Event Agenda

PANIC 2025

Monday, May 19, 2025

Breakfast (provided by PANIC)

8:00 AM – 9:00 AM

Don't PANIC - Subrata Mishra, “The ABC’s of Protein NMR”

9:00 AM – 9:30 AM

Biomolecules, from peptides to monoclonal antibodies, play a critical role in modern therapeutics. For scientists, mastering protein NMR spectroscopy is an invaluable skill, offering unique insights into structure and function. Whether you're new to the field or seeking a solid foundation, join my workshop, *The ABC’s of Protein NMR*. This introductory session covers the fundamentals of protein NMR and includes live demonstrations, interactive exercises, and take-home worksheets for continued learning at your own pace. Expand your expertise and enhance your career with this essential skillset in biomolecular research.

Speaker

Subrata Mishra

Principal Investigator | NIST

JEOL Mini-Symposium on NMR Advancements

9:30 AM – 11:30 AM

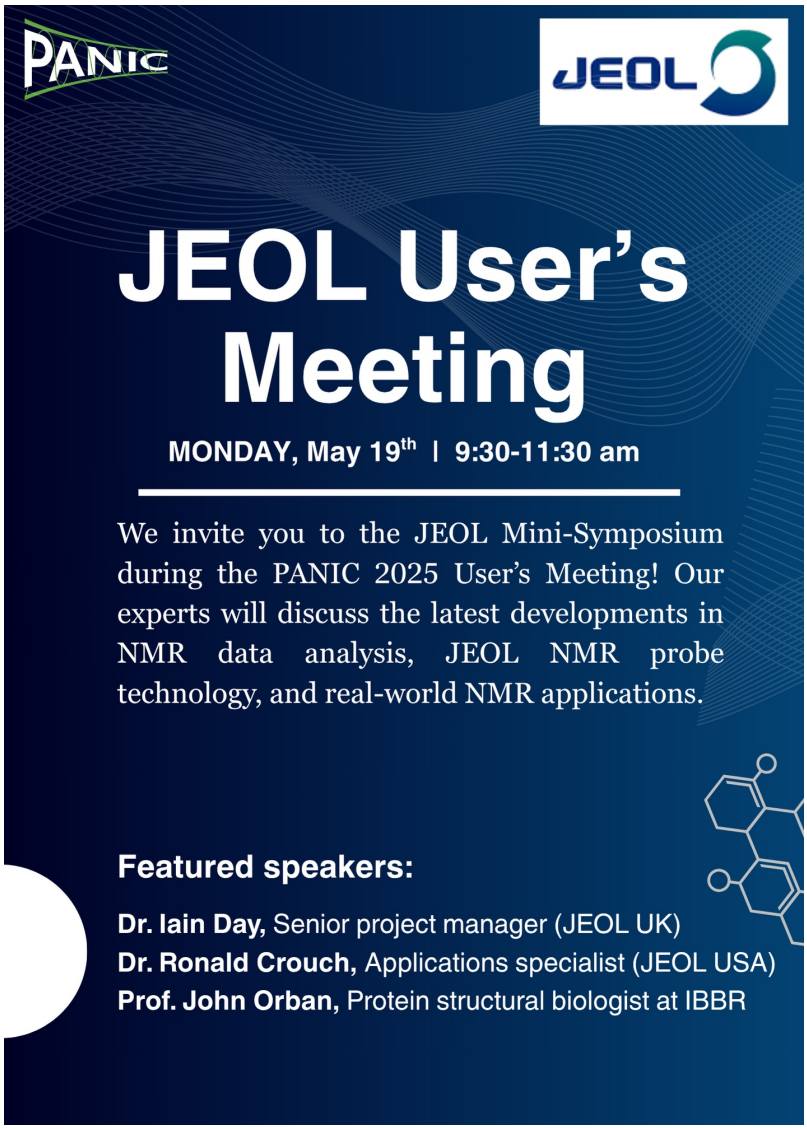
We invite you to the JEOL Mini-Symposium at the IBBR Auditorium on Monday, May 19, from 9:30 AM to 11:30 AM. Our experts will discuss the latest developments in NMR data analysis, JEOL NMR probe technology, and real-world NMR applications.

Featured Speakers:

- Dr. Iain Day (JEOL UK)
- Dr. Ronald Crouch (JEOL USA)
- Prof. John Orban (UMD/IBBR)

Please note this is a hybrid event, meaning you may attend virtually or in-person at 9:30 AM - 11:30 AM.

Register Here



Don't PANIC - Gennady Khirich, "qNMR for the Curious"

11:30 AM – 12:00 PM

NMR is a powerful analytical technology that may be used as a non-destructive quantitative primary measurement technique. The primary aim of this talk is to introduce the audience to the various practical aspects of quantitative NMR – or, qNMR as it is referred to colloquially. Topics covered will include a high-level overview of qNMR applications and the various techniques used for quantifying NMR spectra (with a focus on integration of 1D spectra), how quantification of NMR signals is translated into chemical concentrations/mass/purity, the role of quantitative standards (both internal and external), considerations of acquisition/processing under quantitative conditions, and the origins of systematic and random uncertainty in qNMR measurements. Simulations will be used, as appropriate, to illustrate all the salient points. This tutorial is aimed at both qNMR novices as well as experts who are interested in non-canonical nuances that oftentimes go unmentioned.

Speaker

Gennady Khirich

Associate Principal Scientist | Merck

Lunch (provided by PANIC)

12:00 PM – 1:00 PM

Bruker User Meeting

1:00 PM – 3:00 PM

The Bruker Team is excited to participate in this year's PANIC NMR conference and especially for the first annual Don't PANIC day! Join us for our traditional users meeting in the IBBR auditorium on Monday, May 19, from 1:00 PM – 3:00 PM Connect with fellow NMR enthusiasts, learn about our latest developments, and discover tools to make your job easier. Don't miss out on this opportunity to network and learn. Don't miss out on this chance to elevate your NMR expertise and connect with the brightest minds in the field. See you there!

Featured Bruker Speakers:

- Kate Holub, Global Sales Director
- Bernie O'Hare, Labscape and Regional Sales Manager
- Amy Freund, Senior Applications Scientist

- Alejandro Bara Estaun, Solutions Product Manager

Learn more: https://www.bruker.com/en/news-and-events/events/panic.html

Don't PANIC - Frank Delaglio and Luke Arbogast, "A Spectroscopist's Guide to Principal Component Analysis"

3:00 PM – 3:30 PM

Principal Component Analysis (PCA) is a statistical technique used for dimensionality reduction, pattern recognition, and data visualization. It transforms complex datasets into a set of orthogonal variables called principal components, which capture the most variance in the data. In NMR spectroscopy, PCA is applied to analyze complex spectral data, particularly in metabolomics, food science, pharmaceuticals, and biomolecular research. It helps identify trends, classify samples, and detect subtle differences between spectra. It is a powerful tool across multiple industries, improving efficiency, quality control, and scientific discovery.

Speakers

Luke Arbogast

Director - NMR Spectroscopy | Eli Lilly and Co.

Frank Delaglio

NIST

Break

3:30 PM – 4:00 PM

Mestrelab/SciY User Meeting

4:00 PM – 6:00 PM

Join us for the Mestrelab User Meeting on Monday, May 19, from 4:00 PM to 6:00 PM (EST). You're invited to learn about the latest updates on Mestrelab as part of the SciY family, along with new developments in NMR data analysis, USP-ID and FAIR data management.

Featured Speakers include:

- Farrel Borden, SciY
- Ben Shapiro, US Pharmacopeia

- Vincent Ching, ExxonMobil

And don’t miss Mark Dixon’s talk on May 21:

- Hunting for Reaction Intermediates in Real-Time Using a Combination of NMR Techniques and Other Modalities – 8:55 AM

Register for our User's meeting ? https://lnkd.in/dVnPw-tn

Don't PANIC - John Marino, “From Inspiration to Application: Leading a Successful Collaboration”

6:00 PM – 6:30 PM

Strong leadership skills are essential for guiding a research collaboration between industry and academia because they foster clear communication, align diverse goals, and inspire innovation. A great leader bridges the gap between academic curiosity and industry practicality, ensuring that both sides work toward a shared vision while valuing each other's strengths. By promoting teamwork, adaptability, and a problem-solving mindset, leaders create an environment where groundbreaking discoveries can translate into real-world applications. Their ability to navigate challenges, secure resources, and motivate teams helps turn ideas into impactful solutions that advance not just the field of NMR spectroscopy, but scientific endeavors of all kinds.

Speaker

John Marino

Senior Research Scientist | NIST

Opening Reception

6:30 PM – 8:00 PM

Tuesday, May 20, 2025

Breakfast (provided by PANIC)

7:15 AM – 8:15 AM

Opening Remarks

8:15 AM – 8:20 AM

Spectra of possibilities: Making Sense of Molecular Mixtures

8:20 AM – 9:55 AM

Session Moderators, Alessia Trimigno and Amber Balazs.

Harnessing NMR for analyzing complex mixtures is a powerful approach to gain insights into chemical processes and biochemical pathways. Scrutiny of molecular mixtures over time and circumstance can elucidate interactions and enable higher level insights. Translating these deeper understandings into actions can drive advances in diagnostics, treatments, and best practices. The session will explore advanced NMR methodologies and technologies, offering practical solutions to complex problems.

Speakers

Robert Powers

Charles Bessey Professor of Chemistry | University of Nebraska-Lincoln

Tanvir Sajed

Senior Machine Learning Scientist | University of Alberta

David Rovnyak

Professor of Chemistry | Bucknell University

Metabolomics: the Good, the Bad, and the Ugly

8:25 AM – 8:55 AM

Metabolomics continues to experience an exponential expansion primarily due to its valuable contributions to a diversity of fields ranging from food and the environment to drug discovery and disease diagnostics. A multiplatform, multicohort, and multiomics approach increases the accuracy of a metabolomics study in the same manner that traditional cellular and molecular biology experiments can help validate omics results. Recent examples of this approach will be highlighted that includes our analysis of a metabolic signature for acute radiation syndrome and associated radioprotection treatment, amifostine, a diagnostic biomarker for multiple sclerosis, and the molecular mechanism of a novel fatty acid analogue as treatment for tuberculosis. Despite these and other successes, the field of metabolomics faces a critical inflection point because of the growing concerns regarding the reliability of the thousands of studies populating the scientific literature. Meta-analysis and benchmarking of metabolomics data will also be presented that demonstrate the reproducibility crisis facing the metabolomics field along with some insights of the underlying causes and the need for validated and widely adopted best practices.

Speaker

Robert Powers

Charles Bessey Professor of Chemistry | University of Nebraska-Lincoln

Machine learning tools for accurate NMR spectral prediction and compound identification

8:55 AM – 9:25 AM

NMR is routinely used in organic compound identification, drug metabolite characterization, natural product discovery, and the deconvolution of metabolite mixtures in biofluids (metabolomics and exposomics). Traditionally, identifying compounds via NMR relies on matching experimentally obtained spectra to reference libraries, but these libraries are often limited in size—especially for compounds relevant to medical diagnostics and pharmaceuticals. By leveraging machine learning, it is possible to accurately predict NMR chemical shifts and build extensive spectral libraries. We have developed two machine-learned tools called PROSPRE (PROton Shift PREdictor) and CASPRE (CArbon Shift PREdictor) using a high-quality, solvent-aware experimental dataset to predict 1H chemical shifts (with a mean absolute error below 0.10 ppm) and 13C chemical shifts (with a mean absolute error below 1.8 ppm) in solvents such as water (at neutral pH), chloroform, DMSO, and methanol. PROSPRE outperformed all other known models on an independent dataset of experimental chemical shifts. We have deposited predicted 1H and 13C chemical shifts for over 600,000 molecules in popular metabolomic, drug and natural product databases using the aforementioned machine-learned models. Searching these large databases of predicted chemical shifts facilitates robust and efficient compound identification in complex biological samples, which could potentially aid in drug and biomarker discovery.

Speaker

Tanvir Sajed

Senior Machine Learning Scientist | University of Alberta

A NMR Metabolomic Window on the Progression and Regression of Steatotic Liver Disease

9:25 AM – 9:55 AM

The accumulation of lipids in liver hepatocytes is the initial stage of steatotic liver disease, which affects about 20-30% of the world's population and is termed MASLD (metabolic dysfunction associated steatotic liver disease). Often interpreted as the hepatic expression of metabolic syndrome, MASLD has a discrete progression from an initial steatotic phase, which is phenotypically mild in most subjects, to a more serious state of liver inflammation and scarring termed MASH (SH = steatohepatits) in a smaller number of subjects, which requires intervention. Currently the gold standard for assessing liver health is an invasive biopsy which is costly and samples only about 1/40,000 of the liver volume. Metabolomic methods could offer in principle a low-invasive window to assess liver health. A rigorous tiered suite of studies involving biobanked sera from about 300 subjects has been performed to examine disease pathology, and also to explore the potential of developing an aqueous metabolic profile of MASH that could assess responses to intervention. A candidate metabolic profile resulting from this work will be presented and critically evaluated, while this work will also shed light on fundamental aspects of metabolic research including assessing reproducibility, encountering confounding variables, the increasing pairing of metabolomics with biobanking, and handling complex samples. Additionally, this work yielded several opportunities to examine popular over-the-counter medications in sera, including both fundamental chemistry and also natural experiments which raised hypotheses that suggest that broader metabolomic studies should be open to natural experiments.

Speaker

David Rovnyak

Professor of Chemistry | Bucknell University

Coffee Break (sponsored by Tecmag)

9:55 AM – 10:15 AM

Energy flows where attention goes: Better NMR for better energy materials

10:15 AM – 11:50 AM

Session Moderators, Sarah Mattler and Ryan Nieuwendaal.

How do you make a better battery? You understand the materials that comprise it! In this year's PANIC session "Energy flows where attention goes: Better NMR for better energy materials," our speakers will show us how NMR can help us understand those materials. By quantifying compositions, atomic level structures, and dynamics, our speakers will illuminate us with the role that solid-state NMR has in energy materials investigations. Join us to find out what NMR can tell us!

Speakers

Yanyan Hu

Professor of Chemistry & Biochemistry | Florida State University

Amrit Venkatesh

Assistant Professor | University of Virginia

Mark Bovee

Research Chemist | U.S. Naval Research Laboratory

In-situ magnetic resonance characterizations of rechargeable batteries

10:20 AM – 10:50 AM

Magnetic resonance techniques, including nuclear magnetic resonance spectroscopy (NMR), magnetic resonance imaging (MRI), and electron magnetic resonance (EPR), are non-invasive techniques used to examine both surface chemistry and bulk properties. These techniques employ nuclear or electron spins as probes for interrogating structures and dynamics. We have employed these techniques in situ to understand the working and failing mechanisms of rechargeable batteries. Utilizing in situ 7Li NMR, we determined the lithiation and delithiation sequence and rates at different structural sites in high-voltage transition metal oxide cathodes. Via in situ 17O NMR, we evaluated the reactivity of various oxygen species in these high-voltage transition metal oxide cathodes and the reversibility of these O redox reactions. In conjunction with in situ EPR, we discovered the synergy of the hybridized O2p and TM3d orbitals to deliver additional capacities in Li transition metal oxide materials and the subsequent stabilization of the structures to ensure reversibility. Combined in situ NMR and EPR also prove beneficial to elucidating redox mechanisms in organic cathode materials. Our recent work has demonstrated the efficacy of in situ 7Li MRI in identifying new dendrite formation mechanisms in solid-state batteries and new phenomena in the dendrite formation process. In situ tracer-exchange NMR is useful for mapping out ion transport pathways in complex ion conductors and distinguishing dendrite formation mechanisms at different charge states. In summary, in situ magnetic resonance techniques are useful for uncovering structural and dynamic aspects of energy materials with spatial and temporal resolution.

Speaker

Yanyan Hu

Professor of Chemistry & Biochemistry | Florida State University

In situ chemical shift imaging investigation and first cycle transient effects study of an electrochemical supercapacitor containing a ZIF-67 electrode

10:50 AM – 11:20 AM

In order to reduce fossil fuel consumption with renewable energy, there's been drive to improve the performance of energy storage devices. Supercapacitors represent a category of these devices chosen for applications that demand faster energy delivery than that of a battery and a greater amount of energy than that of a capacitor. Recently, metal-organic frameworks (MOFs) have been considered as electrode materials to bolster the performance of these devices. Metal-organic frameworks offer two potential advantages to these systems: their porosity provides a high surface area that improves energy storage from electrochemical double layer formation, and their metal centers and functionalized organic linkers can participate in reversible redox reactions that provide additional energy storage known as pseudocapacitance. Despite these advantages, MOFs have seen limited use in this application due to their inherent low conductivity and poor chemical stability. Understanding not only the charge storage mechanisms but also the drawbacks of these materials in functioning devices is critical for improving the performance of MOF-based supercapacitors.

Herein, we utilize in situ chemical shift magnetic resonance imaging to investigate the performance of a zeolitic imidazolate framework 67 (ZIF-67) electrode in an electrochemical supercapacitor device with a 1M KOH electrolyte. This technique allows us to separate NMR spectra of the electrolyte as a function of position in the supercapacitor cell, enabling us to monitor the signal of the electrolyte in close proximity to each of the cell's components. Significant changes in the electrolyte's 1H chemical shift are observed near the ZIF-67 electrode upon cell assembly, and they are amplified by the application of voltage during the supercapacitor's first cycle. We connect these changes to the degradation of ZIF-67 in a pH basic environment as previously reported in literature—hydroxide ions displace ZIF-67's 2-methylimidazole linker molecules from its cobalt (II) metal centers. This connection is then verified with ex situ X-Ray Absorption Spectroscopy measurements of pristine and electrochemically cycled ZIF-67 electrodes. Additionally, these images illustrate the migration of free electrolyte towards the electrodes as voltage is applied to the system. We characterize the timescale of this process as well as ZIF-67's decomposition by allowing a pristine cell to rest at 0.20 V while chemical shift images are collected, and we show that this process requires up to six hours at low voltages before changes between images become relatively negligible. Subsequent charging at higher voltages reveals only minor differences among chemical shift images, signifying the majority of change occurred while the voltage of this cell was fixed at 0.20 V for an extended period of time. The observation and characterization of these processes provide insight on this MOF's behavior in a device-like configuration, guiding us in our choice of MOFs for this application as we begin studying and measuring new MOF materials. This presentation will also include recent applications of this technique to other energy storage systems we've studied to better understand their performance.

Speaker

Mark Bovee

Research Chemist | U.S. Naval Research Laboratory

Probing Structure of Heterogeneous Materials using High Field and DNP-Enhanced Solid-State NMR

11:20 AM – 11:50 AM

Solid-state NMR spectroscopy is increasingly recognized as a valuable tool to investigate complex heterogeneous materials that cannot be well-characterized using standard diffraction and microscopy techniques. While solid-state NMR can be used to assess nuclei from across the periodic table that are present in materials, its low intrinsic sensitivity limits its application. To address this sensitivity problem, we use high magnetic fields, fast magic angle spinning (MAS), and dynamic nuclear polarization (DNP). High magnetic fields provide high sensitivity and resolution which can be particularly useful for quadrupolar nuclei, which make up for more than 70% of the periodic table. The enormous sensitivity gains provided by DNP is particularly useful to tackle unreceptive nuclei and investigate surfaces and interfaces of complex heterogeneous materials.

In this talk we will demonstrate examples of the application of sensitivity-enhanced solid-state NMR in catalysis, sustainable energy and environmental remediation. We will focus on the characterization of amorphous aluminosilicates, which are promising catalyst support materials, and MgAl layered double hydroxides (MgAl-LDH), which are promising sorbents for recovery of phosphate from wastewater due to their high anion exchange capacity. We use multi-nuclear one- and two-dimensional solid-state NMR spectroscopy to assemble atomic-structure puzzles, that allow us to better understand the properties exhibited by these materials.

A combination of high-field 1H, 17O, 27Al and DNP-enhanced 15N solid-state NMR spectroscopy reveals insights into the structure of defected amorphous aluminosilicates, which have recently shown to provide improved catalytic activity. In case of the LDH materials, a combination of fast MAS, high field and DNP-enhanced solid-state NMR of 1H, 25Mg, 27Al and 31P nuclei reveals a significant breakdown of MgAl-LDH upon phosphate uptake and reveals phosphate binding sites. These applications demonstrate the versatility of solid-state NMR in materials structure determination.

Speaker

Amrit Venkatesh

Assistant Professor | University of Virginia

Lunch (provided by PANIC)

11:50 AM – 12:50 PM

Posters - Session 1 (even-numbered)

12:50 PM – 2:00 PM

Poster 2: “NMR spectroscopy to aid the discovery of non-nucleoside inhibitors of the flavivirus RNA-dependent RNA polymerase” (Adam Lewis)

Poster 4: “NMR polymorphism in drug design” (Damjan Makuc)

Poster 6: “Development of a Fecal Metabolite Solution (RGTM10212)” (Sandra Da Silva)

Poster 8: “Development of a Vesicle Model to Study Solvent PRE-Effects on Lipoprotein Particles” (Almira Ahmed)

Poster 10: “Metabolomics effect of microplastics and Bisphenol A contamination in Kidney cell line” (Giselle Gouveia)

Poster 12: “Towards characterizing lipoprotein particle size using solvent PRE effect” (Mary Starich)

Poster 14: “An NMR-based fragment screening approach to identify LCAT modulators” (Elena Hausmann)

Poster 16: “Deriving molecular motion parameters in soft materials with DF-MSE, VFT/Arrhenius, and Anderson-Weiss models” (Bruno Trebbi)

Poster 18: “Solid state NMR characterization on interaction of organic solvents and lipid membrane” (Yunqiao Pu)

Poster 20: “Monitoring Chemical Processes with Benchtop NMR” (Blake Fonda)

Poster 22: “Observation of pH-Dependent Residual structure in the pmel17 repeat domain and the implication for its amyloid formation” (Daniel Morris)

Poster 24: “Developing two-dimensional solution NMR strategies for difficult targets in the autophagy and endolysosomal pathways” (David Nyenhuis)

Poster 26: “Empowering structure verification and quantification through digital innovation” (Albert Farre Perez)

Poster 28: “Quantifying populations and exchange rates of ligands at quantum dot surfaces using NMR spectroscopy and diffusometry” (Veera Venkata Shravan Uppala)

Poster 30: “Quantifying aluminum adjuvant adsorption capacity through lipid adsorption with solid-state NMR” (Patrick Keating)

Poster 32: “Dipolar-Filtered Magic Sandwich Echo as an Approach to NMR Cryoporometry” (Bruno Trebbi)

Poster 34: “Innovative utilization of portable time-domain nuclear magnetic resonance (TD-NMR) spectroscopy for accurate in-field citrus raw juice quality analysis.” (Javier Aztiazarain)

Spin Doctors: Using NMR to Diagnose Stability Issues in Biologics Before They Go Viral

2:00 PM – 3:35 PM

Session Moderators, Subrata Mishra and Luke Arbogast.

From vaccine adjuvants to monoclonal antibodies, stability is everything in biopharmaceuticals—but biomolecules don’t always behave as expected under different environmental conditions. NMR spectroscopy provides a powerful toolkit to diagnose and resolve critical stability challenges at the atomic level. This session highlights cutting-edge advances in solid- and solution-state NMR and new advances in isotopic labeling strategies, to characterize complex mAbs, fine-tune formulations, prevent aggregation, and ensure biologics stay in peak condition before reaching the market.

Speakers

Jaekyun Jeon

Assistant Research Professor | University of Maryland College Park

Anupreet Kaur

Post Doctoral Fellow | Institute for Bioscience & Biotechnology Research

Yves Aubin

Research Scientist | Health Canada

Advancing the characterization of aluminum adjuvant-based vaccines using solid-state NMR techniques

2:05 PM – 2:35 PM

Aluminum adjuvant (alum)-based vaccines are among the most widely used vaccine types due to their ability to enhance immune responses effectively. However, despite their extensive application, our understanding of alum-based vaccines remains limited, particularly regarding the structural and dynamic properties of aluminum adjuvants and adsorbed antigens. This gap in knowledge hinders the optimization of vaccine formulations. Solid-state Nuclear Magnetic Resonance (ssNMR) provides a powerful tool for characterizing critical material attributes (CMAs) of alum-based vaccines. Our research focuses on using ssNMR to investigate these CMAs, including surface characterization of alum, conformations of adsorbed antigens, and their interactions with alum.

In this presentation, I will introduce a solid-state NMR approach for directly measuring the adsorption capacities of alum by adsorbing phospholipid molecules onto the adjuvant and utilizing 27Al and 31P ssNMR to quantify the lipid-to-alum adsorption ratios. Phospholipid molecules can adsorb onto various solid surfaces, forming uniform bilayers with tunable charge properties by adjusting the charged-to-neutral lipid ratios, making them excellent probes for quantifying alum's adsorption capacity. Additionally, I will briefly outline other ssNMR methods for characterizing the conformational states of antigens adsorbed onto alum and for studying their adsorption kinetics.

Speaker

Jaekyun Jeon

Assistant Research Professor | University of Maryland College Park

Excipient-Induced mAb Dynamics Unveiled by NMR: Fast-Tracking Biotherapeutic Formulations

2:35 PM – 3:05 PM

Monoclonal antibodies (mAbs) are currently the leading platform for development of protein-based biological drugs due to their high specificity, binding properties, and developability. They are used widely in the treatment of many illnesses, including inflammatory diseases, viral infections, autoimmune disorders, and cancer. These protein therapeutics are particularly prone to physicochemical degradation, making formulation critical for enhancing conformational, colloidal, and chemical stability by minimizing aggregation, lowering viscosity, and improving chemical integrity, bioactivity, and bioavailability. Currently, optimizing formulations relies heavily on trial-and-error experimentation, making the process time-consuming and expensive. Likewise, traditional biophysical techniques, which offer low to moderate structural resolution, only provide a limited mechanistic understanding of how excipients influence mAb dynamics at the atomic level, and how such dynamics correlate to macroscopic observations such as aggregation or stability. Solution NMR provides a powerful way to capture protein dynamics across a wide range of timescales, offering atomic-level detail along with global insights into protein structure, size, and inter-domain motion. In this study, NMR is applied to the 50 kDa Fab domain of the NISTmAb as a model drug substance (DS) to characterize excipient-induced motions. We examine the effects of sodium chloride, sucrose, and polysorbate 80 on the local bond motions and reveal their correlation to altered Fab domain dynamics and surface accessibility. This work highlights the importance of integrating protein dynamics at all scales with HOS analyses to gain a more complete understanding of protein behavior, offering valuable insights for the development of stable biotherapeutics.

Speaker

Anupreet Kaur

Post Doctoral Fellow | Institute for Bioscience & Biotechnology Research

Generic therapeutic mAbs are closer than they appear - How NMR spectroscopy could bring them there

3:05 PM – 3:35 PM

Over 200 therapeutic monoclonal antibodies, where 125 are of the IgG1 subclass, have been approved or are under review in the world, and more than 1000 are under development, which exemplifies the importance of this class of protein therapeutics. Amongst the innovator products, eleven have lost patent protection and have entered competition with their biosimilar counterparts. This class of protein therapeutics is very complex and very challenging to characterize. In the past few years, a number of nuclear magnetic resonance spectroscopy-based approaches have been proposed to characterize mAbs. In this presentation, I will share our latest contributions in the area of labelling strategies of mAbs and their fragments. In particular, a new simple and low-cost protocol that allows near complete resonance assignment of therapeutic monoclonal antibodies in a matter of a few hours. Applied to therapeutics, this method will help bridging the gap between biosimilar and bio-generic products and provide new tools to better understand excipient-mAbs interactions.

Speaker

Yves Aubin

Research Scientist | Health Canada

Coffee Break (sponsored by Tecmag)

3:35 PM – 3:55 PM

Relaxometry

3:55 PM – 5:30 PM

Session Moderators, Matt Augustine and Ryan Nieuwendaal.

Relaxation. It affects you, me and spins. In the case of spins, relaxation manifests as signal decay rates in the time domain and line widths in the frequency domain. An understanding of these “loss” parameters provides intimate details regarding the dynamics of interacting spins. This session explores the relaxation of spins and the use of that information to provide a better understanding of solids and liquids.

Speakers

David Faux

Emeritus Professor of Physics | University of Surrey

Jamal Hassan

Associate Professor | Khalifa University of Science and Technology

Westley Pawloski

Postdoctoral Researcher | National Heart Lung and Blood Institute

NMR investigation of ionic liquid dynamics in confined silica nanopores

3:55 PM – 4:25 PM

The behavior of confined ionic liquids (ILs) within nanoporous materials presents a fascinating interplay of molecular interactions and mobility. While confined water exhibits rapid and cooperative single-file diffusion, ILs demonstrate similarly complex dynamics when restricted within porous matrices. However, the microscopic mechanisms governing these motions remain elusive.

In this study, we employed nuclear magnetic resonance (NMR) spectroscopy to investigate the dynamics of the ionic liquid [BMIM]+[TCM]- confined within mesoporous silica matrices MCM-41 and SBA-15. Using diffusion-relaxation correlation (2D D-T2eff) and relaxation time measurements, we resolved distinct molecular motion modes within these confined geometries. Diffusion distributions were analyzed using a Tikhonov regularization inversion algorithm.

Our findings reveal that in both MCM-41 and SBA-15, Hahn spin echo decays deviate from simple exponential τ^3 behavior due to the complex interplay of diffusive processes. Two distinct IL components were identified: a mobile fraction and an adsorbed fraction, with an additional minor peak at <100 μs attributed to hydroxyl groups. Notably, in SBA-15, the mobile IL component exhibits near-exponential τ^3 decay, whereas in MCM-41, it follows a single-file diffusion mode. These results were further validated using 2D D-T2eff correlation experiments.

Our conclusions indicate that at room temperature, IL molecules in MCM-41 form an adsorbed layer on pore walls, while free anion-cation pairs undergo constrained axial diffusion. At elevated temperatures, the adsorbed IL molecules desorb from the silica surface, altering the diffusion dynamics. These insights contribute to a deeper understanding of IL transport in nanoconfined environments, with potential implications for energy storage and catalysis applications.

Speaker

Jamal Hassan

Associate Professor | Khalifa University of Science and Technology

Connecting fast field cycling NMR to real world problems with the 3-tau model

4:25 PM – 4:55 PM

Fast field cycling NMR (FFC NMR) relaxometry measures the longitude relaxation rate R_1 as a function of magnetic field strength with emphasis on low magnetic fields. The R_1 (ω) dispersion curve captures information about the nanoscale dynamics of water in porous materials which can be accessed provided a suitable model can be fit the data. Identifying a suitable model for a particular material poses a difficult challenge. In recent years, the 3-Tau Model (3TM) has produced exquisite fits to the R_1 (ω) dispersion curves from rocks, clays, soil, cementitious material, silicas and glasses, foodstuffs, hydrogels, creams and pastes, catalysts and biomaterial including blood and cancerous tissues. Each fit yields a set of physically meaningful parameters including three dynamical time constants, a pore size parameter, and surface water and paramagnetic ion densities. Importantly, we have demonstrated that the 3TM can statistically associate fit parameters to the large-scale properties of a material. We show that two 3TM fit parameters obtained from sets of FFC NMR experiments on tumorous murine muscle tissue are statistically correlated to tumor fraction.

It is shown that the pore size parameter can be used to monitor the ageing of cheese. Pore size is also an important quantity for characterizing hydrogels, used for diapers and slow-release drug delivery systems. The 3TM determination of hydrogel pore size may eliminate the need for costly and time-consuming neutron scattering experiments. Lamellar structures are used in personal care products and here 3TM fitting may eliminate the need for X-ray scattering measurements of pore size.

Cement is second only to water as the most consumed material by humans. It is also the third largest contributor to global CO2 emissions (6-8%). The carbon footprint of cement production may be reduced by incorporating additives such as fly ash or recycled powdered cement and concrete from demolished buildings. However, this is only useful if product strength is retained.

We show that the pore size determined by 3TM for a gray cement sample post-hydration decreases exponentially with a time constant T. As cement hardens the ultimate strength depends on several factors, including the curing rate characterized by T and the surface chemistry characterized by the 3TM dynamical time parameters. We show that, in principle, executing many trials with different amounts and type of additive will allow the 3TM parameters to be statistically related to the ultimate strength of the product. Not only would this enable promising additives to be identified at an early stage but would also provide insight into the complex chemistry of cement hydration.

Speaker

David Faux

Emeritus Professor of Physics | University of Surrey

Evaluating the use of lanthanide containing dendrimers for solvent paramagnetic relaxation enhancement

4:55 PM – 5:25 PM

Paramagnetic relaxation enhancement (PRE) is widely utilized in biomolecular NMR spectroscopy to obtain long-range distance and orientational information for intra- or intermolecular interactions. In contrast to conventional PRE measurements, which require tethering small molecules containing either a radical or paramagnetic ion to specific sites on the target protein, solvent PRE (sPRE) experiments utilize paramagnetic cosolutes to induce a delocalized PRE effect. Compounds utilized as contrast agents in magnetic resonance imaging (MRI) applications typically consist of Gd3+ chelated by a small molecule. Tethering these Gd-containing small molecules to larger complexes has been shown to increase the PRE-effect and produce more effective contrast agents in MRI. Inspired by their use as MRI contrast agent, in this work we evaluate the effectiveness of using a functionalized polyamidoamine (PAMAM) dendrimer for sPRE measurements. Using ubiquitin as a model system, we measured the sPRE effect from a generation 5 PAMAM dendrimer (G5-Gd) as a function of temperature and pH and compared to conventional relaxation agents. We also demonstrated the utility of G5-Gd in sPRE studies to monitor changes in the structures of two proteins as they bind their ligands. These studies highlight the attractive properties of these macromolecular relaxation agents in biomolecular sPRE.

Speaker

Westley Pawloski

Postdoctoral Researcher | National Heart Lung and Blood Institute

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Wednesday, May 21, 2025

Breakfast (provided by PANIC)

7:15 AM – 8:15 AM

Opening Remarks

8:15 AM – 8:20 AM

Idea to Execution: NMR Innovations Unveiled

8:20 AM – 9:55 AM

Session Moderators, Samantha Miller and Savanah Shumaker.

Have you ever wondered how groundbreaking NMR innovations come to life? This session pulls back the curtain on the creative process behind cutting-edge hardware and software developments in the field. Hear from spectroscopists at various stages of innovation—whether they're conceptualizing bold new ideas or sharing the journey of turning concepts into creations. From inspiration to execution, discover how these advancements are shaping the future of NMR workflows and technology.

Speakers

Richard Lewis

Principal Scientist | AstraZeneca

Mark Dixon

Mestrelab Research

Ben Reiner

Associate Research Scientist | Dow Chemical

Fit for the future ASV (Automated Structure Verification): Combining techniques and data

8:25 AM – 8:55 AM

Automatic systems to interpret analytical data have been in development for decades. Despite some success they have not produced the step change in productivity needed to keep up with synthetic output that is increasingly coming from automated methods. Recent heightened interest in AI and machine learning methods together with the unabated increase in computational power opens up new opportunities and the field is the most exciting it has been for a decade.

The talk will start with an brief overview of ASV, CASE and machine-learning models. Each technique has strengths and weaknesses but each has the same ultimate aim to generate a structure with a high probability of being correct and consistent with the data. It is likely therefore that the “ultimate” verification system will incorporate different types of approach integrating them into a whole that is more than the sum of the individual components. The talk describes progress towards achieving this goal.

Here we describe our recent work with ASV validated with 100 pairs of structural isomers, one correct and one incorrect (42 distinct compounds) on which diverse analytical data was collected. Proton NMR data was scored using both the ACDlabs verification tool and DP4. We developed an automated algorithm that scores experimental infrared spectra against ab initio calculated spectra. We show using appropriate metrics, that comparing the scores of candidate structures is a far superior technique than relying on a single “ASV” score. Furthermore this technique naturally produces an “unknown” category – structures that score the same or that are not distinguished by a sufficient margin – indicating when further data or manual interpretation is required. We find that, surprisingly, infrared is as powerful as proton NMR at distinguishing the isomeric compounds, and furthermore that the combined techniques outperform either proton NMR or infrared alone suggesting a complementarity in the information content of both.

The talk concludes by showing how the data visualization techniques developed can be used to rank different analytical methods with a hint at what other analytical data might improve the process still further. We also show how machine learning models may give valuable input to the process by suggesting reaction products or suggesting alternative products consistent with the analytical data.

Speaker

Richard Lewis

Principal Scientist | AstraZeneca

Hunting for Reaction Intermediates in Real-Time Using a Combination of NMR Techniques and Other Modalities

8:55 AM – 9:25 AM

Reaction Monitoring is ubiquitous in the study of chemical transformations. The appearance of unexpected byproducts in significant enough amounts can trigger additional investigations into alternative reaction mechanisms. While byproducts can be analyzed after the reaction is completed, intermediates that hold vital clues may have come and gone unnoticed. While use of NMR, IR, and chromatographic methods, such as LC/MS are the main toolbox for a chemist to figure out the constitution of components in a final mixture, in-line or at-line techniques have been largely biased towards IR measurements, especially in a Development and/or Manufacturing environment.

This presentation will focus on two related subjects: the combination of various 2D NMR pulse sequences in ways not used before, to continuously sample a chemical reaction; and secondly, the combination of orthogonal measurement techniques, such as LC/MS and/or IR, alongside NMR, to enable more insightful identification of intermediate species, possibly in real-time, that should be of interest to the PAT community as well as the curious experimentalist.

Speaker

Mark Dixon

Mestrelab Research

DiVeRT NMR: A joint relaxometry/chemometrics approach for predicting material properties from only NMR spectra

9:25 AM – 9:55 AM

The discovery phase of any materials development campaign can be hampered by the slow development of quantitative structure-property relationships. While modern informatics techniques can accelerate such models, the bevy of analytical and computational data required to support a QSAR model is often cumbersome in practice. Disrupted Variable temperature Relaxometry (DiVeRT) NMR was developed to support material development in the discovery phase. DiVeRT is designed as an automated joint spectroscopy/chemometrics approach which provides key insight into macromolecular dynamics with minimal experimental burden. DiVeRT leverages simple spectroscopic principles, iterative statistical methods, and robust selection algorithms to enable use across a wide range of materials. A specific use case of DiVeRT will be presented with sightlines to deployment with other material families.

Speaker

Ben Reiner

Associate Research Scientist | Dow Chemical

Coffee Break

9:55 AM – 10:15 AM

There is strength in being Soft Matter

10:15 AM – 11:50 AM

Session Chairs, Ryan Nieuwendaal

Just because it’s squishy, doesn’t mean it isn’t important. Polymers, gels, suspensions and fluids are all critical to our everyday life, and

in this session, we will see how NMR can shed light on the complex inner workings of soft matter. By measuring chemistry, dynamics, structure, and transport our speakers will show us that great strength can be seen in soft matter.

Speakers

Eduardo de Azevedo

Professor | Universidade de São Paulo - Instituto de Física de São Carlos

Hattie Ring

Research Specialist - NMR Spectroscopist | 3M

Louis (Lou) Madsen

Professor of Chemistry | Virginia Tech

Materials characterization with 1D MRI measurements

10:20 AM – 10:50 AM

T2 NMR relaxation measurements are a useful tool to identify changes in molecular mobility. Bulk measurements of T2 relaxation have been demonstrated to measure polymer differences in cure, crosslinking, degradation, or additives. Layered samples or cases where the sample properties change across the sample can be challenging to evaluate with bulk methods.

Low-field NMR profile equipment has the potential to be used as a magnetic resonance imaging alternative for materials characterization in analytical labs. Low-field magnetic resonance equipment is appealing for materials characterization at manufacturing sites, because of the low cost of equipment (<$100k), reduced maintenance, and small footprint compared to high field NMR. An additional advantage for low-field NMR profile equipment is the non-destructive sample preparation.

Over the past year, we have been integrating NMR profile measurements into our suite of analytical methods for materials characterization and troubleshooting. The measurements that will be discussed were acquired using a 19.51MHz NMR Mobile Universal Surface Explorer (MOUSE). Most of the application opportunities identified with polymers are focused on leveraging T2 profile or T2-weighted 1D images acquired with a CPMG pulse sequence. We intend to discuss the practical limitations of incorporating NMR profile measurements into our analytical lab workflow.

Speaker

Hattie Ring

Research Specialist - NMR Spectroscopist | 3M

Dipolar-based low-field TD-NMR: Insights from molecular structure to macroscopic behavior of Organic Matter

10:50 AM – 11:20 AM

Over the past years, low-field Time-Domain Nuclear Magnetic Resonance (TD-NMR) has emerged as a versatile technique across various applications. Initially recognized for relaxometry—probing relaxation and diffusion processes to characterize fluid properties—TD-NMR has found widespread use in materials science, as well in the food, pharmaceutical, and oil industries. Recent advancements have extended TD-NMR beyond traditional relaxometry, particularly in the study of solid and soft materials, where through-space dipolar coupling between ^{1}H nuclear spins provides sensitivity to molecular packing and mobility. This presentation will explore a class of ^{1}H TD-NMR experiments based on ^{1}H-^{1}H dipolar interactions for investigating organic matter. We will discuss dipolar echoes, dipolar filters, dipolar relaxation, and multiple quantum correlation experiments, demonstrating their effectiveness in assessing key molecular properties such as the onset temperatures of molecular motions, crystallinity, and crosslink density in polymers, as well as distinguishing polymorphic forms in solid pharmaceuticals. Additionally, we will highlight ^{1}H TD-NMR applications in studying macroscopic phenomena, such as fertilizer dissolution in soils and also the use of ^{1}H dipolar TD-NMR as an alternative approach for characterizing mesoporous structures.

Speaker

Eduardo de Azevedo

Professor | Universidade de São Paulo - Instituto de Física de São Carlos

Understanding transport and nanoconfinement in materials by combining multimodal NMR with molecular simulations

11:20 AM – 11:50 AM

Polymer-based materials form essential and rate-limiting components in a wide range of technologies that include water purifiers, batteries, fuel cells, gas separators, and electrolyzers. Our group has uncovered new aspects of nanoconfined transport in such systems by combining temperature- and composition-dependent NMR with molecular dynamics (MD) simulations, leading to new paths of thought for design of polymers and other soft materials. Electrophoretic NMR (ENMR) along with NMR spectroscopy and diffusometry give unprecedented access to chemically specific transport processes and the coupling between local ion dynamics and the surrounding matrix. I will discuss example systems that include lithium battery electrolytes and polymer electrolyte membranes for gas or liquid separations. These systems build bridges between liquid-like and solid-like transport, thus motivating new compositions and new morphologies for electrolytes and other separations technologies. One specific recent example involves quantification of CO2 uptake and diffusion (at 13C natural abundance) in composite gas sorption membranes by NMR spectroscopy and diffusometry, and with the aid of tailored T1 relaxation agents.

Speaker

Louis (Lou) Madsen

Professor of Chemistry | Virginia Tech

Lunch (provided by PANIC)

11:50 AM – 12:50 PM

Posters - Session 2 (odd-numbered)

12:50 PM – 2:00 PM

Poster 1: “Detrimental Solvent Effect on Quantitative NMR Analysis” (Yiyong He)

Poster 3: “MicroNMR for non-invasive embryo selection: a case study” (Kathryn Marable)

Poster 5: “Application of NMR spectroscopy for the authentication of American ginseng” (Aaron Urbas)

Poster 7: “NMR Spectroscopy as a PAT tool: Field integration of a laboratory instrument” (Klas Meyer)

Poster 9: “Miniature Magnetic Resonance Spectroscopy for Early Diagnosis of Diabetes” (Jacob Yoder)

Poster 11: “Using NMR and Chemometrics as a Tool to Investigate Degradation Patterns in Monoclonal Antibodies” (Mark-Adam Kellerman)

Poster 13: “Characterization of highly-crosslinked epoxy resins for advanced semiconductor packaging via quantitative 13C CP-MAS spectroscopy” (Andrew Korovich)

Poster 15: “UEVLD as a potential tool to study Tsg-101 and an application model for pseudocontact shift experiments” (Jose Vazquez)

Poster 17: “Investigating lipid-protein interactions in odorant-binding proteins: insights from NMR and biophysical studies” (Rashmi Puja)

Poster 19: “Liquid- and Solid-State 19F NMR in the Analysis of Food Packaging Materials” (Jennifer Janovick)

Poster 21: “Exploring the future potential and practical limits of NMR: advancing quality control in pharmaceuticals and traditional medicine to protect consumer health in Vietnam.” (Duong Le Tran Thai)

Poster 23: “Probing morphology and transport in self-assembled polymeric materials for sustainable energy” (Nicholas Pietra)

Poster 25: “NMR-Based structural and dynamic insights into acyl carrier proteins: A target for antimicrobial drug discovery” (Mandeep Kaur)

Poster 27: “Optimizing efficient NMR sample preparation and data analysis workflows through innovative automation solutions” (Samuel Kotler)

Poster 29: “Quality control assays of polyurethane raw materials using benchtop NMR spectroscopy” (Matt Leclerc)

Poster 31: “Purity of biosynthesized eumelanin via solid-state NMR” (Nishani Jayakody)

Poster 33: “NMR characterization of complex higher alcohol mixtures” (Vincent Ching)

Coffee With Exhibitors

2:00 PM – 3:00 PM

Reference Materials and Calibrations

3:00 PM – 4:35 PM

Session Chair, Frank Delaglio

Calibrations and reference materials are foundational to practical NMR, and are especially critical for analyzing complex systems, and for high-precision applications. Learn about solutions to address these issues for high-pressure NMR, biomanufacturing, and more.

Speakers

Samantha Miller

Post Doctoral Researcher | National Institute of Standards and Technology

Ioannis Karageorgos

Research Chemist | NIST

Michael Judge

NIST IBBR

Sunil Paudel

qNMR Scientist | U.S. Pharmacopeia (USP)

New Considerations for Nuclear Magnetic Resonance (NMR) Referencing at High-Pressures in Polar Solutions

3:05 PM – 3:35 PM

Despite widespread use of variable pressure nuclear magnetic resonance (NMR) spectroscopy, the standardization and a codified use of chemical referencing in these experiments has remained elusive. Here, we describe a novel methodology to measure the pressure dependent chemical shift of a common reference material used in protein NMR, sodium trimethylsilylpropanesulfonate (DSS) in D2O over a range of 1 – 13,000 psi (0-89.63 MPa) at three distinct experimental temperatures: 10, 25, and 80 °C. Much of our methodology extends upon the foundational work of Hoffman et al., who pointed out the dearth of information available to make pressure-dependent corrections. By measuring the chemical shift of the DSS in D2O standard reference material in relation to a sealed glass capillary containing the identical solution, we isolate the effect of pressure and lay a foundation for variable pressure experiments that require high accuracy, low uncertainty chemical shift reporting.

Speaker

Samantha Miller

Post Doctoral Researcher | National Institute of Standards and Technology

NISTCHO & cNISTmAb: open access biopharmaceutical reference materials

3:35 PM – 4:05 PM

The NIST Biopharmaceutical Reference Material program was established as part of the NIST Biomanufacturing Initiative to support pre-competitive engagement across academic, government and commercial biopharmaceutical organizations and stakeholders and spur innovation in the biomanufacturing industry. NISTmAb Reference Material 8671, the first monoclonal antibody reference material has served as an industry wide-test metric to evaluate performance of emerging technologies and foster collaboration since its release in 2016. Building upon the NISTmAb body of knowledge, several new materials are currently under development to expand available standards through this program, including NISTCHO, a first of its kind, open access living reference material, CHO-K1 producer of non-originator NISTmAb and cNISTmAb, the non-originator product expressed by NISTCHO. These cells present a unique opportunity for the development of both traditional and novel process analytical technologies suitable for next-generation biomanufacturing. In particular, NMR provides detailed quantitative measurements of media components and metabolites in intact samples, and can continuously monitor of metabolic processes and inform digital twins. We present initial results using low field (LF) NMR to monitor bioreactor growth of NISTCHO cultures toward (1) validating LF-NMR as a process analytical technology and (2) providing valuable reference data for NISTCHO.

Speakers

Ioannis Karageorgos

Research Chemist | NIST

Michael Judge

NIST IBBR

A Digital Platform for Automated Analysis of 1H NMR Data: Prototype Framework of Digital Reference Standard

4:05 PM – 4:35 PM

This study introduces an innovative approach to automatically analyzing 1H nuclear magnetic resonance (NMR) data, integrating a quantum mechanical spectral analysis (QMSA) to enhance efficiency over manual data analysis in NMR. This proposed digital platform features a standardized quantitative NMR (qNMR) procedure, digital Reference Spectra within a spectral library, and a visualized interactive interface for streamlined, automated NMR data analysis. This digital platform significantly reduces the need for manual intervention and shows promise in using spectral fitting to compare the calculated spectrum derived from a digital Reference Spectrum with an experimental spectrum. The digital platform excels in processing data of both single chemical and mixture, delivering accurate results, and positioning it as an essential tool for automatic 1H qNMR analyses. Case studies highlight the digital platform's effectiveness, demonstrating its wide-ranging applicability. This shows that the proposed digital platform, based on a qNMR-based QMSA approach, offers reliable qualitative and quantitative analyses and paves the way for integrating digital reference standards into future compendial tests.

Speaker

Sunil Paudel

qNMR Scientist | U.S. Pharmacopeia (USP)

Coffee Break

4:35 PM – 4:45 PM

Benchtop NMR: From Superconducting to Super Convenient

4:45 PM – 6:20 PM

Session Moderators, Gennady Khirich and Matt Augustine.

The past decade has seen a rapid rise in the adaptation of benchtop NMR spectroscopy due to the combination of analytical power, versatility, affordability, and the conveniencethat it offers. It is no wonder why it has found diverse applications across government, academia, and industry, and spans fields as varied as food science, manufacturing, pharmaceuticals, and quality control. Just as the scope of applicability of benchtop NMR continues to grow, so does the need to develop cutting edge methods to truly unleash the power of these analytical workhorses. This session highlights recent practical application of benchtop NMR in the pharmaceutical industry within the biologics and vaccines manufacturing spaces, as well as the development and implementation of pure-shift methods for simplifying complex spectra.

Speakers

Ken Skidmore

Senior Principal Scientist | Genentech

Joris Mandral

PhD student | Nantes Université

Jessica Roth

Senior Scientist | Merck

Benchtop NMR for formulation component testing of protein-based therapeutics

4:50 PM – 5:20 PM

Measuring the concentrations of formulation components is a critical process control and QC requirement for the production of protein-based therapeutics. Evolving regulatory requirements, extended shelf lives, and the need to reduce costs via multi-attribute methods have led to an increased interest in leveraging benchtop NMR for these purposes.

Here, we show an approach using a benchtop NMR system that enables fast, accurate, and precise multi-attribute monitoring of formulation components, even in the presence of relatively large concentrations of protein. Intended for deployment to QC labs or routine users, a simple pre-calibrated benchtop NMR assay provides results equivalent to several resource-intensive process control and release assays, and is capable of testing a single sample of drug product for buffer, sugar, surfactant, and antioxidant concentrations. In certain formulations, pH may also be determined.

As an example, we show results from an 80 MHz benchtop system, using a CPMG-based method to suppress 65 mg/mL protein drug resonances and measure the concentrations of histidine, sucrose, methionine, and polysorbate 80 in the formulation. At typical formulation concentrations (240 mM sucrose, 20 mM histidine, 10 mM methionine, and 0.5 mg/mL polysorbate 80), accuracy is within a relative +/- 5% for the component with the lowest signal-to-noise ratio (polysorbate 80), and better for the buffering species, sugar, and antioxidants. This assay performance is well within the specifications needed for process control and product release. Total measurement time per sample is relatively short, typically varying from 10 to 30 minutes, depending on the particular formulation composition.

To reduce complexity and enable transferability a one-time calibration to a sealed tube of 2 mg/mL dimethyl sulfone is used for quantitation, allowing for accurate measurements of these components without the need to prepare direct standards during each assay session. Thus, rather than a direct proton-to-proton quantitative strategy, we find that for benchtop systems a pre-calibration of the "response factor" of each component relative to the DMS is the preferable and most efficient approach for assessing the formulation components in protein-based therapeutics, and compensates for the use of a CPMG filter and the relatively poor peak separation compared to high-field NMR.

Methods used to process the data also play a key role in the performance of these tests. Given the well-defined analytes targeted, a variety of processing approaches are possible. A comparison of manual processing (baseline correction, phasing and integration), automated processing, and peak fitting algorithms will be shown, and the merits of each discussed.

Speaker

Ken Skidmore

Senior Principal Scientist | Genentech

Pure shift NMR methods for the analysis of complex biological mixtures with a benchtop NMR spectrometer

5:20 PM – 5:50 PM

The analysis of complex mixtures can be a challenge for the analytical chemist, as they may contain a wide variety of molecules of different nature, size and concentration. Liquid-state nuclear magnetic resonance (NMR) spectroscopy is a powerful analytical tool capable of providing a lot of information even in such complex mixtures.

In the 2010s, cryogen-free, maintenance-free and less expensive benchtop NMR spectrometers have appeared, but their capabilities remain limited by the weaker magnetic fields of permanent magnets, reducing their sensitivity and ability to separate overlapped resonances. Over the past decade, manufacturers have sought to minimize these drawbacks by building more powerful instruments, and the magnetic fields of benchtop NMR spectrometers have rapidly increased (from 43 to over 80 MHz). As a result, benchtop NMR spectrometers have become increasingly attractive for the analysis of complex mixtures, and the prospects for new applications offered by their growing capabilities motivate the need to develop methods for complex mixture analysis on compact NMR systems.

The advent of gradient coils on benchtop NMR spectrometers has led to a number of pulse sequence developments. We have recently implemented solvent-suppressed pure shift (PS) NMR strategies on an 80 MHz benchtop NMR spectrometer. PS NMR consists in eliminating the signal multiplicity induced by the homonuclear J-couplings observed in 1D 1H NMR, thereby simplifying the spectral information. We evaluated several PS methods (derived from PSYCHE, Zangger-Sterk and J-resolved pulse sequences) combined with a solvent suppression scheme on a model mixture of metabolites in pure water. We compared their performance considering important analytical criteria for the analysis of complex biological mixtures: sensitivity, resolution, spectral purity and repeatability.

Thanks to pulse sequence optimization improved by processing strategies, we managed to achieve optimum results, and significantly increase the sensitivity of some existing PS strategies. Among the PS techniques we explored, 1D projections of 2D J-resolved double-echo spectra (J-RES DE) gave the most promising results, with the highest sensitivity (27% of WET 1D 1H sensitivity), repeatability (CV = 4%) and spectral purity (no baseline distortions and almost no strong coupling artefacts). The multiplicity suppression provided by J-RES DE PS spectra enables significant spectral simplification compared to WET 1D 1H spectra by considerably reducing the amount of overlap. In addition, this spectral simplification is enhanced by the excellent resolution of the method, which yields singlets with an average linewidth of just 4.1 Hz at 10% of maximum intensity.

We illustrated its better signal recognition capabilities by easily annotating a J-RES DE projection of a challenging complex sample for benchtop NMR spectrometers: a fish feed of commercial formulation. We believe that this J-RES DE strategy could open up prospects for metabolomic / lipidomic profiling on compact NMR spectrometers. Future work will aim to establish whether an untargeted 1H NMR metabolomic analysis of complex biological mixtures can be achieved using the JRES DE strategy on an 80 MHz benchtop NMR spectrometer, and whether its greater separation power is advantageous compared 1D 1H spectroscopy.

Speaker

Joris Mandral

PhD student | Nantes Université

At-line benchtop qNMR for the real time characterization of in-situ STAB in vaccine manufacturing

5:50 PM – 6:20 PM

Benchtop qNMR rapidly quantifies a key reagent used in-situ in vaccine manufacturing. Sodium triacetoxyborohydride (STAB) is synthesized per-use from sodium borohydride, along with the corresponding species of mono-acetoxyborohydride (SMAB) and di-acetoxyborodydride (SDAB). The composition of the substituent ratios was suspected to change with hold time, hold temperature, and reaction temperature. Benchtop qNMR was applied as a new technology within the large molecule commercialization as a non-destructive, linearly responsive, and user-friendly technique implemented at-line. In less than 5 minutes, the substituent ratios are measured from a neat reaction sample. Variation in the acetoxy substituent ratios were monitored and correlated to subsequent vaccine outcomes in a proportional fashion. With this data the risk of process deviations was mitigated.

Speaker

Jessica Roth

Senior Scientist | Merck

PANIC BBQ Happy Hour

6:30 PM – 8:00 PM

Networking event with complimentary BBQ and drinks.

Thursday, May 22, 2025

Breakfast (provided by PANIC)

7:15 AM – 8:15 AM

Opening Remarks

8:15 AM – 8:20 AM

Navigating the ‘Tides with NMR in Pharma

8:20 AM – 9:55 AM

Session Chairs, Gennady Khirich and Luke Arbogast.

NMR has a long and storied history in the pharmaceutical industry owing to its unrivaled capabilities in structural elucidation, quantitative analysis, and qualitative characterization at atomic resolution. With roots in small molecule pharmaceutics, NMR is quickly expanding its scope to include all modalities of pharmaceutical interest, including peptide- and nucleic acid-based therapeutics. This session highlights recent advances in NMR for the characterization of multi-dose peptide formulations, for monitoring real-time kinetics of peptide in solution, and for structural fingerprinting and similarity analysis of oligonucleotides.

Speakers

Dan Xie

Advisor, R&D | Eli Lilly and Company

Akanksha Manghrani

Postdoctoral research associate | IBBR

Qi Gao

Associate Principal Scientist | Merck

Applications of NMR for the Development of Multi-dose Drug Products: A Case Study

8:25 AM – 8:55 AM

Developing multi-dose drug products is a valuable strategy in pharmaceutical development as it offers benefits in terms of drug product supply, patient convenience and environmental sustainability. From a regulatory standpoint, transitioning from a single dose to a multi-dose formulation requires thorough scientific evaluation to ensure that the change does not adversely affect the drug's quality, safety, or efficacy. This involves rigorous testing and validation to demonstrate that the new formulation maintains the same standards as the original single-dose product. We present a case studies that explores the development of a multiple-dose peptide formulation containing preservatives, transitioning from a prior single-dose formulation. We utilized 1D and 2D NMR approaches to understand interactions between preservatives and the peptide drug substance and assess the impact of new excipients on critical quality attributes of the system, including effects on the product's quality and potency. Results from the study illustrate the utility of applying NMR in the development of preserved multi-dose peptide presentations.

Speaker

Dan Xie

Advisor, R&D | Eli Lilly and Company

Development of NMR-based tools for structural fingerprinting of oligonucleotide therapeutics

8:55 AM – 9:25 AM

Oligonucleotide therapeutics represent an emerging class of therapeutics that utilize short sequences to target disease-associated mRNA and non-coding RNAs, triggering their degradation. Their facile sequence design and high specificity for disease targets highlight their utility as a promising therapeutic modality. However, as this class of drugs is still in its early stages, comprehensive and generalized frameworks for characterizing their biochemical properties and structure are still evolving. These therapeutics often include various chemical modifications to the backbone, sugar, and base moieties, which can impact safety, structure, and stability. Therefore, ensuring consistency in both the primary and secondary structures of these oligonucleotides across different manufactured drug lots is essential. To facilitate effective chemical and structural similarity analysis, high-resolution analytical techniques are required to detect small changes in the biochemical properties and structure of these oligonucleotides. Current methods, such as chromatography, UV and CD spectroscopies provide only coarse insights into these complex molecules, limiting our ability to assess subtle structural perturbations and perform similarity assessments. Here, we present 1D and 2D NMR techniques for structural fingerprinting and similarity assessment of RNA oligonucleotide drugs. Using multi-nuclear NMR methods, we investigate the secondary structure and develop statistical tools for analyzing biochemical properties of these drugs. Our work demonstrates NMR as a powerful tool for high resolution fingerprinting of important quality attributes of oligonucleotide therapeutics, paving the way for more robust characterization and quality assessment of this emerging class of therapeutics.

Speaker

Akanksha Manghrani

Postdoctoral research associate | IBBR

Development of flow-NMR spectroscopy for real-time monitoring and kinetics studies of novel therapeutics

9:25 AM – 9:55 AM

Nuclear magnetic resonance (NMR) has long been the method of choice for identifying solution conformation ensembles and studying kinetics for small molecules and biomolecules. Being an intrinsically quantitative analytical technique that delivers atomistic-level structural and dynamic information, NMR enables structural identification and time-course monitoring of reaction components in molar ratios. The NMR data from mixture analysis can provide comprehensive insight into mechanistic or process development understanding. Flow-NMR spectroscopy, involving continuous (continuous-flow) or periodic (stopped-flow) introduction of the sample solution into the NMR probe from an external reaction vessel through a specially designed flow cell, enables non-destructive real-time monitoring of reactions and high-resolution data acquisition via various NMR experiments. It offers the benefits of general accessibility, ease of setup, and relatively fast acquisition.

In this presentation, I will introduce the development of a flow-NMR setup and associated methods to modulate sample conditions and investigate the kinetics of different therapeutics. These experiments collectively yield comprehensive insights into reaction mechanisms without resorting to combining multiple other techniques. The relative ease of setting up and executing our flow-NMR experiments holds significant promise for extending their application to the characterization of other complex therapeutic systems.

Speaker

Qi Gao

Associate Principal Scientist | Merck

Coffee Break

9:55 AM – 10:05 AM

Awards Ceremony

10:05 AM – 10:20 AM

Small Molecules Are Still Hot (SMASH at PANIC)

10:20 AM – 12:00 PM

Session Chairs, Ken Skidmore, Amy Freund, and Mark Dixon.

SMASH NMR unites the latest advancements in NMR methodology with their applications in both academic and industrial settings, focusing on small molecules and hybrid modalities. Key areas of interest include the use of the natural products magnetic resonance database (NP-MRD), NMR studies of catalytic hydrosilylation using multinuclear NMR, and the analysis of molecular configurations through J-coupling constants exhibiting non-Karplus behavior.

Speakers

Magdalena Grochowska-Tatarczak

Centre of New Technologies, University of Warsaw

John Cort

Senior Research Scientist | Pacific Northwest National Laboratory

Roberto Gil

Professor | Carnegie Mellon University

The Natural Products Magnetic Resonance Database (NP-MRD) and the importance of spectroscopic databases and repositories

10:25 AM – 10:55 AM

The Natural Products Magnetic Resonance Database (NP-MRD, np-mrd.org) is a database and repository for NMR data of natural products and specialized metabolites. NP-MRD contains experimental and predicted data, structures, search tools, a chemical shift prediction tool, synonyms, links to other databases, and more for some 400,000 natural products. NP-MRD is also a repository for raw NMR data (FIDs) collected in support of structure elucidation or mixture analysis; anyone can deposit such data through a simple deposition interface. Raw data deposition is increasingly required by journals and funding agencies. NP-MRD is open and FAIR-compliant, a community-focused database resource whose mission is to facilitate natural products research, and aspires to repose NMR data for all natural products, from crude mixtures to reference-quality standard samples.

During the five years since NP-MRD began in 2020, as its size and user base has grown, we have gained insights into the critical value that spectroscopic database resources hold for the natural products research community. For example NP-MRD facilitates dereplication and mixture analysis, and enables validation of structure determination and correction of misassignments. Databases can enable unexpected new research: recent success in artificial intelligence and machine learning for chemical shift prediction attest to this. Furthermore, we can speculate that similar NMR databases for other classes of organic compounds and biomolecules (synthetic intermediates, drugs and xenobiotics, and so on) would have similar value to their research communities. These conceivably could be linked to form a comprehensive NMR database for all organic compounds and metabolites.

We will highlight some specific points about spectroscopic databases and NMR databases in particular: how they are used, how the cost and effort required to build and maintain them is easily underestimated, and how it is easy for them to stagnate or even disappear when not supported and maintained. We argue that data deposition is essential and must be incentivized or mandated by journals and funding agencies. While published chemical shift tables in the literature have value, we suggest that archived raw data is far preferrable insofar as this becomes an enabling resource, whether to facilitate structure validation and revision, to train AI/ML models, or for some as-yet unanticipated use. Unfortunately, much of the raw NMR data collected for natural products over the decades is gone, and more becomes lost each year as researchers retire and old computer systems are shut down. The importance of spectroscopic databases is such that research communities and funding agencies should view them as critical pieces of infrastructure and support and sustain them.

Speaker

John Cort

Senior Research Scientist | Pacific Northwest National Laboratory

Little cation and big consequences. On NMR studies of hydrosilylations

10:55 AM – 11:25 AM

Hydrosilylation is one of the most fundamental reactions in silicone chemistry, that leads to the formation of functional siloxanes and silanes, widely used in today's industry. Hydrosilylations that are performed at an industrial scale often proceed with an addition of a platinum-based catalyst, such as Speier's or Karstedt's catalyst, owing to their high performance and versatility. The process is usually anti-Markovnikov and follows the so-called Chalk-Harrods mechanism, in which the silane molecule is activated by the oxidative addition of a Si-H bond to the metal center. However, it is not free from side reactions, that result in unwanted side products, and often requires a cocatalyst for greater regioselectivity. What is more, high prices and low abundance of platinum urge to seek a new class of catalysts, that would lower the cost of production, while maintaining the high yields.

In my research, I present a novel approach to hydrosilylations, that are performed with the use of Lewis acid. The pseudobinary calcium salt of tertbutoxyperfluorobuthyl anion {Al[OC(CF3)3]4}−, further denoted as PF, forms a highly acidic Ca(C6H4F2)6 2+ complex, that is able to catalyze hydrosilylations with sterically demanding substrates effectively. The superior activity of Ca2+ is attributed to the presence of weakly solvating solvent – here 1,2-difluorobenzene - and the PF anion, which thanks to its perfluorinated surface lacks relevant coordination centers, thus being very loosely bound with its counterion.

Nuclear Magnetic Resonance has proven to be an indispensable tool in exploring the catalytic performance of CaPF2. The air- and water-sensitive nature of a catalyst, which requires preparation in the glovebox and on the Schlenk line significantly hampers studying those reactions by other widely used techniques. On the other hand, the relative tightness of an NMR tube and the non-invasive nature of experiments has made NMR our method of choice. In order to fully examine product structures we have designed a set of 1- and 2-dimensional experiments performed for every reaction. 1-dimensional 29Si and 13C measurements were performed in a quantitative manner (and with sufficiently long d1), that allowed for precise yield determination. Real-time 1H monitoring, carried out in a quasi-rapid-injection way allowed us to observe the significant shift of a double bond signal. Such a shift was in alignment with DFT calculations, that favored a mechanism where a Ca-C=C complex is being formed before the silane binding. All this shows the power of quantitative NMR that when coupled with theoretical calculations allows for precise examination of an emerging new class of catalysts.

Speaker

Magdalena Grochowska-Tatarczak

Centre of New Technologies, University of Warsaw

Discriminating Configuration in Small Molecules Using J-Coupling Constants with Non-Karplus Behavior

11:25 AM – 11:55 AM

J-coupling constants are a cornerstone of NMR-based structural elucidation in small molecules. While the relationship between three-bond couplings and dihedral angles—captured by the Karplus equation—is well established, less attention has been given to coupling constants that do not follow this classical angular dependence. In this presentation, I will focus on the use of such non-Karplus-type J-couplings for the discrimination of configuration in small organic molecules, a critical but often underexplored aspect of structure determination.
Specifically, I will present recent work on two- and three-bond proton-carbon couplings (^{2}JCH and ^{3}JCH) and one-bond carbon-carbon couplings (^{1}JCC). These couplings, while traditionally considered less informative for stereochemical assignments, can in fact provide powerful configuration-sensitive parameters when analyzed properly. I will illustrate how these constants vary depending on molecular configuration, and how their behavior cannot be represented by semi-empirical equations like the dihedral-angle dependence seen in conventional Karplus-type couplings. The key to predicting these J-coupling constants lies in the use of density functional theory (DFT) calculations.

In addition to our own findings, I will highlight complementary studies from other research groups that have also explored the configurational sensitivity of these couplings. Although this area remains relatively limited in scope, the emerging evidence suggests that non-Karplus J-couplings represent a valuable (and often underutilized) tool in the NMR toolbox for small-molecule structural analysis.
This talk will emphasize practical examples, interpretive strategies, and the broader implications for the design of NMR experiments aimed at unambiguous configuration assignments.

Speaker

Roberto Gil

Professor | Carnegie Mellon University

Lunch (provided by PANIC)

12:00 PM – 1:00 PM

The Biopharma Frontier – Exploring strange new molecules and seeking out new applications

1:00 PM – 2:35 PM

Session Chairs, Subrata Mishra and Luke Arbogast.

In the last decade, the application of NMR to biopharmaceutical development has moved beyond a promising emerging technology to an established an essential tool for large molecule characterization. As biotherapeutic portfolios grow in complexity, moving beyond simple protein/monoclonal antibody modalities, and regulatory expectations for characterization of these molecules increase, the essential utility of NMR has become more apparent. This session will highlight us of NMR as integrated tool for biophysical characterization in drug development, new applications of solid-state NMR in the biopharmaceutical context, and characterization of novel lipid nanoparticle platforms

Speakers

Mats Wikstrom

Associate Director | Amgen, Inc

Eric Munson

Professor and Head | Purdue University

Yongchao Su

Senior Principal Scientist | Merck & Co, Inc.

Deploying NMR for the product characterization of protein therapeutics

1:05 PM – 1:35 PM

Nuclear Magnetic Resonance (NMR) spectroscopy has proven to be an indispensable tool in the structural and functional analysis of proteins. When compared to traditional biophysical methods, NMR offers unique advantages, especially in studying proteins in their native, dynamic state, providing superior sensitivity and information richness. In this presentation, we will provide examples of the NMR methods currently employed, and comparisons between NMR and traditional biophysical methods for the characterization of protein therapeutics. Deploying NMR strategically in the regulatory process not only enhances the robustness of the drug characterization but also ensures compliance with rigorous regulatory standards. As the biopharmaceutical industry continues to evolve, the integration of NMR in drug development and regulatory filings will undoubtedly play a critical role in bringing innovative protein-based therapies to market.

Speaker

Mats Wikstrom

Associate Director | Amgen, Inc

Applications of solid-state NMR spectroscopy to pharmaceuticals

1:35 PM – 2:05 PM

Solid-state NMR spectroscopy (SSNMR) is uniquely suited to provide insights into a variety of pharmaceutical problems that cannot be addressed using other analytical techniques. Specifically, both structural and mobility information can be obtained about pharmaceutical formulations, but the challenge is to relate that information to functional properties such as physical and chemical stability. Three very different applications will be highlighted where SSNMR provides unique information about the systems. In the first application, SSNMR has been used to predict the formation of nitrosamines in pharmaceutical formulations, as 1H T1 relaxation times are related to the presence of crystal defects, which are correlated to likelihood of nitrosamine formation. The formation of nitrosamines in pharmaceuticals are of critical importance to the pharmaceutical industry, as the allowed daily intake can be sub ppm, with nitrosamines being formed when the drug product is placed on stability. In the second application, the relative concentration of monomer vs. dimers in drugs loaded into an amorphous solid dispersion (ASD) provides unique insight into the dynamics of molecules diluted into polymeric matrices. Specifically, the monomer/dimer ratio changes with temperature and time can be used to investigate structural relaxation and properties of polymeric materials as much as 70 oC below the glass transition temperature (Tg) of the ASD. This information is critical to being able to model the ability of drugs to crystallize in polymeric matrices such as those found ASDs. In the third application, SSNMR can provide unique information about whether mRNA remains encapsulated in an LNP upon lyophilization, which is critical knowledge to the development of stable mRNA LNP formulations in the solid state. Specifically, the interaction of the mRNA with the lipids is very different when it is inside vs. outside the LNP, which can be observed in the NMR lipid signal.

Speaker

Eric Munson

Professor and Head | Purdue University

Structural and dynamic insights into lipid nanoparticles through solution and solid-state NMR

2:05 PM – 2:35 PM

Lipid nanoparticles (LNPs) have emerged as a leading drug delivery system for oligonucleotide vaccines and therapeutics. Despite significant advancements in research and clinical applications, their molecular-level assembly remains poorly understood. LNPs typically consist of a dense core structure, composed of lipids and oligonucleotide cargo, surrounded by a surface enriched with poly(ethylene glycol) chains that interact with the bulk aqueous environment. This complex architecture exhibits a wide range of molecular motion, enabling the study of its pharmaceutical and physicochemical properties through polarization transfer techniques based on scalar and dipolar couplings. In our studies, we combined solution and solid-state NMR to elucidate the local structures and interactions of LNP components across multiple motional regimes. Specifically, 1H, 13C, and 31P solid-state NMR under static and magic angle spinning conditions provided key insights into the internal structure and dynamics of the LNP core. Meanwhile, 1H-based correlation and diffusion NMR techniques offered valuable information on molecular populations within the interfacial domain between the core and bulk solution. We examined real-world siRNA-encapsulated LNP formulations with variations in composition, manufacturing processes, and storage conditions down to -50°C. These studies revealed critical molecular details that improve our understanding of lipid-based drug delivery systems and the influence of particle engineering on stability and performance. Our work emphasizes the complementary strengths of solution and solid-state NMR in probing the intricate structure and dynamics of complex drug products, demonstrating the value of structural biophysical approaches in addressing pharmaceutical challenges.

Speaker

Yongchao Su

Senior Principal Scientist | Merck & Co, Inc.

Coffee Break

2:35 PM – 2:45 PM

Relax, Slice, and Monitor

2:45 PM – 4:20 PM

Session Moderators, Klas Meyer and Gennady Khirich.

In the face of current and future challenges within the process industry, a comprehensive understanding of underlying (chemical) processes has never been more relevant. Process Analytical Technology (PAT) is not limited to the production floor, but happens a lot in the laboratory for acquiring process knowledge, which is invaluable for optimization and enhancing sustainability.

This session explores the diversity of PAT applications of NMR spectroscopy from various perspectives. It begins with Relaxometry of moving samples, progresses to slice-selective NMR for evaluating complex biphasic systems, and concludes with applications in pharmaceutical development utilizing rather uncommon nuclei selection.

Speakers

Junhe Ma

Associate Scientific Director | Bristol Myers Squibb

Hans Gaensbauer

PhD Student | Massachusetts Institute of Technology

Yael Ben-Tal

Postdoctoral Research Associate | University of British Columbia

Flow-agnostic inline process monitoring with magnetic resonance relaxometry

2:50 PM – 3:20 PM

NMR relaxometry and spectroscopy find many uses in industrial process monitoring, especially in the fields of food production and biomanufacturing where noninvasive contaminant detection and product quality analysis are critical. In practice, it can be challenging to retrofit NMR monitoring into existing industrial processes because many NMR experiments do not tolerate movement of the sample. As a result, it is often necessary to add pumps or valves that stop the flow of the sample during an experiment, which is often expensive or incompatible with existing processes that are sensitive to the flow behavior of the product. In this work, we present a novel extended solenoidal coil geometry that suppresses the effect of sample movement on relaxometry measurements. We show that measurements taken with this coil geometry on a range of sample flow rates match those taken with a conventional coil on a static sample and demonstrate our ability to retrofit our system to existing processes without additional pumps or sequencing by monitoring the cell density of a bioreactor.

Speaker

Hans Gaensbauer

PhD Student | Massachusetts Institute of Technology

Industrially-relevant applications of slice-selective NMR

3:20 PM – 3:50 PM

Liquid-liquid biphasic systems are ubiquitous in chemistry. Many different types of reaction, from cross-couplings to cyclisations and beyond, utilise biphasic conditions. Furthermore, the tendency of compounds to preferentially partition in one phase over the other forms the key operating principle of liquid-liquid extraction, one of the most common techniques for workup and product purification.

Despite their prevalence, however, biphasic systems remain challenging to monitor with process analytical technology (PAT). Nuclear Magnetic Resonance (NMR) spectroscopy is a particularly appealing form of PAT, ubiquitous across almost all disciplines of chemistry as a non-invasive analytical technique capable of providing detailed structural information. Additionally, simple pulse-acquire experiments allow for reaction monitoring on relatively short time-scales. However, biphasic systems are uniquely challenging to monitor by conventional NMR methodology, and this field has thus remained underexplored.

In this work we utilise z-slice selective NMR to overcome several of the challenges intrinsic to monitoring biphasic systems by NMR; including the difficulty in distinguishing between phases and magnetic field inhomogeneity. Slice selective NMR has long been a well-established technique, yet its application remains limited, especially outside the NMR community. Notably, there has been minimal adoption within the broader field of organic chemistry. In this work, we explore several straightforward applications of slice-selective NMR in industrially-relevant contexts, demonstrating its utility in the rapid optimization of liquid-liquid extraction processes and in reaction monitoring.

Speaker

Yael Ben-Tal

Postdoctoral Research Associate | University of British Columbia

The role of NMR in modern process analytical technologies: innovations and applications

3:50 PM – 4:20 PM

Nuclear Magnetic Resonance (NMR) has emerged as a pivotal tool in modern process analytical technology (PAT) for examining starting materials, transient intermediates, and reaction mixtures in pharmaceutical production. Its distinctive capability to provide kinetic information through NMR-active nuclei facilitates a deep understanding of reaction dynamics. While benchtop NMR systems are increasingly favored as mobile PAT tools, traditional high-field NMR remains indispensable in scenarios requiring the analysis of starting materials or offline analysis of samples collected during production. This is due to its superior sensitivity and versatility. In particular, high-field NMR plays a crucial role in quantification, delivering universally quantitative response for all detectable solution-phase species without the need for individual calibration curves for each component. This presentation will showcase recent advancements in solution NMR and its transformative applications in pharmaceutical development, by leveraging not only commonly utilized nuclei such as 1H and 13C nuclei but also the less commonly employed nuclei such as 19F, 31P, 35Cl or 2H.

Speaker

Junhe Ma

Associate Scientific Director | Bristol Myers Squibb

Closing Remarks

4:20 PM – 4:30 PM