

# SMOOTH 14 NMR

Université de Sherbrooke, September 29-30, 2001

## Final Program

### Saturday, September 29

8:00 to 9:00: Registration, Lobby Building C1

#### 9:00 to 10:35: Morning Session I: C1-565 *Pierre Lavigne, Chair*

9:00 to 9:10: Welcoming Comments

*Serge Lacelle,*  
*Université de Sherbrooke*

9:10 to 9:40: NMR and Bicelle Surface Charge,

*Peter Macdonald,*  
*University of Toronto at Mississauga*

9:40 to 10:10: Solid-state NMR approaches to determine the conformation of  
enkephalins in lipid bilayers,

*Michèle Auger, Isabelle Marcotte and Marie-Josée Paquet,*  
*Université Laval*

10:10 to 10:40: Direct Detection of Alkali Cations in DNA Related Systems  
by Solid-State NMR,

*Alan Wong and Gang Wu,*  
*Queen's University*

10:40 to 11:00: Coffee Break, C1-564

#### 11:00 to 12:00: Morning Session II: C1-565 *Linda Reven, Chair*

11:00 to 11:30: Dynamics and Morphology of Adsorbed Random  
Copolymers: A Solid-State NMR and FTIR-PAS Study,

*Victor Nasreddine, Sachiko Chijiwa, and Linda Reven,*  
*McGill University*

11:30 to 12:00: Bifunctional Self-Assembled Monolayers: A Solid State  
NMR Study,

*Shane Pawsey, Susan De Paul and Linda Reven,*  
*McGill University*

**12:00 to 13:30: Lunch, C1-564**

**13:30 to 15:00: Afternoon Session: C1-565 *Stéphane Gagné, Chair***

13:30 to 14:00: Rotational Diffusion Anisotropy and Conformational Exchange in the Dimer of the MAX B-HLH-LZ domain,  
*Simon Sauvé,, Luc Tremblay, Frédéric Gagnon, Jean-François Naud, and Pierre Lavigne,*  
*Université de Sherbrooke*

14:00 to 14:30: Hetero-TOCSY and Selective TOCSY-DEPT - useful derivations of the TOCSY experiment,  
*Valerie Robertson, James H. Davis and Christophe Fares,*  
*University of Guelph*

14:30 to 15:00: Mechanistic Diversity on Square Planar Complexes: Variable Pressure Kinetic Investigations by Heteronuclear NMR,  
*Florence J. Monlien , Lothar Helm, Amira Abou Hamdan and André E. Merbach,*  
*University of Toronto*

**15:00 to 15:20: Coffee Break, C1-564**

15:20 to 16:00: Round-Table Discussion "NMR in Perspective"  
*Serge Lacelle,*  
*Université de Sherbrooke*

**16:00 to 19:00: Cocktail and Poster Session, C1-564 *Luc Tremblay, Chair***

**19:00 Dinner at the Faculty Room, Building B5 (Upstairs in Cafeteria)**

## Sunday, September 30

### 9:00 to 10:30: Morning Session I: C1-565, *Michèle Auger, Chair*

9:00 to 9:30: The  $^{129}\text{Xe}$  Chemical Shift Tensor in a Silicalite Single Crystal,  
*Igor L. Moudrakovski, Victor V. Terskikh, Hongbin Du,*  
*Christopher I. Ratcliffe and John A. Ripmeester,*  
*Stacie Institute for Molecular Sciences*

9:30 to 10:00: Quadrupolar nuclei: so you thought you understood the rotating  
frame of reference,  
*Randall Dumont and Alex Bain,*  
*McMaster University*

10:00 to 10:30: On the Quantumness of NMR,  
*Serge Lacelle,*  
*Université de Sherbrooke*

### 10:30 to 10:45: Coffee Break, C1-564

### 10:45 to 12:15: Morning Session II: C1-565, *Yves Aubin, Chair*

10:45 to 11:15: Study of High amylose Starch tablets by nuclear magnetic  
resonance imaging,  
*Cedric Malveau., E. W. Baille and X.X. Zhu,*  
*Université de Montréal*

11:15 to 11:45: Diffusion measurements of poly(propylene imine) dendrimers  
with TEG amides end groups in PVA solutions and gels by PFG  
NMR spectroscopy,  
*Emmanuel Wilms Baille, C.Malveau, X.X Zhu. and W.T. Ford,*  
*Université de Montréal*

11:45 to 12:15: Applications of LC-NMR in Drug Discovery,  
*Laird A. Trimble,*  
*Merck Frosst Canada & Co.*

### 12:15 to 12:20: Closing Comments

*Serge Lacelle,*  
*Université de Sherbrooke*

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## POSTER SESSION

1. Interaction between cerebroside bilayers: 2H and 31P NMR study.  
*T.Zaraiskaya and K.Jeffrey*  
*University of Guelph*
2. Insights into the Max homodimer BHLHLZ  
*Simon Sauvé, Frédéric Gagnon, Luc Tremblay, Jean-François Naud, and Pierre Lavigne*  
*Université de Sherbrooke*
3. Structural homology of TM006 (*Thermotoga maritima*) and EC005 (*E.coli*) proteins  
**G.Finak**, **A.Denisov**, P.Gutierrez, G.Kozlov, A.Yee, C.Arrowsmith and K.Gehring  
*McGill University*
4. A theoretical study of nitrogen electric field gradients in nucleic acid bases  
**Ramsey Ida and Gang Wu**  
*Queen's University*
5. Intermolecular Recognition in the Ternary PBX-DNA-HOXA1 Complex  
**Tara Sprules, Nancy Green, Mark Featherstone and Kalle Gehring,**  
*McGill University*
6. Biosynthesis and Characterization of Metabolites from *Penicillium crustosum*  
**B.A.Blackwell, M. W. Sumarah, L. Trimble and J.D. Miller**  
*Agriculture and Agrifood Canada*
7. Automated Structure Elucidation of Cryptolepine Derivatives  
**Antony Williams, Sergey Molodtsov, Kirill Blinov, Eduard Martirosian, Mikhail Elyashberg, Gary Martin and Chad Hadden**  
*Advanced Chemistry Development*
8. J-Coupler - A Tool for Automated First Order Multiplet Analysis  
**Antony Williams, Sergey Golotvin and Eugene Vodopianov**  
*Advanced Chemistry Development*
9. NMR Studies of self-assembled polyelectrolyte multilayers  
**Rashida Smith, Christopher Barrett and Linda Reven**  
*McGill University*

10. Dynamics of Fatty-Acid Self-Assembled Monolayers on High Surface Area Substrates: Solid-State NMR Study  
*Kimberly Yach and Linda Reven*  
*Ottawa University*
11. Solid state NMR studies of partially fluorinated SAMS  
*Andrew O'Donnell and Linda Reven*  
*McGill University*
12. NMR of alkali metals deposited in controlled pore glasses  
*V.V. Terskikh, I.L. Moudrakovskii, C.I. Ratcliffe, J.A. Ripmeester C.J. Reinhold, P.A. Anderson and P.P. Edwards*  
*Steacie Institute for Molecular Sciences NRC Canada*
13. Diffusion and Interactions of Oligo(ethylene glycol) in Polymer Hydrogels as Studied by PFG NMR  
*W.E. Baille, C. Malveau and X.X. Zhu*  
*Université de Montréal*
14. Study of High amylose Starch tablets by nuclear magnetic resonance imaging  
*C. Malveau, W. E. Baille and X.X. Zhu*  
*Université de Montréal*
15. Detection of Spin Gravity Interaction with NMR: Fantasy or Reality?  
*Serge Lacelle*  
*Université de Sherbrooke*
16. Polyacrylamide-stabilized Pfl phage liquid crystal for protein NMR  
*Jean-Francois Trempe and Kalle Gehring*  
*McGill University*