

# LAKE LOUISE XXVI

## 26<sup>th</sup> Workshop on Tandem Mass Spectrometry

### Thursday, December 5, 2013, Morning Session

8:00 Introductory Remarks: **Lars Konnermann**

#### Chair: Peter Verhaert *MS/MS Imaging 1*

8:10 Hyphenated activation methods for de novo sequencing, applications to complex samples and imaging MS, **Edwin De Pauw**, Mass Spectrometry Laboratory, University of Liege, Belgium.

8:50 High resolution tandem MS Imaging, **Bernhard Spengler**, University of Giessen, Germany.

9:10 Mass spectrometry imaging under ambient conditions, **Demian Ifa**, York University, Toronto.

9:30 Correlating molecular changes of prostheses material to biomolecule adsorption by MALDI-TOF imaging mass spectrometry, **Martina Marchetti-Deschmann**, Technical University of Vienna, Austria.

9:50 Discussion  
Coffee Break

#### Chair: Peter Verhaert *MS/MS Imaging 2*

10:20 Tandem mass spectrometry imaging on modern ion mobility Q TOF systems, **Emmanuelle Claude**, Waters, Manchester.

10:40 Tandem MS of new antibiotics from Bacillus guided by MALDI MS imaging, **Delphine Debois**, University of Liege, Belgium.

11:00 3-D imaging mass spectrometry, molecular insight into atherosclerosis, **Martin Dufresne**<sup>1</sup>, Heath Patterson<sup>1</sup>, Francois Roubille<sup>2</sup>, Eric Phéaume<sup>2,3</sup>, David Busseuil<sup>2</sup>, Jean-Claude Tardif<sup>2,3</sup> and Pierre Chaurand<sup>1</sup>, <sup>1</sup>Department of Chemistry, University of Montreal, Quebec, <sup>2</sup>Montreal Heart Institute, Montreal, Quebec, <sup>3</sup>Department of Medecin, University of Montreal, Montreal, Quebec.

11:20 Tandem mass spectrometry imaging of small molecular drugs and neurotransmitters, **Per Andréén**, Uppsala University, Sweden.

11:40 Imaging MALDI MS/MS of microarrays as a platform for high throughput biomaterials discovery, **John D. Brennan**, McMaster University, Hamilton, Ontario.

12:00 Discussion

12:10 **Workshop group picture**

12:30 Lunch (in the Fairview Room)

### Afternoon Session

#### Chair: Albert Heck *Lipids and Metabolites*

14:00 Multiplexed lipid quantitation via isobaric mass tagging and multistage MS/MS, **Gavin E Reid**, Michigan State University.

14:20 Recent advances in the development of high performance isotope labeling mass spectrometry for metabolomics applications, **Liang Li**, University of Alberta, Edmonton.

14:40 Mass spectrometric analysis of antineoplastic lipid-based nanoparticles, McDonald Donkuru, Hanan Awad and **Anas El-Aneed**, University of Saskatchewan, Saskatoon.

15:00 Metabolomics and lipidomics using UPLC with ion mobility MS/MS, **Giuseppe Astarita**, Waters Corporation.

15:20 Monitoring reactive metabolite induced covalent modification of proteins, **Lekha Sleno**, André LeBlanc and Makan Golizeh, Université de Quebec à Montréal.

- 15:40 Analyzing modern and ancient lipids using differential mobility spectrometry, **Larry Campbell**, AB Sciex.
- 16:00 Discussion  
Coffee Break

Chair: Kristina Hakansson **Protein Conformations and Interactions**

- 16:30 Expanding the detectable peptide repertoire using electron-transfer/higher-energy collision dissociation (EThD), Christian K. Frese<sup>1,2</sup>, Geert P. M. Mommen<sup>1,2,3</sup>, Maarten Altaar<sup>1,2</sup>, Shabaz Mohammed<sup>1,3</sup> and **Albert Heck**<sup>1,2</sup>, <sup>1</sup>Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht University, The Netherlands, <sup>2</sup>Netherlands Proteomics Centre, Utrecht, The Netherlands, <sup>3</sup>Formulation and Analytical Research, Institute for Translational Vaccinology, Bilthoven, The Netherlands.
- 16:50 Nanodiscs: a novel tool for identifying native protein-glycolipid interactions by ESI-MS, **Aneika Leney**, University of Alberta, Edmonton.
- 17:10 Conformational analysis of transient protein folding intermediates by ESI-MS/MS, **Siavash Vahidi** (CSMS Travel Award Winner, sponsored by Waters), Bradley B. Stocks and Lars Konermann, University of Western Ontario, London.
- 17:30 Mass spectrometric analysis reveals the formation of a highly stable, active-site sulfenic acid in human GAPDH, **Ann English**, Concordia University, Montreal, Quebec.
- 17:50 Discussion
- 18:00 Dinner: Mt. Temple C

**Evening Session**

Chair: Lars Konermann **Instrumentation**

- 20:00 NeuCode SILAC, the one hour yeast proteome, and the orbitrap fusion, **Anne Merrill**, on behalf of Thermo Fisher Scientific.
- 20:20 Development of a new high resolution ion mobility-quadrupole time-of-flight mass spectrometer for structural analyses, **Ruwan Thushara Kurulugama**, Agilent Technologies.
- 20:50 The resonance activation and collision-induced-dissociation of ion by dipole DC waveform frequency in a digital ion trap mass spectrometer, **Chuan-Fan Ding**, Fudan University, China.

21:10 **Poster Session –authors are required to be present until 23:00**

Characterization of unknown variable composition phthalates using GC/MS/MS, **Mehran Alaei**, Environment Canada.

HPLC-MS/MS analysis of novel dipeptide Gemini surfactant, **Mays Al-Dulaymi**, College of Pharmacy and Nutrition, University of Saskatchewan.

Analysis of paralytic shellfish toxins by LC-FAIMS-MS, **Daniel Beach**, Jeremy E. Melanson and Michael Quilliam, National Research Council Canada, Halifax, Nova Scotia.

14N15N SXMSMSM match software for the data analysis of the crosslinking experiments using 15N metabolically-labeled proteins, **Evgeniy V. Petrotchenko** and Christoph H. Borchers, UVic-Genome BC Proteomics Centre, Victoria, British Columbia.

Quantification of hemoglobin A 1 c in clinical dried blood spots by MALDI-TOF, **Andrew Chambers**, UVic-Genome BC Proteomics Centre, Victoria, British Columbia.

Mass spectrometric analysis of Gemini surfactants in mouse epidermal keratinocytes, **McDonald Donkuru**, University of Saskatchewan.

Heme-mediated oxidation of residues in cytochrome c peroxidase as revealed by mass spectrometry provide mechanistic insights into its remarkable H<sub>2</sub>O<sub>2</sub> sensing role, Meena Kathiresan and **Ann M. English**, Dept. of Chemistry and Biochemistry and Center for Biological Applications of Mass Spectrometry (CBAMS), Concordia University, Montreal, Canada.

Miniature condensed phase membrane introduction mass spectrometry (CP-MIMS) probes for the direct measurement of pharmaceuticals and contaminants in complex samples, Kyle D. Duncan<sup>1,3</sup>, Gregory W. Vandergrift<sup>2,3</sup>, Erik T. Krogh<sup>1,2,3</sup> and **Chris G. Gill**<sup>1,2,3</sup>, <sup>1</sup>University of Victoria, British Columbia, <sup>2</sup>Vancouver Island University, Nanaimo, British Columbia, <sup>3</sup>Applied Environmental Research Laboratories (AERL), Nanaimo, British Columbia.

Ion-electron reactions for carbohydrate structural characterization, **Kristina Hakansson**, University of Michigan.

EPA 539 analysis of hormones in drinking water: improved sensitivity and separation, **Ralph Hindle**, Vogon Labs.

Nontarget screening of transformation products formed in biological wastewater treatment using multivariate analysis, Jennifer Schollée, Emma Schymanski, Heinz Singer and **Juliane Hollender**, Environmental Chemistry, Eawag, Swiss Federal Institute of Aquatic Science and Technology, Institute of Biogeochemistry and Pollution Dynamics, Department of Environmental Systems Science (d-USYS) ETH Zurich, Switzerland.

Target, suspect and non-target screening of lake sediments using HR-MS/MS, Aurea C. Chiaia-Hernandez, Kumar Praveen, Emma L. Schymanski and **Juliane Hollender**, Environmental Chemistry, Eawag, Swiss Federal Institute of Aquatic Science and Technology, Institute of Biogeochemistry and Pollution Dynamics, Department of Environmental Systems Science (d-USYS) ETH Zurich, Switzerland.

Protein ID & location in bovine eye lens, Sergei Dikler and Jane Kowalski, attended by **James Kapron**, Bruker.

Atmospheric pressure GC/MS/MS for the analysis of petroleum biomarkers, **Patrice Lemire**<sup>1</sup>, Douglas Stevens<sup>2</sup> and Peter Hancock<sup>3</sup>, <sup>1</sup>Waters Corp, <sup>2</sup>Waters Corp, Milford, MA, USA, <sup>3</sup>Waters Corp, Manchester, UK.

Anionic metalloporphyrin complexes: structure and binding, **Paul Mayer**<sup>1</sup>, and Oliver Hampe<sup>2</sup>, <sup>1</sup>Chemistry Department, University of Ottawa, Ontario, <sup>2</sup>Karlsruhe Institute for Technology.

Applying differential mobility spectrometry with unique gas phase separations to the analysis of naphthenic acids, Larry Campbell<sup>1</sup>, Takeo Sakuma<sup>1</sup>, Andre Schreiber<sup>1</sup>, Paul Winkler<sup>1</sup>, Kerry M. Peru<sup>2</sup>, John V. Headley<sup>2</sup>, attended by **Michael McDonell**, <sup>1</sup>AB Sciex, <sup>2</sup>Water Science and Technology Directorate, Environment Canada, Saskatoon, SK, Canada.

Comprehensive structural characterization of biopharmaceuticals and biosimilars by top-down HDX-MS, **Jingxi Pan** and Christoph H. Borchers, UVic-Genome BC Proteomics Centre, Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada.

Kits for standardizing MRM-based quantitative plasma proteomic analyses, **Andrew Percy**, Andrew G. Chambers, Juncong Yang, Darryl Hardie, and Christoph H. Borchers, UVic-Genome BC Proteomics Centre, Victoria, British Columbia.

Analysis of veterinary antimicrobials in stockpiled feedlot manure using LC-ESI/MS, Srinivas Sura<sup>1,2</sup>, Dani Degenhardt<sup>3</sup>, **Kerry Peru**<sup>2</sup>, Jon Bailey<sup>2</sup>, Allan J. Cessna<sup>1,2</sup>, Francis J. Larney<sup>4</sup>, Tim A. McAllister<sup>4</sup> and John V. Headley<sup>2</sup>, <sup>1</sup>Agriculture and Agri-Food Canada, Saskatoon Research Centre, Saskatoon, Saskatchewan, <sup>2</sup>Environment Canada, National Hydrology Research Centre, Saskatoon, Saskatchewan, <sup>3</sup>Alberta Innovates Technology Futures, Edmonton, Alberta, Agriculture and Agri-Food Canada, Lethbridge Research Centre, Lethbridge, Alberta.

The development of an automated immuno-MALDI assay for the clinical measurement of plasma renin activity, **Robert Popp**<sup>1</sup>, David Malmström<sup>1</sup>, Alexander G. Camenzind<sup>1</sup>, Daniel T. Holmes<sup>2</sup>, J. Grace van der Gugten<sup>2</sup>, Christoph h. Borchers<sup>1</sup>, <sup>1</sup>UVic-Genome BC Proteomics Centre, Victoria, BC, Canada, <sup>2</sup>St. Paul's Hospital, University of BC, Vancouver, British Columbia.

Custom database searching to reveal differences in the haustorial proteomes of three races of wheat leaf rust, *Puccinia triticina*, **Christof Rampitsch**<sup>1</sup>, Eva Beimcik<sup>1</sup>, Aslihan Günel<sup>2</sup>, Guus Bakkeren<sup>3</sup>, Rob Linning<sup>3</sup>, David Joly<sup>3,4</sup>, Brent McCallum<sup>1</sup> and Tao Fan<sup>1</sup>, <sup>1</sup>Agriculture and Agri-Food Canada, Winnipeg, Manitoba, <sup>2</sup>Ahi Evran University, Kirsehir, Turkey, <sup>3</sup>Agriculture and Agri-Food Canada, Summerland British Columbia, <sup>4</sup>Université de Moncton, Moncton, New Brunswick.

Identification of a novel MADS-box phosphorylation motif by phosphopeptide mapping using CID and ETD, Joseph W. Gordon<sup>1</sup>, Donald Chapman<sup>1</sup>, Min Du<sup>2</sup>, Nathaniel Nowacki<sup>2</sup>, John C. McDermott<sup>2</sup> and **Christof Rampitsch**<sup>3</sup>, <sup>1</sup>University of Manitoba, Manitoba Institute of Child Health, Department of Human Anatomy and Cell Science, Faculty of Nursing, Endocrinology and Metabolic Disease Research Group, <sup>2</sup>York University, Department of Biology, Centre for Research in Mass Spectrometry, Muscle Health Research Centre, and Centre for Research in Biomolecular Interactions, <sup>3</sup>Cereal Research Centre, Agriculture and Agri-Food Canada, Winnipeg Manitoba.

Protein dynamics of STAT3: characterization of the SH2 domain binding site of small molecule dimerization inhibitors, **Diana Resette**<sup>1</sup>, Sina Haftchenary<sup>2</sup>, Patrick T. Gunning<sup>2</sup> and Derek J. Wilson<sup>1,3</sup>, <sup>1</sup>York University, Chemistry Department, Toronto, Ontario, <sup>2</sup>Department of Chemical and Physical Sciences, University of Toronto Mississauga, Mississauga, Ontario, <sup>3</sup>Center for Research in Mass Spectrometry, Department of Chemistry, York University, Toronto, Ontario.

A multiplexed kinase assay for screening of small molecule modulators via MALEI-tandem mass spectrometry, **Anne Marie Smith** and John D. Brennan, Biointerfaces Institute and Department of Chemistry and Chemical Biology, McMaster University, Hamilton, Ontario.

Sensitive proteomics for cell surface proteins, Gilbert Lee, Jurgan Sanes, Lisa Lin and **Bingyun Sun** Dept. of Chemistry, Simon Fraser University, Burnaby, British Columbia.

## Friday, Dec. 6, Morning Session

Chair: Kerry Peru *Environmental Applications*

8:00 Strategies to characterize polar organic contamination in the aquatic environment; exploring the capability of high resolution mass spectrometry, **Juliane Hollender**, Philipp Longrée, Martin

- Loos, Matthias Ruff, Jennifer Schollée, Amma Schymanski, Michael Stravs and Heinz Singer, Swiss Federal Institute of Aquatic Science and Technology, Dübendorf, Switzerland.
- 8:40 Use of time-of-flight and triple quadrupole mass analyzers for the analysis of pharmaceuticals and pesticides, **Imma Ferrer**, University of Colorado, Boulder.
- 9:00 Accurate mass tools for the identification of pesticide metabolites in plants by LC/QTOF-MS, **Michael Thurman**, University of Colorado, Boulder.
- 9:20 Membrane introduction tandem mass spectrometry: recent advances and applications, **Christopher G. Gill**, Dept. of Chemistry, Vancouver Island University, Nanaimo, British Columbia.
- 9:40 Tandem mass spectrometry for real-time analysis of compounds in organic aerosol particles, **Sandra E. Spencer (Winner of a Lake Louise Travel Award, sponsored by Research Scientific Services)** and Gary Glish, Dept. of Chemistry, University of North Carolina.
- 10:00 Discussion  
Coffee Break

Chair: Paul Mayer **Gas Phase Reaction Mechanisms**

- 10:30 Coupling liquid chromatography to in-line ozonolysis mass spectrometry (LC/O3-MS) – a new dimension of structure determination for lipid mixtures, **Chenxing (Angela) Sun (CSMS Travel Award Winner, sponsored by Sciex)**, Yuan-Yuan Zhao and Jonathan M. Curtis, University of Alberta, Edmonton.
- 10:50 Systematic mechanistic exploration of negative ion electron capture dissociation (niECD) with synthetic peptides, **Ning Wang (Winner of a Lake Louise ‘ALL SPONSOR SUPPORTED’ Student Travel Award)** and Kristina Håkansson, Dept. of Chemistry, University of Michigan, Ann Arbor.
- 11:10 Radical additions to aromatic residues in peptides facilitate unexpected side chain and backbone losses, **Xing (Vic) Zhang (Winner of a Lake Louise ‘ALL SPONSOR SUPPORTED’ Student Travel Award)** and Ryan R. Julian, Dept. of Chemistry, University of California, Riverside.
- 11:30 Structural characterization of b-type ions and their fragments by collision-induced dissociation-MSn of a series of synthetic hexapeptides containing aromatic amino acids, **Declan Williams**, Justin Kai-Chi Lau, Stefanie Mädler, Yating Wang, Junfang Zhao, Irine Saminathan, Alan C. Hopkinson and Michael Siu, York University, Toronto, Ontario.
- 11:50 Understanding the chemistry in the interface of atmospheric sources with mass spectrometers using DIMS/MS, Samantha Isenberg, Brandon Santiago, Kyle Stevens and **Gary Glish**, University of North Carolina.
- 12:10 Discussion
- 12:15 Lunch
- 13:30 Geology of Lake Louise, with Bob Davidson, in lobby
- 14:00 Informative walk up the lake with Bob Davidson
- 16:30 Broomball: Canada vs. The World – meet in lobby at 4:15 P. M.
- 18:00 Cocktails – Victoria Ballroom
- 19:00 Banquet – Victoria Ballroom

**Sat., Dec. 7, Morning Session**

Chair: Lars Konermann **Proteomics I**

- 8:00 Finding more answers in your proteomics data, **Cassandra Wigmore**, Bioinformatics Solutions Inc. PEAKS Software, Simon Fraser University, Burnaby, British Columbia.
- 8:20 N-glycoproteome of mouse embryonic stem cells, **Bingyun Sun**, Simon Fraser University, Burnaby, British Columbia.
- 8:40 Strategies for preclinical screening of proteins derived from exosomes through tandem MS, **Alan Doucette**, Dalhousie University, Halifax, Nova Scotia.
- 9:00 Composition dependent sorting of peptides: a novel approach to enrichment of N-terminal and C-terminal peptides in bottom-up proteomic LC-MS experiments, **Oleg Krokhin**, University of Manitoba, Winnipeg.
- 9:20 An automated tool for generating curated spectral libraries, **Bernhard Delanghe**, Thermo Fisher Scientific (Bremen) GmbH.
- 9:40 Pulsed electric field cell disruption as a sensitive and clean sample preparation protocol to study microbial proteomes, **Yuanjie Yu** and Peter Verhaert, TU Delft, Netherlands.
- Discussion
- 10:00 Coffee Break

Chair: Gary Glish **Proteomics 2**

- 10:30 A dual LC/MS platform for high throughput proteomics with application to biomarker discovery, **Dennis J. Orton (CSMS Travel Award Winner, sponsored by Thermo Fisher Scientific)** and Alan A. Doucette, Dept. of Chemistry, Dalhousie University, Halifax, Nova Scotia.
- 10:50 XIM cross species immunoassays – analyzing proteins across the barrier, **Oliver Poetz**, Natural and Medical Sciences Institute, University of Tuebingen, Germany.
- 11:10 Exploring the possibilities of a novel quadrupole-orbitrap tandem mass spectrometer in new ‘Red Biotechnology’ projects at Delft University of Technology, **Peter Verhaert** and Martijn Pinkse, TU Delft, Netherlands.
- 11:30 Studying cell-cell interactions by mass spectrometry, **Juergen Kast**, University of British Columbia, Vancouver.
- 11:50 Conformational changes and inter-subunit contacts in prion oligomers studied by crosslinking of <sup>15</sup>N-metabolically labeled prion proteins, **Christoph Borchers**, University of Victoria, British Columbia, Vancouver.
- 12:10 Discussion
- 12:30 Lunch