



Monday 23rd October

- 09.00 – 17.00 Workshop A: Training school for cross-linking (IMBA lecture hall, Dr. Bohrgasse 3)
- 13.00 – 17.00 Workshop B Hydrogen-deuterium exchange. (GMI lecture hall -orange floor, Dr. Bohrgasse 3)
- 17.15-18.15 Key Note Lecture; **Clemens Plaschka** (MRC Laboratory of Molecular Biology, UK), Structural studies of pre-mRNA splicing. (IMP lecture hall, Vienna Bio-Center 1)
- 18.15 Welcome Mixer

Tuesday 24th October

- 08.30-09.00 **Registration**
- 09.00-09.15 Welcome
- 09.15-09.50 **T1 Kasper Rand** (University of Copenhagen, Denmark). Analysis of the conformation and interactions of complex proteins by HDX-MS – expanding the HDX-MS toolbox
- 09.50-10.10 **T2 Riccardo Pellarin** (Institute Pasteur, Paris, France). Title TBC.
- 10.10-10.30 **T3 Alexander Leitner** (IMSB ETH, Zurich, Switzerland), Structural insights into the architecture of the human importin-4 – histone H3/H4 – Asf1a complex using an integrative modeling strategy
- 10.30-10.50 **T4 Franz Herzog** (University of Munich, Germany). Title TBC.
- 10.50-10.55 **PT1 Michal Rosulek** (Charles University, Prague), Limited proteolysis on MALDI compatible biochip
- 10.55-11.00 **PT2 Eleanor Dickinson** (University of Copenhagen, Denmark), Thiol-ene microfluidic chip for sub-second timescale HDX-MS analyses and efficient

pepsin digestion of proteins.

- 11.00-11.30 **Coffee**
- 11.30-12.05 **T5 Andrea Sinz** (Martin-Luther University Halle-Wittenberg, Germany), Cross-Linking/Mass Spectrometry for Investigating Protein Complexes: Where Are We Now and Where Should We Go?
- 12.05-12.25 **T6 Terry Zhang** (Thermo), Electron Transfer Dissociation for Hydrogen/Deuterium Exchange Mass Spectrometry to the Study of Protein Conformation
- 12.25-12.45 **T7 Petr Novak** (Charles University, Czech Republic), Impact of Chemical Cross-Linking on Protein Structure and Function.
- 12.45-12.50 **PT3 Claudio Iacobucci** (Martin Luther University Halle-Wittenberg, Germany), Novel solution- and gas phase-chemistry of "old" protein cross-linkers
- 12.50-12.55 **PT4 Christian Stieger** (Institute for Molecular Pathology, Austria) Monitoring the structural rearrangement of Cas9 via multiplexed quantitative cross-linking MS
- 12.55-13.00 **PT5 Christoph Hage** (Martin Luther University Halle-Wittenberg, Germany), The First "Zero-Length" Mass Spectrometry-Cleavable Cross-Linker for Protein Structure Analysis.
- 13.00-13.05 **PT30 Elena L. Rudashevskaya** (ISAS, Dortmund, Germany), Revealing mitochondrial protein interactome by in organello chemical crosslinking and mass spectrometry
- 13.00-14.30 **Lunch and poster presentations**
- 14.30-15.05 **T8 Philip Andrews** (University of Michigan, USA). Protean proteins: Crosslinking and ion mobility MS provide complementary information on protein structural changes.
- 15.05-15.25 **T9 Nir Kalisman** (The Hebrew University of Jerusalem, Israel), Hybrid computational approach for cross-link identification at the proteome level.
- 15.25-15.30 **PT6 Carolin Sailer** (University of Konstanz, Germany), Using quantitative crosslinking mass spectrometry to study structural dynamics of the ubiquitin ligase E6AP
- 15.30-15.35 **PT7 Alexandra Stützer** (Max Planck Institute for Biophysical Chemistry, Göttingen, Germany) Analysis of protein-DNA cross-links in a chromatin model.
- 15.35-15.55 **Coffee**
- 15.55-16.35 **T10 Jim Bruce** (University of Washington, USA), In vivo cross-linking and mass spectrometry: new opportunities for systems structural biology.
- 16.35-16.40 **PT8 Steve Hessmann** (University of Strasbourg, France), Benchmarking mAb bioconjugation strategies using a combination of native MS and peptide mapping approaches
- 16.40-16.45 **PT9 Julia Lockhauserbäumer** (Leibniz Institute for Experimental Virology, Hamburg, Germany) Native MS demonstrates the supportive impact of carbohydrates on norovirus infection.
- 16.45-16.50 **PT10 Bright D. Danquah** (University Medicine Rostock, Germany) Intact Transition Epitope Mapping - Thermodynamic Weak-force Observation

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- 16.50-16.55 **PT11 Sabine Wittig** (Martin Luther University Halle-Wittenberg, Germany) Native Mass Spectrometry to Identify Stoichiometries and Stability of Protein-Ligand Complexes
- 16.55-17.00 **PT12 Dietmar Hammerschmid** (University of Antwerp, Belgium) Characterization of a membrane-bound globin coupled sensor using native mass spectrometry

Wednesday 25th October

- 09.00-09.35 **T11 Lan Huang** (UC Irvine, California, USA), Uncovering the molecular details underlying the regulation of the Human 26S Proteasome by cross-linking mass spectrometry
- 09.35-09.55 **T12 Carla Schmidt** (Martin Luther University Halle-Wittenberg, Germany), The synaptic vesicle cycle is governed by heterogeneous and macromolecular protein microdomains.
- 09.55-10.00 **PT13 Yi Shi** (University of Pittsburgh School of Medicine, Pittsburgh, PA) Integrative Structural Proteomics of an Organelle Sized Assembly
- 10.00-10.05 **PT14 Lukas Slavata** (Institute of Microbiology CAS, Prague, Czech Republic), Transcription factor-DNA interaction studied by structural mass spectrometry
- 10.05-10.10 **PT15 Antonio Calabrese** (University of Leeds, UK), Insights into outer membrane protein biogenesis from structural mass spectrometry
- 10.10-10.15 **PT16 Julian Bender** (Martin Luther University Halle-Wittenberg, Germany), Structural dynamics and flexibility of the neuronal calcium-sensor Synaptotagmin-1
- 10.15-10.20 **PT17 Kai-Michael Kammer** (University of Konstanz, Germany), Using cross-linking mass spectrometry and integrated modelling to study the architecture of macromolecular complexes
- 10.20-10.25 **PT18 Cecilia Emanuelsson** (Lund University, Sweden), Structural model of the oligomeric human molecular chaperone DNAJB6 comprised of dimers and a site for interaction with aggregation-prone peptides at the dimer interface
- 10.25-10.30 **PT19 Gianluca Degliesposti** (University of Cambridge, UK) Structural, biochemical and XL-MS investigation of Timeless-Tipin interactions
- 10.30-11.00 **Coffee**
- 11.00-11.35 **T13 Kostantinos Thalassinoss** (University College London, UK). Combining native, ion mobility and crosslinking mass spectrometry to study protein structure and dynamics.
- 11.35-11.55 **T14 Fan Liu** (FMP, Berlin, Germany), Developing structural interactomics and its application in cell biology.
- 11.55-12.15 **T15 Charlotte Uetrecht** (Heinrich Pette Institute, Hamburg, Germany), Hitting proteins with a sledgehammer - structural characterization in XFELs.
- 12.15-12.20 **PT20 Manuel Matzinger** (University of Vienna, Austria) Enrichment strategy for cleavable cross-linking technology in living cells
- 12.20-12.25 **PT21 Andreas Linden** (Max Planck Institute for Biophysical Chemistry, Göttingen, Germany) Elucidating the Interactome of B-cell signaling proteins SYK and SLP65 of Homo sapiens and Gallus gallus by Cross-Linking Mass

Spectrometry

- 12.25-12.30 **PT22 Moriya Slavin** (The Hebrew University of Jerusalem, Israel) The use of LC-SDA for cross-linking and mass-spectrometry (XL-MS)
- 12.30-12.35 **PT23 Casimir Bamberger** (The Scripps Research Institute, USA) Covalent Protein Painting Evaluates Protein Surface Accessibilities in vivo
- 12.35-12.40 **PT24 Ebsen Trabjerg** (University of Copenhagen, Denmark), HDX-MS reveals a common binding surface for endogenous peptide- and protein ligands to the Sortilin receptor
- 12.40-12.45 **PT25 Mark Skehel** (MRC Laboratory of Molecular Biology, Cambridge, UK) Analysis of Escherichia coli ProQ RNA binding by HDX-MS
- 12.45-12.50 **PT26 Dominika Coufalova** (Regional Centre for Applied Molecular Oncology, Czech Republic) Study of structural changes of Reptin in dependence on ATP and Liddean (ATP-mimetic) by hydrogen deuterium exchange coupled to mass spectrometry.
- 12.50-12.55 **PT27 Martin Eisinger** (Max Planck Institute of Biophysics, Frankfurt am Main, Germany) New Insights into Secondary Active Transporters by Hydrogen/Deuterium - Mass Spectrometry
- 12.55-13.00 **PT28 Jasmin Dülfer** (Heinrich Pette Institute, Hamburg, Germany), Structural effects of glycan binding to norovirus capsid proteins studied by HDX MS
- 13.00-13.05 **PT29 Srinath Krishnamurthy** (KULeuven, Belgium) Structural basis of quiescence and activation of the translocase motor SecA: A paradigm for the regulation of molecular motors.
- 13.05-14.30 ***Lunch and posters***
- 14.30-15.05 **T16 Frank Sobott** (University of Leeds, UK), Dynamic protein structure: from protein disorder to membrane pores.
- 15.05-15.25 **T17 Dana Reichmann** (The Hebrew University of Jerusalem, Israel), Insights into (un)structure-function relationships of intrinsically disordered chaperones.
- 15.25-15.45 ***Coffee***
- 15.45-16.20 **T18 Jurgen Cox** (MPI for Biochemistry, Munich, Germany), Identification and quantification of cross-linked peptides in the MaxQuant software.
- 16.20-16.40 **T19 Saiful M. Chowdhury** (The University of Texas at Arlington, USA), Dual Cleavable Crosslinking Technology (DUCCT): A High Confidence Approach for Identifying Protein Crosslinking by Differential Tandem Mass Spectrometry
- 16.40-17.00 **T20 Florian Stengel** (University of Konstanz, Germany) Using cross-linking mass spectrometry to structurally probe protein complexes involved in signaling.
- 17.00 Concluding remarks

Poster Presentations

P1 Joanna Zamel (The Hebrew University of Jerusalem, Israel) Cross-Linking and Mass Spectrometry in Living Yeast Cells

P2 Antonia Vogel (IMP, Vienna), Structural and functional studies of the UNC45-myosin complex

P3 Ronja Pogan (Heinrich Pette Institute, Hamburg, Germany), Indications for strain dependent stability profiles in norovirus virus-like particles

P4 Anne Rehkamp (Martin Luther University Halle-Wittenberg, Germany) Structural Insights into Retinal Guanylyl Cyclase/GCAP-2 Interaction Obtained by Cross-linking/Mass Spectrometry

P5 C. Arlt (Martin Luther University Halle-Wittenberg, Germany) An Integrated Mass Spectrometry Based Approach to Probe the Structure of the Full-Length Wild-Type Tetrameric p53 Tumor Suppressor

P6 Marie Barth (Martin Luther University Halle-Wittenberg, Germany) Covalent labelling of proteins for structure elucidation

P7 Christian H. Ihling (Martin Luther University Halle-Wittenberg, Germany), Evaluation of a Deuterated (D12) Version of the MS/MS-Cleavable Cross-Linker Disuccinimidyl Dibutyric Urea (DSBU)

P8 Petra Darebná (Czech academy of sciences) In-situ enrichment and detection of biotinylated molecules using functionalized MALDI chips

P9 Gizem Dinler-Doganay (Istanbul Technical University, Turkey) Bag-1 isoforms interact differentially with cell survival pathway regulators and ERAD mechanism players to modulate cancer progression in breast cancer cells

P10 Marie V. Lukassen (Aarhus University, Denmark), Employing Liquid Chromatography, NH₂-Terminal Sequencing and Mass Spectrometry to Solve a Disulfide Bond Pattern

P11 František Filandr (Czech academy of sciences) How Cellobiose Dehydrogenase and Lytic Polysaccharide Monooxygenase Orchestrate Cellulose Degradation

P12 Petr Halada (Czech academy of sciences) Deciphering the influence of cellobiose dehydrogenase glycosylation pattern on its structure and function.

P13 Caroline Haupt (Martin Luther University Halle-Wittenberg, Germany), Proteoliposomes as a tool for structural analyses of membrane protein complexes

P14 Tommy Hofmann (Martin Luther University Halle-Wittenberg, Germany), Quantification of lipids in protein-lipid complexes

P15 Janine Kopicki (Heinrich Pette Institute, Hamburg, Germany), Investigating assembly of Ebola virus nucleoprotein and accessory proteins with native mass spectrometry

P16 Ruzena Liskova (Czech academy of sciences), Comparison of interactions of TEAD transcription factor with its DNA response elements from C-MYC exon and enhancer

P17 Jana Lorenz (Martin Luther University Halle-Wittenberg, Germany), Mass Spectrometry-Based Interaction Studies of FocA from Escherichia coli to Study its Influence for Formate Transport

P18 Petr Man (Czech academy of sciences), The utility of aspartic proteases in protein phosphorylation mapping

P19 **Eugen Netz** (MPI for developmental biology, Tübingen, Germany) OpenProXL: a fast and versatile XL-MS identification tool

P21 **Zsuzsanna Orbán-Németh** (IMP, Vienna) Structural prediction of protein models using distance restraints derived from chemical cross-linking mass spectrometry data

P24 **Pavla Vankova** (Czech academy of sciences), The role of hydrophobic interactions in the regulation of Hsp70 conformational transition

P25 **Dale Cooper-Shepherd** (Waters Corporation, UK), Native Ion Mobility Mass Spectrometry for the Characterization of Biotherapeutics

P26 **Malcolm Anderson** (Waters Corporation, UK), Implementation of hydrogen-deuterium exchange mass spectrometry for characterisation of peptide-receptive Major Histocompatibility Complex class I molecules

P27 **Şule Yılmaz** (MPI for Biochemistry, Munich, Germany), Development of software packages to MaxQuant for mass spectrometry-based chemical cross-linking studies

P28 **Federica Marini** (Catholic University, Rome) The Human Mitochondria Proteome: state of art and new challenges for Mass Spectrometry

P29 **Jaroslav Srp** (AS CR Prague) Potato Kunitz inhibitors evolved a novel non-canonical binding mode for serine proteases

P30 **Zhuo Chen** (TU Berlin) What more can cross-linking/Mass spectrometry tell us

P31 **F. O'Reilly** (TU Berlin) High-resolution protein structures by mass spectrometry and computational biology – science fiction or science reality?

P32 **Yulia Pivovarova** (Medical University of Vienna, Austria), Structural studies of a dimeric SET domain lysine methyltransferase from *Toxoplasma gondii*

P33 **Christine Piotrowski** (Martin Luther University Halle-Wittenberg, Germany), Cross-Linking and Mass Spectrometry Shed New Light on the bMunc13-2/Calmodulin Interaction

P34 **Iwan Parfentev** (MPI for biophysical chemistry, Goettingen, Germany), Characterization of protein-protein interactions in the synapse by chemical cross-linking mass spectrometry

P35 **Emma Stepanic** (MFPL, Vienna), Structural studies of centriole assembly in *Drosophila*

