

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 (ITEM-TWO)
- 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
- 17.00-18.00 First meeting of the Society for Structural Proteomics (Only PI)
- 18.15 Social Evening at Schweizerhaus (Buses are waiting at Viehmarktgasse)

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 Yilmaz** (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*