LAKE LOUISE XII The 12th Lake Louise Workshop on Tandem Mass Spectrometry

Thursday 2nd December

8:15 Opening Remarks

Chair: Gary Glish

- 8:20 Alan Marshall (Florida State University): Mass Spectrometric Techniques for Identifying Sites and Strength of Binding in Biomacromolecular Complexes
- 9:10 **Don Douglas** (University of British Columbia): Monte Carlo Simulation of the Tandem Mass Spectrometry of Protein-Protein Noncovalent Complexes
- 9:35 Discussion
- 9:45 Break
- 10:10 **Joe Loo** (Parke-Davis): Tandem MS of Proteins and Protein Complexes: Splitting Subtle Associations for Fun and Profit
- 11:00 Paul Kebarle, M. Peschke and A.J. Blades (University of Alberta): Production of Metal-Ligand Complexes by Electospay, Bond Energies of Metel Ligands and Significance in Biocomplexes
- 11:25 George R. Agnes and Mike Bogan (Simon Fraser University): He Bath Gas Thermalized Dissociation of Weakly Bound Metal Ions from the Ligand Poly-ethylene Glycol
- 11:50 Discussion
- 12:00 Break for Lunch

Chair: Orval Mamer

- 13:30 Gordón McKay (University of Saskatchewan): The Use of LC-MS-MS as a High Throughput Quantitative Tool
- 14:20 **J. Paul Speir**, Gary H. Kruppa, Christian Berg, Bruker Daltonics, Inc.; Frank Pullen, George Perkins, Pfizer Central Research: *On-line FTMS/MS Methods Compatible with Fast Chromatographic Separations*
- 14:45 **Daniel Boismenu**, Orval A. Mamer, McGill University, Julie Roy and France Varin, Universite de Montreal: *Determination of Succinylcholine in Plasma by Electrospray Tandem Mass Spectrometry*
- 15:10 Discussion
- 15:20 Break

- 15:35 **Peter Verhaert**, University of Leuven: Peptidomics: A Valuable Complement to .

 Proteomics
- 16:00 **Ken Standing**, University of Manitoba: Protein Sequencing on a Maldi-QqTOF Instrument
- 16:25 John Klassen, University of Alberta: Hydration of DNA Anions in the Gas Phase
- 16:50 **Simon J. Gaskell**, Michael Chalmers, Myriam Ferro, Ileana Cristea, UMIST; Les Gora, Charles Smith, Micromass: New derivatives of peptides and first results from a new instrument for SID
- 17:15 Discussion
- 17:25 Break for Dinner

Chair: John Klassen

- 20:00 Tanya N. Gamble, University of Waterloo: Deuterium Isotope Effects on the Energetics of Clustering Reactions of Small Organic Ions
- 20:30 Cherokee Hoaglund Hyzer, Indiana University: Development of a Gas-Phase Parallel Sequencing Technique Based on Ion Mobility/MS/MS Methods
- 21:00 Posters
- 22:30 Break for Bar

Friday 3rd December

Chair: Pierre Thibault

- 9:00 **Gerald Hart**, Johns Hopkins University: Structural Diversity and Abundance of Protein-Bound Glycans: A Challenge to Proteomic Analyses by Tandem MS
- 9:50 **Helene Perreault**, University of Manitoba: Oligosaccharide Determination using Different HPLC/MS Modes
- 10:15 Discussion
- 10:30 Break
- 10:50 **David Schriemer**, INH Technologies: High Throughput Drug Discovery Strategies Using FAC-MS; Approaches and Applications



- 11:15 **Pierre Thibault**, NRC Institutes for Biological Sciences: Monitoring Glucosylation and Glycosylation in Complex Glycoproteins Using Tandem Mass Spectrometry
- 11:40 Discussion
- 11:50 Lunch

Saturday 4th December Chair: Simon Gaskell

- 8:30 Carolyn J. Cassady, Miami University: Dissociation of Deprotonated Peptide Ions
- 9:20 Ivan K. Chu, Tamer Shoeib, Christopher F. Rodriquez, Alan C. Hopkinson and K.W. Michael Siu, York University: Tandem Mass Spectrometry of Argentinated Oligopeptides
- 9:45 Paul M. Mayer, University of Ottawa: Competition Between Dissociation and Isomerization in Proton Bound Cluster Ions: Using Mass Spectrometry and Theory to Gain Information about Complex Reaction Surfaces
- 10:10 Discussion
- 10:20 Break
- 10:40 **John Holmes**, University of Ottawa: Tandem Mass Spectrometers and the Determination of Ion Energies and Entropies
- Bruce Collings, University of British Columbia: Characterization of a Novel Linear Ion
 Trap Time-of-Flight Mass Spectrometer
 - 11:30 Jennifer M. Campbell, Anatoli Verenchikov, Peter Juhasz, Marvin L. Vestal, PE Biosystems: Development of a High Performance MALDI-TOF/TOF Tandem Mass Spectrometer
 - 11:55 Anne Payne and **Gary Glish**, University of North Carolina: *Chemical Interpretation of Peptide MS/MS Spectra*
 - 12:15 Close

Posters

James I. Langridge and **Guenter K. Eigendorf**, University of British Columbia: Accurate mass, MS2 and MS3 experiments in API modes on a QqTOF system

Richard Ochran et al., University of Ottawa: Competition Between Dissociation and Isomerization in the CH3CN - CH3CH2OH proton bound dimer

Julie McCormack et al., University of Ottawa: Using a Quadrupole Ion Trap to Study Ion-molecule Reactions Involving Complex Potential Energy Surfaces

D. Boismenu, L. Ste-Marie, C. Bomeur, O. Mamer and **J. Montgomery**, McGill University and Notre Dame Hospital, Montreal: The Electrospray-MS/MS Quantitation of 3-Nitro-4-hydroxybenzoate, a Marker of Peroxynitrite Formation, in Microdialysis Samples Following Cerebral Ischemia in the Rat

Anthony K. Ziberna, Finnigan MAT: High Resolution Precursor Selection and ESI-MSn for Polypeptide Sequencing

Anthony K. Ziberna, Finnigan MAT: Automated LC-MS/MS on a Hybrid Tandem Mass Spectrometer

Chunyan Hao, Timothy R. Croley, Raymond E. March, Brenda G. Koenig and Chris D. Metcalfe, Trent University: A GC/MS Study of Persistent Acid Metabolites of Nonionic Surfactant Nonylphenol Ethoxylates

Paul A. D'Agostino, James R. Hancock and Lionel R. Provost, DRES, Suffield, AB: Analysis of Chemical Warfare Agents with a Time-of-Flight Instrument

Y-M She, J.B. Westmore, A. Loboda, A. Krutchinsky, W. Ens, and K.G. Standing, University of Manitoba: Further Observations On The Loss Of C-Terminal Amino Acid Residues From Peptide [M + H]+ Ions, As Recorded By MALDI Qq/TOF Mass Spectrometry

Lawrence Hogge and Gordon McKay, University of Saskatchewan: Development of a quantitative LC-MS-MS method for the analysis of guanfacine

Xiao Feng and George R. Agnes, Simon Fraser University: Single Isolated Droplets with Net Charge: As source of Ions, and as a (Potentially) Interesting Containment Vessel

Mark A. Olsen, Priscilla Offen, Charles W. DeBrosse, Lewis Killmer, Gary Zuber, William M. Clark, SmithKline Beecham Pharmaceutical: Using LC/ES/MS, LC/NMR, NMR And IR Spectroscopic Tools To Determine the Structure Of Process Impurities In Stage 4 And Stage 5 Of Sb 207499

Elena Kitova, John Klassen, University of Alberta: Binding of Single Chain Antibody Variable Domain Fragment to Oligosaccharides Studied by ES-FT-MS

Chungang Gu, C. Martin, E. Nikolaev, G. Samuelson, A. Somogyi and V. Wysocki, JOEL USA and University of Arizona: Sector-TOF Hybrid In-Line Coaxial Design for Low Energy SID and High Energy CID MS/MS

Daniel Boismenu, Francois Lepine and Orval Mamer, McGill University and Institut Armand-Frappier-INRS, Nanospray Tips

I.V. Soulimenkov, V.I. Kozlovski, A.V. Loboda, A.V. Pikhtelev, A.F. Dodonov, V.V. Raznikov, V.V. Trukhan, A.A. Steinman, Institute of Energy Problems in Chemical Physics TAS, PE SCIEX, Institute of Problems in Chemical Physics: Study of Bi- and Tetranuclear Iron-oxo Complexes Using High-Resolution ESI O-TOF MS with a Molecule-Ion Reactor (MIR)