LAKE LOUISE XXIII

23RD Workshop on Tandem Mass Spectrometry

Thursday, December 2, 2010, Morning Session

Chair: Paul Mayer

8:00 Introductory Remarks: **Gordon McKay**

8:10 LC-tandem ion mobility separations and mass spectrometry for extending the sensitivity of pan-omics measurements, ***Richard D. Smith***, Erin S. Baker, Yehia M. Ibrahim, David C. Prior, William F. Danielson III, Anuf R. Shah, Gordon A. Anderson & Yu Chen, Biological Sciences Division, Pacific Northwest National Laboratory.

8:50 Sub-attomole detection limits using enhanced ion-funnel technology on a triple quadrupole mass spectrometer, ***Paul Momoh***, Life Sciences Group, Agilent Technologies, Santa Clara, CA.

9:10 MS-based structural proteomics: first applications to solve clinical and biomedical problems, ***Christoph Borchers***, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

9:30 Increasing depth of coverage in complex “systems” utilizing UPLC-HDMS^{E}, ***Michael Nold***, Scott Geromonos & Jim Langridge, Waters Corporation, Milford, MA.

9:50 Discussion

10:00 Break

Chair: Paul D’Agostino

10:20 Orbitrap based LC MS/MS identification of signalling (poly)peptides secreted by human T-cells, ***Inez Finoulst***[1] **(Winner of a Lake Louise Workshop ‘All Sponsor Supported’ Student Travel Award)**, Paul Vink[2], Mervin Pieterse[1], Martijn Pinkse[1], Ebo Bos[2] & Peter Verhaert[1], [1]Dept. of Biotechnology, Analytical Biotechnology Section & the Netherlands Proteomics Centre, Delft University of Technology, Delft, The Netherlands, [2]Department of Immune Therapeutics, Merck Research Laboratories, MSD, Oss, the Netherlands.

10:40 Non-specific covalent modifications of proteins with carbenes: peptide and residue mapping, ***Chanelle C. Jumper*** & David C. Schriemer, Health Sciences Center, University of Calgary, AB.

11:00 Investigating the folding and assembly of a protein complex by pulsed oxidative labelling and ESI-MS/MS, ***Bradley Stocks*** **(Winner of the Waters Canada supported CSMS Student Travel Award)**, Gary Shaw & Lars Konermann, Dept’s of Biochemistry & Chemistry, The University of Western Ontario, London, ON.

11:20 De novo protein sequencing using MALDI top-down-sequencing, ***Shannon Cornett*** , Anja Resemann, Dirk Wunderlich, Jens Fuchser & Detlev Suckau, Bruker Daltonics, Billerica, MA .

11:40 Comprehensive phosphoproteomics analyses of insulin signalling pathways in *Drosophila melanogaster* using high field asymmetric waveform ion mobility spectrometry and CID/ETD ion activation on a LTQ-Orbitrap, ***Gaëlle Bridon***[1,2], Eric Bonneil[1], Tara Muratore-Schroeder[1], Brenda Kessler[3], & Pierre Thibault[1,2,4], [1]Institute of Research in Immunology and Cancer, Université de Montréal, Montréal, Canada, [2]Department of Biochemistry, Université de Montréal, Montréal, Canada, [3]Thermo Fisher Scientific, San Jose, CA, [4]Department of Chemistry, Université de Montréal, Montréal, Canada.

12:00 Discussion
12:30 Lunch (in the Fairview Room)

Afternoon Session
Chair: Lars Konermann

14:00 The structure of b_3 ions: can such small, isomeric ions really be that different? ***Gary L. Glish***[1] Alessandra L. Ferzoco[1], Julia M. Allen[1], Jefferey Steill[2], Jos Oomens[2], Benjamin Bythell[3] & Bela Paizs[3], [1]University of North Carolina, Chapel Hill, NC, [2]FOM Institute for Plasmaphysics Rijnhuizen, Nieuwegein, Netherlands, [3]German Cancer Research Center, Heidelberg, Germany.

14:20 Peptide group specific immunoaffinity enrichment for mass spectrometric protein quantification, ***Oliver Poetz***[1], Anke Schnabel[2], Hannes Planatscher[3], Dieter Stoll[1], Markus F. Templin[1], Katrin Marcus[2] & Thomas O. Joos[1], [1]NMI Natural and Medical Sciences Institute, University of Tübingen, Germany, [2]Functional Proteomics, Medizinisches Proteom-Center, Ruhr-Universität Bochum, Germany, [3]University of Tübingen, Centre for Bioinformatics, Tübingen, Germany, [4]Medical Proteomics/Bioanalytics, Medizinisches Proteom-Center, Ruhr-Universität Bochum, Germany.

14:40 Quantitative proteomics analysis of TNF-α activated macrophages reveals the selective degradation of mitochondria proteins, ***Christina Bell***[1,2] **(Winner of the Thermo Fisher supported CSMS Student Travel Award)**, Matthias Trost[3], Luc English[4], Michel Desjardins[4] & Pierre Thibault[1,2], [1]Proteomics and Bioanalytical Mass Spectrometry, Institut de recherché en immunology et en cancérologie, Université de Montréal, Montréal, Canada, [2]Department of Chemistry, Université de Montréal, Montréal, Canada, [3]MRC Protein Phosphorylation Unit, University of Dundee, Dundee, Scotland, [4]Department of Pathology and Cell Biology, Université de Montréal, Montréal, Canada.

15:00 The Extent and effects of Peptide sequence scrambling via formation of macrocyclic b ions in model proteins, Irine S. Saminathan, X. Simon Wang, Yuzhu Guo, Olga Krakovska, Sebastien N. Voisin, Alan C. Hopkinson & ***K. W. Michael Siu***, Department of Chemistry and Centre for Research in Mass Spectrometry Toronto, ON.

15:20 Discussion
15:30 Break

Chair: Gary Glish

16:00 Oil sands process water: beyond naphthenic acids, ***Mark P. Barrow***, J. V. Headley, Matthias Witt, K. M. Peru & D. McMartin, Environment Canada, Saskatoon, SK.

16:20 Application of electron-based ion activation methods and multivariate statistical approaches to determine chondroitin sulfate glycosaminoglycan hexuronic acid stereochemistry, ***Franklin E. Leach III***[1] **(Winner of the Research Scientific Services supported Lake Louise Student Travel Award)**, Mellisa Ly[2], Tatiana N.Laremore[2], Jeremy J. Wolff[5], Jacob Perlow[1], Robert J. Linhardt[2,3,4] & I. Jonathan Amster[1], [1]University of Georgia, Department of Chemistry, Athens, GA, [2]Department of Chemistry and Chemical Biology, [3]Chemical and Biological Engineering, and [4]Biology, Rensselaer Polytechnic Institute, Troy, NY, [5]Bruker Daltonics, Billerica, MA.

16:40 Fixed charge derivatization and data dependent CID- and ETD-MS/MS for the enhanced phosphopeptide quantitation and phosphorylation site characterization, ***Gavin E. Reid***, Department of Chemistry, Michigan State University.

17:00 Recent advances in hydrogen exchange mass spectrometry of proteins, ***Lars Konermann***, Department of Chemistry, The University of Western Ontario, London, ON.

17:20 Discussion
18:00 Dinner

Evening Session
Chair: Kerry Peru

20:00 Exploring amphibian biodiversity for novel peptide drug candidates, the tandem MS connection, ***Peter Verhaert***[1], Geisa Caprini-Evaristo[1], Martijn Pinkse[1], Daniel Carvalho Pimenta[2], Celio Haddad[3], Tianbao Chen[4] & Chris Shaw[4], [1]Biotechnology Department, Delft University of Technology, Delft, Netherlands, [2]Butantan Institute, Sao Paulo, SP, Brazil, [3]University of Sao Paulo, Rio Claro, SP, Brazil, [4]School of Pharmacy, Queens University of Belfast, Belfast, UK.

20:40 About FAIMS right now: food safety, proteomics and sport doping, ***Keeley Murphy***, Vertical Marketing – Drug Discovery and Development, Thermo Fisher Scientific.

21:00 Acquisition of ion mobility and tandem mass spectrometric data for the confirmation of organophosphorus chemical warfare agents, ***Paul A. D'Agostino*** & Claude L. Chenier, DRDC Suffield, AB.

20:20 Discussion

20:25 Poster Session – please man posters until 23:00

Detection and sequencing of small peptides from enzymatically hydrolysed flaxseed protein using LC-MS/MS and immonium precursor ion scanning, ***Steve Ambrose***[1], Harsha Marambe[2], Janitha Wanasundara[3], Phyllis Shand[2] & Randy Purves[1], [1]Plant Biotechnology Institute, National Reaserch Council, Saskatoon, SK [2]Food and Bioproduct Sciences, University of Saskatchewan, Saskatoon, SK, [3]Department of Chemistry, Agriculture and Agri-Food Canada, Saskatoon, SK.

Enhanced sensitivity for protein quantitation using a triple quadrupole with a dual ion funnel, ***Richard C. Barry***[1], Christine A. Miller[1], Yanan Yang[1], Derek Smith[2] & Christoph H. Borchers[1], [1]Agilent Technologies, Santa Clara, CA, [2]UVic-Genome BC Proteomics Centre.

LC-MS/MS method development for the quantification of a novel Gemini surfactant within PAM212 cells, ***Joshua Buse***[1], Ildiko Badea[1], Ronald Verrall[2] & Anas El-Aneed[1], [1]University of Saskatchewan, Saskatoon, SK, [2]Department of Chemistry, University of Saskatchewan, SK.

MRM quantitation of human blood plasma following antibody depletion of high abundant proteins, ***Alex Camenzind***, Juncong Yang, Angela Jackson, Dominik Domanski, Derek Smith & Christoph H. Borchers, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

Development of a method for quantitative MALDI imaging by MRM for absolute and spatial quantitation of proteins, ***Elizabeth Clemis***, Derek Smith, Ryan M. Danell, Tyra J. Cross & Christoph H. Borchers, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

Reduction of double oxidation in peptides containing tryptophan, ***Elizabeth Clemis***, & Christoph H. Borchers, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

Development of a new MALDI-TOF-TOF tandem mass spectrometer utilizing a spiral ion trajectory TOFMS and an offset parabolic reflectron, Takaya Satoh, Yoshiyuki Itoh, Takafumi Sato, Jun Tamura, Yoshihisa Ueda & ***Robert B. Cody***, JEOL, USA, Inc.

A stress response comparison: LC/MS metabolomics analysis of *Saccharomyces cerevisiae* exposed to the immunosuppressant drugs FK506 and Cyclosporin A, ***Linda Côté***[1], Theodore R. Sana[2], Stefan Jenkins[2,3], Lily Chen[4], [1]Agilent Technologies, Montréal, [2]Agilent Technologies, Santa Clara, CA, USA, [3]Cell and Molecular Biology MS Program, [4]San Francisco State University.

BIRD and computational studies of $Ca(Uracil)_n^{2+}$ complexes (n=5-14): stuctures, energetics and evidence for isomers for n=5, Elizbeth E. A. Gillis, Maria Demireva, Kashuk Nanda, Evan Williams, Greg Beran & ***Travis D. Fridgen***, Memorial University, Newfoundland.

Towards understanding the differential mass spectral fragmentation of triacylglycerol reioisomers, Lisandra Cubero Herrera, ***J. Stuart Grossert*** & Jeremy E. Melanson, Institute of Marine Biosciences, National Research council of Canada, Halifax, NS.

Tandem ion traps – a novel technique to analyze large populations of ions, ***Mircea Guna***, AB Sciex.

Characterization of oil sands acids in aquatic plant tissue using orbitrap ultra-high resolution mass spectrometry with electrospray ionization, ***J. V. Headley***, ***K. M. Peru***, A. Janfada & ***B. Fahlman***, water Science and Technology Directorate, Saskatoon, SK.

Fullerenes from polycyclic aromatic hydrocarbons in a MALDI TOF mass spectrometer, ***Robert E. Haufler***, AB Sciex.

Non-specific covalent modifications of proteins with carbenes: peptide and residue mapping, ***Chanelle C. Jumper*** & David C. Schriemer, University of Calgary, AB.

Overalkylation of protein digest with iodoacetamide during proteomic experiments: consequences for IDA LC-MS/MS analyses, Peter McQueen, Janice Reimer, Vic Spicer & ***Oleg Krokhin***, Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, Canada.

Tandem mass spectrometric analysis of novel amino acid/peptide substituted Gemini surfactants used as non-viral delivery agent, ***Waleed Mohammed-Saeid***[1], Joshua Buse[1], Ronald Verrall[2] Ildiko Badea[1] & Anas El-Aneed[1], [1]Drug design and Discovery Research Group, College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, SK, [2]Department of Chemistry, University of Saskatchewan, SK.

Resolving alternative structures of intact proteins by high-field asymmetric ion mobility spectrometry, ***Keeley Murphy***, Julian Sabaa & Tonya Pekar Second, Vertical Marketing – Drug Discovery and Development, Thermo Fisher Scientific, San Jose, CA, USA.

Less is more: improved sensitivity of plasma protein MRM quantitation with reduced sample loading, ***Leanne Ohlund***, Christine A. Miller, Yanan Yang, Derek Smith & Christoph H. Borchers, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

Multiplexed iMALDI for the detection of angiotensin I and angiotensin II, ***Carol Parker***, D. Randal Mason, Jennifer D. Reid, Daniel T. Holmes & ***Christoph H. Borchers***, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

A MALDI MS assay for the determination of glycated hemoglobin and hemoglobin variants, ***Evgeniy V. Petrotchenko*** & Christoph H. Borchers, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

Redox signalling through cysteine modification in *Fusarium graminearum* NADPH oxidase deletion mutants revealed by LC-MS, Manisha Joshi, Rajagopal Subramaniam, Tao Fan & ***Christof Rampitsch***, Agriculture and Agrifood Canada.

A diagnostic test for detection of prion aggregates by crosslinking and mass spectrometry, ***Jason J. Serpa***, Evgeniy V. Petrotchenko & Christoph H. Borchers, University of Victoria – Genome BC Proteomics Centre, Victoria, BC.

Quantitative mass spectrometry of *Brachypodium distachyon* proteins form stressed and unstressed plants, ***David B. Shearer***, Victor Spicer, Oleg Krokhin, Steve Haber

& Kenneth G. Standing, Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, Canada.

The formation of $[M-H]^+$ species during matrix assisted laser desorption ionization mass spectrometric analysis of nitrogen-containing curcumin analogs, ***Lindsey Usher***[1], A. Cohen[2], U. Das[1], D. Dimmock[1], D. Pinto[2] & Anas El Aneed[1], [1]Drug Design and Discovery Research Group, University of Saskatchewan, College of Pharmacy and Nutrition, Saskatoon SK, Canada, [2]NRC, Institute for Marine Bioscience, Halifax, NS, Canada.

Friday, Dec. 3, Morning Session
Chair: Michael Siu

8:20 Fluorescence and fluorescence resonance energy transfer (FRET) measurements of trapped ions, ***Rebecca A. Jockusch*** **,** Francis O. Talbot, Matthew W. Forbes, Qunzhou Bian & Martin F. Czar, Chemistry Department, University of Toronto, Toronto ON.

9:00 Probing the structure and stability of the covalently bound HCN and HNC dimers using tandem mass spectrometry and computational chemistry, ***Karl J. Jobst*** & Johan K. Terlouw, Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON.

9:20 Teaching old metals new tricks: the generation and reactions of metal anions, Sharon Curtis, Justin Renaud, Jason DiMuzio & ***Paul Mayer***, Chemistry Department, University of Ottawa, Ottawa, ON.

9:40 Information-dependent MS/MS acquisition with exclusion/inclusion lists generated on-the-fly, Peter McQueeen, Janice Reimer, Vic Spicer & ***Oleg Krokhin***, Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, Canada .

10:00 Discussion
10:10 Break

Chair: Michael Siu

10:30 Structures of electrosprayed complexes formed between Pb^{2+} and the conjugate bases of amino acids, Mike B. Burt, Sarah G. A. Decker & ***Travis D. Fridgen***, Memorial University, Newfoundland.

11:10 The importance of structure in understanding fragmentation of polyfunctional anions in tandem mass spectrometry – a study assisted by isotopic labelling and density functional computations, ***J. Stuart Grossert***, Lana E. Greene & Robert L. White, Department of Chemistry, Dalhousie University, Halifax, NS.

11:30 Adventures in time-resolved mass spectrometry: the hunt for 'Sticky Conformers' and teeny-tiny kinetic isotope effects, ***Derek J. Wilson***, York University, Toronto, ON.

11:50 Elucidating the specificity of the formaldehyde cross-linking reaction by LC-MS/MS, Xuan Ding, Jason Rogalski & ***Juergen Kast,*** The Biomedical Research Centre and Department of Chemistry, University of British Columbia, Vancouver, BC, Canada.

12:10 Cex in a vacuum: solution and gas-phase hydrogen deuterium exchange studies of protein inhibitor noncovalent complexes, ***Don Douglas***, Peran Terrier & Chuanfan Ding, Department of Chemistry, The University of British Columbia.

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. 4, Morning Session
Chair: Orval Mamer

8:30 Mass spectrometry applications in biochemical genetics: current trends, ***Christiane Auray-Blais***, René Gagnon & Joe T. R. Clarke, Service of Genetics, Department of Pediatrics, Faculty of Medicine and Health Sciences, Université de Sherbrooke.

9:10 Characterization of seafood aero allergenic proteins and determining their levels in the air of fish plants using tandem mass spectrometry, ***Anas M. Abdel Rahman*** **(Winner of a Lake Louise Workshop 'All Sponsor Supported' Student Travel Award)** & Robert J. Helleur, Memorial University of Newfoundland.

9:30 A simple strategy for acquiring products *of All* using TOF; in application to lipid characterization, ***Brigitte Simons***, Stephen Tate & Eva Duchoslav, AB Sciex.

9:50 Gas-phase ions of variant human hemoglobins, ***Yang Kang***[1] **(Winner of the AB Sciex supported CSMS Student Travel Award)**, Peran Terrier[2] & D. J. Douglas, [1]Department of Chemistry, The University of British Columbia, [2]Adocia, Lyon, France.

10:10 Discussion
10:20 Break

10:40 Metabolomic signatures in disorders of mitochondrial protein import and lysosomal amino acid transport, ***Floyd F. Snyder***, University of Calgary, AB.

11:20 Non-targeted screening and quantification of marine biotoxins by high resolution mass spectrometry, ***Jeremy E. Melanson***[1], Pearl Blay[1], Joseph Hui[1], Ruth Perez[1] & James Chang[2], [1]NRC Institute for Marine Biosciences, Halivax, Nova Scotia, Canada, [2]Thermo Scientific, San Jose, CA.

11:40 Quantitative LC/MS/MS of progesterone; trials and tribulations, ***G. McKay***[1], W. Schwab[1], C. Ebert[2] & M. Hetherington[1], [1]Pharmalytics Ltd, Saskatoon, SK, [2]Watson Pharmaceuticals Brand division, Salt Lake City, UT.

12:00 Discussion
12:15 Adjourn and Lunch

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