The 36th MOOT NMR Symposium

Memorial University of Newfoundland

September 27-28, 2025

Friday September 26

5:30 - 8:30 informal mixer at Quidi Vidi brewery

Saturday September 27

8:15 - 9:00 Registration and Coffee/Pastries

9:00 - 12:15 Morning talks

12:15 - 1:30 Lunch

1:30 - 4:30 Afternoon talks

4:30 - 6:00 Poster Session

6:30 Banquet at Emera Innovation Exchange Conference Centre, on Signal Hill

Sunday September 28

8:30 - 9:00 Coffee/Pastries

9:00 - 12:10 Sunday talks

12:10 Closing remarks and Award Presentations

Saturday, 27 September 2025

8:00 AM - 9:00 AM - Whale Atrium
Registration and Morning Coffee

9:00 AM - 9:10 AM - CSF 1302
Welcome

9:10 AM - 9:55 AM - CSF 1302
Plenary Session 1

9:10 AM - 9:55 AM **20 YEARS OF ENVIRONMENTAL NMR DEVELOPMENT: TRANSFERABLE TECHNOLOGIES AND TECHNIQUES FOR EVERYONE** Andre Simpson[1]. [1]University of Toronto.

9:55 AM - 10:35 AM - CSF 1302
Short Talks 1

9:55 AM - 10:15 AM **Harnessing Water-Suppression NMR Technique for Precise Quantification of Liquid Products in Electrocatalytic CO2 Reduction** Oforbuike Egbe[1]. [1]Memorial University of Newfoundland.

10:15 AM - 10:35 AM **Real-Time 13C-Detection, Multi-Receivers NMR-Based Assay for Site-Specific Prolyl-Hydroxylation: Regulation of HIF-1α** Genevieve Seabrook[1]. [1]Princess Margaret Cancer Centre.

10:35 AM - 10:55 AM - Whale Atrium
Morning Coffee Break

10:55 AM - 12:15 PM - CSF 1302
Short Talks 2

10:55 AM - 11:15 AM **A Variable-Temperature Operando 7Li NMR Study of Lithium Plating in Si-C Composite Anode Material.** Aiman Quadiri[1]. [1]McMaster University.

11:15 AM - 11:35 AM **On the robustness of DFT-calculated 13C isotropic chemical shifts of organic solids when involving a 'simple molecular correction'** Sadam Adebayo[1]. [1]University of Regina, Regina, Saskatchewan.

11:35 AM - 11:55 AM **A Local Structure Analysis of Defects in UiO-66: Insights from Solid-state NMR and XAFS** Jiabin Xu[1]. [1]Western University.

11:55 AM - 12:15 PM **Advancements in Ultra-High Field NMR: Enhancing Spectral Resolution and Sensitivity** Martine Monette[1]. [1]Bruker Canada Ltd..

12:15 PM - 1:30 PM - Whale Atrium
Lunch

1:30 PM - 2:15 PM - CSF 1302
Plenary Session 2

ION DYNAMICS IN LITHIUM and ZINC ION CELLS REVEALED BY MAGNETIC RESONANCE SPECTROSCOPY and RELAXOMETRY Gillian R. Goward[1]. [1]Department of Chemistry & Chemical Biology, McMaster University, Hamilton, Canada.

2:15 PM - 2:55 PM - CSF 1302
Short Talks 3

2:15 PM - 2:35 PM **Assessing Compound-Membrane Interactions by NMR** Paul White[1]. [1]NMX Research and Solutions.

2:35 PM - 2:55 PM **Sherlock Holmium and the Case of the Shifty Isotopes** David Bryce[1]. [1]University of Ottawa.

2:55 PM - 3:15 PM - Whale Atrium
Afternoon refreshment Break

3:15 PM - 3:30 PM -
The contributions of Bill Reynolds

3:30 PM - 4:15 PM - CSF 1302
Panel Discussion

4:15 PM - 6:00 PM - Whale Atrium
Poster session and cocktail

6:00 PM - 6:30 PM -
Shuttle to Signal Hill

6:30 PM - 11:00 PM -
Banquet

Sunday, 28 September 2025

8:15 AM - 9:00 AM - Whale Atrium
Morning Coffee

9:00 AM - 9:05 AM - CSF 1302
Introduction

9:05 AM - 9:50 AM - Whale Atrium
Plenary Talk 3

From bacteria to red blood cells - understanding the action of antimicrobial peptides by in-cell solid-state NMR
Isabelle Marcotte[1]. [1]Université du Québec à Montréal.

9:50 AM - 10:30 AM - Whale Atrium
Short Talk 4

9:50 AM - 10:10 AM **Exploring Microcoils and Microcoil Arrays for Environmental Nuclear Magnetic Resonance** Daniel Lysak[1]. [1]University of Toronto.

10:10 AM - 10:30 AM **Understanding Electrolyte Decomposition and SEI Formation in Lithium-Ion Batteries Using 19F NMR Spectroscopy** Emma Magee[1]. [1]McMaster University.

10:30 AM - 10:50 AM - Whale Atrium
Morning Coffee Break

10:50 AM - 11:50 AM - CSF 1302
Short Talk 6

10:50 AM - 11:10 AM **Structural Basis of Protein Kinase G Inhibition for Retinal Degeneration Therapy** Karla Martinez Pomier[1]. [1]Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON.

11:10 AM - 11:30 AM **Optimization and Characterization of an Aptamer Targeting the p47/p97 Interaction for Therapeutic and Diagnostic Applications in Neurodegenerative Disorders and Cancer** Peter Kim[1]. [1]Student Researcher.

11:30 AM - 11:50 AM **Diffusion in crowded environments** Anand Yethiraj[1]. [1]University of Guelph.

12:10 PM - 12:30 PM - CSF 1302
Awards and Closing words

12:30 PM - 1:00 PM - Whale Atrium
Box lunch

12:50 PM - 1:00 PM -
Optional Sunday Afternoon Activity

Plenary Session 1

20 YEARS OF ENVIRONMENTAL NMR DEVELOPMENT: TRANSFERABLE TECHNOLOGIES AND TECHNIQUES FOR EVERYONE

Andre Simpson[1]

[1]University of Toronto

Practically all environmental research involves working with ultra-complex natural mixtures. Over my career environmental questions have required the development of a wide range of novel technologies and techniques. The presentation will cover a range of approaches with a focus on those that have the largest potential for widespread NMR application, some examples include:

Comprehensive Multiphase (CMP) NMR: CMP NMR, combines all the electronics from solution-state, semi-solid and solid-state NMR into a single NMR probe. The resulting technology permits an uncompromised analysis of liquid, semi-solid and solid components within unaltered samples in their natural swollen state. As well as unravelling the binding orientation, and receptors for contaminants/drugs CMP-NMR is also capable of monitoring the kinetic transfer between and across interfaces providing an unprecedented window into otherwise inaccessible molecular information.

In-vivo NMR and Targeted Experiments: The living organism becomes the “ultimate biosensor” responding in real time to its environment, while the NMR spectrometer interprets the biochemical changes, providing information explaining sub-lethal toxicity at the molecular level. The special techniques needed to extract information *in-vivo,* hold great potential for many areas of research.

Digital Microfluidics NMR and “Easy” Microcoil Technology: Microcoils are required for the study of mass limited samples (tiny organisms, eggs, cells, etc.), but sample handling becomes challenging. Digital Microfluidics involves the movement of droplets over an open array of electrodes, essentially a tiny computer-controlled laboratory. When inside the NMR and integrated with micro coils, separations, titrations, reactions, even chromatography can be performed on chip and the products analyzed in real-time.

Short Talks 1

Harnessing Water-Suppression NMR Technique for Precise Quantification of Liquid Products in Electrocatalytic CO2 Reduction

Oforbuike Egbe[1], Celine Schneider[2], Francesca Kerton[1], Jane Stockmann[1]

[1]Memorial University of Newfoundland, [2]CCART, Memorial University

The electrocatalytic reduction of carbon dioxide (CO_2R) into value-added products powered by renewable energy offers a promising pathway for carbon capture and utilization (CCU). Catalyst design is central to this process, enabling high efficiency and product selectivity while reducing energy requirements. Copper-based catalysts are especially promising for producing multi-carbon (C_{2+}) products such as ethanol, ethylene, and propanol. However, accurate quantification of these small molecules remains challenging. Conventional techniques like LC, GC-MS, and HPLC can detect low concentrations but often face limitations due to overlapping retention times and difficulty in distinguishing isomers. Nuclear Magnetic Resonance (NMR) spectroscopy provides a powerful alternative, simultaneously identifying unknown products and quantifying known ones with detection limits below 5 μM.[1,2] In particular, ^{1}H-NMR offers high sensitivity but is hindered by the intense water resonance (~4.7 ppm) in aqueous systems.[3] In this study, we employed pre-saturation and WATERGATE pulse sequences to suppress the water signal without compromising adjacent CO_2R product peaks. This enabled reliable detection of liquid products at concentrations below 0.1 μM, corresponding to Faradaic efficiencies under 1%. Our findings establish water-suppression NMR as a robust and precise tool for CO_2R studies, supporting catalyst evaluation, product identification, and mechanistic insights.

References

(1) Pander III, J. E. *et al*., *Catal. Sci. Technol.* **2017**, *7* (24), 5820-5832.

(2) Bertheussen, E. *et al*., *Catal. Today* **2017**, *288*, 54-62.

(3) Preikschas, P. *et al*., *Commun. Chem.* **2023**, *6* (1), 147.

Real-Time 13C-Detection, Multi-Receivers NMR-Based Assay for Site-Specific Prolyl-Hydroxylation: Regulation of HIF-1α

Genevieve Seabrook[1]

[1]Princess Margaret Cancer Centre

Post-translational modifications (PTMs) are key regulators of many cellular processes, leading to a variety of cellular events. While some PTMs such as phosphorylation are extensively studied, proline hydroxylation, an oxygen-dependent and rare PTM, remains poorly understood due to a lack of site-specific detection methods. Hypoxia-Inducible Factor (HIF) proteins are a family of transcription factors. The modulation of cellular HIF levels is regulated by prolyl-hydroxylation, which induces degradation. Maintaining oxygen homeostasis is critical for cellular processes. Abnormal levels lead to severe human diseases, including cancer. HIF proteins degradation domain lacks 3D structure making them quite challenging to study. However, new NMR assays can be developed to study these proteins. Here, we present for the first time, a real-time 13C-detection NMR-based assay allowing the thorough analysis of HIF-1α hydroxylation at two proton-less residues, P402 and P564, by the prolyl hydroxylase enzyme PHD2. NMR technological advancement allowed us to directly monitor at the atomic level the hydroxylation of both prolines with the use of a cold probe optimized for 13C-detection combined with the exploitation of multiple receivers (CON//HSQC). This allowed us to simultaneously acquire snapshots of backbone amide (1H-15N HSQC) and carbonyl-nitrogen (13C-15N CON) chemical

shifts while monitoring changes occurring during the process of HIF-1α prolyl-hydroxylation. The site-specific prolyl-hydroxylation rates revealed a better understanding of the molecular mechanisms of HIF-1α regulation. This real-time 13C-detection multi receivers NMR-based assay can be applied to other IDPs/IDRs and others PTMs. Ultimately, it can help discover new therapeutic targets and develop new treatments related to human diseases.

Short Talks 2

A Variable-Temperature Operando 7Li NMR Study of Lithium Plating in Si-C Composite Anode Material.

Aiman Quadiri[1], Kevin J. Sanders[1], Gillian Goward[1]

[1]McMaster University

Lithium-ion batteries (LIBs) have been the leading energy storage technology since their commercialization in the early 1990s, enabling portable electronics and electric transportation. Despite their widespread acceptance across various fields, improvement in specific energy density and battery life is needed to optimize their use in electric and hybrid vehicles, where fast charging and low temperatures often compromise performance. A major drawback under these conditions is lithium plating, which accelerates cell degradation.[1]

Operando ^{7}Li Nuclear Magnetic Resonance (NMR) spectroscopy has emerged as a particularly powerful method for probing lithium nuclei in functioning cells. It provides an unambiguous identification of metallic lithium and allows detection even at low concentrations.[2] Additionally, *operando* studies under low-temperature and high-rate operation of the battery can be performed, providing information crucial for real-life LIB applications.

In this work, we use a parallel-plate resonator radio frequency (RF) probe in combination with a cartridge-type cell design for *operando* ^{7}Li NMR spectroscopy.[3] We examine the plating behaviour of Si-C composite anode material at temperatures as low as -30 °C, under fast-charge conditions, with graphite serving as a reference point. This work provides a detailed insight into the impact of anode materials on the performance of LIBs and a better understanding of their performance in cold-climate and fast-charging applications.

References:

Waldmann, T., et al., *Journal of Power Sources*. 384 (2018).

O. Pecher, J. et al., *Chem. Mater.* 29 (2017).

Sanders, K. J., et al. *J. Am. Chem. Soc.* 145, (2023).

On the robustness of DFT-calculated 13C isotropic chemical shifts of organic solids when involving a ‘simple molecular correction’

Sadam Adebayo[1], Cory M Widdifield[1]

[1]University of Regina, Regina, Saskatchewan

NMR crystallography protocols involving gauge-including projector augmented-wave (GIPAW) density functional theory (DFT) computations use crystal structure models to predict solid-state NMR observables, such as isotropic chemical shifts (), for crystal structure characterization and determination.[1] This process may be resource-intensive when compared against alternative approaches. Hence, there is value in determining if DFT-quality computations of ^{13}C values can be performed more efficiently. Using GIPAW DFT, we computed carbon isotropic magnetic shielding () values using 12 crystal structures at various and k-point grid values. Thereafter, we applied a ‘simple molecular correction’ (SMC)[2] to adjust GIPAW DFT-computed (C) values. The SMCs are intended to improve upon the exchange-correlation (XC) functional and/or quality of relativistic contributions to values. After a linear mapping, the SMC protocols unsurprisingly enhanced the accuracy of our calculated (^{13}C) values for the selected crystals. The optimal linear mapping was determined by minimizing the root mean square deviation (RMSD) between computed and experimental (^{13}C) values for the 12 systems. We find that the (^{13}C) values arrived at after the SMC are robust to degradation in the GIPAW DFT computation to about = 400 eV. The Inclusion of scalar relativistic effects in the SMCs were found to dominate over spin-orbit relativistic effects for the selected systems.

References

(1) Hartman, J. D.; Monaco, S.; Schatschneider, B.; Beran, G. J. O. *J. Chem. Phys.,* **2015**, *143*, 102809.

(2) Dračínský, M.; Unzueta, P.; Beran, G. J. O. *Phys. Chem. Chem. Phys*., **2019**, *21*, 14992.

A Local Structure Analysis of Defects in UiO-66: Insights from Solid-state NMR and XAFS

Jiabin Xu[1], Amrit Venkatesh[2], Ivan Hung[3], Zhehong Gan[3], Tsun-Kong Sham[1], Yining Huang[1]

[1]Western University, [2]University of Virginia, [3]National High Magnetic Field Laboratory

Defect engineering in metal-organic frameworks (MOFs) offers a promising approach to modify material properties by introducing controlled structural imperfections. Zr-based MOFs, particularly the well-known UiO-66, hold significant potential for diverse applications. Defects in UiO-66 can be generated using monocarboxylic acids as modulators, among other methods. However, resolving the atomic-level local structures of these defects remains a considerable challenge. In this study, the local structures of these defects are carefully characterized by multinuclear solid-state NMR spectroscopy (SSNMR) in combination with X-ray absorption fine structure

(XAFS). In-situ heating XAFS analyses at Zr K-edge reveal critical changes in the local structure of Zr during the removal of trifluoroacetic acid (TFA), including the decreased Zr-O coordination numbers and alterations in Zr-Zr bond distances. Multinuclear ^{1}H, ^{13}C, ^{19}F, ^{35}Cl, ^{17}O solid-state NMR methods are used to identify capping species and defect-associated species. Subsequently, the engineered defects are found to significantly improve the catalytic performance of Pt nanoparticles (NPs) integrated into the defective UiO-66 framework. Pt-UiO-66 with defects exhibits much improved hydrogen evolution reaction (HER) activity and stability compared to the Pt-UiO-66 without defects.

Advancements in Ultra-High Field NMR: Enhancing Spectral Resolution and Sensitivity

Martine Monette[1], Patrick Wikus[2]

[1]Bruker Canada Ltd., [2]Bruker Switzerland AG

Ultra-high field Nuclear Magnetic Resonance (NMR) spectroscopy, operating at magnetic fields of 1.0 GHz and above, represents a significant advancement in the field of analytical chemistry and structural biology. These high-field NMR systems, such as those utilizing 1.2 GHz magnets, offer unprecedented spectral resolution and sensitivity. In this presentation, we will review the history of high-field NMR magnets. We will also discuss Bruker's R&D initiative for developing NMR magnets beyond 28 Tesla, and present preliminary results from these efforts.

Plenary Session 2

ION DYNAMICS IN LITHIUM and ZINC ION CELLS REVEALED BY MAGNETIC RESONANCE SPECTROSCOPY and RELAXOMETRY

Gillian R. Goward[1]

[1]Department of Chemistry & Chemical Biology, McMaster University, Hamilton, Canada

Li-ion batteries (LIBs) have become ubiquitous in society, ranging from hand-held portable electronics to widespread adoptions in electric vehicles. Beyond mobile devices, a Net-Zero future requires appropriate energy storage for the grid, for which LIBs are impractical. Alternative chemistries are composed of abundant materials and utilize aqueous electrolytes, which are environmentally friendly, sustainable, and cost-effective. Aqueous Zinc-Ion Batteries (ZIBs) are lower energy density than LIBs, but offer higher safety and cost effectiveness. Magnetic resonance spectroscopy and imaging techniques are powerful tools for probing dynamic processes in lithium-ion batteries.[1] We have recently reported the application of a parallel-plate resonator to the *real-time* ^{7}Li *operando* NMR monitoring of Li metal deposition on a graphite

anode during repeated charging and discharging of a single layer prismatic cell.[2] The method allows the quantification of the lithiation of the anode material as well as the early detection of plated metallic lithium throughout the duration of cell charging. Optimized ^{1}H and ^{7}Li PPRs are utilized to enable high sensitivity *in situ*and *operando* NMR experiments with fine temporal resolution. We have combined ^{1}H spectroscopy and relaxaometry to evaluate Mn^{2+}(aq) dissolution and re-deposition during cycling of aqueous zinc-ion batteries. We will discuss the performance of these cells as a function of the cycling conditions, including the influence of buffering the electrolyte. This work is a collaboration with Salient Energy, a Halifax-based start-up company.

Short Talks 3

Assessing Compound-Membrane Interactions by NMR

Paul White[1], Ludmilla Guduff[1], Steven LaPlante[1]

[1]NMX Research and Solutions

The penetration of pharmaceuticals through the cell membrane by passive diffusion is estimated to be the dominant mechanism of transport into cells for over 90% of pharmaceuticals. Rapid screening methods to assess membrane permeability of fragments & leads are critical to identifying promising scaffolds and guide synthetic efforts. Current assays for membrane permeability are often performed by PAMPA. However, long incubation times, functional group requirements for detection, and limited available membrane formulations reduce the versatility of this technique. By employing liposomes and NMR spectroscopy, we demonstrate that membrane interactions and permeability can be assessed as soon as the sample is mixed. The versatility of liposome formulations furthermore opens the possibility for quickly developing custom membrane compositions more reflective of the cell-type of interest.

Sherlock Holmium and the Case of the Shifty Isotopes

Alireza Nari[1], Patrick Szell[2], David Bryce[1]

[1]University of Ottawa, [2]Quadrufy Inc.

Nuclear quadrupole resonance (NQR) is a radiofrequency spectroscopy that provides a chemical fingerprint in the absence of a magnetic field. Materials may present NQR spectra featuring multiple overlapping isotopic resonances, like isotopes all trying to talk over each other at a party, leading to ambiguous spectral assignments. We show how the application of a weak magnetic field (≤ 50 mT) allows for measurement of the nuclear gyromagnetic ratio associated with each resonance with sufficient precision for isotopic identification. The technique is demonstrated on

pure and impure powdered samples and the concept of multisite multinuclear Zeeman-perturbed NQR spectral fitting is introduced. New insights are thereby gained into the sensitivity of the Zeeman-QSR response and into the characterization of complex samples. This approach creates new opportunities in NMR/NQR spectroscopy and provides a sustainable cryogen-free alternative to the helium-cooled superconducting magnets associated with high-field NMR that's easy on the planet and your budget.

Plenary Talk 3

From bacteria to red blood cells - understanding the action of antimicrobial peptides by in-cell solid-state NMR

Isabelle Marcotte[1]

[1]Université du Québec à Montréal

Antimicrobial peptides are part of the defense arsenal of many living organisms. They serve as an inspiration for the development of new antibiotics, as they act by disrupting bacterial membranes riched in anionic lipids—a mechanism that makes the emergence of resistance difficult. To gain deeper insight into their mechanism of action, we have been developing in-cell solid-state NMR approaches to investigate molecular-level interactions while preserving cellular complexity. Using specific deuterium labeling of bacterial membranes and fluorine-19 labeling of red blood cell ghost membranes, we revealed differences in modes of action. By combining non-specific carbone-13 labeling of bacteria with dynamic filters, we identified interactions with specific constituents of the Gram(+) *Bacillus subtilis* cell wall. Altogether, this talk will outline our progress toward a deeper understanding of AMP interactions with the cellular membrane and the cell wall.

Short Talk 4

Exploring Microcoils and Microcoil Arrays for Environmental Nuclear Magnetic Resonance

Daniel Lysak[1], Carl Michal[2], Kathryn Marable[3], Reza Farsi[3], Marco Grisi[3], Peter Costa[1], Jacob Pellizzari[1], William Wolff[1], Katelyn Downey[1], Kiera Ronda[1], Katrina Steiner[1], Andre Simpson[1]

[1]University of Toronto, [2]University of British Columbia, [3]Annaida Technologies

Microcoil NMR is a powerful approach for the analysis of small, mass limited samples. However, despite the mass sensitivity advantages offered by microcoils, throughput can still be low for complex biological samples. For example, studying the eggs of *Daphnia magna*, (typically <400 µm) still results in long experiment times and challenging analysis. Given the ecological importance of this species, the study of *D. magna* (and their eggs) can be very powerful in

establishing the biochemical impacts of stressors and monitoring environmental health as a whole. Here, recent advances utilizing microcoil NMR to study environmental samples and developments facilitating the application of microcoil arrays (e.g., inexpensive (<$300) NMR receivers and “receive-only” microcoils) are described. These approaches were used to study *D. magna* eggs (by tracking a fluorinated contaminant in an intact egg, for example), along with other environmentally relevant samples. Microcoil arrays provide two key advantages: improved throughput due to the ability to simultaneously study multiple samples and the ability for a unique study design where control and exposed organisms are studied concurrently, reducing day-to-day variability and improving data confidence. Receive-only microcoils (which use external excitation, to overcome microcoil nutation challenges) were combined into an array and used to analyze three *D. magna* eggs simultaneously. This approach showed both excellent nutation behaviour and an improved signal-to-noise ratio compared to standard “transceiver” microcoils, demonstrating the potential of this approach on a complex sample. Overall, both microcoils and microcoil arrays have considerable potential for environmental analysis.

Understanding Electrolyte Decomposition and SEI Formation in Lithium-Ion Batteries Using 19F NMR Spectroscopy

Emma Magee[1], Gillian Goward[1], Kevin Sanders[1]

[1]McMaster University

Lithium ion batteries (LIBs) continue to find themselves at the forefront of rechargeable batteries used in electric vehicles (EVs) due to their high energy density despite their limited performance range and slow charge times, particularly as they age. For practical performance output, LIBs are cycled at a voltage beyond the stability window of the electrolyte. This causes reduction of the electrolyte at the anode, leading to the formation of an electronically insulating but ionically conductive layer called the solid electrolyte interface (SEI). The SEI is a complicated matrix composed of a variety of compounds, including some of which contain lithium. Pulverization of the SEI due to anode volumetric changes or lithium plating leads to the layer’s reformation, which borrows lithium that otherwise would contribute to cell capacity, and continuous reduction of the electrolyte which produces unwanted and performance-limiting by-products. Characterization of the SEI components using nuclear magnetic resonance (NMR) is well known; however, the mechanism of formation of the SEI, as well as its composition change during battery cycling is not well understood. Herein, we discuss using *Operando* ^{19}F NMR to study the formation of the SEI and its continual evolution during cell cycling.

Short Talk 6

Optimization and Characterization of an Aptamer Targeting the p47/p97 Interaction for Therapeutic and Diagnostic Applications in Neurodegenerative Disorders and Cancer

Peter Kim[1], Rui Huang[2], Derek O'Flaherty[2]

[1]Student Researcher, [2]PI

p97 is an AAA+ ATPase that is crucial for a variety of cellular processes, including protein quality control, membrane fusion, and chromatin-associated regulation. Dysregulated p97 activity is implicated in cancer and neurodegenerative disorders. Thus, p97 has emerged as a promising target for interventions for these diseases.

p97 engages with diverse cofactors to orchestrate its various functions. One such cofactor is p47, which directs p97 to assist in membrane fusion events within the cell. Our lab has been exploring specific binders of the p47 cofactor to provide a pathway-specific inhibitor of p97 function. In collaboration with Dr. Juewen Liu's group, we identified the first aptamer for p47, a 42-base-pair oligonucleotide, using capture-SELEX. Aptamers are short, single-stranded DNA or RNA sequences selected for their high affinity and specificity to a target.

Using ITC, we determined the binding affinity between the selected aptamer and p47 to be approximately 4 μM. Further analysis using NMR identified that the aptamer interacts with the SEP domain, one of the three folded domains on p47. Through chemical shift perturbations, we mapped out the binding interface on p47 and found that the aptamer may contain multiple binding sites for p47.

Future work will involve evaluating the aptamer's binding within the p47-p97 complex and optimizing the aptamer sequence to increase its binding affinity based on structural insights. By combining these complementary biophysical approaches, we aim to establish a detailed characterization of these aptamers and their mechanisms of target recognition, laying the foundation for their development as novel cancer therapeutics.

Diffusion in crowded environments

Anand Yethiraj[1]

[1]University of Guelph

It is valuable to have label-free methods to study macromolecular motions in environments that are crowded, such as that in the living cell. Pulsed field gradient NMR (pfg-NMR) methods occupy an important niche in such studies. In our group, we have shown that we can extract detailed information of motions in complex- and aggregate-forming systems using pfg-NMR. In this work, I will describe methods to study simple polymer-colloid binary aqueous systems. We have also begun developing ways to studying increasingly more complex systems, with the goal being to approach the complexity of molecular motions in living matter via a bottom-up approach.

Structural Basis of Protein Kinase G Inhibition for Retinal Degeneration Therapy

Karla Martinez Pomier[1], Mariia Khamina[2, 3], Giuseppe Melacini[1, 4]

[1]Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON, [2]Department of Medical Biophysics, The University of Toronto, Toronto, ON, [3]Molecular Medicine Program, The Hospital for Sick Children, Toronto, ON, [4]Department of Biochemistry and Biomedical Sciences, McMaster University, Hamilton, ON, Canada

Hereditary retinal degeneration (RD) conditions such as Retinitis Pigmentosa and Leber's Amaurosis, are untreatable disorders leading to photoreceptor cell death and blindness. These diseases usually start with the degeneration of rod photoreceptors, causing the subsequent loss of cone photoreceptors and severe vision decline. cGMP (cyclic guanosine-3', 5'-monosphosphate) signaling pathways have emerged as critical disease drivers common to different types of RD. Elevated cGMP levels within photoreceptors result in the over-activation of cGMP-dependent protein kinase G (PKG), leading to photoreceptor apoptosis. Therefore, the inhibition of PKG by cGMP-based analogs that compete with cGMP has emerged as a promising therapeutic route against RD. Specifically, the cGMP analog CNO3 preserves *in vivo* retinal function and reduced photoreceptor degeneration in different RD models, emerging as a lead to target RD-type diseases. However, translating leads like CNO3 into drugs requires optimizing their potency while preserving selectivity for PKG *vs*. other retinal kinases and cGMP-effectors. By using Nuclear Magnetic Resonance (NMR) and docking, we seek to determine the molecular mechanism underlying the allosteric inhibition of PKG by CNO3 and other cGMP-analogs. Our study shows, at atomic resolution, that when bound to CNO3, PKG adopts an intermediate conformation that resembles the inactive conformation. The CNO3's inhibitory mechanism targets key allosteric hotspots of PKG and the capping lid keeping the kinase inactive, while retaining high affinity. Using a ligand-substituent cycle approach, we established which substitutions of CNO3 are key to inhibit PKG and/or enhance binding affinity, a crucial step for the identification of a pharmacophore model for selective and potent PKG allosteric inhibition.

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POSTER ABSTRACTS

7 - Investigating the Interactome of Arabidopsis thaliana MPKs: An Integrative Approach Using Multiple Sources of Evidence and Machine Learning-Based Structural Modeling

Tim Xing[1], Sameer Khan[1]

[1]Carleton University

The *Arabidopsis thaliana* mitogen-activated protein kinase (MPK) signaling network plays a role in various cellular processes. This study integrated protein-protein interaction, genetic interaction, and co-expression data from the STRING, BioGRID, and ATTED-II databases to provide a comprehensive dataset of interactions within the network. The key MPK network components from this set were identified and subjected to functional enrichment analysis, which revealed their involvement in diverse biological processes and pathways. The 3D structure of MKK2 was predicted using AlphaFold2, and protein-protein docking simulations were performed between MPK6 and MKK2. The docking analysis identified important residues mediating their interaction. This integrative approach, combining multiple sources of evidence, structural predictions, and protein-protein docking, provides a comprehensive approach for understanding the *A. thaliana* MPK signaling network. The findings demonstrate the complex regulatory mechanisms that play a role in plant stress responses and development.

8 - Magnetic resonance imaging to measure maternal brain plasticity

Haley Adams[1], Melanie Lapierre[1], Katie Wadden[1], Lindsay Cahill[1]

[1]Memorial University of Newfoundland

The female brain is an exceptionally dynamic organ that changes in response to female-specific experiences such as pregnancy and menopause. Despite the discovery made over 30 years ago linking changes in estradiol levels to alterations in the structure and function of the brain, female-centric research represents less than 4% of neuroscience studies. Further, little research has focused on the benefits of non-pharmaceutical lifestyle interventions such as physical activity and exercise during reproduction to improve brain outcomes.Using a scoping review, our group found that few human and animal studies have examined the influence of exercise on maternal brain plasticity, with the majority of the literature focusing on the brain health of the offspring.The animal studies lacked consistency in methods and revealed knowledge gaps in the brain outcome measures such as 3D high-resolution brain imaging. While magnetic resonance imaging (MRI) has revealed significant changes in the male mouse brain with exercise, no study has used MRI to

study the impact of exercise in females (non-pregnant and pregnant).This motivated our group to: (i) develop the Consensus on Exercise Report Template for animal research, including questions about biological sex and pregnancy status and (ii) measure brain plasticity using MRI in a mouse model of pregnancy to understand the effect of an exercise intervention on brain health during late pregnancy and postpartum. We hope that this project will lay the groundwork for future studies to examine the relationships between brain plasticity during pregnancy and postpartum depression and whether physical exercise can protect the maternal brain.

10 - Exploring Microcoils and Microcoil Arrays for Environmental Nuclear Magnetic Resonance

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Microcoil NMR is a powerful approach for the analysis of small, mass limited samples. However, despite the mass sensitivity advantages offered by microcoils, throughput can still be low for complex biological samples. For example, studying the eggs of *Daphnia magna*, (typically <400 µm) still results in long experiment times and challenging analysis. Given the ecological importance of this species, the study of *D. magna* (and their eggs) can be very powerful in establishing the biochemical impacts of stressors and monitoring environmental health as a whole. Here, recent advances utilizing microcoil NMR to study environmental samples and developments facilitating the application of microcoil arrays (e.g., inexpensive (<$300) NMR receivers and “receive-only” microcoils) are described. These approaches were used to study *D. magna* eggs (by tracking a fluorinated contaminant in an intact egg, for example), along with other environmentally relevant samples. Microcoil arrays provide two key advantages: improved throughput due to the ability to simultaneously study multiple samples and the ability for a unique study design where control and exposed organisms are studied concurrently, reducing day-to-day variability and improving data confidence. Receive-only microcoils (which use external excitation, to overcome microcoil nutation challenges) were combined into an array and used to analyze three *D. magna* eggs simultaneously. This approach showed both excellent nutation behaviour and an improved signal-to-noise ratio compared to standard “transceiver” microcoils, demonstrating the potential of this approach on a complex sample. Overall, both microcoils and microcoil arrays have considerable potential for environmental analysis.

12 - Solution-phase NMR - a tool for understanding MOF formation

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Metal-Organic Frameworks (MOFs) are a class of porous materials composed of metal nodes/clusters bridged by organic linkers. Due to the seemingly infinite combination of metals and linkers, MOFs have been explored extensively for a wide range of applications including gas capture/separation, catalysis, and chemical sensing. Despite the large amount of research done on MOFs over the last thirty years, mechanistic information about the formation of MOFs is poorly understood.

In a typical synthesis of a MOF, ligands, solvent, and modulators are all binding with the metal node or metal node precursor. This is affected by solvent, and its decomposition products (e.g., formic acid and dimethylamine from N,N-dimethylformamide), pH, water content, and temperature, to name a few. Determining how each component affects the mechanism of MOF formation may be unique to a particular system (e.g., kinetically inert vs. labile metal) or could result in some more universal observations.

To address this, it's important to develop readily available inter-laboratory techniques so that new methodologies can be rapidly compared to one another. In this presentation, I will discuss how solution-phase NMR can be used to track MOF synthesis and give useful mechanistic insights. With this information, we can develop new synthetic protocols to improve crystallinity, yield, and even target some new systems.

14 - Impact of Computational Input Variations on The Accuracy of Predicted 1H Isotropic Chemical Shifts in NMR Crystallography

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Nuclear magnetic resonance (NMR) crystallography combines solid-state NMR experiments and quantum-chemical calculations (and on occasion data from crystallography techniques) and can be useful for the identification and precise characterization of organic crystal structures. NMR crystallography is advantageous in situations where obtaining sufficiently large single crystals to pursue single-crystal X-ray diffraction (XRD) for structure determination is not possible.[1] Here, we will describe our recent investigations on enhancing the efficiency and/or accuracy of NMR crystallography when characterizing the crystal structures of molecular organics. Specifically, we consider the robustness of ^{1}H isotropic chemical shift root-mean-squared deviation (RMSD) metrics by performing gauge-including projector-augmented-wave (GIPAW) density functional theory (DFT) calculations on a set of 24 benchmark crystal structures with known experimental chemical shift values. We explore how these metrics change as functions of key computational parameters such as the plane wave basis set energy cut-off value and the k-point grid density.[2]

Subsequently, we apply a 'simple molecular correction' (SMC)[3] by augmenting the quality of the DFT exchange-correlation (XC) functional *via* ORCA DFT calculations. The SMC was done in theory to enhance the precision and accuracy of computed ^{1}H isotropic chemical shift parameters.

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16 - The Influence of Nanoconfinement Effects on Dynamics and Diffusion in ε-Poly-L-lysine Systems for Controlled Drug Delivery

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A new class of molecules, genetic materials (DNA and RNA) are emerging as effective treatments for various diseases, including cancer, heart disease, and the development of the mRNA vaccine for COVID-19. These molecules are fragile and the current drug delivery methods that exist are inefficient. For example, the COVID-19 RNA vaccines needed to be kept at ultra low temperatures, and their short shelf-life caused the wastage of billions of dollars of vaccines.

Polymer systems have the potential to solve these problems by protecting fragile genetic materials. Polymer nanosystems can encapsulate the materials and respond to physiochemical cues, for controlled and targeted release in the body. This project investigates how size of the delivery system affects polymer chain dynamics which in turn influences diffusion and release from the polymer delivery nanosystems.

As a model system, ε-Poly-L-lysine, a polymer that breaks down in the body overtime, was functionalized and combined with oxime reversible bonds through polymer chain crosslinking to form nanogels of different sizes. The size of the resulting nanogels was controlled during their preparation by miniemeulsion polymerization. The effect of the degree of nanoconfinement on the performance of the nanogels was investigated by studying the relaxation of the network and the local displacement of the network and the payload was probed through their self-diffusion.

17 - Structural Basis of Protein Kinase G Inhibition for Retinal Degeneration Therapy

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Hereditary retinal degeneration (RD) conditions such as Retinitis Pigmentosa and Leber's Amaurosis, are untreatable disorders leading to photoreceptor cell death and blindness. These diseases usually start with the degeneration of rod photoreceptors, causing the subsequent loss of cone photoreceptors and severe vision decline. cGMP (cyclic guanosine-3', 5'-monosphosphate) signaling pathways have emerged as critical disease drivers common to different types of RD. Elevated cGMP levels within photoreceptors result in the over-activation of cGMP-dependent protein kinase G (PKG), leading to photoreceptor apoptosis. Therefore, the inhibition of PKG by cGMP-based analogs that compete with cGMP has emerged as a promising therapeutic route against RD. Specifically, the cGMP analog CNO3 preserves *in vivo* retinal function and reduced photoreceptor degeneration in different RD models, emerging as a lead to target RD-type diseases. However, translating leads like CNO3 into drugs requires optimizing their potency while preserving selectivity for PKG *vs*. other retinal kinases and cGMP-effectors. By using Nuclear Magnetic Resonance (NMR) and docking, we seek to determine the molecular mechanism underlying the allosteric inhibition of PKG by CNO3 and other cGMP-analogs. Our study shows, at atomic resolution, that when bound to CNO3, PKG adopts an intermediate conformation that resembles the inactive conformation. The CNO3's inhibitory mechanism targets key allosteric hotspots of PKG and the capping lid keeping the kinase inactive, while retaining high affinity. Using a ligand-substituent cycle approach, we established which substitutions of CNO3 are key to inhibit PKG and/or enhance binding affinity, a crucial step for the identification of a pharmacophore model for selective and potent PKG allosteric inhibition.

18 - Detection and quantification of PFOA in murine tissue samples using 19F solid-state MAS NMR

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Per- and polyfluoroalkyl substances (PFAS) are known to be highly environmentally persistent and bioaccumulate within tissues by binding to serum albumin. As a result of environmental exposure, PFAS has been associated with a number of health impairments including liver and kidney disease as well as reproductive and developmental complications. Various mass spectrometry and nuclear magnetic resonance (NMR) methodologies have been utilized to detect and quantify PFAS in environmental and biological samples. However, the investigation of PFAS in biological samples using ^{19}F solid state magic angle spinning (MAS) NMR has not been conducted. In this study, we utilized ^{19}F solid-state MAS NMR to detect and quantify perfluorooctanoic acid (PFOA) in tissue samples from healthy pregnant (n=5) and non-pregnant (n=4) CD1 mice that were exposed to 50 ppm of PFOA via their drinking water. PFOA was detected and quantified above the LOD (10 ug/g) in liver (n=9/9), placenta (n=6/24), and adipose tissues (n=2/8). The detection and quantification of PFOA in placenta samples illustrated sex differences, with a higher detection frequency and average concentration in placentas from male

fetuses than females. These findings provide evidence to support the use of ^{19}F solid-state MAS NMR as a method for detection and quantification of PFAS in tissue samples and implore continued investigation of PFAS detection and links to adverse health effects.

19 - Understanding Electrolyte Decomposition and SEI Formation in Lithium-Ion Batteries Using 19F NMR Spectroscopy

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[1]McMaster University

Lithium ion batteries (LIBs) continue to find themselves at the forefront of rechargeable batteries used in electric vehicles (EVs) due to their high energy density despite their limited performance range and slow charge times, particularly as they age. For practical performance output, LIBs are cycled at a voltage beyond the stability window of the electrolyte. This causes reduction of the electrolyte at the anode, leading to the formation of an electronically insulating but ionically conductive layer called the solid electrolyte interface (SEI). The SEI is a complicated matrix composed of a variety of compounds, including some of which contain lithium. Pulverization of the SEI due to anode volumetric changes or lithium plating leads to the layer's reformation, which borrows lithium that otherwise would contribute to cell capacity, and continuous reduction of the electrolyte which produces unwanted and performance-limiting by-products. Characterization of the SEI components using nuclear magnetic resonance (NMR) is well known; however, the mechanism of formation of the SEI, as well as its composition change during battery cycling is not well understood. Herein, we discuss using *Operando* ^{19}F NMR to study the formation of the SEI and its continual evolution during cell cycling.

20 - NMR metabolomics to investigate placental biomarkers of pregnancy complications

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Introduction: Pregnancy complications such as preterm birth, gestational hypertension, preeclampsia, and gestational diabetes remain leading causes of maternal and neonatal morbidity and mortality worldwide. Despite their prevalence, reliable methods for early detection are lacking, and their underlying molecular mechanisms remain poorly understood. The placenta, central to maternal-fetal exchange, provides a window into the metabolic disruptions driving these conditions. This study aimed to identify placental biomarkers and understand molecular mechanisms of pregnancy complications using NMR-based metabolomics.

Methodology: Placental tissue was collected from individuals recruited from Eastern Health (St. John's, Newfoundland). The first cohort included 9 individuals with healthy term pregnancies and 9 with preterm pregnancies (<37 weeks' gestation). An additional cohort included 8 individuals with gestational diabetes, 6 with pregnancy-induced hypertension, and 9 with healthy pregnancies. Following delivery, placental tissue (~1 cm^3) was snap-frozen in liquid nitrogen. Comprehensive multiphase NMR experiments were performed on a 500 MHz Bruker Avance III spectrometer (MAS = 2.5 kHz) for the preterm birth cohort. Additional samples were analyzed on a 600 MHz Bruker Avance III spectrometer using an HRMAS iProbe (MAS = 4 kHz). Data were processed using MestReNova and analyzed with MetaboAnalyst

Findings and Significance: Twenty-three low molecular weight metabolites were identified using ^{1}H and ^{13}C literature values and correlations from 2D ^{1}H-^{1}H COSY and ^{1}H-^{13}C HSQC experiments. Distinct metabolic profiles were observed between complication groups and controls, suggesting potential biomarkers of altered placental function. This work highlights NMR metabolomics as a tool for early detection of pregnancy complications and revealing underlying biochemical disruptions.

21 - A Variable-Temperature Operando 7Li NMR Study of Lithium Plating in Si-C Composite Anode Material.

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Lithium-ion batteries (LIBs) have been the leading energy storage technology since their commercialization in the early 1990s, enabling portable electronics and electric transportation. Despite their widespread acceptance across various fields, improvement in specific energy density and battery life is needed to optimize their use in electric and hybrid vehicles, where fast charging and low temperatures often compromise performance. A major drawback under these conditions is lithium plating, which accelerates cell degradation.[1]

Operando ^{7}Li Nuclear Magnetic Resonance (NMR) spectroscopy has emerged as a particularly powerful method for probing lithium nuclei in functioning cells. It provides an unambiguous identification of metallic lithium and allows detection even at low concentrations.[2] Additionally, *operando* studies under low-temperature and high-rate operation of the battery can be performed, providing information crucial for real-life LIB applications.

In this work, we use a parallel-plate resonator radio frequency (RF) probe in combination with a cartridge-type cell design for *operando* ^{7}Li NMR spectroscopy.[3] We examine the plating behaviour of Si-C composite anode material at temperatures as low as -30 °C, under fast-charge conditions, with graphite serving as a reference point. This work provides a detailed insight into the impact of anode materials on the performance of LIBs and a better understanding of their performance in cold-climate and fast-charging applications.

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24 - Perezone, α and β pipitzols, diperezone: chemistry, X-Ray and NMR. New answers to old questions.

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Perezone is the first secondary metabolite from plants isolated in America back in 1852 by Leopoldo Río de la Loza. Since then, a large number of structurally related natural products have been isolated or synthesised, including the early detected mixture of α and β pipitzols, aiming to understand the fascinating chemistry of perezone and its derivatives. To date, the unambiguous NMR assignment and detailed J-couplings of pure pipitzols were unknown, and no X-ray characterisation of pure pipitzols has been performed. This work provides total, unambiguous NMR assignments and J-coupling measurements of α and β pipitzols at 800 MHz, crystal structures of both isomers, and the synthesis, crystal structure, and NMR data of the dimer diperezone.

25 - Assessing Compound-Membrane Interactions by NMR

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The penetration of pharmaceuticals through the cell membrane by passive diffusion is estimated to be the dominant mechanism of transport into cells for over 90% of pharmaceuticals. Rapid screening methods to assess membrane permeability of fragments & leads are critical to identifying promising scaffolds and guide synthetic efforts. Current assays for membrane permeability are often performed by PAMPA. However, long incubation times, functional group requirements for detection, and limited available membrane formulations reduce the versatility of this technique. By employing liposomes and NMR spectroscopy, we demonstrate that membrane interactions and permeability can be assessed as soon as the sample is mixed. The versatility of liposome formulations furthermore opens the possibility for quickly developing custom membrane compositions more reflective of the cell-type of interest.

26 - Milk and cream composition by time-domain nuclear magnetic resonance (TD-NMR) relaxometry

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Conventional methods for the determination of dairy composition are generally laborious, time-consuming, and destructive to the samples, which therefore are not suited for on-line applications. This work investigated the possibility of determining milk and cream composition in fresh samples using TD-NMR relaxometry.

By performing leave-one-out cross-validation and partial least squares regression, calibration models were established using NMR signals from 72 (24 cream, 48 milk) samples of known composition. The best result was achieved with calibration correlation coefficient R_C^2 of 0.99961, 0.98613, and 0.99949 for fat, crude protein, and total solids content, respectively. Separate calibrations for cream and milk gave comparable values for fat and total solids with cream samples (R_C^2 = 0.99970), slightly lower values for crude protein in both groups (R_C^2 ~ 0.93), and much lower values for fat and total solids with milk samples (R_C^2 ~ 0.81-0.89). These results correlated well with the coefficient of variation in each calibration group. Except for fat and total solids in milk, ratio of performance to deviation (RPD) values were sufficient (> 3) for industrial use. For milk samples, additional calibrations were obtained for casein and lactose content, yielding RPD > 3 for casein but not lactose.

These NMR results were compared with those obtained on the same samples using a dedicated dairy analyzer based on Fourier-transform infrared spectroscopy. Except for lactose, high regression coefficients were obtained, as expected more so for cream than for milk.

This work can help the dairy industry to better control the composition of dairy products.

27 - Optimization and Characterization of an Aptamer Targeting the p47/p97 Interaction for Therapeutic and Diagnostic Applications in Neurodegenerative Disorders and Cancer

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p97 is an AAA+ ATPase that is crucial for a variety of cellular processes, including protein quality control, membrane fusion, and chromatin-associated regulation. Dysregulated p97 activity is implicated in cancer and neurodegenerative disorders. Thus, p97 has emerged as a promising target for interventions for these diseases.

p97 engages with diverse cofactors to orchestrate its various functions. One such cofactor is p47, which directs p97 to assist in membrane fusion events within the cell. Our lab has been exploring

specific binders of the p47 cofactor to provide a pathway-specific inhibitor of p97 function. In collaboration with Dr. Juewen Liu's group, we identified the first aptamer for p47, a 42-base-pair oligonucleotide, using capture-SELEX. Aptamers are short, single-stranded DNA or RNA sequences selected for their high affinity and specificity to a target.

Using ITC, we determined the binding affinity between the selected aptamer and p47 to be approximately 4 μM. Further analysis using NMR identified that the aptamer interacts with the SEP domain, one of the three folded domains on p47. Through chemical shift perturbations, we mapped out the binding interface on p47 and found that the aptamer may contain multiple binding sites for p47.

Future work will involve evaluating the aptamer's binding within the p47-p97 complex and optimizing the aptamer sequence to increase its binding affinity based on structural insights. By combining these complementary biophysical approaches, we aim to establish a detailed characterization of these aptamers and their mechanisms of target recognition, laying the foundation for their development as novel cancer therapeutics.

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