

MOOT XXIII

MINI NMR SYMPOSIUM

Dalhousie University, Halifax, Nova Scotia

All talks to take place in the Scotia Auditorium of the Marian McCain Arts & Social Sciences Building.
Posters located in the McInnis Room of the Dalhousie Student Union Building.

SCIENTIFIC PROGRAM

Friday, October 15th

7:00 – 9:00 pm: Mixer & Pre-Registration (Tupper Link)

Saturday, October 16th

8:00 - 9:00 Registration and Poster Setup

9:00 – 9:10 Welcoming Remarks & Announcements (Joe Zwanziger – Director NMR³)

Morning Session

Chair: Prof. Rob Schurko, University of Windsor

9:10 – 9:40 Interdomain Regulation in a Neuronal Signaling Protein
Logan Donaldson* and Jamie Kwan
Department of Biology, York University

9:40 – 10:10 Molecular Basis of E2A-PBX1 Induced B-cell Leukemia: Structural and Functional Studies of the E2A-CBP Interaction
Chris Denis, Seth Chitayat, Michael Plevin, S. Lui, Holly Spencer, Mitsu Ikura, David LeBrun and Steven Smith*
Department of Biochemistry, Queen's University

10:10 – 10:40 Structural and Functional Characterization of the N-terminus and First Transmembrane Segment of the Apelin Receptor
David N. Langelan* and Jan K. Rainey
Department of Biochemistry and Molecular Biology, Dalhousie University

10:40 – 11:00 Refreshment Break

11:00 – 11:30 Functional Characterization of Proteins Utilizing STD-NMR
Andrew W. Robertson* and David L. Jakeman
Department of Chemistry, Dalhousie University

11:30 – 12:00 Probing Electrostatic Interactions within Liquid Crystals
Ray Syvitski*¹, Karen Cheng², James Polsen², and Elliott Burnell²
¹Institute for Marine Biosciences, NRC, Halifax
²Department of Chemistry, University of British Columbia

12:00 – 1:30 Lunch (McInnis Room of Student Union Building)

Afternoon Session

Chair: Prof. David Bryce, University of Ottawa

1:30 – 2:00 Structure and Photoelastic Response of Lead-Borate Glasses
Vincent Martin*, Bryanna Wood, Ulrike Werner-Zwanziger, Josef W. Zwanziger
Department of Chemistry, Dalhousie University

2:00 – 2:30 New advances in ¹⁴N solid-state NMR
L.A. O'Dell¹, S. Veinberg², C. Mireault², B.E.G. Lucier², M. Hildebrand² and R.W. Schurko*²
¹ Steacie Institute for Molecular Sciences, NRC, Ottawa, Ontario
² Department of Chemistry & Biochemistry, University of Windsor, Windsor, Ontario

2:30 – 2:50 Refreshment Break

2:50 – 3:20 Quadrupolar Halogen (³⁵Cl, ⁸¹Br & ¹²⁷I) Solid-State NMR Spectroscopy of Haloanilinium Salts Exhibiting Halogen Bonding
Robert Attrell*, Cory Widdifield, David Bryce
Department of Chemistry, University of Ottawa

3:20 – 3:45 *In situ* Electrochemical NMR
Xiaocan Zhang and Josef Zwanziger*
Department of Chemistry, Dalhousie University

3:45 – 4:05 Elucidating the Relative Stereochemistry of Organic Molecules Using NMR Spectroscopy
Vanessa Marx*, Mike Lumsden, and Jean Burnell
Department of Chemistry, Dalhousie University

4:05 – 5:30 Poster Session and Refreshments (McInnis Room of Student Union Building)

6:00 Banquet (Halifax Citadel National Historic Site) & Presentation of Student Poster Prizes

Sunday, October 17th

8:55 - 9:00: Announcements

Morning Session

Chair: Dr. Mike Lumsden, Dalhousie University

9:00 – 9:25 Structures and Interactions of Lung Surfactant Protein B (SP-B) Peptides
Muzaddid Sarker*¹ and Valerie Booth^{1,2}
¹Department of Physics and Physical Oceanography, Memorial University
²Department of Biochemistry, Memorial University

9:25 – 9:50 Solid-state NMR as a Probe of HIV-1 Vpu Protein Oligomerization and Local Mobility in Lipid and Detergent
Dave Davidson* and Simon Sharpe
University of Toronto / Hospital for Sick Children

9:50 – 10:15 Computer Simulation and Dynamic NMR of Cationic Catena-Phosphorus Frameworks
Yuen-Ying Carpenter*, Mike Lumsden, and Neil Burford
Department of Chemistry, Dalhousie University

10:15 – 10:35 Refreshment Break

10:35 – 11:00 A ZORA-DFT and NLMO Study of the One-Bond Fluorine-X Indirect Nuclear Spin-Spin Coupling
Tensors for Various VSEPR Geometries
Frédéric A. Perras* and David L. Bryce
Department of Chemistry, University of Ottawa

11:00 – 11:25 ¹³C NMR study of Gymnospermous Cuticles and Associated Coals from Late Pennsylvanian Seed
Ferns and Cordaites
Ulrike Werner-Zwanziger*¹, Banghao Chen¹, and Erwin Zodrow²
¹Department of Chemistry, Dalhousie University
²Department of Geology, Cape Breton University

11:25 – 11:50 Crystal Structure Based Design of Signal Enhancement Schemes for Solid-State NMR of
Half-integer Quadrupolar Nuclei
Luke A. O'Dell* and Christopher I. Ratcliffe
Steacie Institute for Molecular Sciences, NRC, Ottawa

11:50 – 12:00 Closing Remarks

POSTERS

A total of three prizes of \$75 each will be awarded to the three best posters paid for by the Suraj Manrao Student Science Fund.

- 1. CSChameleon: Predicting Protein Secondary Structure in Disparate Environments Using Random Coil Chemical Shifts**
Banks, A. W.*, Tremblay, M.-L., Rainey, J.K.
Department of Biochemistry and Molecular Biology, Dalhousie University
- 2. Exact Calculation of the Response of a Quadrupolar Nucleus to RF Irradiation**
T.L. Spencer, G.R. Goward, A.D. Bain*
Department of Chemistry, McMaster University
- 3. Application of Continuous Optimization Techniques to 2D INADEQUATE Spectra**
S. Watson, C.K. Anand, A.D. Bain*
Department of Chemistry, McMaster University
- 4. Diffusion Ordered Spectroscopy of the GPCR Ligand Apelin and Mutant Analogues**
Christopher A. Doyle* and Jan K. Rainey
Department of Biochemistry and Molecular Biology, Dalhousie University
- 5. Fibril Structure of Human Prion Protein Fragments Characterized by Solid-State NMR**
Jason Yau* and Simon Sharpe
Department of Molecular Structure and Function – Hospital for Sick Children
And Department of Biochemistry – University of Toronto
- 6. From Single Proteins to Fibers: Spider Silk Structural Studies**
Tremblay, M.-L.*, Xu, L., Liu, P., Rainey, J.
Department of Biochemistry and Molecular Biology, Dalhousie University
- 7. Structure Determination of the Phosphate-Containing Polysaccharide from *Lactococcus lactis* subsp. *lactis* NCIMB 700966**
Marie-Rose Van Calsteren*, Fleur Gagnon, Nancy Guertin
Food Research and Development Centre, Agriculture and Agri-Food Canada
- 8. Structure and Function of Targeted Antimicrobial Peptides against *S. mutans***
Nadine Merkley*¹, Zakia Biswasz¹, Junni Mai², Susan E. Douglas¹, Yung-Hua Li² and Raymond T. Syvitski¹
¹Institute of Marine Biosciences, National Research Council of Canada
²Department of Applied Oral Sciences, Department of Microbiology and Immunology, Dalhousie University, Halifax, NS.
- 9. Biophysical Characterization of the Conformation Induced Binding of the First Extracellular Loop of the Apelin Receptor in Lipid Environment**
Pascaline Ngweniform* and Jan Rainey
Department of Biochemistry and Molecular Biology, Dalhousie University
- 10. Structural Characterization of a Syrian Hamster Prion Protein Misfolding Intermediate**

Patrick Walsh*, Karen Simonetti, Carlene Starck and Simon Sharpe
Department of Molecular Structure and Function – Hospital for Sick Children and Department of
Biochemistry – University of Toronto

11. **P31 Chemical Shift Tensors in Tri-tolylphosphines**
Rebecca Jamieson*, Matthew White, and Glenn Penner
Department of Chemistry, University of Guelph
12. **Structure and Dynamics in Solid Trimethylammonium Chloride**
Renee Webber*, Luke O'Dell² and Glenn Penner¹
¹Department of Chemistry, University of Guelph
²Steacie Institute for Molecular Sciences, NRC, Ottawa
13. **qNMR Using External Standards: Method Validation**
Sheila Crain*, Ian Burton, Michael Quilliam, John Walter, Ray, Syvitski, Tobias Karakach
Institute for Marine Biosciences, NRC, Halifax
14. **Quebec/Eastern Canada High Field NMR Facility**
Tara Sprules*, Kalle Gehring^{1,2}
¹Quebec/Eastern Canada High Field NMR Facility
²Department of Biochemistry, McGill University
15. **Coordination Complexes of Organozinc Reagents with Ionic Ligands**
Ian S. MacIntosh*, Cody N. Sherren¹, Katherine N. Robertson², Jason D. Masuda¹, Cory C. Pye¹, and
Jason A. C. Clyburne¹
¹Department of Chemistry, Saint Mary's University, Halifax, NS, Canada
²Department of Chemistry, Dalhousie University, Halifax, NS, Canada
16. **Triglyceride Regiospecificity on Lipase Catalyzed Transesterification of Ethyl Ester and
Esterification of Fatty Acid Hydrolysates of Varying EPA/DHA Concentrations – A 13C NMR Study**
Erick Reyes-Suarez*, Paul F. Mugford¹, Alfred J. Rolle¹, Ian W. Burton², John A. Walter², and Jaroslav A.
Kralovec¹
¹Ocean Nutrition Canada Ltd.
²Institute for Marine Biosciences, NRC, Halifax
17. **Probing the Effects of Slow-Exchange Conformational Sampling Upon Dynamics Determined by
Peptide Backbone 15N Relaxation**
Tyler Reddy¹, Brian D. Sykes², and Jan K. Rainey*^{1,3}
¹Department of Biochemistry and Molecular Biology, Dalhousie University, Halifax, NS
²Department of Biochemistry, University of Alberta, Edmonton, AB
³Department of Chemistry, Dalhousie University, Halifax, NS
18. **Evidence for Membrane-Catalyzed Apelin-Receptor Binding**
David N. Langelaan*, E. Meghan Bebbington¹, Tyler Reddy¹, and Jan K. Rainey^{1,2}
¹Department of Biochemistry and Molecular Biology, Dalhousie University, Halifax, NS
²Department of Chemistry, Dalhousie University, Halifax, NS

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