



MOOT XX NMR Symposium
Hôtel Le Chantecler, Sainte-Adèle, Québec
(All talks and posters will be presented in Seigneurie I)

Organizers: Laird A. Trimble and Dan Sørensen.

Final Program

Saturday, September 29

8:00 – 8:45 Registration and Poster Setup.

8:50 – 9:00 Welcoming Remarks and Announcements.

Chair: Bob Berno

9:00 – 9:10 News from McMaster University.
Bob Berno
MCMASTER UNIVERSITY

9:15 – 9:40 Learning More and More About Less and Less Until You Know Almost Everything
About Almost Nothing.
Tim Burrow, Raul Enriquez, Daivd McNally and Bill Reynolds*
UNIVERSITY OF TORONTO

9:40 – 10:05 A Study of Proton Dynamics in Imidazole Based Compounds.
Jason W. Traer* and Gillian R. Goward
MCMASTER UNIVERSITY

10:05 – 10:55 Refreshment Break

10:55 – 11:20 Protein-protein interactions by NMR.
Kalle Gehring*, Alexey Denisov and Guennadi Kozlov
MCGILL UNIVERSITY

11:20 – 11:45 NMR structural studies of the interaction between the p62/Tfb1 subunit of the general
transcription factor IIH (TFIIH) and acidic domains from p53, VP16 and the alpha
subunit of TFIIIE.

Di Lello, P., Miller Jenkins, L. M., Mas, C., Langlois, C., Appella, E., Legault, P. and Omichinski, J. G.*

UNIVERSITY OF MONTREAL

11:45 – 12:15 Uncovering the Role of Dimerization in S100 Proteins by utilizing NMR Amide Exchange, Chemical Shifts and Rotational Diffusion.
Nicole M. Marlatt* and Gary S. Shaw
UNIVERSITY OF WESTERN ONTARIO

12:15 – 13:45 Lunch

Afternoon Session

Chair: Robert Schurko

13:45 – 14:10 Probing the structure of the Ff bacteriophage major coat protein transmembrane helix dimer by solution NMR.
Yanqiu Wu, Steve Shih and Natalie Goto*
UNIVERSITY OF OTTAWA

14:10 – 14:35 Solution NMR study of solubilised natural and recombinant spider silk proteins.
J r mie Leclerc, Fabien Pottier, St phane Gagn , Michel P zolet and Mich le Auger
LAVAL UNIVERSITY

14:35 – 15:00 SAM Domain : Functional Diversity from a Simple Protein Fold.
Jamie J Kwan, Arwa Kurabi, Philip Johnson, Ferenc Evanics and Logan Donaldson*
YORK UNIVERSITY

15:00 – 16:00 Refreshment Break

16:00 – 16:25 Bicelles: disks or perforated lamellae?
Mohamed N. Triba, Philippe F. Devaux and Dror E. Warschawski*
UQAM

16:25 – 16:50 Diffusion of PEG confined between lamellae of magnetically aligned bicelles: Pulse field gradient ¹H NMR Measurements.
Ronald Soong* and Peter Macdonald
UNIVERSITY OF TORONTO

16:50 – 17:15 NMR Studies of Polymer Multilayer Capsules and Films.
Dr. Linda Reven, Blythe Fortier-McGill*
MCGILL UNIVERSITY

17:15 Closing Remarks.

17:30 – 19:00 Poster Session and Refreshments

19:45 Bus arrives at hotel for transportation to Banquet.

19:55 Bus departs for Banquet (Restaurant Maestro, 339 Principale, Saint-Sauveur).

22:30 Bus departs from Restaurant Maestro to return to hotel.

Sunday, September 30

8:55 – 9:00 Announcements.

Chair: Mike Lumsden

9:00 – 9:25 Measuring molecular order in DOPC:DPPC:Cholesterol mixtures.
James H. Davis, Jesse J. Clair and Janos Juhasz*
UNIVERSITY OF GUELPH

9:25 – 9:50 Dipolar Chemical Shift Correlation Spectroscopy for Homonuclear Carbon Distance Measurements in Proteins in the Solid State: Application to Structure Determination and Refinement.
Xiaohu Peng*, David Libich, Rafal Janik, George Harauz and Vladimir Ladizhansky
UNIVERSITY OF GUELPH

9:50-10:15 Solid state NMR studies of a 62 kDa MBP-actin complex.
Mumdooh A.M. Ahmed*, Vladimir V. Bamm, Marta Steiner-Mosonyi, John F. Dawson, George Harauz, Vladimir Ladizhansky
UNIVERSITY OF GUELPH

10:15 – 11:00 Refreshment Break.

11:00 – 11:25 Multinuclear solid state NMR studies on proton conducting solid acid materials.
Vijayakumar Murugesan*, Jason W. Traer and Gillian R. Goward
MCMASTER UNIVERSITY

11:25 – 11:50 Solid-state NMR of metal nuclei in nanoparticles.
Robert W. Schurko* and Andy Y.H. Lo
UNIVERSITY OF WINDSOR

11:50 – 12:15 A High-Field Solid-State ^{35/37}Cl NMR and Quantum Chemical Investigation of the Chlorine Quadrupolar and Chemical Shift Tensors in Amino Acid Hydrochlorides.
Rebecca P. Chapman*, Gregory D. Sward and David L. Bryce
UNIVERSITY OF OTTAWA

Posters

1. Quebec/Eastern Canada High Field NMR Facility. Tara Sprules* and Kalle Gehring, Quebec/Eastern Canada High Field NMR Facility.
2. Ultrahigh-field NMR Studies of Nitrogen Doping and Spin-lattice Relaxation in Two Polytypes of Silicon Carbide. Alex D. Bain, Bob. Berno and Steven. Hartman*, Brock University.

3. Listening to Your Spectrometer: The Charms of Spin Noise. Alex D. Bain* and Timothy R. Field, McMaster University.
4. Preparation and Characterization of Polyelectrolyte-Coated Gold Nanoparticles. Annie Dorris*, Linda Reven, Christopher Barrett and R. Bruce Lennox, McGill University.
5. Solid State NMR Studies of Li-ion Intercalation Materials. Linda J. M. Davis*, Rebecca P. Chapman, Lindsay S. Cahill and Gillian R. Goward, McMaster University.
6. Au Nanoparticle Liquid Crystal Dispersions. Jonathan Milette*, Linda Reven, Bruce Lennox and Tara Yacovitch, McGill University.
7. Measurement and calculation of ^{13}C chemical shift tensors of Push-Pull Ethylene. Alex D. Bain, Gillian R. Goward, Mohsen Tafazzoli and Saeed K. Amini*, Sharif University of Technology.
8. Cation- π interactions studied by solid-state NMR spectroscopy. Philip K. Lee, Becky P. Chapman, Samyuktha Adiga, Lei Zhang, George W. Gokel and David L. Bryce*, University of Ottawa.
9. $^{6,7}\text{Li}$ 2D Exchange NMR to Study Lithium Ion Dynamics in Phosphates and Fluorophosphates for Cathode Materials. Lindsay S. Cahill*, Yasutoshi Iriyama, Linda F. Nazar and Gillian R. Goward, McMaster University.
10. Solid-State ^{91}Zr , $^{47/49}\text{Ti}$ and ^{35}Cl NMR Studies of Organometallic Complexes Utilized in Heterogeneous Olefin Polymerization Catalysis. Aaron J. Rossini*, Ivan Hung, Ryan W. Mills, Graham A. Briscoe and Robert W. Schurko, University of Windsor.
11. Structural and dynamic studies of natural spider silk by solid state NMR. Isabelle Cloutier, Jérémie Leclerc, Michèle Pézolet and Michèle Auger, Laval University.
12. Probing hydrogen bonding and ion-carbonyl interactions of G-ribbon and G-quartet using solid-state ^{17}O NMR spectroscopy. Irene C.M. Kwan*, Xin Mo and Gang Wu, Queen's University.
13. Solid-State NMR Study of the Membrane Interaction of a 21-mer Cytotoxic Model Peptide. Marise Ouellet*, Normand Voyer and Michèle Auger, Laval University.
14. Solid state NMR and spectroscopic characterization and assignments in a novel proton pump proteorhodopsin. Lichi Shi*, Vladimir Ladizhansky and Leonid Brown, University of Guelph.
15. Study of the interactions between Alzheimer's amyloid-beta peptide and model membranes by solid-state NMR. Jean-François Labbé* and Michèle Auger, Laval University.
16. Isolation and Analysis of Arctic Dissolved Organic Matter using NMR Spectroscopy. Jimmy Yuk*, Gwen Woods*, Bu Lam and Andre Simpson, University of Toronto.
17. Structural characterization of a new anthraquinone isolated from noni (*Morinda citrifolia*) fruits from Vietnam. Bui, T.K.A.; Sabik, H.; Gagnon, F.; Van Calsteren, M.-R.*, Agriculture and Agri-Food Canada.
18. Structure determination of the exopolysaccharide produced by *Lactococcus lactis* subsp. *cremoris* strain SMQ-461. Van Calsteren, M.-R.*; Gagnon, F.; Guertin, N.; Moineau, S.; LaPointe, G., Agriculture and Agri-Food Canada.

19. Sugar sequence determination of the exopolysaccharide produced by *Streptococcus thermophilus* strain NCFB 2393 by high-resolution NMR. Van Calsteren, M.-R.*; Gagnon, F.; Guertin, N.; Roy, D., Agriculture and Agri-Food Canada.
20. Functional study of an intramembrane protease by solution NMR. Allison R. Melhuish* and Natalie K. Goto, University of Ottawa.
21. Structural Characterization of E2A Activation Domain 1 Bound to the KIX Domain of CREB-Binding Protein. Chris M. Denis*, Seth Chitayat, Michael J. Plevin, Shuang Liu, Holly L. Spencer, Mitsuhiro Ikura, David P. LeBrun and Steven P. Smith, Queen's University.
22. Solution structure of the bb' domains of the human protein disulfide isomerase. Alexey Denisov*, Pekka Maattanen, Guennadi Kozlov, David Thomas and Kalle Gehring, McGill University.
23. NMR assignments and dynamics analysis of HCV-C82 in 100% water and in 90% TFE. Jean-Baptiste Duvignaud, D. Leclerc and Stéphane M. Gagné, Laval University.
24. NMR Characterization of Protein-Based Biologics. Simon Sauvé*, Geneviève Gingras and Yves Aubin, Health Canada.
25. Measurement of residual dipolar couplings in aligned proteins using rotor-synchronized REDOR recoupling. Jean-François Trempe*, Ekaterina Pomerantseva and Kalle Gehring, McGill University.
26. NMR study of multiple timescale dynamics for PSE-4, a 30 kDa beta-lactamase. Sébastien Morin* and Stéphane M. Gagné, Laval University.
27. The Impact of Transferrin on the Mechanism of the Early Stages of A-beta Oligomerization. Annie V. Raditsis, Julijana Milojevic and Giuseppe Melacini*, McMaster University.
28. Backbone dynamics of β -lactamases TEM-1 and PSE-4 - At the crossroads of molecular mechanics and NMR spectroscopy. Olivier Fisette*, Patrick Lagüe and Stéphane M. Gagné, Laval University.
29. Using Saturation Transfer Difference Epitope Mapping to Understand the Mechanistic Interactions of Organic Contaminants. Azadeh Shirzadi* and Andre Simpson, University of Toronto.
30. Structural studies and dynamics of the cementoin domain of pre-elafin. Audrey Bellemare*, Yves Bourbonnais and Stéphane M. Gagné, Laval University.
31. Interaction studies of the E3-ligase Parkin with Ubiquitin-Interacting Motifs. Susan S. Safadi* and Gary S. Shaw, University of Western Ontario.
32. The NMR Solution Structure of the Prohormone Convertase 1 C-terminal Dense Core Secretory Granule Sorting Domain Reveals a Calcium binding site. Dikeakos J.D.*, Di Lello P., Lacombe M.J., Legault P., Reudelhuber, T.L and Omichinski J.G, University of Montreal.
33. Structural Basis for the cAMP Signal Translation in PKA by NMR. E. Tyler McNicholl* and Giuseppe Melacini, McMaster University.
34. Structural Mapping of the Myo1B IQ motif interactions with Calmodulin and MlcB. Janine Liburd*, Seth Chitayat, Chris Denis, Scott Crawley, Graham Cote and Steven P. Smith, Queens's University.
35. Epitope mapping of contaminant interactions with dissolved organic matter using saturation transfer double-difference NMR. Buuan Lam* and Andre J. Simpson, University of Toronto.