Organizing committee: Andrea Sinz Evgeniy Petrotchenko Christoph Borchers

Thursda	v November	19 <sup>th</sup> .	2015
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9:00 – 9:15	Welcome; <b>Michael Bron</b> , vice Principal Martin Luther University Halle-Wittenberg & Andrea Sinz, local organizer			
9:15 - 10:00	Michal Sharon (Weizmann Institute, Rehovot), Discovering a new subunit for an old complex by native mass spectrometry			
10:00 - 10:30	Petr Novak (Academy of Sciences, Prague), When X-ray crystallography fails: CD302 Antigen Structure via Mass Spectrometry			
	and NMR spectroscopy			
10:30 - 11:00	Coffee Break			

- 11:00 11:15 Charlotte Uetrecht (Leibniz Inst. Exp. Virol., Hamburg), Studying viral assemblies with mass spectrometry
- 11:15 11:30 **Carla Schmidt** (University of Oxford), Dimeric 13-Subunit Cytochrome C Oxidase is Stabilised by Lipids and Regulated by Post-translational Modifications
- 11:30 11:45 **Janne Jänis** (University of Eastern Finland), Ligand Binding Preference of a Macrolide Specific Repressor Protein MphR(E)
- 11:45 12:00 Nina Morgner (Frankfurt University), LILBID-MS on membrane protein complexes
- 12:00 12:15 Knut Kölbel (University of Antwerp), Conformational Properties of Gas Phase Protein Molecular Ions from a Thermodynamic Perspective
- 12:15 12:30 Marc Kipping (Waters), Extensive Charge Reduction and Dissociation of Intact Protein Complexes Following Electron Transfer on a Quadrupole-lon Mobility-Time-of-Flight MS
- 12:30 12:35 Poster Talk: **Dietmar Hammerschmid** (University of Antwerp), Structural characterization of the globin coupled sensor from Geobacter sulfurreducens (GsGCS) by using native mass spectrometry
- 12:35 12:40 Poster Talk: **Jingzhi Yang** (Proteome Center Rostock), From antibody structure function correlation to multiplexed immuno-assays
- 12:40 12:45 Poster Talk: Albert Konijnenberg (University of Antwerp), Extending structural proteomics to integral membrane proteins
- 12:45 14:30 Lunch and Poster Session
- 14:30 15:10 Franz Herzog (LMU Munich), Cross-Linking and Mass Spectrometry: Architecture and Mechanism of Chromatin-Associated Complexes
- 15:10 15:40 **Olaf Jahn** (MPI Exp. Med. Göttingen), Structural characterization of synaptic calmodulin complexes by photoaffinity labeling and mass spectrometry: the (everlasting) Munc13 story
- 15:40 16:00 Coffee Break
- 16:00 16:15 Nir Kalisman (Hebrew University of Jerusalem), Two years later The XL-MS model of the transcription pre-initiation complex revisited
- 16:15 16:30 **Alexander Leitner** (ETH Zurich), Monitoring large conformational changes in protein complexes with a dedicated quantitative cross-linking software pipeline
- 16:30 16:45 Jens Meiler (Vanderbilt University), De novo protein structure prediction from crosslinking data
- 16:45 16:50 Poster Talk: **Valentina D'Atri** (Univ. Bordeaux, INSERM), Structural characterisation of human telomeric G-quadruplexes by using Ion Mobility Mass Spectrometry (IM-MS) and Molecular Dynamics (MD) simulations
- 16:50 16:55 Poster Talk: Pavel Reichmann (IPB Halle), Description of an N-End Rule E3 Ligase Substrate Binding Site
- 16:55 17:00 Poster Talk: **Verena Tinnefeld** (ISAS Dortmund), Enrichment of cross-linked peptides from complex samples by charge-based fractional diagonal chromatography
- 17:45 18:45 City Night Tour through Halle (meet at Händel statue)
- 19:00 Dinner Palais S (Address: Ankerstraße 3c, 06108 Halle) with Live Music

## Friday, November 20th, 2015

9:00 – 9:40	Perdita Barran (The University of Manchester), Adventures with Disorder and Charge
9:40 - 10:10	Julia Chamot-Rouke (Institut Pasteur, Paris), Application of top-down mass spectrometry to microbial proteomics

- 10:10 10:40 Coffee Break
- 10:40 10:55 **Philip Lössl** (University of Utrecht), Integrating native (ion mobility) MS, cross-linking/MS and top-down proteomics to decipher the interplay between phosphorylation and interactions of the mitotic regulators Aurora A, Bora, and Plk1
- 10:55 11:10 **Stéphanie Deroo** (University of Brussels), Towards the receptor-active conformation of apolipoprotein E: a combined XL/MS and molecular dynamics study
- 11:10 11:25 **Nadine Harrer** (LMU Munich), The structural architecture of the chromatin remodeler ISWI determined by cross-linking and mass spectrometry
- 11:25 11:40 **Giambattista Guaitoli** (DZNE Tübingen), Crosslinking-MS analysis combined with molecular modelling provides novel insight into the domain architecture of the PD-associated protein kinase LRRK2
- 11:40 11:55 **Gert von Helden** (Fritz Haber Institute Berlin), Unzipping of gas phase proteins similar secondary structures at high charged states
- 11:55 12:10 **Tam Nguyen** (University of Copenhagen), A novel CE-MS interface for top-down MS analysis of proteins
- 12:10 12:15 Poster Talk: **Waldemar Hoffmann** (Fritz Haber Institute Berlin), Gas-Phase Infrared Spectroscopy of Ion Mobility-Selected Amyloid Intermediates
- 12:15 12:20 Poster Talk: **Melanie Göth** (Free University Berlin), Gas-Phase Microsolvation of Ubiquitin: Identification of Crown Ether Complexation Sites
- 12:20 12:25 Poster Talk: **Patrick Knight** (University of Leeds), Characterising the interaction of ataxin-3 and the poly-glutamine aggregation inhibitor QBP1
- 12:25 14:30 Lunch and Poster Session
- 14:30 15:00 **Kevin Pagel** (Free University Berlin), Separation of Oligosaccharide and Glycopeptide Isomers using Ion Mobility-Mass Spectrometry
- 15:00 15:15 Mathias Müller (Thermo Fisher Scientific), Analysis of Native Protein Complexes on a Benchtop Orbitrap Mass Spectrometer
- 15:15 15:30 **Dana Reichmann** (Hebrew University of Jerusalem), The nature and role of stress-regulated protein disorder in cellular proteostasis
- 15:30 15:45 **Pernille Foged Jensen** (University of Copenhagen), Dissecting the FcRn binding mode of antibodies with different pharmacokinetic profiles by hydrogen/deuterium exchange mass spectrometry

16:35 17:00	Farewell Coffee End of Symposium
16:30	WrbA multimerization Goodbye
16:25 – 16:30	assembly" algorithm Poster Talk: <b>Michal Rosulek</b> (Charles University Prague), From monomer to tetramer: Mass spectrometric study of protein
16:20 – 16:25	conformations of plant HOP2/MND1 Poster Talk: <b>Gabriel Mazzucchelli</b> (University of Liege), De novo sequencing using MELD proteolysis coupled to "sequence
16:15 – 16:20	resolution techniques Poster Talk: <b>Zsuzsanna Orban-Nemeth</b> (IMP Vienna), Comprehensive XL-MS reveals parallel orientation and versatile
16:10 – 16:15	and Peptide-Bound Major Histocompatibility Complexes by Hydrogen/Deuterium Exchange Mass Spectrometry Poster Talk: <b>Marcus Nagel</b> (UFZ Leipzig), First full-length Thyroid stimulating Hormone-Receptor structure elucidated by low
16:05 – 16:10	a Hydrogen/ Deuterium exchange Mass Spectrometry workflow Poster Talk: <b>Patrick Merkle</b> (University of Copenhagen) Studying the Interaction between Affinity Enhanced T-Cell Receptors
15:45 – 16:00 16:00 – 16:05	Ales Hnizda (Academy of Sciences, Prague), Integrative structural biology of relapsed-ALL specific cN-II mutants Poster Talk: Rasmus Jakobsen (University of Copenhagen), Implementation of online electrochemical reduction of proteins into

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Po	ost	eı	'S

S. Chatterjee

Fan Liu Biörn Häupl

**Konstanze Bosse** 

Michael Götze

**Lutz Fischer** 

D. Hammerschmid Structural characterization of the globin coupled sensor from Geobacter sulfurreducens (GsGCS) by using native mass

spectrometry

Jingzhi Yang From antibody structure - function correlation to multiplexed immuno-assays

Albert Konijnenberg Extending structural proteomics to integral membrane proteins

Valentina D'Atri Structural characterisation of human telomeric G-quadruplexes by using Ion Mobility Mass Spectrometry (IM-MS) and

Molecular Dynamics (MD) simulations

**Pavel Reichman** Description of an N-End Rule E3 Ligase Substrate Binding Site

Verena Tinnefeld Enrichment of cross-linked peptides from complex samples by charge-based fractional diagonal chromatography

**Waldemar Hoffmann** Gas-Phase Infrared Spectroscopy of Ion Mobility-Selected Amyloid Intermediates Melanie Göth Gas-Phase Microsolvation of Ubiquitin: Identification of Crown Ether Complexation Sites Characterising the interaction of ataxin-3 and the poly-glutamine aggregation inhibitor QBP1 Patrick Knight

Rasmus U. Jakobsen Implementation of online electrochemical reduction of proteins into a Hydrogen/ Deuterium exchange Mass

Spectrometry workflow

Merkle P.S. Studying the Interaction between Affinity Enhanced T-Cell Receptors and Peptide-Bound Major Histocompatibility

Complexes by Hydrogen/Deuterium Exchange Mass Spectrometry

First full-length Thyroid stimulating Hormone-Receptor structure elucidated by low resolution techniques M. B. M. Nagel Z. Orban-Nemeth Comprehensive XL-MS reveals parallel orientation and versatile conformations of plant HOP2/MND1

De novo sequencing using MELD proteolysis coupled to "sequence assembly" algorithm Gabriel Mazzucchelli From momomer to tetramer: Mass spectrometric study of protein WrbA multimerization M. Rosůlek

J. Lockhauserbäumer Norovirus infection pathway: glycan binding triggers structural changes

Johannes Heidemann Structural investigation of co-assembled clathrin adaptor protein complexes by native mass spectrometry **Boris Krichel** Quaternary structure of endolysin reveals how its activity is regulated by a secondary translation product Gili Ben-Nissan Native mass spectrometry as a tool to discover structural impairment of Parkinson's disease related proteins

Improving desolvation on q-tof instruments for native applications Jan Commandeur

Characterisation of Rip-2 kinase autophosphorylation and oligomeric state by mass spectrometry and crystallography Elisabetta Boeri Erba

IM-MS characterisation of protein therapeutics

Josephine Abi-Ghanem Effect of the non-canonical G•U wobble base pair on the binding mechanism of RNA kissing complexes Natàlia Carulla

SDS-PAGE analysis of Aβ oligomers is disserving research into Alzheimer's disease: appealing for ESI-IM-MS

E.Grifnée, G.Mazzuchelli Strutural characterisation of protein by using enzymatic reactor

**Tomas Jecmen** Expression of photo-reactive cytochrome b5 reductase for mapping its interaction surface with redox partner

cytochrome b5

Photo cross-linking via L-Photo-Met and MS to study the interaction of 14-3-3 with phosphorylated Raf peptide R. Ptackova

Miroslav Šulc The photo-initiated cross-linking via pMet and MS; the tool to study the protein-protein interactions

**Moritz Fischer** Synthesis of less hydrophobic Derivatives of MS/MS-Cleavable Cross-Linkers: Synthesis and Evaluation of Reactivity

for effective Protein Structure Analysis

**Christoph Hage** Dissociation behavior of bifunctional TEMPO-benzyl active ester for peptide structure analysis by free radical initiated

peptide sequencing (FRIPS) mass spectrometry in negative ion mode

Rico Schwarz Monitoring Conformational Changes in Peroxisome Proliferator-Activated Receptor β/δ by Cross-Linking/Mass

Spectrometry

**Christine Piotrowski** Structural Analysis of the bMunc13-2/Calmodulin Interaction by Cross-Linking and Mass Spectrometry

Proteome-wide profiling of the structure and interaction of protein assemblies by cross-linking mass spectrometry

Characterization of protein kinase D2 complexes by chemical cross-linking and mass spectrometry

SILAC-Based Secretome Analysis of Non-Small Cell Lung Cancer Cell Lines

C. U. Schräder A comprehensive look at the cross-linking pattern of human, bovine and frog elastin

Production and characterization of elastin-like biomaterial in vitro cross-linked by lysyl oxidase like 2 protein J. Wang

A.C. Mora Huertas Insights into the age-related changes in elastic fibers from skin

G. Rutsdottir, K. Bernfur Characterization of V181A, a dimeric Hsp21 mutant by SAXS and CXMS

Efficient Identification of Cross-Linked Peptides with StavroX and MeroX in Structural Proteomics

False Discovery Rate Estimation in Cross-Linking/Mass Spectrometry and application in Protein Structure

Determination

Möller, I.R. Applying Hydrogen-Deuterium Exchange Mass Spectrometry to Analyze the Dynamics and Drug Binding of the Human

Serotonin Transporter

Expanding the acid protease toolbox for H/D exchange Petr Halada

Michael O. Glocker Ion Mobility and Surface Topology Mapping Reveals the Cause of the Protein G'e - IgG Affinity Switch

Peter Højrup An Integrated Approach for Probing Protein Structure by Mass Spectrometry

Petr Man Transcription factor – DNA interaction studied by structural mass spectrometry Alan Kadek Maxime Bourguet Nicholas J. Bond Sandra Richter

Edwin De Pauw Leonhard H. Urner Gerard Comamala Sabrina Pfennig Christian Arlt Jiří Hausner Electrostatics-driven conformational dynamics of cellobiose dehydrogenase probed by structural mass spectrometry Structural MS for the characterization of yeast U3 snoRNP assembly

Structural and molecular studies of IL-33 disulphide isoforms

Proteomic identification of reinforcement- polarity dependently regulated synaptic proteins in an auditory learning paradigm in mice

Bottom-up and top-down high-throughput sequencing of toxins with pharmacological interest

Photoswitchable Nanocarriers for Gas Phase Membrane Protein Analysis

Studying Back-exchange Effects on Protein Analysis by Hydrogen/Deuterium exchange Mass Spectrometry

Regulation of the Chromatin Remodeler ISWI by its N-terminal domain

3D-Structural Characterization of the N- and C-terminal Regions of p53 by Combining Cross-Linking/MS and Native MS

Dynamics of chloride channel from E. coli studied by hydrogen/deuterium exchange



























