

Chemical Cross-Linking and Covalent Labeling: from Proteins to Cellular Networks

Organized by

Lan Huang
University of California, Irvine

Andrea Sinz Martin-Luther University Halle-Wittenberg, Germany

Richard Vachet
University of Massachusetts, Amherst

31st ASMS Sanibel Conference on Mass Spectrometry January 24 – 27, 2019 St. Petersburg, FL

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eSpectra

THURSDAY, JANUARY 24

4:00 - 7:00 pm **Setup all posters**, *Grand Bay Ballroom South*

6:00-7:00 pm **Registration**

7:00 – 7:05 pm

Opening Remarks, Lan Huang, Andrea Sinz & Richard Vachet *Grand Bay Ballroom North*

7:05 - 8:05 pm KEYNOTE LECTURE

Session Chair: Andrea Sinz

7:05-8:05 pm "Alternative Ways to Study Protein Interactions"; **Carol Robinson**, *University of Oxford*

8:05-10:00 pm Reception

Grand Bay Ballroom South

The following students received an ASMS Student Travel Award. Congratulations!

Jayanta Kishor Chakrabarty

University of Texas at Arlington

Hope Flaxman

Harvard University

Danté T. Johnson

University of Maryland Baltimore School of Pharmacy

Jin Joo Kang

Montreal Clinical research Institute/McGill University

Julia Kitaygorodsky

University of Toronto

Oleg Klykov

Utrecht University

Andrew Norris

The Ohio State University

Daniel Polasky

University of Michigan

Esben Trabjerg

ETH Zurich

Sabine Wittig

Universität Halle-Wittenberg, Halle (Saale)

Bingqing Zhao

Indiana University Bloomington

Daniel Ziemianowicz

University of Calgary

FRIDAY, JANUARY 25

7:00 - 8:30 am **Continental Breakfast**, *Grand Bay Ballroom South*

8:30-10:00 am Developing Cross-linking Mass Spectrometry to Delineate Protein Structures Session Chair: Philip Andrews Grand Bay Ballroom North	
8:30-9:00 am	"Protein Structure Prediction by the Combined Approach of Short Distance Crosslinking and Discret Molecular Dynamics"; Christoph Borchers , <i>University of Victoria</i> , <i>Canada</i>
9:00-9:30 am	"Improving Mass Spectrometry Analysis of Protein Structures with Arginine-Selective Chemical Cross-linkers"; Meng-Qiu Dong , <i>National Institute of Biological Sciences</i> , <i>China</i>
9:30-10:00 am	"Cross-linking/Mass Spectrometry Workflows Based on MS-Cleavable Cross-Linkers and the MeroX Software for Studying Protein Structures and Protein-Protein Interactions"; Andrea Sinz , <i>Martin Luther University Halle-Wittenberg</i>
10:00-10:15 am	Coffee Break, Grand Bay Ballroom South

10:15-11:45 am
Developing Cross-Linking Mass Spectrometry to Delineate Protein Structures
Session Chair: James Bruce

Session Chair: James Bruce	
10:15-10:45 am	"Cross-Linking Mass Spectrometry Strategies to Define Interaction and Structural Dynamics of Protein Complexes"; Lan Huang , <i>University of California</i> , <i>Irvine</i>
10:45-11:15 am	"Kinetochore Assembly and Function: Insights by Chemical Crosslinking and Mass Spectrometry"; Franz Herzog , <i>Ludwig-Maximilians-Universität München</i>
11:15-11:45 am	"Compositional Dynamics of Protein Complexes"; Natalie Romanov , <i>EMBL Heidelberg</i>
11:45-Noon	Group Photo
Noon - 1:15 pm	Group Lunch, provided by ASMS St. Petersburg I & II

FRIDAY, JANUARY 25

	1:15-3:15 pm Oxidative Labeling Session Chair: Ian Webb
1:15-1:45 pm	"Oxidative Footprinting and Crosslinking for Determining Protein/Protein and Protein/Peptide Interfaces"; Michael Gross , <i>Washington University</i>
1:45-2:15 pm	"Structure and Dynamics of Macromolecules Using Footprinting"; Mark Chance, Case Western Reserve University
2:15-2:45 pm	"Reproducibility and Robustness in FPOP: the Need for Community Standards for Radical Dosimetry"; Josh Sharp , <i>University of Mississippi</i>
2:45-3:15 pm	"Functional Implications of Protein Oxidation: Turning Cytochrome C into an Apoptotic Peroxidase"; Lars Konermann , <i>Western University, Canada</i>
3:15-7:00 pm	Free Time, we recommend the world-renowned Dali Museum, even if you do not like his art the venue is worth a visit, located two blocks south of the Hilton.
	7:00-7:45 pm KEYNOTE LECTURE Session Chair: Richard Vachet
7:00-7:45 pm	"Surveying and Mapping Macromolecular Cellular Terrains"; Brian Chait , Rockefeller University
	7:45-8:00 pm 3-Minute Poster Flash Talks Session Chair: Richard Vachet
7:45-7:48 pm	Heather O'Neill ; Poster #31: "Aptamer-Based Affinity Labeling Identifies a Surface Spliceosomal Complex that When Internalized Induces Aberrant Splicing and Cell Death in B-Cell-Lymphoma Cells"
7:48-7:51 pm	Esben Trabjerg ; Poster #35: "Feasibility of Succinimidyl-Based Crosslinking at Slightly Acidic Conditions"
7:51-7:54 pm	Sabine Wittig; Poster #41: "Cross-Linking Intact Synaptic Vesicles Reveals Protein Interactions Networks that Mediate Membrane Fusion in the Neuronal Synapse"
7:54-7:57 pm	Jayanta Kishor Chakrabarty ; Poster #11: "High Confidence Identification of Protein Cross-Linking by Next Generation Dual Cleavable Cross-Linking Technology (DUCCT)"
7:57-8:00 pm	Bingqing Zhao ; Poster #45: "Multiple Dissociation Methods in Conjunction with an ETD Cleavable Cross-Linker Facilitate the Identification of Cross-Linked Peptides"

8:00-10:00 pm
Poster Session I & Reception
Odd-Numbered Posters Present
Grand Bay Ballroom South

SATURDAY, JANUARY 26

7:00 - 8:30 am Continental Breakfast, Grand Bay Ballroom South

	8:30-10:30 am Software Development and Structural Modeling Session Chair: Carla Schmidt Grand Bay Ballroom North
8:30-9:00 am	"Incorporating XlinkX into Integrative Structural Biology"; Albert Heck , <i>University of Utrecht</i>
9:00-9:30 am	"The MaxQuant Software for Cross-Linking/Mass Spectrometry"; Jürgen Cox , MPI Martinsried
9:30-10:00 am	"Reliable Identification of Cross-Links with Non-Cleavable Linkers", Robert Chalkley , <i>University of California, San Francisco</i>
10:00-10:30 am	"Macromolecular Structure and Dymamics Based on Cross-Links"; Dina Schneidman , <i>Hebrew University</i>
10:30-10:45 am	Coffee Break, Grand Bay Ballroom South
	10:45-11:45 am 15-Minute Short Talks Session Chair: Michael Sussman
10:45-11:00 am	Mark Larance; Poster #28: "Global Liver Protein Crosslinking Reveals a Direct Interaction between the RISC Complex and the Ribosome"
11:00-11:15 am	Rosa Viner ; Poster #38: "Protein Complex Dynamics Using Quantitative Cross-Linking Mass Spectrometry"
11:15-11:30 am	Saiful Chowdhury ; No Poster "Toll-Like Receptor 2 Interactome by Mass Spectrometry-Based Co-Immunoprecipitation (Co-IP) Crosslinking Proteomics"
11:30-11:45 am	Julian Mintseris ; Poster #30: "High-Density Chemical Cross-Linking for Modeling Protein Interactions"
11:45-1:00 pm	Lunch on your own

We recommend the eclectic Saturday Market, located one block north of the Hilton.

SATURDAY, JANUARY 26

1:00-2:30 pm in vivo Labeling and Analysis of Cellular Networks Session Chair: Henning Urlaub Grand Bay Ballroom North	
1:00-1:30 pm	"Quantitative Interactome Dynamics: A Look under the Hood"; Jim Bruce , <i>University of Washington, Seattle</i>
1:30-2:00 pm	"In-Cell Footprinting for Proteome-Wide Structural Biology"; Lisa Jones , <i>University of Maryland</i>
2:00-2:30 pm	"Proximity Proteomics: from Organelles to Complexes"; Anne-Claude Gingras , Lunenfeld-Tanenbaum Research Institute, Canada

	2:30-3:00 pm 15-Minute Short Talks Session Chair: Meng-Qiu Dong
2:30-2:45 pm	Casimir Bamberger ; Poster #4: "Covalent Protein Painting Reveals Aberrant Protein Folding in Cells and Tissues <i>in vivo</i> "
2:45-3:00 pm	Haiyuan Yu ; Poster #46: "MaXLinker: an Innovative "MS3-Centric" Proteome-Wide Cross-Link Search Engine with High Specificity and Sensitivity"
3:00-7:00 pm	Free Time

SATURDAY, JANUARY 26

7:00-7:30 pm		
	15-Minute Short Talks	
	Session Chair: Huilin Li	
7:00-7:15 pm	Ryan Bomgarden ; Poster #8: "Right Tools for the Job: New compounds and Sample Preparation Reagents for Studying Chemically Cross-Linked Proteins"	
7:15-7:30 pm	Gianluca Degliesposti ; Poster #16: "Cross-Linking and Mass Spectrometry for the Structural and Functional Investigation of the 3'-End mRNA Cleavage and Polyadenylation Factor (CPF)"	

7:30-7:51 pm		
3-Minute Poster Flash Talks Session Chair: Huilin Li		
7:30-7:33 pm	Therese Dau ; Poster #14: "Sequential Digestion with Trypsin and Elastase Improves Sequence Coverage in Cross-Linking/Mass Spectrometry"	
7:33-7:36 pm	Christian Tüting; Poster #36: "Structural Insight into the Polyadenylation Complex"	
7:36-7:39 pm	Laurence Angel ; Poster #2: "Weak Acid-Base Interactions of Histidine and Cysteine Affect the Charge States, Tertiary Structure, and Zn(II) Labeling of HeptaPeptides"	
7:39-7:42 pm	Mowei Zhou ; Poster #48: "Pseudo-Enzyme PDX1.2 and Its Interaction with Active Analogs Explored with Native Mass Spectrometry"	
7:42-7:45 pm	Marshall W. Bern; Poster #6: "How the Flu Takes Off Its Coat: Cross-Linking Study of pH-Induced Changes of the Influenza A Virus Matrix Layer"	
7:45-7:48 pm	Ann English ; Poster #18: "Profiling Oxidative Proteoforms to Discover New Redox Functions of Proteins in Cells: the Case of Cytochrome C Peroxidase".	
7:48-7:51 pm	Oleg Klykov; Poster #26: " <i>in-situ</i> Crosslinking Mass Spectrometry Provides a High-Resolution Structural Model of Fibrin Clots"	

8:00-10:00 pm
Poster Session II & Reception
Even-Numbered Posters Present
Grand Bay Ballroom South

SUNDAY, JANUARY 27

7:00 - 8:30 am **Continental Breakfast**, *Grand Bay Ballroom South*

7.00 - 0.30 am	Continental Dicartast, Grana Bay Banroom Soun
	8:30-10:00 am Defining Protein Aggregates/Complexes Session Chair: Anne-Claude Gingras Grand Bay Ballroom North
8:30-9:00 am	"Insight into beta-2-Microglobulin Amyloid Formation and Inhibition Using Covalent Labeling Mass Spectrometry"; Richard Vachet , <i>University of Massachusetts</i>
9:00-9:30 am	"Diazirine-Based Reagents for Structural Mass Spectrometry of Complex Systems"; David Schriemer , <i>University of Calgary, Canada</i>
9:30-10:00 am	"Methods and Applications for the Thermodynamic Analysis of Protein-Ligand Complexes on the Proteomic Scale"; Michael Fitzgerald , <i>Duke University</i>
10:00-10:15 am	Coffee Break, Grand Bay Ballroom South
10:15-11:15 am	
	Defining Protein Aggregates/Complexes (Continued)
	Session Chair: Anne-Claude Gingras

	Defining Protein Aggregates/Complexes (Continued) Session Chair: Anne-Claude Gingras
10:15-10:45 am	"Structural Basis of Cullin-RING E3 Ligase Regulation by the COP9 Signalosome Using Integrative Mass Spectrometry"; Argyris Politis , <i>King's College London</i>
10:45-11:15 am	"Integrating Surface-Induced Dissociation into a Native MS Workflow"; Vicki Wysocki , <i>Ohio State University</i>

11:15-12:15 pm	
KEYNOTE LECTURE	
Session Chair: Lan Huang	

11:15-12:15 pm	"Towards the Modular Proteotype", Ruedi Aebersold , <i>ETH</i>
12:15-12:30 pm	Closing Remarks, Lan Huang, Andrea Sinz & Richard Vachet
12:30 pm	Remove all posters

- Utility of Covalent Labeling Mass Spectrometry Data in Protein Structure Prediction with Rosetta; Melanie Aprahamian¹; Emily Chea²; Lisa Jones²; Steffen Lindert¹; ¹Ohio State University, Columbus, OH; ²University of Maryland, Baltimore, MD
- Weak Acid-Base Interactions of Histidine and Cysteine Affect the Charge States, Tertiary Structure, and Zn(II) Labeling of HeptaPeptides; Laurence Angel¹; Yu-Fu Lin¹; Enas N Yousef¹; ¹Texas A&M University Commerce, Commerce, TX
- 3 Energy Barriers to the Pre-amyloid Structural Change of β-2-microglobulin under Amyloid Forming Conditions Studied by Covalent Labeling and Mass Spectrometry; Robert Vaughan¹, Akshada Abhyankar¹, Jamie Canderan¹, Eric Graban², John Hale³; ¹Indiana University, Bloomington, IN, ²QuarryBio, LLC, Tallahassee, FL, ³QuarryBio, LLC, Klamath Falls. OR
- 4 Covalent Protein Painting Reveals Aberrant Protein Folding in Cells and Tissues in vivo;

 <u>Casimir Bamberger</u>¹; Sandra Pankow¹; Salvadore Martínez-Bartolomé¹; John R Yates III¹;

 <u>Iscripps Research Institute</u>, La Jolla, CA
- Chemical Labelling of Proteins for Structure Elucidation and Determination of the Protein Orientation within Membranes; Marie Barth¹; Julian Bender¹; Andy Lau²; Argyris Politis²; Carla Schmidt¹; Interdisciplinary Research Center HALOmem, Charles Tanford Protein Center, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany; ²Department of Chemistry, Kings College London, London, United Kingdom
- How the Flu Takes Off Its Coat: Cross-Linking Study of pH-Induced Changes of the Influenza A Virus Matrix Layer; Lisa Selzer¹; Jasmine Moshiri¹; Ryan Leib¹; Allis Chien¹; Fang Liu¹; Kratika Singhal¹; Rowan Matney¹; Wilfred Tang²; Marshall W. Bern²; Karla Kirkegaard¹; Istanford University, Stanford, CA; Protein Metrics, Cupertino, CA
- Protein Interactions in Bacterial Biofilm Matrix Studied by Cross-Linking Mass Spectrometry; Chengzhi Cai¹; Guoting Qin¹; Pengzhi Zhang¹; ¹University of Houston, Houston, TX
- Right Tools for the Job: New Compounds and Sample Preparation Reagents for Studying Chemically Cross-Linked Proteins; Ryan Bomgarden¹; Leigh Foster¹; Erum Raja¹; Chris Etienne¹; Rosa Viner²; John Rogers¹; ThermoFisher Scientific, Rockford, IL; ²ThermoFisher Scientific, San Jose, CA
- 9 **Quantitative, Comprehensive, and Ultra-Sensitive Protein Footprinting in Living Cells**; Jenna G. Caldwell; Joshua E. Elias; Pehr A. B. Harbury; *Stanford University, Stanford, CA*
- 10 Electrochemistry-Assisted Mass Spectrometric Absolute Quantification without the Use of Standards; <u>Hao Chen</u>; New Jersey Institute of Technology, Newark, NJ
- High Confidence Identification of Protein Cross-Linking by Next Generation Dual Cleavable Cross-Linking Technology (DUCCT); Jayanta Kishor Chakrabarty¹; Abu Hena M Kamal¹; Saiful M. Chowdhury¹; ¹University of Texas, Arlington, Arlington, TX

- Implementation of Single Residue Resolution HDX-MS Data for Protein Modeling in SURPASS and CABS Algorithms; Dominik Cysewski¹; Aleksandra Badaczewska-Dawid²; Michal Burdukiewicz³; Michal Kistowski¹; Katarzyna Dabrowska¹; Michal Dadlez¹; ¹Institute of Biochemistry and Biophysics, Polish Academy of Sciences, Warsaw, Poland; ²Faculty of Chemistry, University of Warsaw, Wroclaw, Poland; ³Warsaw University of Technology, Warsaw, Poland
- Sequential Digestion with Trypsin and Elastase Improves Sequence Coverage in Cross-Linking/Mass Spectrometry; Therese Dau¹; Kapil Gupta²; Imre Berger²; Juri Rappsilber^{1, 3}; ¹University of Edinburgh, Edinburgh, United Kingdom; ²University of Bristol, Bristol, United Kingdom; ³Technische Universität Berlin, Berlin, Germany
- Protein Visualization Using Trihalo Compounds; Rabab ElMergawy¹; Gianluca Triolo¹; Michael Myers¹; Protein Networks Group, International Centre for Genetic Engineering and Biotechnology (ICGEB), Trieste, 34149, Italy
- Cross-Linking and Mass Spectrometry for the Structural Investigation of the 3'-end mRNA Cleavage and Polyadenylation Factor (CPF); Gianluca Degliesposti¹; Sarah L Maslen¹; Chris H Hill²; Lory A Passmore¹; Mark J Skehel¹; ¹MRC Laboratory of Molecular Biology, Cambridge, United Kingdom; ²Department of Pathology, University of Cambridge, Cambridge, United Kingdom
- 17 **Structural Proteomics through Photo-Affinity Labeling Mass Spectrometry: Studies with the FKBP12-rapamycin-FRB Ternary Complex**; <u>Hope A Flaxman</u>¹; Chia-Fu Chang¹; Hung-Yi Wu¹; Carter Nakamoto¹; Christina M Woo¹; ¹Harvard University, Cambridge, MA
- Profiling Oxidative Proteoforms to Discover New Redox Functions of Proteins in Cells: the Case of Cytochrome c Peroxidase; Ann M English; Concordia University, Montreal, QC
- 19 **Developing Quantitative Chemical Labeling Strategies to Characterize Biopharmaceutical Protein Aggregation Using Mass Spectrometry Analysis**; M. Cyndell Gracieux; Sarah
 Ballance; Jack Thomas, Michael B. Goshe; *North Carolina State University, Raleigh, NC*
- An Integrated One-Week Protocol for Proteome-Wide Cross-Linking/Mass Spectrometry Studies Based on the MS-Cleavable Cross-linker DSBU and the MeroX 2.0 Software; Claudio Iacobucci¹; Michael Götze¹; Christine Piotrowski¹; Christian Ihling¹; Andrea Sinz¹;

 *Imartin Luther University Halle-Wittenberg, Halle (Saale), Germany
- Evaluation of an Isotope-Labeled MS/MS-Cleavable Cross-Linker for Protein Structure Analysis; Patrizia Springorum¹; Michael Götze²; Christoph Hage¹; Christian Ihling¹; Mathias Schäfer³; Andrea Sinz¹; ¹Martin Luther University Halle Wittenberg, Halle (Saale), Germany; ²ETH Zurich, Zürich, Switzerland; ³University of Cologne, Cologne, Germany
- The Role of Aliphatic Side Chains in Sculpting the Folding Free Energy Landscape of TIM Barrel Proteins across Evolutionary Time; Rohit Jain¹; Khaja Muneeruddin^{1, 2}; Scott A Shaffer^{1, 2}; C. Robert Matthews¹; Department of Biochemistry and Molecular Pharmacology, University of Massachusetts Medical School, Worcester, MA; Proteomics and Mass Spectrometry Facility, University of Massachusetts Medical School, Shrewsbury, MA

- Innovation of a Novel Pulse-Chase in Cell Footprinting Method for the Study of Protein Folding Phenomena; <u>Dante T Johnson</u>¹; Lisa M Jones¹; Benjamin Punshon-Smith²; Anne Gershenson³; ¹University of Maryland Baltimore School of Pharmacy, Baltimore, MD; ²University of Maryland Baltimore County, Baltimore, MD; ³University of Massachusetts Amherst, Amherst, MA
- Functional and Structural Mechanism of Drosophila PRC1 with Chromatin Assembly across the Cell Cycle; Jin Joo Kang; IRCM, Montreal, QC
- Mapping of Protein Interactions through Protein Crosslinking Coupled to in vivo Protein Tagging.; Julia Kitaygorodsky^{1, 2}; Brett Larsen¹; Cassandra Wong¹; Payman Samavarchi Tehrani¹; Amber Couzens¹; Anne-Claude Gingras^{1, 2}; ¹Lunenfeld-Tanenbaum Research Institute, Toronto, ON; ²Department of Molecular Genetics, University of Toronto, Toronto, ON
- *in-situ* Crosslinking Mass Spectrometry Provides a High-Resolution Structural Model of Fibrin Clots; Oleg Klykov^{1, 2}; Sander A. B. Meijer^{1, 3}; Albert J.R. Heck^{1, 2}; Ricahrd A. Scheltema^{1, 2}; ¹Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht, Netherlands; ²Netherlands Proteomics Center, Utrecht, Netherlands; ³Depar
- Hydroxyl Radical Footprinting with PLIMB (Plasma-Induced Modification of Biomolecules) Identifies Structural Changes upon EGFR Dimerization; Benjamin Minkoff¹; Joshua M. Blatz¹; Daniel Benjamin¹; Faraz A. Choudhury¹; J. Leon Shohet¹; Michael R. Sussman¹; ¹University of Wisconsin, Madison, WI
- Global Liver Protein Crosslinking Reveals a Direct Interaction between the RISC complex and the Ribosome; Isobel Tenison-Collins¹; Dylan J Harney¹; Andrew Giltrap¹; Richard Payne¹; Mark Larance¹; ¹The University of Sydney, Sydney, Australia
- 29 Enrichment of Crosslinked Peptides Post-Digestion Using Desthiobiotin Tagged
 Symmetrical Crosslinker; Victoria Sanchez¹; Stephan Uebel¹; Nagarjuna Nagaraj¹; MaxPlanck
 Institute for Biochemistry, Munich, Germany
- 30 **High-Density Chemical Cross-Linking for Modeling Protein Interactions**; <u>Julian Mintseris</u>¹; Steven P Gygi¹; ¹Harvard Medical School, Boston, MA
- Aptamer-Based Affinity Labeling Identifies a Surface Spliceosomal Complex that When Internalized Induces Aberrant Splicing and Cell Death in B-Cell-Lymphoma Cells; Heather O'neill¹; Vaishali Pannu¹; Sonal Tonapi¹; Janet Duncan¹; Mathew Rosenow¹; Anthony Helmstetter¹; Daniel Magee¹; Qing Zhang¹; Teresa Tinder¹; Melissa Richards¹; Michael Famulok²,³; David Spetzler¹; Mark Miglarese¹; Günter Mayer²,⁴; ¹Caris Life Sciences, Phoenix, AZ; ²LIMES Program Unit Chemical Biology & Medicinal Chemistry, University of Bonn, Bonn, Germany; ³Chemical Biology Max-Planck-Fellowship Group, Center of Advanced European Studies and Resea
- Use of Chemical Modification and Native Mass Spectrometry to Investigate the Assembly of Archaeal RNase P, a Catalytic Ribonucleoprotein Complex; Andrew Norris¹; Hong-Duc Phan¹; Stella Lai¹; Venkat Gopalan¹; Vicki Wysocki¹; ¹The Ohio State University, Columbus, OH
- Global Profiling of Protein-Protein Interactions in *E. coli* Biofilms Using Crosslinking-based Mass Spectrometry; Lolita Piersimoni¹; Janet Price¹; Matthew Chapman¹; Peter Freddolino¹; Philip C Andrews¹; *¹University of Michigan, Ann Arbor, MI*

- 34 Broadening the Repertoire of CID-Cleavable Crosslinkers: MC4 Characterization and Structural Analysis of GPCR Complexes; Manolo David Plasencia¹; Qiuyan Chen²; Lolita Piersimoni¹; John JG Tesmer²; Philip C Andrews¹; ¹University of Michigan, Ann Arbor, MI; ²Purdue University, West Lafayette, IN
- Feasibility of Succinimidyl-Based Crosslinking at Slightly Acidic Conditions; Esben <u>Trabjerg</u>¹; Alexander Leitner¹; Institute of Molecular Systems Biology, Department of Biology, ETH Zurich, Zurich, Switzerland
- 36 **Structural Insight into the Polyadenylation Complex**; Christian Tüting; Martin Luther University Halle Wittenberg, Halle (Saale), Germany
- Covalent Labeling Modulates Intact Protein Fragmentation: Towards a Combined Analysis of Intact Protein Sequence and Structure; <u>Daniel A Polasky</u>¹; Michael Keating^{1, 2}; Sugyan M Dixit¹; Philip C Andrews¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI; ²University of Texas, Austin, Austin, TX
- Protein Complex Dynamics Using Quantitative Cross-linking Mass Spectrometry; Rosa Viner¹; Terry Zhang¹; Leigh A Foster²; Ryan Bomgarden²; Kai Fritzemeier³; Frank Berg³;

 ThermoFisher Scientific, San Jose, CA; ThermoFisher Scientific, Rockford, IL; Thermo Fisher Scientific, Bremen, Germany
- Flash Oxidation (FOX): A New and Improved Platform for Biopharmaceutical Hydroxyl Radical Protein Foot-printing Higher Order Structural Analysis; Scot R Weinberger¹; Ron C Orlando^{1, 2}; Joshua S Sharp^{1, 3}; GenNext Technologies, Inc., Montara, CA; University of Georgia, Athens, GA; University of Mississippi, Oxford, MS
- 40 **Developing Cross-linking Mass Spectrometry (XL-MS) to Delineate Protein Interaction Landscapes in Living Cells**; Andrew Wheat¹; Clinton Yu²; Xiaorong Wang²; Lan Huang²;

 ¹University of California, Irvine, Irvine, CA; ²Department of Physiology and Biophysics, Irvine, CA
- 41 Cross-Linking Intact Synaptic Vesicles Reveals Protein Interactions Networks that Mediate Membrane Fusion in the Neuronal Synapse; Sabine Wittig¹; Marcelo Ganzella²; Susann Kostmann¹; Ángel Pérez-Lara²; Reinhard Jahn²; Carla Schmidt¹; ¹Universität Halle-Wittenberg, Halle (saale), Germany; ²Department of Neurobiology, Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany
- 42 Universal Extraction of Crosslinked Peptides from Linear Peptide Backgrounds via Orthosift; Bjorn-Erik Wulff; Stanford University, Stanford, CA
- Optimized Fragmentation Strategies for Maximizing Identification of Cross-Linked Peptides Using Sulfoxide-Based MS-Cleavable Reagents; Clinton Yu¹; Lan Huang¹;

 Iniversity of California, Irvine, Irvine, CA
- 44 **High-Throughput Quantitative Top-Down Proteomics in Complex Samples using Protein- Level Tandem Mass Tag (TMT) Labeling**; <u>Dahang Yu</u>¹; Zhe Wang¹; Qiang Kou²; Kenneth Smith³; Xiaowen Liu²; Si Wu¹; ¹University of Oklahoma, Norman, OK; ²Indiana University-Purdue University Indianapolis, Indianapolis, IN; ³Oklahoma Medical Research Foundation, Oklahoma City, OK

- Multiple Dissociation Methods in Conjunction with an ETD cleavable Cross-Linker Facilitate the Identification of Cross-Linked Peptides; Bingqing Zhao¹; Colin P. Reilly¹; James P. Reilly¹; Indiana University, Bloomington, IN
- MaXLinker: an Innovative "MS3-Centric" Proteome-Wide Cross-Link Search Engine with High Specificity and Sensitivity; Haiyuan Yu; Cornell University, Ithaca, NY
- 47 A Comprehensive Analytical Routine for Enhanced Mapping of Protein Surfaces Using Carbene-Based Labeling Methods; <u>Daniel S Ziemianowicz</u>¹; David C Schriemer¹; ¹University of Calgary, Calgary
- 48 **Pseudo-Enzyme PDX1.2 and its Interaction with Active Analogs Explored with Native Mass Spectrometry**; Irina V Novikova¹; <u>Mowei Zhou</u>¹; Jared B Shaw¹; Hanjo Hellmann²; James E Evans¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Washington State University, Pullman, WA
- Covalent Labeling and Mass Spectrometry for Epitope Mapping of Monoclonal Antibodies Against TNF; Robert Vaughan¹, Akshada Abhyankar¹, Jamie Canderan¹, Eric Graban², John Hale³; ¹Indiana University, Bloomington, IN, ²QuarryBio, LLC, Tallahassee, FL USA, ³QuarryBio, LLC, Klamath Falls. OR