

LAKE LOUISE X
The Tenth Lake Louise Workshop on Tandem Mass Spectrometry
All meetings to be held in the Tom Wilson Room on the 7th Floor

Thursday 4th December

8.30 Welcome and Announcements

Simon Gaskell, Chair

8:35 *Chrys Wesdemiotis* (University of Akron, OH, USA): Thermochemistry as a probe of biomolecular structures

9:20 *Arpad Somogyi* (University of Arizona, Tucson, USA): Prediction of bond strengths in protonated peptides by quantum chemical calculations, ESI/SID and thermal dissociation measurement

9:40 Discussion

10:00 Break

10:20 *Evan Williams* (University of California, Berkeley, USA): Blackbody infrared radiative dissociation of biomolecule ions

11:05 *Don Douglas* (University of British Columbia, Vancouver): Mechanism of the activation of protein ions in triple quads and an application to homomyoglobin

11:25 *Sharon Shields* (Texas A&M University, College Station, USA): Fragmentation reactions of MALDI formed $[M+Cu]^+$ peptide ions

11:45 Discussion

12:00 Lunch

Gordon McKay, Chair

13:30 *Mark Reimer* (Phoenix International Life Sciences, St Laurent, Quebec): The role of high throughput LC/MS/MS technology in early drug development: new advances in in vitro metabolite profiling

14:15 *Daniel Boismenu* (McGill University, Montreal): Measurement of isotopically labelled sulfate in biological fluids by electrospray tandem mass spectrometry

14:35 *Michael Siu*, V.W.M. Lee, R. Guevremont, T-C. Lau (NRC, Montreal): Determination of the relative gas phase silver(I) basicities of alpha-amino acids using the kinetic method

14:55 Discussion

15:15 Break

15:35 A.J. Bell, J. Murrell, *Peter Watts* (DERA, Porton Down, UK): MS_n analyses of organophosphates using an ion trap

15:55 Y. Ho, *Paul Kebarle* (University of Alberta, Edmonton): Activation energies and reaction mechanisms in CID of deprotonated mononucleotides

16:15 Discussion

16:40 Break

18:00 Dinner

Orval Mamer, Chair

20:00 *Christiane Aubry* (University of Ottawa: recipient of the 1997 Micromass Travel Award): Dimethylcarbene, its radical cation and dication

20:30 *Ray March* (Trent University, Peterborough, Ontario: recipient of the 1997 CSMS Award for Distinguished Contributions to Canadian Mass Spectrometry): A comparison of HMR, QQQ, and IT/MS/MS for the determination of dioxins

21:00 Poster discussion session (Refreshments will be served)

Friday 5th December

Gary Glish, Chair

8:30 *Terry McMahon* (University of Waterloo, Ontario): Novel MS_n experiments using Fourier transform ion cyclotron resonance spectrometry

9:15 *Gary Glish*, M.R. Asam and K.L. Ray (University of North Carolina, Chapel Hill, USA): Improved MS_n analysis using collision-induced signal enhancement

9:35 *Julie Leary* (University of California, Berkeley, USA): Ion trap MS/MS of diastereomeric metal-ligated oligosaccharides: synthesis and analysis

9:55 Discussion

10:10 Break

10:30 B.A. Mansoori, C. Lock, E. Dyer, B. Thomson, *Bob Boyd* (NRC, Halifax, Nova Scotia): Experimental and SIMION investigations of a high pressure RF-only quadrupole collision cell with a controllable axial field

10:50 A. Loboda, A. Krutchinsky, W. Ens, **Ken Standing** (University of Manitoba, Winnipeg): Selective collision-induced dissociation by resonance excitation of the ions in an RF-only quadrupole operating at elevated pressures

11:10 **Bruce Thomson**, I. Chernushevich (Sciex, Concord, Ontario): A new multiply charged ion scan mode

11:30 Discussion

12:00 Lunch

Afternoon Free

19:30 for 20:00 Workshop Dinner

Saturday 6th December

Bob Boyd, Chair

8:30 **Ruedi Aebersold** (University of Washington, Seattle, USA): 2D gel electrophoresis and mass spectrometry: complementary tools for proteome analysis

9:15 **Peter Verhaert** (University of Leuven, Belgium): Tandem MS on unseparated neuropeptides by nanospray-QToF

9:35 **Jim Langridge**, R.S. Bordoli (Micromass UK, Manchester, UK) P. Camilleri, G. Okato (SmithKline Beecham, Harlow, UK): Glycan sequencing by MALDI-MS and electrospray-MS/MS

9:55 Discussion

10:10 Break

10:30 **John Stults** (Genentech, South San Francisco, USA): Strategies for protein differential display and identification

11:15 **Catherine Stacey**, G. Kruppa (Bruker Daltonics, Billerica, MA, USA): Strategies for the identification of proteins from proteolytic digests using nanospray MS and MS/MS

11:35 **Simon Gaskell**, I. Riba (UMIST, Manchester, UK), H. Cho, W.R. Widger, H. Kohn (University of Houston, USA): Mass spectrometric characterization of the interaction between the antibiotic, bicyclomycin, and rho protein

11:55 Discussion

12:15 Close

POSTERS (in alphabetical order of presenting author)

Paul D'Agostino, L.R. Provost, J.R. Hancock (Defence Research Establishment Suffield, Medicine Hat, Alberta): Identification of munitions grade mustard hydrolysis products by LC-ESI-MS and LC-ESI-MS/MS

R.C. Jones, S.G. Summerfield (UMIST, Manchester, UK), R.S. Bordoli (Micromass UK, Manchester, UK), W. Simmons, J. Taurog (University of Texas Southwestern Medical School, Dallas, USA), **Simon Gaskell** (UMIST): Sequencing of peptides bound to MHC molecules using a combined MALDI-ToF and electrospray-QToF strategy

T. Lin and **Gary Glish** (University of North Carolina, Chapel Hill, USA): C-terminal peptide sequencing via multistage mass spectrometry of alkali metal cationized peptides

Steven Hall (Alza Corporation, Palo Alto, CA, USA): Probing thermal induced degradation of a peptide hormone using tandem mass spectrometry

John Headley (NHRI, Saskatoon, Saskatchewan): LC/MS/MS of explosives in water from military sites in Germany

John Klassen, P.D. Schnier, E.R. Williams (University of California, Berkeley, USA): Blackbody infrared radiative dissociation of nucleic acid dimers, oligonucleotides and their duplexes

Jim Langridge, G. Critchley, J. Hoyes, R.S. Bordoli, E. Kapp (Micromass UK, Manchester, UK), M. Sheil (University of Wollongong, Australia): Automated peptide mass screening and protein identification by electrospray and MALDI/TOF mass spectrometry and database search strategies

J.C. Yves Le Blanc (Phoenix International Life Sciences, St Laurent, Quebec), **George Scott**, J. Plomley, W. Stott (PE-Sciex, Concord, Ontario): Improving the transmission of ions through a high-pressure quadrupole collision cell

I.V. Chernushevich (Sciex, Concord, Ontario and University of Manitoba, Winnipeg), S. Haber (Cereal Research Centre, Winnipeg), G. Westmacott, W. Ens, **Ken Standing** (University of Manitoba, Winnipeg): Mass measurement on the coat proteins of some plant viruses with MALDI-TOF, ESI-TOF, and ESI-QqTOF instruments

Phillip Whitfield (Institute of Child Health, University of London, UK): The structural characterization of polar lipids in biological samples and lipid emulsions using electrospray ionization tandem mass spectrometry

Paul Zavitsanos (Hewlett Packard, Mississauga): The Esquire LC/MSn high performance ion trap