

LAKE LOUISE XXIX

29th Workshop on Tandem Mass Spectrometry

THURSDAY, DECEMBER 1

8:00 Introductory Remarks: *Lars Konermann*

Ion Mobility MS/MS Chair: *Kristina Håkansson*

8:10 **Chris Hogan**, Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN
“Monitoring and Modeling Adsorption in the Gas and Liquid Phases via Ion Mobility Spectrometry”

8:35 **Matt Bush**, Department of Chemistry, University of Washington, Seattle, WA
“TBA”

9:00 *Nicole D. Wagner* and **David H. Russell**, Department of Chemistry, Texas A&M University, College Station, TX
“Defining Non-Covalent Ubiquitin Homodimer Interfacial Interactions through Comparisons with Covalently-Linked Diubiquitin”

9:25 **Helen Cooper**, School of Biosciences, University of Birmingham, Birmingham, UK
“Differential ion mobility and top-down mass spectrometry for the analysis of proteins from complex biological samples”

9:50 Coffee Break
Victoria Ballroom

Proteins: Structure and Dynamics (Part 1)

Chair: *Gary Glish*

10:20 **Brandon Ruotolo**, University of Michigan, Ann Arbor, MI
“New Ion Mobility-Mass Spectrometry Techniques for the Rapid Analysis of Protein Sequence, Structure and Stability”

10:40 **Francisco Fernandez-Lima**, Florida International University
“Advantages of TIMS-TOF MS and TIMS-FT-ICR MS for Complex Mixture Analysis and Structural Biology”

11:00 **Lekha Sleno**, Université du Québec à Montréal, Montréal, QC
“Quantitation of acetaminophen protein binding in human plasma”

11:20 **Kristina Hakansson**, University of Michigan, Ann Arbor, MI
“Tandem Mass Spectrometry Approaches to the Elucidation of Sulfur-Associated Protein Modifications”

11:40 **Christoph Borchers**, University of Victoria - Genome BC Proteomics Centre, Victoria, BC
“Solving Protein Structures by Cross Linking - Discrete Molecular Dynamics”

12:00 Discussion and **Workshop group picture**

12:15 to 13:30 Lunch

Fairview Dining Room

Endogenous Peptides Chair: **Peter Verheart**

14:00 Introductory Remarks: **Peter Verheart**

14:05 **Lingjun Li**, University of Wisconsin, Madison, WI
“Enabling Large-Scale Discovery, Characterization and Quantitation of Neuropeptides via Tandem Mass Spectrometry”

14:30 **Paul Thomas**, Northwestern University, Chicago, IL
“Top Down Proteomics in the Age of Proteoforms”

14:55 **Geert Baggerman**, University of Antwerp, Antwerp, Belgium
“Micro peptides as a new class of bio-active peptides in higher eukaryotes”

15:20 **Luuk van Oosten**, Heidelberg University, Heidelberg, Germany
“Tandem MS structure elucidation of disulfide containing peptides from ant venom after determining their S-engendered mass defect and isotope shift using high resolution MS”
Lake Louise Student Travel Award Winner

15:40 Coffee Break

Victoria Ballroom

Bio-Applications, Proteomics Chair: **David Schriemer**

16:10 **Daniel Lopez Ferrer**, Thermo Fisher Scientific, San Jose, CA
“Applications of UVPD for Top Down Proteomics on an Orbitrap Fusion Lumos Mass Spectrometer”

16:30 **Arash Zarrine-Afsar**, University of Toronto, Toronto, ON
“Rapid Detection of Breast Cancer with an Optimized MS Analysis Workflow”

- 16:50 **Dirk Valkenburg**, University of Georgia, VITO, Mol, Belgium
“*PRiSM: A universal search engine for peptidomics and proteomics*”
- 17:10 **Anas El-Aneed**, University of Saskatchewan, Saskatoon, SK
“*Mass spectrometric approaches to assess the cellular fate of lipid-based drug delivery systems*”
- 17:30 Discussion

18:00 Dinner
Mount Temple Ballroom C

Gas Phase Ion Chemistry

Chair: **Paul Mayer**

- 19:30 **Travis Fridgen**, Memorial University, St. John's, NL
“*The structures of Ca^{2+} (Uracil)₄₋₆ and cationized aromatic half-belts*”
- 19:50 **Nicholas Riley** and Joshua Coon, University of Wisconsin, Madison, WI
“*Activated Ion Electron Transfer Dissociation on an Orbitrap Fusion Mass Spectrometer*”
Winner of the Marg Northcott Lake Louise Student Travel Award
- 20:10 **Ivan Chu**, University of Hong Kong, Hong Kong
“*Radical-Mediated Peptide Tyrosine Nitration*”
- 20:30 **Sydney Wellman** and **Rebecca Jockusch**, University of Toronto, Toronto, ON
“*Unravelling environmental effects: Photodissociation action spectroscopy and fluorescence of gaseous Chl a*”
NSERC CREATE Travel Award Winner
- 20:50 **K. W. Michael Siu**, University of Windsor, Windsor, ON
“*Gas-Phase Dehydration of Protonated Polyglycines*”

21:10 Poster Session (Authors are asked to be present until 23:00)
Victoria Ballroom

Xuguang Liu and Shawn Li, The University of Western Ontario, London,
“*An AP-MS method for profiling tyrosine kinase activity in cancer*”

John Sausen, Agilent Technologies, Oconomowoc WI
“*Integrating Highly Accurate Collision Cross Section Measurements into Metabolomic Screening and Discovery Workflows for Increased Identification and Detection Confidence*”

Travis Falconer, U.S. FDA, Cincinnati, OH
“*HCD vs rCID for Qualitatively Significant Product Ions*”

Annie von Eyken, McGill University, Montreal, QC

“Development of a fast screening and quantification method of ten antimicrobials in honey using direct injection in HPLC-QTOF-MS/MS”

Christof Rampitsch, Agriculture & Agrifood Canada, Morden, MB

“Mining the wheat leaf apoplast for effector proteins of Puccinia triticina”

Randy Purves, University of Saskatchewan, Saskatoon, SK

“Semi Quantitative LC-SRM workflow for the analysis of over 100 polyphenols in lentil crops”

Jean Lodge, Jessica Rabuck-Gibbons, Anna K Mapp, Brandon T. Ruotolo, University of Michigan
Ann Arbor, MI

“Dissecting activator-coactivator interactions using collision induced unfolding”

Paul Mayer, Department of Chemistry, University of Ottawa, Ottawa, ON

“Gas phase reaction dynamics of ionized PAHs”

Krishna Anapindi and Jonathan W. Sweedler, University of Illinois, Urbana, IL

“Mass spectrometry based label-free quantitation of peptides involved in opioid-induced hyperalgesia”

Kevin A. Kovalchik¹, M.S. MacLennan¹, Chukwuemeka Ajaero², K.M. Peru³, D.W. McMartin², J.V. Headley³, D.D.Y. Chen¹ ¹University of British Columbia, Department of Chemistry, Vancouver, BC., V6T 1Z1, ²University of Regina, Faculty of Engineering and Applied Science, Regina, SK., S4S 0A2, ³Environment and Climate Change Canada, Science and Technology Branch, Saskatoon, SK., S7N 3H5
“Characterization of Amine-Derivatized Naphthenic Acids by High Resolution Tandem Mass Spectrometry”

David Schriemer, University of Calgary, Calgary, AB

“TBA”

Victor Yin and Lars Konermann, Department of Chemistry, The University of Western Ontario,
London, ON

“Investigating the Effects of In situ Oxidation on the Structure and Non-Canonical Functions of Cytochrome C using Electrospray Mass Spectrometry”

Lars Konermann, Tilo Schachel, Vlad Popa, Department of Chemistry, The University of Western
Ontario, London, ON

“Molecular Dynamics Simulations of Analyte Fragmentation in MS/MS: Bringing Together Theory and Experiment”

Tim Wood, Protechnik Laboratories, Div. of ARMSCOR SOC, Pretoria, South Africa

“The Prevalence of Selected Pharmaceuticals in South African Surface Water”

FRIDAY, DECEMBER 2

Proteins: Structure and Dynamics (Part 2)

Chair: **Susan Richardson**

- 8:00 **Frank Sobott** University of Antwerp, Antwerp, Belgium
"Top-down and native ETD of proteins and complexes"
- 8:20 **Derek J. Wilson**, York University, Toronto, ON
"Translating mass spectrometry enabled hydrogen deuterium exchange to drug development in neurodegenerative disease and cancer"
- 8:40 **Haidy Metwally** and Lars Konermann, Department of Chemistry, The University of Western Ontario, London, ON
"Mechanism of protein supercharging by sulfolane and mNBA"
Winner of a CSMS Travel Award, sponsored by Waters
- 9:00 **Jason J. Serpa**; Evgeniy V. Petrotchenko; Christoph H. Borchers, UVic Genome BC Proteomics Centre, Victoria, BC
"Structure of prion β -oligomers as determined by structural proteomics"
Winner of a CSMS Travel Award, sponsored by Thermo Fisher
- 9:20 **Peter Tieleman** University of Calgary, Calgary, AB
"Computer simulations of membrane proteins"

9:40 *Coffee Break*
Victoria Ballroom

Food, Environment, and other MS/MS Applications

Chair: **Gary Glish**

- 10:10 **Xing-Fang Li**, University of Alberta, Edmonton, AB
"Sweetened Swimming pools"
- 10:30 **Susan Richardson**, University of South Carolina, Columbia, SC
"Hydrofracking Impacts on Drinking Water: High Resolution-MS and Tandem MS Uncovering New Chemical By-Products"
- 10:50 **X. Chris Le**, University of Alberta, Edmonton, AB
"Mass spectrometry characterization of novel arsenic metabolites"
- 11:10 **Stephane Bayen**, McGill University, Montreal, QC
"From targeted to non-targeted analysis: applications to food safety"
- 11:30 **Brigitte Simons**, SCIEX, Concord, ON
"Turning new keys and making money; the demand for LC-MS iMETHODs"

11:50 Discussion

12:15 to 13:30 Lunch

Fairview Dining Room

Friday Afternoon: Free time – Enjoy the Great Outdoors!

18:00 Cocktails

Victoria Foyer / Victoria Ballroom

19:00 Banquet

Victoria Ballroom

SATURDAY, DECEMBER 3

Health and Disease

Chair: **Lars Konermann**

8:10 **John McLean**, Vanderbilt University, Nashville, TN

“Advances in Structural Mass Spectrometry for Metabolomics and Medicine”

8:30 **Mona Hamada**, University of Saskatchewan, Saskatoon, SK

“The development of novel targeted metabolomic methods for the diagnosis of respiratory illnesses”

Winner of a CSMS Travel Award, sponsored by Sciex

8:50 **Mari DeMarco**, Providence Health Care & University of British Columbia, Vancouver, BC

“Alzheimer disease biomarkers in patient care: A mass spec solution to a sticky situation”

9:10 **Bingyun Sun**, Simon Fraser University, Burnaby, BC

“Do biomarker exist?”

9:30 **Per Andrén**, Uppsala University, Uppsala, Sweden

“Mass spectrometry imaging – opportunities for drug discovery and neuroscience”

9:55 Coffee Break

Victoria Ballroom

Saccharides, Lipids, Metabolites

Chair: **Peter Verheart**

10:30 **Jon Amster** University of Georgia, Athens, GA

“Ion Mobility Studies of Glycosaminoglycan-Protein Complexes”

10:50 **Pietro Morlacchi**, Agilent Technologies, Saint Laurent, QC

“Mass Spectrometry as it relates to metabolomics and cell energetics studies”

- 11:10 **Brian Clowers** Washington State University, Pullman, WA
“Frequency Encoded Mobility Separations and Fragmentation Yields for Isomeric Tetrasacharides”
- 11:30 **Gary Glish** University of North Carolina, Chapel Hill, NC
“A Simple Mass Spectrometry Method to Identify Mono and Disaccharides”
- 11:50 **Jeffrey Smith**, Carleton University, Ottawa, ON
“Recent improvements in TrEnDi chemistry: enhancing plasmalogen and sphingomyelin signal and allowing fatty acyl identification”

12:10 Discussion and Adjournment

12:15 to 13:30 Lunch

Fairview Dining Room

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The top category: “Double Black Diamond” is currently vacant.