

# MOOT 33

Guelph, Ontario / Oct 22-23 2022

## Conference Schedule

For abstracts, please visit <https://event.fourwaves.com/moot33/abstracts>

### Saturday October 22<sup>nd</sup>, Alexander Hall

**8:30 – 9:00**     **Registration and Coffee/Pastries**

9:00 – 9:05     Opening Remarks

#### Session A (Chair, Vladimir Ladizhansky), Alexander Hall Room 100

9:05 – 9:50     **Keynote Lecture:** A journey in the solid-state NMR study of microalgal cells  
**Isabelle Marcotte**, *Université du Québec à Montréal*

9:50 – 10:15     Energy landscape for third and second stages of membrane protein folding by  
hydrogen-deuterium exchange solid-state NMR  
**Peng Xiao**, *University of Guelph*

10:15 – 10:40     The effect of recycle delay in analyzing organic soil with paramagnetic  
elements  
**Jeewan Gamage**, *University of Guelph*

10:40 – 11:00     Coffee Break

#### Session B (Chair, Gillian Goward), Alexander Hall Room 100

11:00 – 11:25     Accurate measurements of Li<sup>+</sup> dynamics in solid electrolytes under the  
influence of mechanical compression using <sup>7</sup>Li NMR  
**Mengyang Cui**, *McMaster University*

11:25 – 11:50     Strategy for the production of isotopically labelled Fab fragments of  
therapeutic antibodies in *Escherichia coli* for NMR studies  
**Donald Gagné**, *Health Canada*

11:50 – 12:15     Use of NMR and MD to study photoswitchable proteins  
**P Maximilian M Reed**, *University of Toronto*

## Lunch, Summerlee Science Complex, Atrium

### Session C (Chair, James Longstaffe), Alexander Hall Room 100

- 1:30 – 1:55      Application of NMR-based metabolomics for the health assessment of blue mussels (*Mytilus edulis*)  
**Stéphane Beauclercq**, *Université du Québec à Montréal*
- 1:55 – 2:20      Non-destructive quantification of triacylglycerides in oilseeds by <sup>1</sup>H HR-MAS NMR  
**Leah Gauthier**, *University of Prince Edward Island*
- 2:20 – 2:45      Developing and applying <sup>19</sup>F NMR-based methodologies to understand the mechanisms of apelin-membrane interaction  
**Tran Thanh Tam Pham**, *Dalhousie University*
- 2:45 – 3:05      Coffee Break

### Session D (Chair, R. Scott Prosser), Alexander Hall Room 100

- 3:05 – 3:30      Having fun with the CPMAS cryoprobe  
**Martine Monette**, *Bruker Canada*
- 3:30 – 3:55      Triangulation of non-annular lipids in an integral membrane protein using paramagnetic NMR  
**Raoul Vaz**, *University of Guelph*
- 3:55 – 4:20      An NMR study of lithium transport in liquid-ceramic hybrid solid composite electrolytes  
**Gabrielle Foran**, *Université de Montréal*

## Poster Session & Banquet, Summerlee Science Complex, Atrium

- 4:30 – 6:15      Poster Session (beverages and light snacks served)
- 6:30 – 9:00      Banquet

## Sunday October 23<sup>rd</sup>, Alexander Hall

8:30 – 9:00 Coffee/Pastries

### Session E (Chair, Rui Huang), Alexander Hall Room 100

9:00 – 9:45 **Keynote Lecture:** Allosteric regulation of protein kinases  
**Giuseppe Melacini**, *McMaster University*

9:45 – 10:10 Using NMR to identify the products formed by ridoquinone biosynthesis enzyme A (RquA)  
**Trilok Neupane**, *Dalhousie University*

10:10 – 10:35 Characterization of the subunit exchange rate of hexameric p97 using methyl-TROSY NMR spectroscopy  
**Victoria Muir**, *University of Guelph*

10:35 – 10:55 Coffee Break

### Session F (Chair, Barbara Blackwell), Alexander Hall Room 100

10:55 – 11:20  $^{91}\text{Zr}$  and  $^{47/49}\text{Ti}$  solid-state NMR at high magnetic fields: unraveling local environments of zirconium and titanium based MOFs  
**Wanli Zhang**, *Western University*

11:20 – 11:45 Investigating the interaction between the Rac guanine nucleotide exchange factor, P-Rex 1, and the regulatory subunits of protein kinase A type I (PKA R1 $\alpha$ ) through NMR and fluorescence spectroscopies  
**Karla Martinez Pomier**, *McMaster University*

*10-minute mini-break*

11:55 – 12:20 Probiotics product consistency analysis and bacterial strain differentiation using NMR metabolomics  
**Arun Krishnamurthy**, *Purity-IQ*

12:20 – 12:45 NMR chemical fingerprinting provide quality assurance to authenticate Natural Health Products (NHPs)  
**Thiru Arunachalam**, *University of Guelph*

## Awards Presentation and Closing Remarks

12:45 -12:55 Awards Presentation and Closing Remarks

12:55 “Grab and go” Lunch, Alexander Hall Lobby

# Poster Presentations

1. Development of a comprehensive  $^{19}\text{F}$  NMR-based fragment screening platform for GPCR drug discovery  
**Zuhair Ahmed**, *University of Toronto Mississauga*
2. Investigating the binary adsorption of acetylene and carbon dioxide in metal-organic frameworks using solid-state NMR spectroscopy  
**Tahereh Azizvahed**, *Western University*
3. Use of  $^n\text{J}_{\text{C-H}}$  coupling constants for the conformational analysis of  $\alpha$ -halo propiophenones  
**Camila Botin Francisco**, *University of Toronto Mississauga*
4. Structural basis of co-activator recruitment by the microphthalmia-associated transcription factor  
**Alexandra Brown**, *Dalhousie University*
5. Exploring optimization algorithms for use on NMR spectral peaks  
**Rachel Brown**, *University of Guelph*
6. Exploring the enzymatic and structural properties of human i-AAA YME1L  
**Nicole Chen**, *University of Guelph*
7. Selective amino acid labelling for large protein NMR  
**Elizabeth M Connelly**, *Western University*
8. Investigating the mechanism of cAMP signal termination  
**Leonardo Della Libera**, *McMaster University*
9. Structure elucidation of RNA aptamers bound to derivative Hoechst dyes  
**Natasha Evans**, *University of Waterloo*
10. Molecular basis of KLF15-mediated repression of cardiac hypertrophy  
**Matthew Fishman**, *Queen's University*
11. Development of boron-based inhibitors of the mitochondrial ClpXP protease to combat Acute Myeloid Leukemia  
**Monica Goncalves**, *University of Guelph*
12. Solid-state NMR studies of lithium-ion dynamics in  $\text{LiFeV}_2\text{O}_7$  as a function of lithium content  
**Gillian Goward**, *McMaster University*
13. Role of structural dynamics in controlling platelet factor 4 tetramer asymmetry  
**Jinfeng Huang**, *McMaster University*

14. Investigation of allosteric mechanisms of cGMP-dependent protein kinase Ia activation  
**Mariia Khamina**, *McMaster University*
15. Probiotics product consistency analysis and bacterial strain differentiation using NMR metabolomics  
**Arun Krishnamurthy**, *Purity-IQ*
16. Sequence properties, not structure, influence hydrophobin function  
**David Langelaan**, *Dalhousie University*
17. Molecular basis of PF4 and polyphosphate interactions  
**Giulin Ma**, *McMaster University*
18. Assessing the chemical characteristics of soil organic matter on HF treated soil using DP-MAS  
**Moazame Mesgar**, *University of Guelph*
19. Investigating water and carbon dioxide adsorption in metal-organic frameworks using  $^2\text{H}$  and  $^{13}\text{C}$  solid-state NMR  
**Yan Ham Ng**, *Western University*
20. Sequence context and complex Hofmeister salt interactions dictate phase separation propensity of resilin-like polypeptides  
**James Otis**, *University of Toronto*
21. Use of moderate pressure oxygen to improve quality of the spectrum  
**Dmitry Pichugin**, *University of Toronto Mississauga*
22. Solving the atomic-level structure of recombinant pyriform silk  
**Jan Rainey**, *Dalhousie University*
23. Towards a high-performance pulse EPR Facility at University of Toronto for GPCR research  
**Joerg Reichenwallner**, *University of Toronto*
24. Stress-inducible phosphoprotein 1 (HOP/STI1/STIP1) regulates the accumulation and toxicity of  $\alpha$ -synuclein *in vivo*  
**Benjamin Rutledge**, *University of Western Ontario*
25. Solid-state NMR study of novel sensory rhodopsin from *Thermochromatium tepidum*  
**Sajjad Salimi Nanekharani**, *University of Guelph*
26. Understanding monoclonal antibody-excipient interactions to assist regulation of this class of important therapeutics  
**Muzaddid Sarker**, *Health Canada*

27. Investigating the caspase-9 activation mechanism via Methyl-TROSY NMR  
**Alexander Sever**, *University of Toronto*
28. A study of the structure and CO<sub>2</sub> sorption of metal-organic frameworks based on s-block metals  
**Yihao Shen**, *Western University*
29. MMRF Helium Recovery System  
**Tara Sprules**, *QANUC/McGill University*
30. Mutual protein-ligand conformational selection drives cGMP-vs.-cAMP selectivity in protein kinase G (PKG)  
**Bryan VanSchouwen**, *McMaster University*
31. Investigation of the effect of Mn(II) contaminants on lithium dynamics in manganese-rich Lithium-ion batteries (LIBs)  
**Runze Zheng**, *McMaster University*
32. Comparative Analyses of Surface PF4 Mutations  
**Ellen Mak**, *McMaster University*

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## Keynote Lecturer Biography: Prof. Isabelle Marcotte

Professor Isabelle Marcotte obtained a PhD in chemistry in 2003 at Université Laval, under the supervision of Prof. Michèle Auger. During her PhD, she focused on the study of membrane systems by solid-state NMR. She was especially interested in the interaction of peptides with phospholipid model membranes. She then moved to Zurich (2003-2006) to pursue postdoctoral research under the guidance of Prof. Beat Meier at the ETH, where she gained experience in the solid-state NMR study of complex proteins such as spider silk. In 2006, she was recruited by the Université du Québec à Montréal, and moved back to her hometown, where she established her



laboratory dedicated to the study of complex biological systems by solid-state NMR. With her team, they develop model membranes and study protein fibers such as mussel byssus, also known as sea silk. They also develop strategies to investigate intact cells by solid-state NMR. Her lab is particularly interested in looking at interactions of antimicrobial peptides with intact bacteria, and characterizing microalgae for environment applications. In 2014, she obtained the Young Researcher Award of the Université du Québec à Montréal's Faculty of Sciences. She is Full Professor at the Department of Chemistry since 2015, and Associate Dean of Research of the Faculty of Sciences since 2017.

## Keynote Lecturer Biography: Prof. Giuseppe Melacini

Giuseppe Melacini is a Professor in the Department of Chemistry and Chemical Biology and a joint member of the Department of Biochemistry and Biomedical Sciences. Dr. Giuseppe Melacini received his undergraduate degree in Chemistry (1992) and his Ph.D. in Biophysical Chemistry (1996) from the University of Milan with external research at the University of California, San Diego (UCSD). During his graduate studies, he worked in the area of peptidomimetics under Dr. Murray Goodman at UCSD. Then he moved to the Netherlands for his post-doctoral studies in the laboratories of Dr. Robert Kaptein and Dr. Rolf Boelens at Utrecht University. There he focused on the study of protein hydration by Nuclear Magnetic Resonance spectroscopy (NMR). After returning to UCSD as Lecturer and Assistant Project Scientist, he joined the Departments of Chemistry and Biochemistry at McMaster in 2003.



In 2018-2019 Giuseppe served as Associate Chair of graduate studies in Chemistry, and since July 2019 as Director of the Chemical Biology graduate program. Giuseppe is the recipient of the Biological and Medicinal Chemistry Lectureship Award by the Canadian Soc. of Chem. (2020), the Excellence in Graduate Student Supervision Award (2019), the Natural Sciences and Engineering Research Council - Discovery Accelerator Supplement Award (2014), the McMaster Student Union - Teaching award (2012), the Canadian Institutes of Health Research - Maud Menten Finalist Prize (2007), the Heart & Stroke Foundation of Canada - New Investigator (2006) and Maureen Andrew Awards (2006), the Alzheimer Society of Canada - Young Investigator Award (2005) and the Premier's Research Excellence Award (2005).

Giuseppe has served on multiple grant review panels in Canada and has reviewed US, European and Israeli grant applications. He has been an executive member of the Biophysical Society of Canada for which he chaired the award committee (2014-2019). He has also co-organized and co-chaired several conferences. He has consulted for biopharmaceutical and biotech companies.

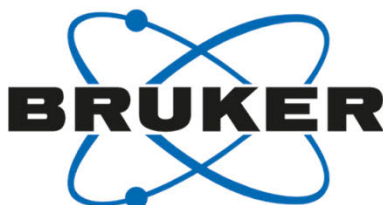
He is the author of over 100 manuscripts and is a member of the editorial boards of the Journal of Biological Chemistry and Nature Scientific Reports. He has served as associate editor for the Journal of Alzheimer's Disease and as invited expert editor for the Proceedings National Academy Science USA (PNAS).

Giuseppe is very proud to have something in common with Jeff Bezos and Bill Gates – he does the dishes every night.



## Sponsors

The organizing committee would like to extend our deepest thanks to this year's MOOT sponsors:



with special thanks to the Suraj Manrao Science Fund.

# Conference Map

