LAKE LOUISE XI

The Eleventh Lake Louise Workshop on Tandem Mass Spectrometry

Thursday 3rd December

8.30 Welcome and Announcements

Simon Gaskell, Chair

- 8.35 P. Iannitti, A. Weimann, J. Beck, J.A. Burgess and Margaret Sheil (University of Wollongong, Australia): *Tandem mass spectrometry of oligonucleolides and drug-DNA adducts*
- 9.20 John Klassen (University of Alberta, Edmonton): Gas-phase acidities of the nucleobases
- 9.40 Discussion
- 10.00 Break
- 10.20 **Gordon McKay** (University of Saskatchewan, Saskatoon): Development of a quantitative analysis for Buproprion and its metabolites using MRM
- 10.40 **Ken Tomer** et al. (NIEHS, Research Triangle Park, NC, USA): *HIV glycopeptide characterization using the QTOF hybrid MS*
- 11.00 Chris Lock (Institute for Marine Biosciences, Halifax): The separation and characterisation of peptides by combined micro-HPLC Qq-TOF
- 11.20 Peter Verhaert et al. (Innogenetics, Gent, Belgium): MALDI-PSD and ESI-TOF MS/MS for de novo sequencing of neuropeptides
- 11.40 Discussion
- 12.00 Lunch

Pierre Thibault, Chair

- 13.30 Frank Turecek (University of Washington, USA): Variable time and photoexcitation studies in NRMS
- 14.15 **Richard Vachet** et al. (Naval Research laboratory, Washington DC, USA): *Using ion-molecule reactions to study the structure of metal complexes*
- 14.35 **John Holmes** (University of Ottawa): An appraisal of the kinetic method for determining proton affinities
- 14.50 Discussion
- 15.10 Break

- 15.30 Kenneth L. Ray and Gary Glish (University of North Carolina, Chapel Hill, NC, USA): Hadamard transform quadrupole ion trap mass spectrometry
- 15.50 Glenn Legault et al. (Trent University, Peterborough): Ion trap analysis of arachidonic acid arising from long-term potentiation in rat brain
- 16.10 Paul Kebarle, Michael Peschke and Arthur T Blades (University of Alberta): Towards a metalloenzyme ion-ligand thermochemistry and what we can learn from it
- 16.30 Discussion
- 16.45 Break
- 18.00 Dinner

Orval Mamer, Chair

- 20.00 Einar K. Fridriksson, Barbara Baird, David Holowka, and Fred W. McLafferty (Cornell University, Ithaca, NY, USA): Studies of IgE antibodies, 190 kDa, with Fourier-transform tandem mass spectrometry
- 20.30 Gabi V. Koellisch (University of Bayreuth, Germany), Peter D. Verhaert (Innogenetics, Gent, Belgium), and Klaus H. Hoffmann (University of Bayreuth, Germany): Tandem mass spectrometry and butterfly neurohormones the TOF connection
- 21.00 Poster session

Friday 4th December

Gary Glish, Chair

- 8.30 Mike Bowers (University of California, Santa Barbara, CA, USA): Conformations of macromolecules in the gas phase: the latest news
- 9.15 Luke Hanley et al. (University of Illinois at Chicago, USA): Shattering of SiMe₃⁺ during surface-induced dissociation
- 9.35 Peter Ver/vaert

 9.35 Jim Scrivens et al. (ICI, Cleveland, UK): Tandem mass spectrometric aspects of polymer microstructure
- 9.55 Discussion
- 10.10 Break
- 10.30 Pierre Thibault, Li Jianjun (Institute for Biological Sciences, Ottawa), Bruce Thomson (Sciex), Nicholas Bings, Cameron D. Skinner, Can Wang, and D. Jed Harrison (University of Alberta): Development of microfabricated devices with low dead volume connection for capillary electrophoresis-electrospray mass spectrometry: enhanced sample throughput for protein identification

- 10.50 Paul D'Agostino, Lionel Provost and James Hancock (DRES, Suffield): Packed Capillary LC-ESI-MS and MS/MS of CWC organophosphorus warfare agents, related compounds and their degradation products
- 11.10 Carmai Seto, J. Stuart Grossert (Dalhousie University, Halifax), David S Waddell, Robert R Boyd and Jonathan M Curtis (Institute for Marine Biosciences, Halifax): Remote-site fragmentation processes in long-chain alkyl ammonium ions from an electrospray source
- 11.30 **J. Stuart Grossert**, Elizabeth Lewis and Robert L White (Dalhousie University, Halifax): MS/MS studies on protonated derivatives of acetanilides
- 11.50 Discussion
- 12.00 Lunch

Afternoon free

19.30 for 20.00 Workshop Dinner

Saturday 5th December

Gordon McKay, Chair

- 8.30 **Ken Standing** (University of Manitoba): *Tandem MS measurements on hybrid quadrupole/time-of-flight instruments*
- 9.15 Robert H. Bateman, Robin Carruthers, John B. Hoyes, Anthony J. Gilbert, James I. Langridge, Kevin Malone, Robert S. Bordoli, and Alan Millar (Micromass UK, Manchester, UK): The novel precursor scanning mode of a quadrupole time-of-flight hybrid tandem mass spectrometer
- 9.35 **Igor Chernushevich** et al. (Sciex): Parent ion scan improvements on a QqTOF tandem mass spectrometer
- 9.55 Discussion
- 10.10 Break
- 10.30 **Don Douglas** et al. (University of British Columbia): A linear ion trap time-of-flight system for MS/MS
- 10.50 Brian Musselman (PerSeptive Biosystems, Framingham, MA, USA): New developments in tandem TOF MS/MS
- 11.10 Ken Tornec 11.10 Gary-Kruppa (Bruker Daltonics, Billerica, MA, USA): Strategies for accurate mass measurement in MSⁿ with FTMS
- 11.30 Alex Harrison (University of Toronto): A comparison of skimmer-cone and quadrupole cell CID
- 11.50 Myriam Ferro, Richard Jones, and Simon Gaskell (UMIST, Manchester, UK): The formation and fragmentation of dimeric peptide ions during electrospray MS
- 12.10 Close of Workshop

POSTERS

- 1. Luke Hanley et al. (University of Illinois at Chicago, USA): Relative energies of peptide ion fragmentation by surface induced dissociation
- 2. Victor Nesati, Don Douglas et al. (University of British Columbia): Tandem MS of non-covalent protein-protein complexes
- 3. Alister Muir, Andrew Aubin and Dana Yurach (Agriculture and Agrifoods Saskatoon Research Centre): LC-MS/MS analysis of lignans in plasma and urine problems and solutions
- 4. Lisa Cousins et al. (MDS-Sciex Canada): Radial excitation MS/MS and MS/MS/MS in continuous beam quadrupoles
- 5. **Anil Shukla**, Helen de Clercq, Atish Sen, Sergey Rakov and Jean Futrell (University of Delaware): Surface-induced dissociations: A crossed-beam study
- 6. **Francois Lépine** et al. (Institut Armand Frappier, Laval, Quebec): Reactions of t-butylcyclohexyl esters with oxygen in the collision cell of an MS/MS
- 7. Yi-Min She, Ken Standing et al. (University of Manitoba): Studies on plant viral strain variation and evolution by tandem mass spectrometry
- 8. **Alexandre Loboda**, Ken Standing et al. (University of Manitoba): *MALDI QqTOF: design and performance*
- 9. **John Headley** et al. (NHRI, Saskatoon): Evaluation of the efficacy of photocatalysis combined with biofilm uptake for the attenuation of organic contaminants
- 10. Gary Kruppa (Bruker Daltonics, Billerica, MA, USA): Automated MSⁿ with FTMS
- 11. George Agnes (Simon Fraser University, Burnaby, BC): Alkali metal ion competition in solution, and in the gas phase, for the ligand poly(ethyl glycol)
- 12. George Agnes (Simon Fraser University, Burnaby, BC): Resonant ion ejection with supplemental AC fields in RF-only linear quadrupoles
- 13. Gord McKay, Lawrence Hogge, T. Gurnsey and R. Mazzei (College of Pharmacy, U of Saskatchewan; MicroPharm Consulting): Reproducability of high sensitivity multiple reaction monitoring (MRM) data obtained using LC/MS/MS with doxazosin gabapentin analysis as examples