernyshev - National Research Nuclear University MEPhl, Linantek Ltd, Russia	nected
Th0S34-3 Membrane inlet Mass Spectrometry for in-field security applications Stamatios Giannoukos, University of Liverpool, UK	
Th0S34-4 Nucleation and chemical reactivity of mixed aerosol particles: new approach based on mass spectrometric det Josef Lengyel - J. Heyrovský Institute of Physical Chemistry, Academy of Science of the Czech Republic, Czech Republic	

Th0S34-5	Synthesis and reactions of atomically precise clusters Michael Wieklinski - Purdue University, USA
09h00 11h00	ThOS35 - Elemental and Isotopic MS, ICP-MS General, Cultural Heritage and Archaeology Room © Chairs: Ryszard Lobinski, Detlef Günther
Th0S35-1	<u>Keynote</u> : Interested in the determination of molecules with a heteroatom in a complex matrix – why not use ICP-MS for speciation and bioimaging? Jörg Feldmann - University of Aberdeen, UK
Th0S35-2	Novel coupling of separations with laser desorption elemental and molecular Mass Spectrometry Jan Preisler - Masaryk University, Czech Republic
Th0S35-3	Investigation of the pharmacological behavior of novel platinum(IV)-based anticancer agents by means of ICP-MS and LA-ICP-MS Sarah Theiner - Institute of Inorganic Chemistry, University of Vienna, Austria
Th0S35-4	Precise quantification and isotope ratio measurement of boron in U3Si2-Al nuclear fuel by ICP-TOF-MS Abhijit Saha - Radioanalytical Chemistry Division, Bhabha Atomic Research Centre, India
Th0S35-5	Isotope ratio mass spectrometry for the study of catalytic reactions of transformation hydrocarbons Olesya Krol - IHP SB RAS, Russia
15h00 17h00	Th0S36 - Advanced MS in Food and Nutrition Chairs: Michel Nielen, Laurent Fay Room Room
Th0S36-1	Keynote: Advanced MS-methods to study toxic secondary metabolites in food crops Rudolf Krska - Universität für Bodenkultur Wien, Austria
Th0S36-2	Improved precision of measured isotope ratio through peak parking and scan-based statistics in IDMS of small organic molecules Andreas Breidbach - EC-JRC-IRMM, Belgium
Th0S36-3	GC-APCI-MS/MS to enhance sensitivity for residues and contaminants analysis in food and biological fluids Emmanuelle Bichon - LABERCA-Oniris, France
Th0S36-4	The power of ion mobility-mass spectrometry for increased selectivity in food analysis: "A new beginning for Collision Cross Section" Séverine Goscinny - Scientific Institute of Public Health, Belgium
Th0S36-5	Non-Target and unknown screening of food samples using accurate mass LC-MS/MS screening techniques Ashley Sage - AB SCIEX, UK
15h00 17h00	ThOS37 - Hyphenated Techniques - Applications Chairs: Gérard Hopfgartner, Marc Suter Room 2
Th0S37-1	<u>Keynote</u> : Digital microfluidic sample processing for separations and Mass Spectrometry Aaron Wheeler - University of Toronto, Canada
Th0S37-2	Online SPE-nano-LC-HRMS for analysis of polar organic micropollutants in environmental samples: method development, validation and applications Michael Andrej Stravs - Eawag, Dübendorf, Switzerland
Th0S37-3	Characterization of bioactive peptides from snake venoms by LC-MS coupled to bioactivity assessment via at-line nanofractionation Marija Mladić - VU Universtiy Amsterdam, The Netherlands
Th0S37-4	Analysis of oligosaccharides in complex samples using MS-based techniques Leon Coulier - DSM Biotechnology Center, The Netherlands
Th0\$37-5	Monoclonal antibodies complete primary structure and biosimilarity assessment in a single analysis by sheathless capillary electrophoresis-mass spectrometry Gahoual, Rabah - Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), CNRS – UMR7140, University of Strasbourg, Strasbourg, France
15h00 17h00	Th0S38 - Non-Covalent Interactions Chairs: Albert Heck, Leopoldo Ceraulo
Th0S38-1	<u>Keynote</u> : Combining advanced native MS techniques for the characterization of non-covalent complexes Sarah Cianferani - CNRS - IPHC - LSMBO, France
Th0S38-2	Opposing charges in ESI-MS of non-covalent complexes explain many observations Rachel Loo - UCLA David Geffen School of Medicine, USA

Th0S38-3	Automated non-covalent mass spectrometry in drug discovery: improved screening of protein-ligand interactions Rebecca Burnley - UCB Celltech, UK
Th0S38-4	Novel application of ion mobility and high resolution mass spectrometry to characterise Ligand binding to a DNA aptamer Chris Nortcliffe - University of Manchester, UK
Th0S38-5	UV-MALDI-MS analysis of non-covalent complexes with a 6-Aza-2-thiothymine-matrix: effect of wavelength and fluence on the detection of the complexes Andreas Schnapp - Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany
15h00 17h00	ThOS39 - Informatic Tools for MS Chairs: Thomas Hankemeier, Ruedi Aebersold Room ◆
Th0S39-1	<u>Keynote</u> : Highly sensitive feature detection for LC-MS-based metabolimics Oliver Kohlbacher - University of Tübingen, Germany
Th0S39-2	Illuminating the 'dark matter' of mass spectrometry Steve Stein - NIST, USA
Th0S39-3	enviMass 2.0 – A workflow for fast spill and trend detection of micropollutants in aquatic systems using LC-HRMS data Martin Loos - Eawag, Switzerland
Th0S39-4	MassTrees to study the evolution of the influenza virus and detect antiviral resistant strains Kavya Swaminathan - University of Sydney, Australia
Th0S39-5	Spectviewer, a software for mass spectrometry Imaging Jean-Pierre Both - CEA, France
15h00 17h00	ThOS40 - 2D and 3D Analysis and Imaging of Inorganic, Organic, and Biological Materials Room 6 Chairs: John Vickerman, Detlef Günther
Th0S40-1	<u>Keynote</u> : 2D and 3D imaging of inorganic, organic, and biological samples John Fletcher - Department of Chemistry and Molecular Biology, University of Gothenburg, Sweden
Th0S40-2	Cellular scale imaging of cancer drugs using a stigmatic MALDI imaging mass spectrometer Hiroki Kannen - Osaka univirsity, Japan
Th0S40-3	High resolution MALDI imaging of tryptic peptides in fresh frozen and FFPE tissue Katharina Huber - Justus Liebig University Giessen, Germany
Th0S40-4	Highly multiplexed imaging of tumor tissues with subcellular resolution by mass cytometry Bernd Bodenmiller - University of Zurich, Switzerland
Th0S40-5	Inspecting the anticancer drugs cisplatin and NKP1339 in tissue sections by LA-ICP-MSI Alexander Egger- Austrian Drug Screening Institute GmbH - ADSI, Austria

Friday,	August 29 th	
09h00 11h00	FOS41 - Gas-Phase Ion Fragmentation Mechanisms Chairs: Gianluca Giorgi, Leopoldo Ceraulo	oom ①
F0S41-1	<u>Keynote</u> : Surface-induced dissociation: characterization of an activation method for large complexes Vicki Wysocki - Ohio State University, USA	
F0S41-2	CO ₂ incorporation in hydroxide and hydroperoxide containing water clusters - unifying mechanism for hydrolysis protolysis Einar Uggerud - Department of Chemistry, University of Oslo, Norway	and
F0S41-3	Post-collision internal energy distributions and PAH ion fragmentation Paul Mayer - University of Ottawa, Canada	
F0S41-4	Peptide fragmentation: energetics, structures, and mechanisms Peter Armentrout - Department of Chemistry, University of Utah, USA	
F0S41-5	Distinction of alpha and beta forms of substituted glucose by tandem mass spectrometry and ion mobility spectre Laurence Charles - Aix-Marseille University, France	ometry
09h00 11h00	FOS42 - Forensics and Doping Chairs: Laurent Bigler, Olivier Laprévote	oom 2
F0S42-1	<u>Keynote</u> : Mass spectrometry in forensic hair testing: example of drug-facilitated crimes Pascal Kintz - X-Pertise Consulting, France	
F0S42-2	Screening for anabolic steroids in sports: new strategy based on the direct analysis of phase I and phase II metaby LC-MS/MS Georgina Balcells - Bioanalysis Research Group, IMIM-Hospital del Mar, Spain	bolites
F0S42-3	New technologies to help facing new challenge for growth promoters' detection Laure Beucher - LABERCA ONIRIS, France	
F0S42-4	Analysis of sexual assault evidence by ambient mass spectrometry: a statistical comparison between DESI-MS a EASI-MS Mario Francesco Mirabelli - Università della Calabria, Italy	nd
F0S42-5	Unambiguous Differentiation of Explosives-related Isomers using Electrospray High-Resolution Mass Spectromet Adrian Schwarzenberg - Université Pierre et Marie Curie, France	try
09h00 11h00	FOS43 - Environmental Analysis Chairs: Marja Lamorée, Marc Suter	oom 3
F0S43-1	<u>Keynote</u> : Wastewater-based epidemiology: the analysis of human biomarkers in sewage Kevin Thomas - NIVA, Norway	
F0S43-2	Suspect and non-target screening of lake sediments: approaches to identify records of organic contaminants in complex matrix Juliane Hollender - Eawag, Swiss Federal Institute of Aquatic Science and Technology, Switzerland	
F0S43-3	Influence of extraction pH upon the FT-ICR MS profiles of water samples from the Athabasca oil sands region Mark Barrow - University of Warwick, UK	
F0S43-4	Tracing genotoxic disinfection by-products after medium pressure UV water treatment using nitrogen labeling an mass spectrometry Annemieke Kolkman - KWR Watercycle Research Institute, The Netherlands	nd
F0S43-5	High resolution mass spectrometry based metabolomics: a new tool to detect and characterize emerging pollutar water and food matrices. Jerome Cotton - CEA/Profilomic, France	nts in
09h00 11h00	FOS44 - Very Large Biomolecules and Structural Biology Chairs: Michal Sharon, Eric Forest	oom 4
F0S44-1	<u>Keynote</u> : Mass Spectrometry and very large biomolecules Albert Heck - Utrecht University, The Netherlands	
F0S44-2	Probing protein structural transitions in complex biological backgrounds and on a large scale Paola Picotti - ETH Zurich, Inst. of Biochemistry, Switzerland	
F0S44-3	Radical probe Mass Spectrometry for high throughput protein footprinting Simin Maleknia - University New South Wales, Australia	

F0S44-4	Rapid and direct MALDI-MS identification of pathogenic bacteria from blood via ionic liquid-modified magnet nanoparticles Hui-Fen Wu - National Sun Yat-Sen University, Taiwan	ic
F0S44-5	Structural analysis of protein complexes by chemical cross-linking and mass spectrometry Alexander Leitner - ETH Zurich, Switzerland	
09h00 11h00	F0S45 - Single Cell MS Chairs: Bernd Bodenmiller, Renato Zenobi	Room 6
F0S45-1	<u>Keynote</u> : Single cell pheno-functional proteomics by mass cytometry Scott Tanner - Fluidigm Canada Inc., Canada	
F0S45-2	Absolute quantification of proteins and protein modifications on the single-cell level Serena Di Palma - Institute of Molecular Life Sciences, Switzerland	
F0S45-3	Profiling of algal populations with aingle-cell MALDI-FT-ICR mass spectrometry Jasmin Krismer - Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland	
F0S45-4	Near-field laser ablation sample capture for mass spectrometry imaging Kermit K. Murray - Louisiana State University, USA	
F0S45-5	Detection of microbial resistance markers in clinical samples using MALDI mass spectrometry Omar Belgacem, SHIMADZU	