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MOOT XXII

MINI **NMR** SYMPOSIUM

CARLETON UNIVERSITY, OTTAWA, ON
(TALKS WILL BE PRESENTED IN STEACIE ROOM 103 AND POSTERS
WILL BE IN THE GALLERIA AT THE UNIVERSITY CENTRE)

ORGANIZER: YVES AUBIN

SCIENTIFIC PROGRAM

SATURDAY, OCTOBER 17

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| 8:00 – 8:45 | Registration and Poster Setup. |
| 8:50 – 9:00 | Welcoming Remarks and Announcements. |
| Chair: | TBD |
| 9:00 – 9:35 | NMR studies of disodium guanosine 5'-monophosphate self-assembly in neutral solution
Irene C.M. Kwan* and Gang Wu
Department of Chemistry, Queen's University |
| 9:35 – 10:00 | Getting the Most out of your HMBC Spectra
Timothy Burrow, Raul Enriquez and William Reynolds*
Department of Chemistry, University of Toronto |
| 10:00 – 10:25 | Structural characterization of inhibitors of HIV-1 nucleocapsid function.
Nathalie Goudreau*, Pierre Bonneau, Anne-Marie Faucher, Chantal Grand-Maitre, Oliver Hucke, Olivier Lepage, Stephen Mason & Steve Titolo
Department of Chemistry, Boehringer-Ingelheim Canada (Ltd) |
| 10:25 – 10:45 | Refreshment Break |

- 10:45 – 11:10 Measurement of $\Delta IJ(199\text{Hg}, 31\text{P})$ in $[\text{HgPCy}_3(\text{OAc})_2]_2$ and Relativistic ZORA DFT Investigations of Mercury-Phosphorus Coupling Tensors
David L. Bryce*, Noemie Manuelle Dorval Courchesne, and Frederic A. Perras
Department of Chemistry, University of Ottawa
- 11:10 – 11:35 A potential role of the membrane in the hERG channel functioning and acquired long QT syndrome
Étienne Chartrand, Alexandre A. Arnold, Andrée Gravel, Sarah Jenna and Isabelle Marcotte*
Département de Chimie, Université du Québec à Montréal
- 12:00 – 13:30 Lunch and Meet the Sponsors (Galleria, University Centre)

AFTERNOON SESSION

Chair: Dr. Barbara Blackwell

- 13:30 – 13:55 An NMR Study of Proton Sponge
Renee Webber*, Glenn H. Penner, David Ben-Israel and Rebecca Jamieson
Department of Chemistry, University of Guelph
- 13:55 – 14:20 Dramatic micelle binding induced conformational change in the bioactive peptide apelin.
David N. Langelaan and Jan K. Rainey*
Department of Biochemistry & Molecular Biology, Dalhousie University
- 14:20 – 14:25 Glycosylation of Interferon Alpha 2a Alters the Dynamics of the Protein Backbone
Pascal Belcourt^{1*}, Simon Sauvé², Denis Brochu³, Michel Gilbert³ and Yves Aubin^{1,2}
1. Department of Biology, Carleton University
2. Centre for Biologics Research, Health Canada
3. Institute for Biological Sciences, National Research Council Canada
- 14:25 – 14:50 Refreshment Break
- 14:50 – 15:05 Na dynamics in 5'-GMP
Parisa Akhshi, Gang Wu
Department of Chemistry, Queen's University
- 15:05 – 15:30 Structure-function studies of the AIDA-1 neuronal signalling scaffolding protein
Arwa Kurabi, Jamie Kwan, Riya Shanbhag and Logan Donaldson*
Department of Biology, York University
- 15:30 – 15:55 A Solid-state B-11 NMR and Computational Study of Boron Electric Field Gradient and Chemical Shift Tensors in Boronic Acids and Boronic Esters: Using NMR Parameters to Probe Local Molecular and Electronic Structure
Joseph Weiss* and David Bryce
Department of Chemistry, University of Ottawa

- 15:55 – 16:00 Closing Remarks.
- 16:00 – 17:30 Poster Session and Refreshments
- 18:00 Banquet (Restaurant Al's Steakhouse 327 Elgin Street, Ottawa).

SUNDAY, OCTOBER 18

- 8:55 – 9:00 Announcements.
- Chair: Prof. Natalie Goto
- 9:00 – 9:25 Structure of the Conserved Hydrophobic Region of the Prion Protein (110-136) in Dodecylphosphocholine by NMR: Surface Interactions are a Prelude to Micelle Insertion
Simon Sauvé*, Daniel Buijs & Yves Aubin
Centre for Biologics Research, Health Canada
- 9:25 – 9:50 NMR Quantumness, Nuclear Spin Statistics and Bulk Matter Nuclear Magnetism
Serge Lacelle*, Luc Tremblay and Jonathan Lussier
Département de Chimie, Université de Sherbrooke
- 9:50-10:15 Solid-State O-17 NMR Study of Organic Compounds
Jianfeng Zhu*, Amada J. Geris, Justin Lau, and Gang Wu
Department of Chemistry, Queen's University
- 10:15 – 10:35 Refreshment Break.
- 10:35 – 11:00 Structure determination of the exopolysaccharide produced by *Lactococcus lactis* subsp. *lactis* CNRZ 151
Marie-Rose Van Calsteren,* Fleur Gagnon and Nancy Guertin
Centre de recherche et de développement sur les aliments Agriculture et Agroalimentaire Canada
- 11:00 – 11:25 Mg-25 Ultra-High Field Solid State NMR Spectroscopy and First Principles Calculations of Magnesium Compounds
Peter J. Pallister¹*, Igor L. Moudrakovski² and John A. Ripmeester²
1. Department of Chemistry, Carleton University
2. Steacie Institute for Molecular Sciences, National Research Council Canada
- 11:25 – 11:50 The effect of detergents on the full-length rhomboid protease using solution NMR.
Allison R. Sherratt*, Michael V. Braganza, Elizabeth Nguyen, Thierry Ducat and Natalie K. Goto
Department of Biochemistry, Molecular Biology and Immunology, University of Ottawa
- 11:50 – 12:00 Closing Remarks

POSTERS

THE SURAJ MANRAO STUDENT TRAVEL FUND WILL OFFER 3 PRIZES OF 50.00\$ EACH TO THE THREE BEST POSTER FROM GRAD STUDENTS

1. Structure determination of the exopolysaccharide produced by *Lactococcus lactis subsp. lactis* NCIMB 700712
Marie-Rose Van Calsteren,* Fleur Gagnon and Nancy Guertin
Centre de recherche et de développement sur les aliments, Agriculture et Agroalimentaire Canada
2. Structure determination of the neutral exopolysaccharide produced by *Lactobacillus delbrueckii subsp. bulgaricus* OLL1073R-1
Marie-Rose Van Calsteren,* Fleur Gagnon, Hassan Sabik and Seiya Makino
Centre de recherche et de développement sur les aliments, Agriculture et Agroalimentaire Canada
3. Solution NMR structure of the parkin Ubl domain bound to the endophilin-A1 SH3 domain
Jean-Francois Trempe*, Carol X.-Q Chen, Karl Grenier, Guennadi Kozlov, Edna M. Camacho, Peter M. McPherson, Kalle Gehring, Edward A. Fon
Department of Biochemistry McGill University
4. National Ultrahigh-Field NMR Facility for Solids
Eric Ye,¹ and Victor Tserkikh²
1. Department of Chemistry, University of Ottawa, Ottawa, Ontario, Canada K1N 6N5
2. Steacie Institute for Molecular Sciences, National Research Council Canada
5. Characterization of Metabolites from Red Spruce Endophytes by LC-MS-SPE/NMR
Mark W. Sumarah^{1*}, Dan Sørensen², Barbara Blackwell³ and J. David Miller¹
1. Chemistry Carleton University
2. Spectroscopy & Analytical Chemistry Merck Frosst Canada Ltd
3. Research Centre, Agriculture and AgriFood Canada Ottawa
6. NMR at the Centre for Chemical Analysis, Research and Training (C-CART)
Céline Schneider*, Sarah Bourbigot, Tsan-Chin Yang, Suliman Barhoum, Rebecca Dean, Zhenzhong Hu, Robert Gendron
7. A Suggested Definition for the Bandwidth of a Pulse
J. Stephen Hartman and Alex D. Bain*
Department of Chemistry McMaster
8. Determining the mode of action responsible for the antimicrobial activity of synthetic peptides by ³¹P and ²H NMR solid-state NMR spectroscopy
Aurélien Lorin*, Mathieu Noël, Vanessa Turcotte, Marie-Ève Provencher, Sébastien Cardinal, Normand Voyer, Michèle Auger
Department of Chemistry Université Laval

9. Characterization of the spider spinning process: Structure and aggregation properties of spider silk proteins
J r mie Leclerc, Fabien Pottier, Andr anne Guay-B gin, Camille Lapointe Verreault, Louis-Phillippe Montrency, St phane Gagn , Michel P zolet, Mich le Auger
D partements de Biochimie et Microbiologie, de Chimie Universit  Laval
10. Study of Group 13 Chloride Catalysts Using Chlorine Solid-State Nuclear Magnetic Resonance and Gauge-Including Projector-Augmented Wave Calculations
Rebecca P. Chapman, David L. Bryce
Department of Chemistry, University of Ottawa
11. The Structure and Dynamics of 2,2'-difluorobiphenyl in Solution
Rebecca Jamieson and Glenn H. Penner
Department of Chemistry, University of Guelph
12. Quebec/Eastern Canada High Field NMR Facility
Tara Sprules*, Kalle Gehring
McGill University
13. Study of critical fluctuations by deuterium Nuclear Magnetic Resonance in DOPC/DPPC-d62/Cholesterol ternary mixtures
Latifa Ziani*, Miranda L. Schmidt, James H. Davis
Department of Physics, University of Guelph
14. Phase Equilibria in DOPC/DPPC: Conversion from Gel to Subgel in Two Component Mixtures
Miranda L. Schmidt*, Latifa Ziani, Michelle Boudreau, and James H. Davis
Department of Physics , University of Guelph
15. Spectroscopic studies of the membrane interactions of TTR10-20, an amyloid peptide from transthyretin
Myriam Laneville*, Joanie Voyer-Desch nes and Mich le Auger
D partement de Chimie, Universit  Laval
16. NMR Studies of the Fatty Acids Present in Flax Seed Development.
Christopher W. Kirby*, Jason L. McCallum, and Bourlaye Fofana
Bio-Based Products and Processes, Agriculture and Agri-Food Canada
17. Solid State NMR Studies of Hydrogen Bonded Multilayers
Blythe Fortier-McGill*, Linda Reven
Department of Chemistry, McGill University
18. Decomposition of Ammonia Borane and Ammonium Borohydride by Solid State NMR
Igor Moudrakovski¹*, Peter Pallister², Roxana Flacau¹ and Chris Ratcliffe¹
1. Steacie Institute for Molecular Sciences, National Research Council Canada
2. Department of Chemistry, Carleton University
19. Doing More with INADEQUATE
A.D. Bain¹, D.W. Hughes¹, V.J. Robertson²
1. Department of Chemistry, McMaster University
2. Department of Physics, University of Guelph