



***PROGRAM***

# **MOOT<sub>30</sub> NMR Conference**

Western University

London, ON | Sept. 29 – Oct. 1, 2017

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## SATURDAY, SEPTEMBER 30

Registration & Breakfast

North Campus Building: Atrium

8:15 – 9:10

Session I

North Campus Building: 113

Session Chair: Gary Shaw

9:10 – 9:20

Opening Remarks

**Mathew Willans – *Western University***

9:20 – 10:05

An NMR Spectroscopist's Perspective of Transcriptional Regulation

**Lawrence McIntosh – *University of British Columbia***

10:05 – 10:25

Combining Ex Situ Na-23 Solid-State NMR and DFT to Study Polyanionic Cathode Materials for Sodium Ion Batteries

**Danielle Smiley – *McMaster University***

10:25 – 10:45

S-Nitrosylation Suppresses Stromal Interaction Molecule-1 Activation by Stabilization of the Calcium Sensing Domains

**Jinhui Zhu – *Western University***

Morning Break

North Campus Building: Atrium

10:45 – 11:10

Session II

North Campus Building: 113

Session Chair: Peter Stathopoulos

11:10 – 11:30

Determination of <sup>17</sup>O NMR Tensors in Epoxides

**Andrew Rinald – *Queen's University***

11:30 – 11:50

Molecular Mechanism for the (-)-Epigallocatechin Gallate-Induced Toxic to Nontoxic Remodeling of the Alzheimer's Disease A $\beta$  Oligomers

**Rashik Ahmed – *McMaster University***

11:50 – 12:10

<sup>35</sup>Cl Solid-State NMR Spectroscopy of Fluoxetine HCl Cocrystals Synthesized Using Solvothermal and Mechanochemical Methods

**Austin Peach – *University of Windsor***

12:10 – 12:30

Structure of Phosphorylated UBL Domain and Insights into PINK<sub>1</sub>-Orchestrated Parkin Activation

**Karen Dunkerley – *Western University***

<b>SATURDAY, SEPTEMBER 30</b>	
<b>Lunch</b> <span style="float: right;"><b>Grad Club, Middlesex College: 19</b></span>	
12:30 – 14:10	
<b>Session III</b> <span style="float: right;"><b>North Campus Building: 113</b></span>	
Session Chair: Gillian Goward	
14:10 – 14:30	Understanding Proton Transport in Perfluorosulfonic Acid Membranes via Solid-State NMR <b>Blossom Yan – <i>McMaster University</i></b>
14:30 – 14:50	Solution Characterization of the Cohesin-Dockerin Dual Binding Mode: A High Affinity Protein-Protein Interaction Critical for Cellulosome <b>Alison Upsdell – <i>Queen's University</i></b>
14:50 – 15:10	Studying Metal-Organic Frameworks via Solid-State NMR: Structure Determination, Host-Guest interactions, and Gas Dynamics <b>Jason Zhang – <i>Western University</i></b>
15:10 – 15:30	Solid-State NMR Provides Evidence for Small-Amplitude Slow Domain Motions in a Multi-Spanning Transmembrane $\alpha$ -Helical Protein <b>Daryl Good – <i>University of Guelph</i></b>
<b>Poster Session</b> <span style="float: right;"><b>Physics &amp; Astronomy Building: Atrium</b></span>	
15:45 – 17:45	
<b>Banquet</b> <span style="float: right;"><b>Delta London Armouries: Gunnery Ballroom</b></span>	
19:00 – 22:00	

**SUNDAY, OCTOBER 1****Session IV****North Campus Building: 113**

Session Chair: Yining Huang

9:30 – 10:15	NMR Across the Periodic Table: Observing "Invisible" Nuclei in Organic, Inorganic and Organometallic Materials <b>Robert Schurko – <i>University of Windsor</i></b>
10:15 – 10:35	Multiplexed Real-Time NMR GEF Assay to Measure Full Length GEFs Activity from Cells and Organoids <b>Teklab Gebregiorgis – <i>Princess Margaret Cancer Centre</i></b>
10:35 – 10:55	Deciphering the Molecular Mechanism of RAF Family Dimerization and Regulation <b>Pierre Maisonneuve – <i>Lunenfeld-Tanenbaum Research Institute</i></b>

**Morning Break****North Campus Building: Atrium**

10:55 – 11:20

**Session V****North Campus Building: 113**

Session Chair: Steven Smith

11:20 – 11:40	Non-Destructive Fatty Acid Profiling of Seeds by <sup>1</sup> H HRMAS <b>Chris Kirby – <i>Agriculture and Agri-Food Canada</i></b>
11:40 – 12:00	Dynamical Basis of cGMP-vs.-cAMP Selectivity of Protein Kinase G <b>Bryan VanSchouwen – <i>McMaster University</i></b>
12:00 – 12:20	NMR-Driven Refinements of Crystal Structures Using Dispersion-Corrected Density Functional Theory <b>Sean Holmes – <i>University of Windsor</i></b>
12:20 – 12:30	Awards Presentation & Closing Remarks <b>Mathew Willans – <i>Western University</i></b>

1. Synthesis of  $^{17}\text{O}$ -Labeled Glucose-6-Phosphate via Enzymatic Reactions  
**Neil Sengupta**, *Queen's University*
2. The NMR and DNP Centre at the University of Guelph  
**M. Sameer Al-Abdul-Wahid**, *University of Guelph*
3. Probing the Metal Centres in Calcium Based Metal-Organic Frameworks by Natural Abundance  $^{43}\text{Ca}$  Solid State NMR  
**Shoushun Chen**, *Western University*
4. Optimizing Fluorotryptophan-Based  $^{19}\text{F}$  NMR to Probe Ligand-GPCR Interactions  
**Jan K. Rainey**, *Dalhousie University*
5.  $^{27}\text{Al}$  Solid State NMR of Calcium-Aluminum Rich Inclusions (CAIs) from the Solar Nebula  
**Victoria Houde**, *Western University*
6. Dissecting the Molecular Basis of Nrf2-p21 Interaction  
**Nadun Chanaka Karunatileke**, *Western University*
7. Methods of Structural Solution of Mixed-Linker Cadmium Imidazolate Frameworks  
**Jacqueline Gemus**, *University of Windsor*
8. Epigenetic, Structural, and Functional Characterization of the E2A-PBX1 Oncogenic Transcriptional Network  
**Marina Lochhead**, *Queen's University*
9. Zeolite Structure Determination Using Solid-State NMR Experiments through the Application of Combinatorial Tiling Theory  
**Chelsey Hurst**, *McMaster University*
10. Conformational Arrangement of the E2-Ubiquitin Conjugate for Parkin Loading  
**Tara EC Condos**, *Western University*

## Posters

11. Lipid Interactions with Anabaena Sensory Rhodopsin  
**Jeff de Vlugt**, *University of Guelph*
12. Solid-State  $^{17}\text{O}$  NMR and Computational Study of Epoxides  
**Andrew Rinald**, *Queen's University*
13. Structural Characterization of the Interaction Between p53 and Plakoglobin  
**Qinyan Song**, *Dalhousie University*
14. Optimal Control of Frequency-Swept Pulses for the Acquisition of Ultra-Wideline Solid-State NMR Spectra  
**Adam R. Altenhof**, *University of Windsor*
15. Stable Isotopic Labeling of Glycine using  $^{17}\text{O}$  and its Incorporation into Yeast Ubiquitin  
**Binyang Lin**, *Queen's University*
16. Pores, Channels, and Cages:  $\text{CO}_2$  Locations and Dynamics in MOFs and Zeolites  
**Bryan Lucier**, *Western University*
17. Calcium Binding to the Dysferlin C2A Domain  
**Yuning Wang**, *Western University*
18. The Acquisition of  $^2\text{H}$  Solid-State NMR Spectra with Frequency-Swept Pulses  
**Lucas Foster**, *University of Windsor*
19. Comparison of HDX Protocols to Probe the Dynamics of Parkin  
**E. Aisha Freeman**, *Western University*
20. Examining the Adsorption of Small Molecules in the Cu(INAIP) MOF via Solid-State NMR  
**Mansheng Chen**, *Western University*

21. An Investigation of Proton Conducting Sites in Solid State Proton Conductors  
**Gabrielle Foran**, *McMaster University*
22. Probing Nitrite Ion Dynamics in  $\text{NaNO}_2$  Crystals by Solid-State  $^{17}\text{O}$  NMR  
**Yizhe Dai**, *Queen's University*
23. Characterization of the MITF Transcription Factor and its Interaction with CBP/p300  
**David Langelaan**, *Dalhousie University*
24. Characterization of a Class IB Hydrophobin Structure by NMR Spectroscopy  
**David Langelaan**, *Dalhousie University*
25. Deducing Adsorbed Gas Behaviour in Ultramicroporous Metal-Organic Frameworks using Solid-State NMR Spectroscopy  
**Bligh Desveaux**, *Western University*
26. NMR Studies to Elucidate Unique Structural Elements in the HK97 gp74 HNH Endonuclease and Define Key Metal Binding Residues  
**Sasha Weiditch**, *University of Toronto*
27. Multinuclear Solid-State NMR Spectroscopy of Halide Salt Cocrystals  
**Cameron Vojvodin**, *University of Windsor*
28. The Drug Discovery Platform (DDP) of the Research Institute of the McGill University Health Center (RIMUHC): Discover and Develop Next-Generation Diagnosis, Prognosis and Therapeutic Approaches  
**Andrée E. Gravel**, *Drug Discovery Platform - Research Institute of the McGill University Health Center*

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