

LAKE LOUISE XXIV

24th Workshop on Tandem Mass Spectrometry

Thursday, December 1, 2011, Morning Session

Chair: Jeff Smith

- 8:00 Introductory Remarks: **Gordon McKay**
- 8:10 Membrane protein structure and function studied using mass spectrometry, **Julian Whitelegge**, The Pasarow Mass Spectrometry Laboratory, The NPI-Semel Institute for Neuroscience and Human Behaviour, David Geffen School of Medicine, University of California, Los Angeles, USA.
- 8:50 LC-MS for membrane proteome profiling, **Liang Li**, University of Alberta.
- 9:10 Membrane protein structure and function studied by tandem mass spectrometry, **Lars Konermann**, The University of Western Ontario.
- 9:30 Discussion
- 9:40 Coffee Break

Chair: Lars Konermann

- 10:00 Shotgun lipidomics on high resolution mass spectrometers, **Andrej Shevchenko** MPI OF Molecular Cell biology and Genetics.
- 10:40 An alternative tandem mass spectrometric approach for lipid analysis: multi-dimensional mass spectrometry-based shotgun lipidomics, **Xianlin Han**, Sanford-Burnham Medical Research Institute.
- 11:00 Development of a metabolomic/lipidomic platform based on a hybrid quadrupole time-of-flight (QToF) ion-mobility mass spectrometer, **John Shockcor**, Waters Corp.
- 11:20 Lipidomics of neurodegenerative diseases, **Daniel Figeys**, University of Ottawa.
- 11:40 A quantitative lipidomics analysis of K562 cells infected with Vesicular Stomatitis Virus, Shira Joudan¹, Lennart Trouborst¹, Girija Waghray², Harold Atkins² and **Jeffrey Smith**¹, ¹Carleton University, ²Ottawa Hospital Research Institute.
- 12:00 Discussion
- 12:30 Lunch** (in the Fairview Room)

Afternoon Session

Chair: Gary Glish

- 14:00 Negative ion electron capture dissociation (niECD): mechanism, analytical improvement, and applications, **Kristina Hakansson**, Ning Wang, Hangtian Song and Katherine E. Hersberger, Dept. of Chemistry, University of Michigan, Ann Arbor, MI, USA.
- 14:40 Differential ion mobility/MS: simplifying complex samples, Samantha L. Isenberg¹, Alice L. Pilo¹, Mark E. Ridgeway¹, Desmond A. Kaplan², Melvin A. Park² and **Gary Glish**¹, ¹University of North Carolina, Chapel Hill, NC, ²Bruker Daltonics, Billerica, MA.
- 15:00 Struggling with space charge effects in linear quadrupole ion traps, Hui Qiao¹, Cong Gao², Dunmin Mao³, Nidolai Konenkov⁴ and **Don Douglas**⁵, ¹Ionics Mass Spectrometry Group, ON, Canada, ²UBC, ³QLT Inc., BC, Canada, ⁴Physical and Mathematical Department, Ryazan State University, Byazan, Svoboda, Russia, ⁵Chemistry, U.B.C.
- 15:20 Discussion
- 15:30 Coffee Break

Chair: Susan Richardson

- 15:50 Non-target analysis of urine using ESI-FAIMS-MS/MS, **Daniel G. Beach (Winner of the AB Sciex supported CSMS Student Travel Award)** and Wojciech Gabryelski, Dept. of Chem., University of Guelph, Guelph, ON, Canada.
- 16:10 Affinity purification and nanoLC coupled to LTQ-Orbitrap analysis of redox signalling by mitochondrial and extra-mitochondrial cytochrome c peroxidase, **Meena Kathiresan**, Dorival Martins, Jean-Pierre Falguyret and Ann M. English, Dept. of Chemistry and Biochemistry, Concordia University. Montreal, Quebec, Canada.
- 16:30 Using CESI to improve LOD & LOQ of pharmaceuticals and their metabolites, **John C. Hudson**, Beckman Coulter Canada.
- 16:50 High resolution analysis of carbene footprints on calmodulin complexes, **Chanelle Jumper**¹ and David C. Shriemer², ¹Dept. of Chemistry, University of Calgary, ²Dept. of Biochemistry and Biomolecular Biology, University of Calgary.
- 17:10 Unique formation of [M-H]⁺ ions during MALDI-MS analysis of curcumin-like antineoplastic agents, L. Usher¹, A. Cohen², S. Das¹, J. Dimmock¹, U. Das¹, D. Pinto³ and **Anas El-Aneed**¹, ¹Drug Design and Discovery Research Group, College of Pharmacy and Nutrition, University of Saskatchewan, ²Proteomics Core Facility, Clinical Research Centre, Dalhousie University, ³NRC, Institute for Marine Bioscience, Halifax.
- 17:30 Discussion
- 18:00 Dinner: Mt. Temple A

Evening Session

Chair: Peter Verhaert

- 20:00 Structure and stability of protein-ligand complexes in solution and the gas phase, **John Klassen, (Winner of the Lossing Award sponsored by Agilent,)** Alberta Innovates Centre for Carbohydrate Science, Dept. of Chem. University of Alberta, Edmonton, Alberta, Canada.
- 20:40 Identification of differentially expressed proteins in direct expressed prostatic secretions of men with organ-confined versus extracapsular prostate cancer, **Yunee Kim**¹, **(Winner of the Thermo Fisher supported CSMS Student Travel Award)**, O. John Semmes^{2,3}, Raymond S. Lance^{3,4}, Julios O. Nyalwidhe^{2,3}, Jeffrey A. Medin^{2,3}, Richard R. Drake^{2,3} and Thomas Kislinger⁵, ¹University of Toronto, Dept. of Medical Biophysics, Toronto, Canada, ²Eastern Virginia Medical School, Dept. of Microbiology and Molecular Cell Biology, Norfolk VA, USA, ³Eastern Virginia Medical School, Cancer Research Center, Norfolk, VA, USA, ⁴Urology of Virginia and Eastern Virginia Medical School, Dept. of Urology, Norfolk, VA, USA, ⁵Ontario Cancer Institute, University Health Network, Toronto, Canada.
- 21:00 Discussion
- 21:05 Poster Session – **‘authors’ are required to be present until 23:00**
- Levels of hexabromocyclododecane (HBCD) in peregrine falcon (*Falco peregrinus*) eggs from Canada and Spain, Paula Guerra¹, Grazina Pacepavicius¹, Begoña Jiménez¹, Chris Marvin¹, Gordia MacInnis¹, Ethel Eljarrat¹, Damià Barceló¹, Louise Champoux¹, Kim Fernie¹ and **Mehran Alaei**¹, ¹Dept. of Environmental Chemistry, Barcelona, Spain, ¹Water Science and Technology, Environment Canada, Burlington, Canada, Dept. of Instrumental Analysis and Environmental Chemistry, Institute of Organic Chemistry, CSIC, Madrid, Spain, ¹Catalan Institute for Water Research (ICRA), Girona, Spain, ¹Wildlife Toxicology and Disease, Environment Canada, Sainte-Foy, Canada, ¹Ecotoxicology and Wildlife Health, Environment Canada, Burlington, Canada.
- Quantitation of 67 putative biomarkers of cardiovascular disease in human plasma by LC-MRM-MS, Dominik Domanski¹, Andrew J. Percy¹, Juncong Yang¹, **Andrew Chambers**¹, John S. Hill^{2,3}, Gabriela V. Cohen Freue² and Christoph H. Borchers¹, ¹Genome BC Proteomics Centre,

University of Victoria, ²PROOF Centre of Excellence, Vancouver, BC, ³Genome B The James Hogg Research Centre, St. Paul's Hospital, University of BC ^ Institute for Heart + Lung Health, Vancouver, BC.

Structural analysis of complex lipids by MALDI-spiralTOF-TOF tandem MS with high precursor-ion selectivity, Ayumi Kubo¹, Yoshiyuki Itoh¹, Masaaki Ubukata², Masahiro Hashimoto¹, Jun Tamura¹, Jyun Onodera¹ and **Robert B. Cody**², ¹JEOL Ltd., Akishima, Tokyo, ²JJEOL USA, Inc., Peabody, MA, USA.

Quantitation of Gemini surfactant nanoparticle constituents by matrix assisted laser desorption ionization mass spectrometry, Joshua Buse¹, Haixia Zhang², Steve Ambrose², Randy Purves², Ildiko Badea¹, Ronald E. Verrall³ and **Anas El-Aneed**¹, ¹Drug Design & Discovery Group College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, SK, Canada, ²Mass Laboratory Plant Biotechnology Institute (PBI), National Research Council of Canada, Saskatoon, Canada, ³Dept. of Chemistry, University of Saskatchewan, Saskatoon, SK, Canada.

Quantification of plasma S-adenosylhomocysteine and S-adenosylmethionine by positive ion ESI LC/MS/MS, **David Hasman**¹, Sheila Innis² and Roger Dyer, ¹Procyon Research and BCIT Forensic Sciences, ²Child and Family Research Institute, Dept. of Paediatrics, University of British Columbia, Canada.

Utilization of high resolution LC-MS for screening and quantitative analysis of pesticides in food matrix using a Q Exactive bench top orbitrap platform, (presented by **Stephen Hassan**), Charles Yang, Dipankar Ghosh, Jia Wang and Kristi Akervik, Thermo Fisher Scientific, San Jose, CA, USA.

HPLC ESI MS characterization of flavonoids and phenolic acids from Caribbean Asteraceae and Lamiaceae plants with bio-accumulator potential, Sonia Peter¹, **John Headley**², Kerry Peru² and Brian Fahlman², ¹Dept. of Chemistry, Barbados Community College, ²Aquatic Ecosystem Protection Research Division, Environment Canada, Saskatoon, SK, Canada.

Conformational isomers of the calcineurin hetero-dimer follow distinctive dissociative pathways, B. Kükler¹, I. M. Barbu¹, J. Copps², S. S. Taylor², E. van Duijn¹ and **Albert J. R. Heck**¹, ¹Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Utrecht, ²U Dept. of Chemistry and Biochemistry, University of California San Diego, La Jolla, California, USA.

Automatic MS/MS characterization of N-linked glycopeptides, presented by **James Kapron**, Andrea Kiehne, Anja resemann, Ulrike Schweiger-Hufnagel, Arndt Asperger and Detlev Suckau, Bruker Daltonics, Germany.

Analysis of short chain chlorinated paraffins with tandem and accurate mass GCMS, **Marcus Kim**¹, Anthony Macherone¹, Sofia Aronova¹, Ed Sverko² and Greg Tomy², ¹Agilent Technologies, Environment Canada, ²Environment Canada.

Measuring kinetic isotope effects in enzyme systems by time-resolved ESI-MS, **Peter Liuni** and Derek J. Wilson, The Centre for Research in Mass Spectrometry, Dept. of Chem, York University.

Extending the linear dynamic range and limits of detection of a quadrupole time-of-flight (TOF) mass spectrometer down to the low parts-per-trillion range, **J. C. Marr**, Bill Barry, Christian Klein, George Stafford, Michael Ugarov and Michael Flannigan, Agilent Technologies, Inc., Santa Clara, CA, USA.

Proteomics phenotyping of human cancer cell lines, **J. C. Marr**¹, Vadiraja B. Bhat², Christine Miller³, Jose Meza³, Suresh Kumar⁴, Vaibhav C. Chumbalkar⁵ and Xiaowei Xu⁴, ¹Agilent Technologies, Mississauga, ON, ²Agilent Technologies Inc., Wilmington, DE, ³Agilent Technologies Inc, Santa Clara, DA, ⁴University of Pennsylvania, ⁵University of Texas MD Anderson Cancer Center, Houston.

In silico construction of a negative ion TW-ion mobility calibration set and its use in investigating the phospholipid content of *Pistacia lintisc*, Jenna Hamilton, **Justin B. Renaud**, ,Hajer Trabelsi and Paul M. Mayer, University of Ottawa.

The proteome of intracellular feeding structures purified from the wheat leaf rust pathogen, *Puccinia triticina*, **Christof Rampitsch**¹, Aslihan Günel², Eva Beimcik¹ and Tao Fan¹, ¹Agriculture and Agrifood, Winnipeg MB, Canada, ²Middle East Technical University, Department of Chemistry, Ankara, Turkey.

Quantitative mass spectrometry of proteins from the model grass *Brachypodium distachyon* by metabolic labelling with nitrogen 15, **David Shearer**, Melodie Budzinsky, Vic Spicer, Oleg Krokhin, Steve Haber and Kenneth G. Standing, University of Manitoba.

Using mass spectrometry to study the ozonolysis of model lipid systems, **Chenxing Sun**, Yuan-Yuan Zhao and Jonathan Curtis, Dept. of Agriculture, Food and Nutritional Science, University of Alberta.

Structural proteomics characterization of prion protein aggregation Evgeniy V. Petrotchenko, **Jason J. Serpa**, Jun Han, Aileen Patterson, David Wishart and Christoph H. Borchers, Genome BC Proteomics Centre, University of Victoria.

Highly specific quantitative profiling of lipids using differential mobility, **J. Bryce Young**, Brigitte Simons, Eva Duchoslov and Paul Baker, AB Sciex, Concord, ON, Canada.

Friday, Dec. 2, Morning Session

Chair: Michael Siu

- 8:00 Time-resolved, spatially resolved measurements of protein conformational dynamics using a microfluidic chip incorporating TRESI and rapid proteolytic digestion, **Derek Wilson**, York University.
- 8:20 Defining amino acid's hydrophobicity using proteomic RP-HPLC/MS experiments, **Oleg Krokhin**, Dmitry Shamshurin and Vic Spicer, Manitoba Centre for Proteomics and Systems Biology, University of Manitoba.
- 8:40 Protein quantification by reductive dimethylation of lysine: isoform identification in mesenchymal stem cells, **Terry D. Cyr**, Yi-Min She, Michael Rosu-Myles and Lisa Walrond, Health Canada.
- 9:00 Isolation and identification of protein-binding ligands in complex mixtures using tandem mass spectrometry, **Erica. M. Forsberg**, (**Winner of the Research Scientific Services supported Lake Louise Student Travel Award**) and J. D. Brennan, Dept. of Chem. And Chemical Biology, McMaster University, Hamilton ON, Canada.
- 9:20 Stoichiometry of adenovirus proteins determined by label free and isotope labelled quantification: from protein quantification to functional insights into host infection, **Marco Benevento**¹, (**Winner of a Lake Louise Workshop 'All Sponsor Supported' Student Travel Award**), Crystal Moyer², Glen Nemerow², Shabaz Mohammed¹ and Albert J. R. Heck¹, ¹Biomolecular MS and Proteomics Group, Netherlands Proteomics Centre, Utrecht Institute for Pharmaceutical Sciences and Bijvoet Center for Biomolecular Research, Utrecht University, Utrecht, the Netherlands, ²The Scripps Research Institute, San Diego CA, USA.
- 9:40 A fully automated workflow for glycopeptide analysis, **Julian Saba** and Rosa Viner, Thermo Fisher Scientific.

10:00 Discussion
10:10 Coffee Break

Chair: Albert Heck

10:30 Structural proteomics analysis of prions, **Christoph Borchers**, Biochemistry & Microbiology, University of Victoria.

10:50 Tandem mass tags to study peptide biology, **Peter Verhaert**¹, Martijn Pinkse¹ and Ian Pike²,
¹Analytical Biotechnology & Innovative Peptide Biology, Delft University of Technology,
²Proteome Sciences, London, U.K.

11:10 Zen and the art of CESI; revealing PTMS & characterizing proteins, **Jeff D. Chapman**, Beckman Coulter.

11:30 Beneficial use of CID, HCD and ETD in proteomics, **A. F. Maarten Altelaar**¹, Christian K. Frese¹, Shabaz Mohammed¹ and Albert J. R. Heck¹, ¹Biomolecular MS and Proteomics Group, Utrecht Institute for Pharmaceutical Sciences and Bijvoet Center for Biomolecular research, Utrecht University, Utrecht, the Netherlands, ²Netherlands Proteomics Centre, Utrecht University, Utrecht, The Netherlands.

11:50 *De Novo* sequencing by a combination of CID with ETD tandem MS reveals the primary structure of 3 novel Kazal-type protease inhibitors from the dorsal skin secretion of the Brazilian walking leaf frog, *Phyllomedusa burmeisteri*, **Geisa Evaristo**¹. (**Winner of a Lake Louise Workshop 'All Sponsor Supported' Student Travel Award**), Martijn Pinkse¹, Chris Shaw², Albert Heck³ and Peter Verhaert¹, ¹Analytical Biotechnology/Innovative Peptide Biology Group and Netherlands Proteomics Centre, Dept. of Biotechnology, TUDELFT, Delft, The Netherlands, ²Laboratory of Natural Drug Discovery, School of Pharmacy, Queen's University of Belfast, Belfast, United Kingdom, ³Netherlands Proteomics Centre, Utrecht University, Utrecht, the Netherlands.

12:10 La³⁺/small peptide complexes and their fragmentation to give dipositively charged protonated ions in the gas phase, **K. W. Michael Siu**, York University.

12:30 Discussion
12:45 Lunch

13:30 Geology of Lake Louise, with Bob Davidson, in lobby
14:00 Information walk, with Bob Davidson, up lake
16:30 Broomball: Canada vs. The World
18:30 Banquet – Mount Temple Ballroom A

Sat., Dec. 3, Morning Session

Chair: Kerry Peru

8:30 Olive oil authentication using GC/Q-TOF MS and multivariate software, **Stephan Baumann**, Agilent Technologies.

8:50 LC/MS investigation of Devil's Club, a medicinal plant of the Pacific Northwest, **David Hasman**¹, Joe Tai² and Susan Cheung³, ¹Procyon Research and BCIT Forensics, ²Child and Family Research Institute Dept. of Pathology-Laboratory Medicine, UBC, ³Dept. of Pediatrics and Surgery, UBC.

9:10 Structural analysis of glycosaminoglycan carbohydrates by FTMS/MS, John Muchena¹, Josh Driver¹, Mellisa Ly², Robert Linhardt² and **Jon Amster**¹, ¹University of Georgia, ²Rensselaer Polytechnic Institute.

9:30 RRKM modeling of the energy-resolved collision-induced dissociation of β -cyclodextrin/drug complexes, **Justin B. Renaud**, (**Winner of the Waters Canada supported CSMS Student Travel Award**), Gleb G. Mironov, Maxim V. Berezovski and Paul M. Mayer, University of Ottawa, Ottawa, Canada.

09:50 Discussion

10:00 Break

Chair: Gordon McKay

10:30 Application of ion mobility and tandem mass spectrometry for the identification of organophosphorus chemical warfare agent hydrolysis products, **Paul A. D'Agostino**, Claude L. Chenier, Carmela R. Jackson Lepage and Stephanie D. Huelin, DRDC Suffield, Canada.

10:50 LC-MS-MS in water and health research, **Xing-Fang Li**, Yuli Zhao, Rongfu Huang, Jessica Boyd and Wei Wang, University of Alberta.

11:10 High resolution mass spectrometry and its applications to molecular biomarkers in cardiovascular disease, **Jose Castro-Perez**², Douglas G. Johns¹, David McLaren², Stephen Previs², Vinit Shah², Karen Gagen¹, Vivienne Mendoza¹, Sheng-Ping Wang¹, Alan Millar⁴, Henry Shion⁴, Nathan Hatcher³, Nana Kofi Karikari³, Brian Hubbard¹ and Thomas P. Roddy², ¹Merck & Co., Inc. Atherosclerosis Research, Rahway, NJ, USA, ²Merck & Co., Inc. Molecular Biomarkers, Rahway, NJ, USA, ³Merck & Co., Inc. Molecular Biomarkers, West Point, PA, USA, ⁴Waters Corp, Milford, MA, USA.

11:30 Discussion

11:45 Adjourn

12:15 Lunch