

08:30-09:00 Registration for workshops

Workshops Part I (parallel)

09:00-10:30 **Johannes Rainer**, EURAC Bozen

Workshop 1 - Exploring and analyzing LC-MS data with Spectra and xcms

Corinna Brungs and Robin Schmid, IOCB Prague

Workshop 2 - Feature finding and molecular networking in MZmine

Dominik Kopczynski, Nils Hoffmann, Robert Ahrends, University of Vienna

Workshop 3 - Lipidomics-LIFS Bioinformatics Training

Joao Mokochinski, ThermoFisher Scientific

Workshop 4 - Small molecule workflows with Thermo Scientific™ Compound Discoverer™ software

10:30-11:00 **Coffee break**

Workshops Part II

11:00-12:30 Continuation of the workshops 1, 2, 3 and 4

12:30-13:30 **Lunch break (for workshop participants only)**

13:30-14:30 Registration MassSpec-Forum 2024

14:30-14:45 **Gunda Köllensperger & Christopher Gerner**, University of Vienna, Austria

Welcome and Opening

Session 1 - MS Imaging Techniques

14:45-15:20 **Klaus Dreisewerd**, University of Münster, Germany

T01 *MALDI MS - From the early years and fundamentals to new developments*

15:20-15:55 **Jens Soltwisch**, University of Münster, Germany

T02 *MALDI-MS imaging at high spatial resolution coupled to fluorescence microscopy for sub-cellular resolving power*

15:55-16:15 **Caroline Jones**, Shimadzu / Kratos Analytical Ltd., UK

T03 *tba (MALDI-TOF)*

16:15-16:30 **Daniel Skoczowsky**, TU Dortmund, Germany

T04 *Investigation of the Distribution of Pesticides and Their Metabolites in Plants After Root Uptake Using HPLC-HR-MS and MALDI-MSI*

16:30-16:40 **Short break**

16:40-17:15 **Martin Šala**, National Institute of Chemistry, Slovenia

T05 *Calibration, the Achilles heel of LA-ICPMS*

17:15-17:30 **Laura Kronlachner**, TU Wien, Austria

T06 *A novel strategy for sample preparation and calibration for nanoparticle analysis using laser ablation single particle-ICP-MS*

17:30-19:00 **Poster Session ground floor (beer/wine/snacks)**

Session 2 - Interactomics and Multiomics

08:30-09:05 **Fan Liu**, FMP Leibniz, Germany

T07 *Developing structural interactomics and its application in biology*

09:05-09:25 **Katharina Paschinger / Iain Wilson**, University of Natural Resources and Life Sciences Vienna, Austria

T08 *Highly branched immunogenic N-glycans of the porcine whipworm*

09:25-09:45 **Robert Ahrends**, University of Vienna, Austria

T09 *Multiomics reveals critical shifts in lipid metabolism during megakaryocyte differentiation and proplatelet formation*

09:45-10:05 **Eva Rauch**, University of Innsbruck, Austria

T10 *Linking acetyl-CoA labelling and histone acetylation dynamics for accurate determination of acetylation rates via ordinary differential equations*

10:05-10:25 **Jan Bucek**, Plasmion GmbH, Germany

T11 *SICRIT®- Seeing the Invisible & Connecting Unlinkable*

10:25-11:00 **Coffee break/Exhibition 2nd floor**

Session 3 - Ion Mobility

11:00-11:35 **Valerie Gabelica**, University of Geneva, Switzerland

T12 *Mass Spectrometry for Biophysics: Challenges and Perspectives*

11:35-11:55 **Jennifer Krone**, MOBILion Systems, USA

T13 *Revealing the Unseen with the High-Resolution Ion Mobility MOBIE Platform: A 13 Meter Serpentine Journey to the Future of Separations*

11:55-12:15 **Victor Weiss**, TU Wien, Austria

T14 *Differential mobility analysis (nES GEMMA instrumentation) applied for virus-like particle research*

12:15-13:15 **Lunch break/Exhibition 2nd floor**

Session 4 - Metabolomics

13:15-13:50 **Justin van der Hoof**t, Wageningen University, Netherlands

T15 *Computational Metabolomics Strategies to Gain Insights from Untargeted Mass Spectrometry*

13:50-14:05 **Kevin Mildau**, University of Vienna, Austria

T16 *msFeaST: a feature-set testing and visualization workflow for LC-MS/MS untargeted metabolomics data*

14:05-14:25 **André Müller**, Thermo Fisher Scientific, USA

T17 *Simultaneous Quantitation and Discovery (SQUAD) Analysis: Combining the Best of Targeted and Untargeted Mass Spectrometry-Based Metabolomics*

14:25-14:45 **Xiaobo Tian**, University of Geneva, Switzerland

T18 *Improved Quantification of Carbonyl Sub-metabolome by LC-MS Using a Fragmentation-Controlled Multiplexed Isotopic Tag*

14:45-15:00 **Veronika Fitz**, University of Vienna, Austria

T19 *Internal one-point calibration using isotopically labeled biomass for IDMS-metabolomics*

15:00-15:15 **Stefanie Rubenzucker**, University of Vienna, Austria

T20 *Analyzing bioactive lipids in complex biological matrices using LC-MS/MS*

15:15-15:55 **Coffee break/Exhibition 2nd floor**

Session 5 - Glycomics and Structure Elucidation

15:55-16:15 **Friedrich Altmann**, University of Natural Resources and Life Sciences Vienna, Austria

T21 *Can mass spectrometry of N-glycans topple microalgae taxonomy?*

16:15-16:30 **Johannes Helm**, University of Natural Resources and Life Sciences Vienna, Austria

T22 *Non-targeted high-resolution N-glycomics reveals new layers of organ-specific glycan diversity in mouse*

16:30-16:50 **Márkó Grabarics**, University of Oxford, UK

T23 *Electrospray deposition combined with scanning probe microscopy reveals the atomic structure of cyclic oligosaccharides*

16:50-17:10 **Ernst Pittenauer**, TU Wien, Austria

T24 *Tandem mass spectrometry of pincer ligands and their pincer complexes (Ni, Co): apparently the same precursor ions with a mass difference of one electron*

17:10-17:25 **Richard Gruseck**, University of Vienna, Austria

T25 *Elucidating biotransformation pathways of flavonoids in soils*

17:30-18:30 **Poster Session ground floor**

18:30 **Get Together/Dinner, ground floor**

Session 6 - Proteomics

08:30-09:05 **Katrin Marcus-Alic**, Ruhr-Universität Bochum, Germany

T26 *Identification of crime scene samples – a "very different" project*

09:05-09:40 **Karl Mechtler**, Vienna BioCenter, Austria

T27 *Unprecedented sensitivity, coverage, and quantitative accuracy for single-cell proteomics using the Astral mass analyzer, reveals more than 7500 proteins from single-cell level bulk samples & up to 5200 proteins from single cells*

09:40-09:55 **Daria Emekeeva**, Moscow Institute of Physics and Technology, Russia

T28 *Mass spectrometry de novo sequencing for identification of amino acid substitutions in Alzheimer's Disease*

09:55-10:10 **Yan Yan Beer**, Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

T29 *Improving Viral Load Measurements through Complementary Peptide- Based Protein Quantification and Digital Droplet PCR*

10:10-10:30 **Holger Stalz**, Agilent Technologies, Switzerland

T30 *Forever Chemicals – Workflows to detect PFAS in Water, Soil and Food*

10:30-11:00 **Coffee break/Exhibition 2nd floor**

Session 7 - Glycoproteomics and Exposomics

11:10-11:45 **Christian Huber**, Paris Lodron University of Salzburg

T31 *Glycoproteomics of a single protein: digging into the universe of protein isoforms*

11:45-12:05 **Lilla Turiák**, Research Centre for Natural Sciences, Budapest, Hungary

T32 *Glycoproteomics analysis of triple wild-type lung adenocarcinoma tissue samples*

12:05-12:20 **Thomas Berger**, Paris Lodron University of Salzburg

T33 *Characterization of critical quality attributes of therapeutic monoclonal antibodies from different CHO cell line subclones – a case study*

12:20-12:40 **Vinicius Verri Hernandes**, University of Vienna, Austria

T34 *Development of a combined targeted (MRM) and untargeted (SWATH) methodology for integrated exposomics and metabolomics.*

12:40-12:55 **Thomas Contini**, University of Rennes, France

T35 *DECRIPIT - Deciphering the human prenatal chemical exposome using high-resolution mass spectrometry*

12:55-13:00 **Closing**