Odd-numbered posters present Mon and Wed; Even-numbered posters present Tues & Thurs.
*Missing poster numbers represent late withdrawals.*

**POSTER TOPICS-OVERVIEW**

**Biomolecular Solids NMR** (Posters 001 – 032)

**Biomolecular Solution NMR** (Posters 033 – 113)

**Eclectica in Magnetic Resonance** (Posters 114 – 121)

**Hyperpolarization Methodologies** (Posters 122 – 168)

**Instrumentation** (Posters 169 – 193)

**Metabolomics** (Posters 194 – 209)

**MRI MRS** (Posters 210 – 226)

**Organic Inorganic and Hybrid Materials** (Posters 227 – 253)

**Small Molecules Natural Products** (Posters 254 -271)

**Theory Computation and Data Processing in NMR** (Posters 272 – 302)

**Late** (Poster 303)

**POSTER 001**
**Molecular Mechanisms of Survival at Low Temperatures and Drastic Dehydration for Antarctic Lichen**
Presenting Author: Aleksandra Andrzejowska

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*Aleksandra Andrzejowska (Jagiellonian University); Karol Kubat (Jagiellonian University); Kazimierz Strzaka (Jagiellonian University); Angelica Casanova-Katny (Catholic University of Temuco); Hubert Haraczyk (Jagiellonian University)*

Lichens can survive severe desiccation and extreme cold. Therefore, they are excellent models for studying resistance to these. This study attempts to determine changes in molecular behaviors of bound water in Antarctic endemic lichen, Umbilicaria antarctica, when exposed to stresses.
The dependence of low-temperature water behavior on hydration level was investigated by 1H-NMR temperature measurements for thalli at three different hydration levels. Liquid water was observed in the thalli at temperatures as low as -17˚C. These findings were confirmed by DSC scans. Moreover, we recorded photosynthetic activity even at -12˚C.
Additionally, non-cooperative immobilization of water was discovered, suggesting the presence of supercooled water. Thanks to the BPP theory the average distance between relaxing proton pairs and activation energies were determined.

**POSTER 002**
**SASSY NMR: SimultAneous Solid and Solution spectroscopY**
Presenting Author: Rajshree Ghosh Biswas

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*Rajshree Ghosh Biswas (University of Toronto); Ronald Soong (University of Toronto); Amy Jenne (University of Toronto); Monica Bastawrous (University of Toronto); Myrna Simpson (University of Toronto); Andre Simpson (University of Toronto)*

Traditional NMR spectroscopy has evolved as separate fields of research (solid or solution/gel) each with specialised probes, experiments, and sample preparation techniques. However, it is the synergism between all phases (solutions, gels, solids) that gives rise to environmental and biological reactivity. Traditional monitoring methods involve sequential experiments which miss information in the non-observed phase. Here, a simple, easy-to-use technique known as SASSY is introduced to simultaneously observe all phases using standard, solid-state equipment. SASSY uses alternating in-phase (IP) and anti-phase (AP) slices with a stepped decoupling regime to isolate all fractions, ranging from crystalline solids to gels and dissolved material, with each scan. This study introduces SASSY to monitor processes and observe complex samples such as a living freshwater shrimp.

**POSTER 003**
**13C-13C J-Coupling Measurements in the Sup35p Segment GNNQQNY Using Solid State NMR**
Presenting Author: Edward P. Saliba

Complete Author List:
*Edward Saliba (MIT); Robert G. Griffin (MIT)*

We present 13C-13C J-coupling measurements in the Sup35p segment GNNQQNY using the in-phase anti-phase (IPAP) pulse sequence developed by Cadars, et al. The doubly selective nature of IPAP allows nearly all of GNNQQNY's J-couplings to be measured in pseudo-2D experiments. The knowledge of accurate homonuclear J-couplings is necessary when fitting TEDOR buildup data, as evolution of the carbon magnetization takes place under both the dipolar couplings to the 15N spins, and the homonuclear J-couplings to other 13C spins. We use this information to fit representative TEDOR buildup curves in GNNQQNY. Furthermore, we use this information to illustrate the ability of a frequency selective J-based double quantum filter to produce high resolution 1D spectra of peptide samples.

**POSTER 004**
**Studying cell interfaces with solid-state NMR**
Presenting Author: Thomas Kress

Complete Author List:
*Thomas Kress (University of Cambridge); Astrid Berge (University of Cambridge); Marie Juramy (University of Cambridge); Melinda Duer (University of Cambridge)*

In this work, we present improved Goldman-Shen experiments to study cell interfaces between bovine vascular smooth muscle cells (VSMCs) and their surrounding 13C-enriched extra-cellular matrix. These experiments rely on relaxation filters and proton spin diffusion that can transport proton magnetisation up to 10 nm away from cell membranes which enabled us to record interface-edited CP (1D) and PDSD (2D) spectra.

**POSTER 005**
**Drug Binding and Oligomeric Structure of the SARS-CoV-2 Envelope Protein Studied by Solid-State NMR**
Presenting Author: Noah H Somberg

Complete Author List:
*Noah Somberg (MIT); Joao Medeiros-Silva (MIT); Westley W. Wu (MIT); Hyunil Jo (University of California); Jun Wang (University of Arizona); William F. DeGrado (University of California); Mei Hong (MIT)*

As of January 2023, COVID-19 has caused over six million deaths worldwide. SARS-CoV-2, the causative virus of the global pandemic, has four structural proteins. Among these, the envelope protein E is responsible for the acute respiratory symptoms of the disease. E is therefore a potential antiviral drug target. Structural information about E remains scarce, and no approved drugs targeting E currently exist. Using the 19F CODEX technique, we determine that E forms a homopentamer, and under certain conditions these pentamers cluster in the membrane. The drug binding of the channel blocker hexamethelene amiloride (HMA) is probed using 19F spin diffusion, 1H{19F} and 13C{19F} REDOR experiments, which together reveal complex dynamics of HMA in the lipid membrane.

**POSTER 006**
**Solid-state NMR Exchange Spectroscopy: Characterizing Site-Specific Water Exchange in Biological Systems**
Presenting Author: Riqiang Fu

Complete Author List:
*Riqiang Fu (National High Magnetic Field Lab); Rongfu Zhang (Florida State University); Timothy A. Cross (National High Magnetic Field Lab); Shenlin Wang (Peking University)*

Understanding water dynamics and structure is an important topic in biological systems, as many essential biological processes take place with the aid of water. In this presentation, we extend our previously reported one-dimensional (1D) method for water-protein 1H chemical exchange measurements via indirect detection into a two-dimensional (2D) scheme, allowing for the probing of site-specific water exchangeable sites in the biological systems. Since those sites that are not in exchange with water are largely suppressed in the resulting 2D spectra, the characterization of the site-specific water exchange dynamics becomes possible in such much simplified spectra. Here we demonstrate the feasibility of using this method for studying water exchange dynamics in biological systems (e.g., dynamics of RNA base pairs).

**POSTER 007**
**Elucidating the hydration effect on structure and dynamics of hyaluronic acid in extracellular matrix hydrogels studied by solid state NMR**
Presenting Author: Pushpa

Complete Author List:
*Pushpa Rampratap (University of Groningen); Alessia Lasorsa (University of Groningen); Marthe Walvoort (University of Groningen); Patrick Van der Wel (University of Groningen)*

Hyaluronic acid (HA) is a highly abundant natural polysaccharide and a fundamental component of the extracellular matrix (ECM). The macromolecular size of the HA polymer regulates tissues macro- and micro-environments, and its up-regulation is a hallmark feature of certain tumors. Probing the molecular structure and dynamics of high molecular weight (HMW) polysaccharides in a physiological-like environment is crucial but also technically challenging. Thus, isotopically enriched HMWHA was produced enabling systematic investigations by multidimensional ssNMR spectroscopy. We identify different conformations and dynamics in HA polymer, as a function of hydration level and site-specific changes when HA is interacting with ECM. The developed methods apply similarly to further studies of HA-based hydrogels and biomaterials, in wide use in pharmaceutical and cosmetic industries.

**POSTER 008**
**Chirp Mixing Schemes for Broadband Homonuclear Correlations**
Presenting Author: Sungsool Wi

Complete Author List:
*Neeraj Sinha (Centre of Biomedical Research, SGPGIMS Campus); Tuo Wang (Michigan State University); Frederic Mentink-Vigier (National High Magnetic Field Laboratory, Florida State University); Sungsool Wi (National High Magnetic Field Laboratory/FSU); Lucio Frydman (Weizmann Institute of Science)*

A chirp pulse mixing scheme, Adiabatic Linearly FREquency Swept reCOupling (AL FRESCO) method, was employed to establish two-dimensional (2D) homonuclear dipolar 13C-13C, 15N-15N, and 1H-1H correlations. This scheme uses a remarkably low rf power even under a ultrafast magic-angle spinning (MAS) rate by employing a single or a series of weak frequency-chirped pluses on the nuclei that constitute heteronuclear dipolar couplings with those homonuclear dipolar pairs under consideration for recoupling. Key considerations required for optimizing these mixing schemes are discussed and experimental results were demonstrated on uniformly 13C,15N-labeled protein samples. Also discussed were 2D homonuclear 13C-13C correlations demonstrated on natural abundant 13C samples by incorporating a double-quantum filter while utilizing the signal enhancement effect from the dynamic nuclear polarization (DNP).

**POSTER 009**
**Simultaneous Recoupling of Chemical Shift Tensors of Two Nuclei by R-Symmetry Sequences**
Presenting Author: Gal Porat-Dahlerbruch

Complete Author List:
*Gal Porat-Dahlerbruch (University of Delaware); Tatyana Polenova (University of Delaware)*

Chemical shift tensors (CSTs) are sensitive probes of structure and dynamics. R-symmetry pulse sequences (RNCSA) can efficiently recouple CSTs in MAS NMR experiments, for a broad range of conditions and MAS frequencies. We introduce dual-channel R-symmetry (DORNE-CSA) pulse sequences for simultaneously recording CSTs of two different nuclei, in a single experiment. We demonstrate DORNE-CSA performance for simultaneous measurement of 13C and 15N CSTs, on a U-13C,15N-labeled microcrystalline L-histidine. We show that the DORNE-CSA method is robust, provides accurate CST parameters, and takes only half of the measurement time compared to a pair of RNCSA experiments otherwise required for recording the CSTs of individual nuclei. DORNE-CSA approach is broadly applicable to a wide range of biological and inorganic systems.

**POSTER 010**
**Characterization of TDP43 C-terminal Disease-Associated Aggregates with MAS Solid-state NMR**
Presenting Author: Blake Fonda

Complete Author List:
*Blake Fonda (UC Davis); Dylan T. Murray (UC Davis)*

TDP43 is a human transcription factor protein whose pathological aggregation is associated with neurodegenerative disorders, including ALS. Previous characterization by other researchers on ex-vivo ALS-patient derived fibrils with cryo-electron microscopy yielded a characterization of the fibril rigid core region. To better understand TDP43 fibril structural variants as well as the behavior of the rest of the pathologically associated TDP43 C-terminal domain, in-vitro formed C-terminal fibrils are generated and studied with ssNMR. CP and INEPT based MAS ssNMR allows for a structural comparison versus the previously identified ex-vivo ALS TDP43 fibrils. A major goal of this work is to better understand TDP43 structural variant selection as a result of formation conditions such as phoshomimetic substitution.

**POSTER 011**
**Withdrawn**

**POSTER 012**
**Monitoring Lignification in Model Plant Arabidopsis thaliana by Solid-State NMR**
Presenting Author: Wancheng Zhao

Complete Author List:
*Wancheng Zhao (Michigan State University); Fabien Deligey (Michigan State University); Sarah A. Pfaff (Pennsylvania State University); Daniel J. Cosgrove (Pennsylvania State University); Tuo Wang (Michigan State University)*

Plant cell walls formed by complex carbohydrates and lignin constitute the majority of lignocellulosic biomass and serve as an inexhaustible resource of biomaterials and biofuel. Lignin is a polyphenolic biopolymer deposited during secondary cell wall formation, which provides strength, assists water transporting, and resists microbial attacks. The mechanism of lignification is only partly understood. Here, we employ solid-state NMR to monitor the lignification process in the model plant Arabidopsis thaliana. Our results showed that lignin deposition is fully completed for the mature stems above 20 cm height, and the lignification process relates to the position of the stem. Molecular insight is obtained on the formation of lignin-carbohydrate interface. These findings are beneficial to the rational design of efficient biomass-conversion pathways.

**POSTER 013**
**Characterization of Kindlin-2 Binding to Phosphatidylinositol Phosphates**
Presenting Author: Andrew Nieuwkoop

Complete Author List:
*Tom Osborn Popp (Rutgers University); Ashley Bernstein (Rutgers University); Robert D. Palmere (Rutgers University); Insha Chhabra (Rutgers University); Zainab O. Mustapha (Rutgers University); Andrew Nieuwkoop (Rutgers University)*

Kindlin-2 (K2) is a peripheral membrane protein regulated in part through its binding to phosphatidylinositol phosphates (PIPs). The Nieuwkoop lab works to understand the PIP binding sites of K2 PIP binding domains and characterize the effects of PIP binding on the structure and dynamics of K2. We use solution and solid-state NMR to investigate the binding sites of the F0 and PH PIP binding domains of K2. 1H detected solid-state NMR experiments at 100+ kHz MAS pair with solution NMR titrations with IP4 and PIP liposomes and solid-state experiments on PIPs in lipid bilayers. 1H, 13C, 15N and 31P-detected experiments acquired at static, 15, and 40 kHz MAS are also used to fully characterize the K2-PIP binding event.

**POSTER 014**
**Comparing the Cell Wall of Aspergillus Species and Investigating Their Responses to Antifungals**
Presenting Author: Isha Gautam

Complete Author List:
*Isha Gautam (Michigan State University); Malitha Widanage (Louisiana State University); Frederic Mentink-Vigier (National High Magnetic Field Laboratory, Florida State University); Ping Wang (Louisiana State University); Tuo Wang (Michigan State University)*

The fungal cell wall contains polysaccharides that are absent in humans, making it a promising target for antifungal agents. Here we compare the cell wall of two opportunistic pathogens Aspergillus fumigatus and Aspergillus nidulans using solid-state NMR and Dynamic Nuclear Polarization (DNP). Both fungal species showed similar composition in the rigid portion of the cell wall but A. nidulans have a higher percentage of galactosaminogalactan in the mobile shell. When treated with the antifungal drug caspofungin, A.

fumigatus exhibited higher hydrophobicity with increased chitin content to compensate for the loss of β-glucan caused by drug inhibition. These findings will provide a foundation for discovering promising antifungal drugs.

**POSTER 015**
**Unique Structural Features of Covid-19-Associated Rhizopus Species Revealed by Solid-State NMR**
Presenting Author: Qinghui Cheng

Complete Author List:
*qinghui cheng (Chemistry department, Michigan State University); Malitha C. Dickwella Widanage (Michigan State University); Ping Wang (Microbiology, Immunology & Parasitology, Louisiana State University); Tuo Wang (Department of Chemistry, Michigan State University)*

Recently the covid-19-associated mucormycosis caused by fungi such as Rhizopus species has emerged globally as a challenge to our health system, and it leads to a severe increase in mortality rate during the pandemic. Here we employed 2D 13C-13C/15N correlation solid-state NMR to characterize the dynamics and structure of cell-wall polysaccharides in the Rhizopus delemar. Data on the dynamics, water-contact, and intermolecular contacts suggest a framework formed by rigid chitin and semi-rigid chitosan. However, the content of mobile β-1,3-glucan, the major target of almost all wall-targeting antifungal drugs, became very minor. This unique structural feature requires and assists the development of novel antifungal agents targeting other carbohydrate components in the cell wall to combat against these fungal infections.

**POSTER 016**
**Cryo-stopped flow methodology for the investigation of prenucleation species: first steps towards time-resolved solid-state NMR**
Presenting Author: Ieva Goldberga

Complete Author List:
*Ieva Goldberga (LCMCP); Tristan Geroges (LCMCP); Thierry Azas (LCMCP)*

In this work, we show the potential of the cryo-stop flow methodology to follow the formation of calcium phosphate ' prenucleation species' (PNS) at a different time in a biomineralization context. This cryo-stop flow methodology enables the addition and mixing of independent Ca2+ and phosphate solutions at controlled concentrations, volumes and rates. Then The subsequent freezing at defined time points enables to stop the precipitation reaction and analyze transient PNS by low-temperature solid-state NMR in order to follow their formation step-by-step. Here, we describe the set-up and condition optimization to study these PNS at the early stages of hydroxyapatite (Ca10(PO4)6(OH)2) formation, the main component of bones and teeth.

**POSTER 017**
**Combined Effects of Calcium and Phosphatidylserine on the Dynamics of PIP3-Containing Lipid Bilayers**
Presenting Author: Ashley D Bernstein

Complete Author List:
*Ashley Bernstein (Rutgers University); Tom Osborn Popp (Rutgers University); Andrew Nieuwkoop (Rutgers University)*

Phosphatidylinositol phosphates (PIPs) play a large role in cellular processes by binding with extreme specificity to partner proteins. Regions of the cytosolic side of the human cellular membrane have elevated levels of phosphatidylinositol triphosphate (PIP3) and phosphatidylserine (PS), both of which are anionic. MAS ssNMR was used to study calcium titrations of PIP3-containing liposomes with and without PS. The presence of calcium has a significant effect on the 31P and 1H chemical shifts, T1 and T2 of the PIP3-containing lipid bilayers. We attribute these differences in relaxation to changes in the dynamics and observe distinct results for each phosphate species present. The effect of a certain concentration of calcium on these phosphates is altered in the presence of PS.

**POSTER 018**
**19F DNP-Enhanced Fast (25-40 kHz) MAS NMR of Protein/RNA Complexes**
Presenting Author: Kumar Tekwani Movellan

Complete Author List:
*Kumar Tekwani Movellan (University of Delaware); Tatyana Polenova (University of Delaware); Angela Gronenborn (University of Pittsburgh School of Medicine); Daniel Banks (Bruker Biospin Corporation); James Kempf (Bruker Biospin Corporation); Brent Runge (University of Delaware)*

We present the first demonstration of 19F DNP combined with fast (25-40 kHz) MAS frequencies for studies of protein/RNA assemblies. We report remarkably high, up to 128-fold signal enhancements in DNP MAS NMR spectra of nucleocapsid protein (NP) assemblies with RNA fragments, both containing fluorine labels. We discuss the resolution gains and the overall benefits of high MAS frequencies. Our work establishes the power of 19F DNP-enhanced fast MAS NMR spectroscopy for structural characterization of biological assemblies.

**POSTER 019**
**DNP NMR Assisted 'In-Cell' Structural Characterization of Mitochondria localized α-Synuclein Toxic Conformers**
Presenting Author: Swapna Bera

Complete Author List:
*Swapna Bera (Postdoctoral researcher)*

The role of α-Synuclein, a major hallmark of Parkinson's disease (PD), in modulating mitochondrial function in both physiological and pathological conditions has long been a topic of intense debate. Multiple studies reported on mitochondrial dysfunction and oxidative stress by α-Syn's aggregation. Unfortunately, the dynamically interchanging heterogenous conformations of α-Syn make the in-cell structural studies very inflexible. With our novel development of a cellular systems platform for in-vivo structural biology (JACS.2021,143,44,18454–18466) I am investigating mitochondria localized α-Syn structure inside mammalian cells and reveal how cellular environments influence protein's amyloid core structure. Collectively, this structural information in live cells will directly link cellular toxicity to protein conformation and will transform our mechanistic understanding of protein misfolding and mitochondrial impairment in PD etiology.

**POSTER 020**
**Solid-state NMR with a CPMAS CryoProbe enables structural studies of human blood protein vitronectin bound to hydroxyapatite**
Presenting Author: Tata Gopinath

Complete Author List:
*Tata Gopinath (Medical College of Wisconsin)*

The low sensitivity of solid-state NMR is a major bottle neck for studying protein samples under dilute conditions, such as, membrane proteins and protein-ligand complexes. Cryogenically cooled probe technology overcomes sensitivity limitations enabling solid-state NMR applications to challenging biomolecular systems. Here we present solid-state NMR data acquired with a CP-MAS CryoProbe for the human blood protein vitronectin bound to hydroxyapatite. Vitronectin is a major blood protein that regulates many different physiological and pathological processes. The high sensitivity of the CP-MAS CryoProbe enabled us to acquire three-dimensional solid-state NMR spectra for sequential assignment of vitronectin bound to hydroxyapatite. We also demonstrate residue specific water-protein interactions that provide structural insights into water coordination in the protein complex.

**POSTER 021**
**Measuring the Fluidity of Deep Sea Hydrothermal Vent Bacterial Membranes at High Pressure with Solid State NMR**
Presenting Author: Thomas Osborn Popp

Complete Author List:
*Tom Osborn Popp (Rutgers University); Ian J. Schlegel (Rutgers University); Costantino Vetriani (Rutgers University); Andrew Nieuwkoop (Rutgers University)*

Thermopiezophiles are microorganisms that grow at high pressures and temperatures (10 - 100 MPa, 50-100 °C), and are typically isolated from deep-sea hydrothermal vents. Currently, little is known about the chemical and biophysical properties of these organisms, due to the technological challenges associated with observing them under conditions that mimic their natural habitat. Here we employ solid state NMR under both static and magic angle spinning (MAS) conditions to study thermopiezophile phospholipid membranes as a function of both pressure and temperature. Our initial results suggest that these organisms modify the lipid composition of their membranes in response to growth pressure in order to maintain a well-defined membrane fluidity.

**POSTER 022**
**Solid-State NMR Investigation of Molecular Attributes in Frozen Solution**
Presenting Author: Yong Du

Complete Author List:
*Yong Du (Merck & Co. Inc.); Yongchao Su (Merck & Co. Inc.)*

Investigating microenvironmental properties and the underlying physiochemical mechanism in frozen solutions is a critical but underexplored task. For example, the physical environment of biologics changes dramatically during freezing which may lead to severe stability issues. However, it is technically challenging to probe the local molecular properties (e.g., phase separation, pH, ionic strength, protein structure and dynamics) in an in situ, high-resolution, and quantitative manner. Our studies aim to explore these molecular attributes in frozen solutions using solid-state NMR spectroscopy.

**POSTER 023**
**Combined use of Solid-State and Solution NMR to Understand Allosteric Transitions in a Ligand-Activated Oligomeric Protein**
Presenting Author: Rodrigo Muzquiz

Complete Author List:
*Rodrigo Muzquiz (The Ohio State University); Cameron Jamshidi (The Ohio State University); Dan Conroy (The Ohio State University); Mark P. Foster (The Ohio State University)*

TRAP is an allosterically regulated protein that is activated by tryptophan (Trp) to bind RNA and terminate tryptophan biosynthesis in Bacilli. We performed solution and solid-state NMR experiments on TRAP to understand how binding of Trp to its 11 identical sites modulates its RNA binding function. We performed methyl CPMG relaxation dispersion experiments in solution on Thr/Ile methyl labeled TRAP in the absence and presence of Trp. These experiments showed strong dispersions indicative of μs-ms time scale exchange in apo-TRAP that are diminished in holo-TRAP. Complementary solid-state INEPT experiments identified residues invisible in solution and CP experiments. These experiments allow us to characterize the structural and dynamic landscape of apo-TRAP and new insights into mechanisms of its regulation by Trp.

**POSTER 024**
**Exploring binding site of MODAG-005 on $\alpha$-Synuclein aggregates as a novel PET tracer**
Presenting Author: Myeongkyu Kim

Complete Author List:
*Myeongkyu Kim (Max Planck Institute for Multidisciplinary Sciences)*

Early detection of a-synuclein (αSYN) aggregates and observing the pathological process has been a challenge. Positron emission tomography (PET) is a non-invasive in vivo imaging technique useful for early diagnosis of aggregates in the human brain. However, a target-specific tracer to detect pathological aggregates of αSYN is missing. Here, we report the development of anle170322 (PET tracer) based on anle138b, a compound shown to have therapeutic activity in animal models of neurodegenerative diseases. The structure of the fibril was determined by cryo-EM and the binding sites (internal and external) of anle170322 were identified through solid-state NMR spectroscopy and dynamic nuclear polarization (DNP). Interestingly, two binding sites are found depending on the preparation protocol.

**POSTER 025**
**CPMAS NMR Platform for Direct Compositional Analysis of Mycobacterial Cell Wall Complexes and Whole Cells**
Presenting Author: Xinyu Liu

Complete Author List:
*Xinyu Liu (Stanford University); Jasna Bri (Stanford University); Gail Cassell (PAI Life Sciences Inc); Lynette Cegelski (Stanford)*

Mycobacteria cause chronic incurable infections and are alarmingly resistant to currently available antibiotics that target cell-wall biosynthesis. Resistance is attributed to assumed differences in cell-wall composition across species, which is challenging to analyze with conventional biochemical methods. We introduce an approach to directly observe chemical composition of mycobacterial cell walls using solid-state NMR. By obtaining 13C CPMAS spectra of cell-wall components, we uncovered a higher arabinogalactan-to-peptidoglycan ratio in M. abscessus, which is noted for its antibiotic resistance, relative to a basic model strain M. smegmatis. Differentiating influences of cell-wall targeting antibiotics were observed in spectra of treated whole cells. Our platform will be valuable in evaluating cell-wall composition and antibiotic activity among different mycobacteria and guiding effective combination treatment regimens.

**POSTER 026**
**Analyzing Biopolymer Motion via Rotating Frame Relaxation in MAS NMR of Large Anisotropy 13C Sites**
Presenting Author: Eric G. Keeler

Complete Author List:
*Eric Keeler (New York Structural Biology Center); Ann E. McDermott (Columbia University)*

The study of biomolecular motions by magic angle spinning NMR rotating frame relaxation measurements has been demonstrated to yield fruitful results. Focusing on systems where modulation of the chemical shift interaction is the driving force for the mechanism of relaxation we demonstrate a strategic approach to extract motional time scales, activation energies, and the order parameters from rotating frame relaxation data. We use both model free analysis and numerical simulations, including treatment of the relaxation data in the time domain, to demonstrate the optimal conditions for obtaining precise and accurate time scales of motions. Furthermore, we extend this exercise to the model ion channel KcsA to provide an example.

**POSTER 027**
**Discovery and Characterization of Natural Modified Polysaccharides in Bacteria Biofilms Using SSNMR.**
Presenting Author: Alexandre Poulhazan

Complete Author List:
*Alexandre Poulhazan (Stanford University); Wiriya Thongsomboon (Stanford University); Lynette Cegelski (Stanford)*

Cellulose is the most abundant biopolymer on Earth and solid-state NMR was uniquely enabling in the discovery of a modified cellulose produced by E. coli– phosphoethanolamine cellulose. Together with curli amyloid fibers, these polymers form remarkable basket-like structures surrounding E. coli. In exploring the production of celluloses in E. coli strains, we discovered another polysaccharide produced in high abundance. This discovery was enabled by our use of genetic modifications to suppress the co-production of curli and enable isolation and characterization of the polysaccharide. I will present our characterization by solid-state and solution-state NMR of this potentially as-of-yet unidentified but with potential relevance in infection polysaccharide. We are expanding our discovery platform to seek out new chemistry and alternately modified polysaccharides.

**POSTER 028**
**Structural Analysis of Membrane-mediated Amyloid Aggregates of human islet amyloid polypeptide (hIAPP)**
Presenting Author: Venus Singh Mithu

Complete Author List:
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Evidence suggests that the interaction between hIAPP and phospholipid membrane is pivotal in causing β cell failure, a hallmark of Type II diabetes mellitus (T2DM) pathology. Thus, structural characterization of this interaction is essential for designing therapeutic interventions. We have investigated the structural fold of full-length recombinant hIAPP fibrils grown in the presence of small unilamellar vesicles (SUVs) composed of zwitterionic POPC and negatively charged POPS phospholipids. Sequence-specific assignment of hIAPP was achieved using 1H-detected correlation spectroscopy at 55 kHz magic-angle-spinning (MAS) and 1H-mediated 13C-13C through-space correlation spectroscopy under slow MAS conditions. Chemical shift-based dihedral angle predictions and long-range inter-residue contacts will be used in conjunction with Cryo-EM-based investigations to obtain the atomic structure of membrane-mediated fibrils.

**POSTER 029**
**New Insights into the Influence of β-lactam Antibiotics against S. aureus by Solid-State NMR Spectroscopy**
Presenting Author: Till Kallem

Complete Author List:
*Till Kallem (Stanford University)*

The mechanism of killing by cell-wall-targeting β-lactam antibiotics against the Gram-positive pathogen S. aureus remains poorly understood. This is partially due to shortcomings in conventional biochemical methods for studying the highly crosslinked S. aureus cell wall. Furthermore, β-lactams can induce an unexplained paradoxical killing trend against S. aureus such that lower doses outperform higher doses (Eagle Effect). We leveraged 13C and 15N CPMAS solid-state NMR analysis of whole cell and cell wall samples to reveal different compositional changes under low and high doses of meropenem against a methicillin susceptible strain, S. aureus 29213. Our results indicate that meropenem induces two distinct lethal pathways, depending on dosage, that correlate with differential killing kinetics and underpin the Eagle Effect in this system.

**POSTER 030**
**NMR Crystallography of Toho-1 β-Lactamase Enabled by Nearly Complete Backbone and Sidechain Assignments**
Presenting Author: Christopher Williams

Complete Author List:
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Nearly complete backbone and sidechain chemical shifts are reported for a microcrystalline sample of the 28 kDa Toho-1 β-Lactamase: using only two 2D and three 3D experiments at 900 MHz, 96% of the backbone and 80% of the nonaromatic sidechains can be assigned, including the mechanistically important active site sidechain residues. These chemical shifts allow preliminary refinement of the structure and protonation states of the active site using NMR crystallography – the integrative combination of solid-state NMR with diffraction and first principles computational chemistry.

**POSTER 031**
**Study of phosphorus clusters in tau fragment fibrils via multiple quantum solid-state NMR under DNP**
Presenting Author: Lokeswara Rao Potnuru

Complete Author List:
*Lokeswara Rao Potnuru (UCSB); Mesopotamia S. Nowotarski (UCSB); Austin Dubose (UCSB); Songi Han (UCSB)*

Multiple quantum spin counting (MQ-SC) is a technique that can identify the formation of clusters by measuring the multi-quantum coherence orders between the coupled spins. MQ-SC has been applied to various glass and solid materials at varying magic angle spinning (MAS) rates. In the present study, we show the utility of MQ-SC on the vitrified solution samples of phosphate-containing species of amorphous calcium phosphate (ACP), and crystalline hydroxyapatite (HAp) and tau fragment fibrils at 100 K under DNP conditions. 31P MQ-SC experiments were carried out by using the SR218 pulse sequence to create multiple even and odd MQCOs at 10 kHz MAS frequency to find out the cluster sizes and clustering of phosphate species.

**POSTER 032**
**Solid-state NMR analyses of Glycera worm jaws and biomimetic analogs**
Presenting Author: Arun Kumar Patel

Complete Author List:
*Arun Patel (Postdoc Researcher); Nathan A. Prisco (Postdoc Researcher); William Wonderly (Graduate Student); Herbert J. Waite (Professor); Bradley F. Chmelka (Professor)*

Glycera (bloodworm) jaws are comprised almost entirely of organic matter; though exhibit robust mechanical properties that are similar to those of inorganic solids. Glycera jaws are unique in that they are composed predominantly of melanin (40–50 wt%), which is typically a soft material and not associated with load-bearing properties. Our objective is to understand the atomic-level origins of this unusual natural material and compare its composition and structure with that of synthetic analogs. Here, we report solid-state two-dimensional (2D) 13C{1H} correlation NMR, 2D 1H{1H} single quantum-double quantum (SQ-DQ), and dynamic-nuclear-polarization (DNP)-enhanced 15N NMR analyses that enable complicated compositional similarities and differences to be established between Glycera worm jaws and polydopamine and which correlate with their respective mechanical properties.

**BIOMOLECULAR SOLUTION NMR** (Posters 033 – 113)

**POSTER 033**
**NMR Structural Studies of an Insect Cytokine: Manduca sexta Stress Responsive Peptide-3**
Presenting Author: Andy Su

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Similar to innate immunity in vertebrates, insects rely on both humoral and cellular responses to defend them from pathogen invasion. Recently, a family of peptides has been identified in many insects including mosquitoes, which may function as insect cytokines to regulate immune responses. Our previous structural studies suggest that these peptides adopt a fold similar to C-terminal sub-domain of EGF, and they may interact with EGFR-like molecules. Manduca sexta stress responsive peptide-3 (SRP3) is predicted to be a 27-residue peptide (FLIKSSGCPKGYVKRGTFCFPDEDYDY), stabilized with a disulfide bond. We have initiated structural/functional and dynamics studies on SRP-3 using homo and hetero-nuclear multi-dimensional NMR spectroscopy to obtain experimental data that will aid in the development of potential EGFR inhibitors useful in cancer treatment.

**POSTER 034**
**Structure Elucidation of an Invisible Excited State with Allosteric Relevance in a KRAS Oncogenic Mutant Using RDCs**
Presenting Author: Gabriel Cornilescu

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Localized dynamics of RAS, including regions distal to the nucleotide binding site modulates the interaction with effectors and regulators. Among several oncogenic mutants, methyl relaxation dispersion experiments revealed highly synchronized conformational dynamics in the active KRAS-G13D, indicative of exchange between two conformational states in solution. Methyl and 31P NMR spectra of active KRAS-G13D in solution also indicate a two-state ensemble, with peaks corresponding to the State 1 conformation and to an intermediate state, different from the known State 2 conformation recognized by RAS effectors. We used residual dipolar couplings to solve and cross-validate the structure of the intermediate state, which shows regions of structural fluctuations with functional relevance and potential for drug discovery.

**POSTER 035**
**Structure of Calmodulin Bound to Two Different Functional Sites in the Retinal Cyclic Nucleotide-Gated Channel Revealed by NMR Spectroscopy**
Presenting Author: Aritra Bej

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*Aritra Bej (Department of Chemistry, University of California); James B. Ames (Department of Chemistry, University of California)*

Retinal cyclic nucleotide-gated (CNG) channels (composed of three CNGA1 and one CNGB1 subunits) exhibit a Ca2+-dependent inactivation mediated by calmodulin (CaM). Defects in the Ca2+-dependent regulation of CNG channels may be linked to retinitis pigmentosa and color blindness. Here, we reported the binding analysis and NMR structures of CaM bound to two distinct cytosolic sites within rod CNGB1 called CaM1 (residues 565-587) and CaM2 (residues 1120-1147). The binding studies revealed that CaM1 prefers binding to Ca2+-bound CaM N-lobe (residues 1-79) whereas CaM2 binds to Ca2+-bound CaM C-lobe (residues 80-149) with higher affinity. We solved separate NMR structures of Ca2+-saturated CaM bound to CaM1 and CaM2, identified the key intermolecular contacts, and proposed a Ca2+-dependent conformational switch in the CNG channel.

**POSTER 036**
**NMR study on the interaction of human ZBP1 with its target Z-DNA**
Presenting Author: Youyeon Go

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*youyeon Go (Gyeongsang national university); Joon-Hwa Lee (Gyeongsang national university)*

ZBP1 functions as a central regulator of cell death and inflammatory responses. ZBP1 is capable of sensing Z-form RNAs produced during IAV infection, cumulating in a form of caspase-independent, inflammatory cell death. ZBP1 interaction with DNA, as well as viral and endogenous RNA via its N-terminal Z-DNA-binding domains of ZBP1, has been reported. The Zα1ZBP1 and Zα2ZBP1 structure are similar to other Z-DNA binding proteins, although it demonstrates an unusual Z-DNA recognition. In this study, we performed HSQC experiments on complexes of hZα1ZBP1 and hZα2ZBP1 with d(CG)3 duplex r(CG)3 duplex at various DNA-to-protein molar ratios. The results from previous studies can produce valuable insights into the distinct molecular mechanism of the DNA duplex B–Z transition induced by hZα1ZBP1 and hZα2ZBP1.

**POSTER 037**
**Structure Characterization of the Lipid Nanoparticle Surface in an mRNA Vaccine using High Field NMR Spectroscopy**
Presenting Author: Maple Wang

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Lipid nanoparticles (LNPs) have been successfully used as a carrier for messenger RNA (mRNA) vaccines. The surface properties of LNPs are important to the stability and function of mRNA vaccines. Polyethylene glycol (PEG) is a functional lipid at the surface of LNPs that improves colloidal stability, increases circulation time, and inhibits cellular uptake. We explore the lipid composition at the surface of the LNPs using high-field nuclear magnetic resonance (NMR) spectroscopy. Our results demonstrate that NMR can detect and resolve PEG chains on the surface of intact LNP and provide quantification of PEG and other lipid components. Comparative NMR analysis of different vaccine preparations and stability samples provides a global view of the mRNA-LNP surface structure for enhanced product understanding.

**POSTER 038**
**Intermediate-state-trapped Mutants Unravel a Sequential Conformational Allostery of G Protein-coupled Receptor**
Presenting Author: Libin Ye

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*Libin Ye (University of South Florida)*

Please see the attachment.

**POSTER 039**
**A 13C Direct-Detect Nuclear Magnetic Resonance Method to Investigate Lysine Acetylation**
Presenting Author: Olivia Fraser

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Lysine N-acetylation is a ubiquitous post translational modification (PTM) that affects proteins involved in a wide range of cellular processes. Despite this, the molecular mechanisms by which acetyl marks are installed, affect protein function, and are removed, are not well characterized in comparison with other PTMs. This is in part due to limitations of current methods, which can require exogenous tags or acetyllysine mimics. We demonstrate the ease and utility of a novel 13C direct-detect method to observe acetyllysine using histone H3 tail acetylation as a model. This method does not require chemical modifications that could alter the modified lysine's properties or interfere with downstream biochemical processes, making it suitable for use in systems where changes beyond acetylation are unacceptable.

**POSTER 040**
**Ranking mAb-excipient Interactions in Biologics Formulations by NMR Spectroscopy and Computational Approaches**
Presenting Author: Chunting Zhang

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Excipients are added to biopharmaceutical formulations for enhancing protein stability and developing robust formulations, but the mechanism by which they confer stability remains not fully understood. Our study aimed at using STD-NMR to provide direct experimental evidence to excipient-mAb binding affinity, and therefore ranking a series of excipients with respect to their dissociation constant and non-specific binding constants. Molecular dynamic and Monte Carlo simulations were done in parallel, to rank the excipient proximity to the proteins and thereby corroborating the ranking. Finally, the excipient ranking was correlated to mAb conformational and colloidal stability, therefore aiding with excipient selection in biologic formulations, by providing insights into mAb-excipient affinities before conducting a conventional excipient screening study which is time-consuming.

**POSTER 041**
**Calcium dissociation and functional unfolding: A discovery by NMR for a 1.1 mDa component of the C. difficile binary toxin**
Presenting Author: Spiridon Sevdalis

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Clostridium difficile infection (CDI) is challenging because treatment options are limited, and high recurrence rates occur in hypervirulent strains. The C. difficile toxin (CDT) has a toxic enzymatic component, termed CDTa, and a pore-forming or delivery subunit termed CDTb. A novel mechanism for CDT delivery is unlike that observed for any other members of the AB toxin family (i.e., anthrax). Specifically, CDTb was shown to be regulated by a Ca2+-dependent unfolding event that is consistent with CDT entry into endosomes. Thus, lowering of free Ca2+ concentration upon entry induces conformational exchange in its receptor binding domain1 (RBD1) to "trigger" protein dynamic features throughout CDTb that allows for delivery of toxic CDTa into the host cell cytoplasm.

**POSTER 042**
**New cross-polarization schemes for heteronuclear transfers involving labile protons in biomolecular NMR**
Presenting Author: Jihyun Kim

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INEPT-based experiments are widely used for $^{1}H\rightarrow^{15}N$ transfers but often fail when involving labile protons due to solvent exchanges. J-based cross-polarization (CP) offers a more efficient alternative to perform such transfers, particularly when leveraging the additional $H^{water}\leftrightarrow H^{N}$ exchange process to boost the $^{1}H\rightarrow^{15}N$ transfer. This demands spin-locking both $^{1}H^{water}$ and $^{1}H^{N}$ by a strong $^{1}H$ RF field, while fulfilling the $\gamma_H B_{1,H}=\gamma_N B_{1,N}$ Hartmann-Hahn condition. Given the low value of $\gamma_N/\gamma_H$, these demands cannot be simultaneously achieved by the power-limited cryogenic probes used in high-field contemporary NMR. Here we introduce two CP alternatives that can alleviate this limitation and demonstrate their performance on double and triple resonance transfer experiments on amino acids and intrinsically disordered proteins, that confirm theoretical expectations.

**POSTER 043**
**Watson-Crick-like Tautomeric and Anionic G•T/U Conformational States in RNA-DNA Hybrids: Context Dependence and Implications for Transcriptional Errors**
Presenting Author: Or Szekely

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G-T/U wobble mismatches in B-DNA and A-RNA can form low-abundance Watson-Crick-like conformations through tautomerization or ionization, having implications in replication and translation errors. Little is known about propensities to form WC-like conformations in RNA-DNA hybrids and their roles in transcriptional errors. Using NMR R1ρ relaxation dispersion we show that hybrid dG-rU and dT-rG wobble mismatches exist in equilibrium with low-populated short-lived tautomeric and anionic WC-like conformations. Tautomeric exchange-kinetics were very similar to those reported previously, while anionic population and forward rate-constant were uncharacteristically ten-fold higher for dG-rU versus rG-dT. Reexamination of prior measurements revealed large variations in anionic apparent pKa, with a strong preference to ionize in cytosine-rich sequence contexts. Our study indicates plausible roles for WC-like conformations in transcriptional errors and indicates that mutagenic dynamics strongly depend on nucleic acid sequence and structural contexts.

**POSTER 044**
**Quantitative analysis of sterol modulated monomer-dimer equilibrium of β1-adrenergic receptor by DEER spectroscopy**
Presenting Author: Nina Kubatova

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GCPRs play a vital role in intracellular signaling pathways and control various physiological processes in eukaryotes. The oligomerization properties of GPCRs, and hence their cellular functions, may be modulated by various components within the cell membrane. Using DEER spectroscopy, we demonstrate different effects of soluble cholesterol analog CHS and cholesterol derivative bile salt sodium cholate on the oligomerization propensities of β1-adrenergic receptor (β1AR) in DDM micelles. Global fitting of DEER echo curves for spin-labeled β1AR upon titration with sodium cholate and CHS demonstrates that saturation of micelles with the former induces receptor dimerization, while specific binding of the latter to β1AR inhibits dimerization and stabilizes the monomeric form.

**POSTER 045**
**Structural Study of the NS2B Membrane Protein from Zika Virus in SDS Micelles by Solution NMR**
Presenting Author: Beatriz Rosa Penna

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Zika virus (ZIKV) emerged as a global public health concern due to its relationship with severe neurological disorders. NS2B is a viral membrane protein responsible for regulating viral protease activity and critical for virus replication, making it an attractive antiviral drug target. This work aims to elucidate the structure and study the dynamics of the full-length ZIKV NS2B in SDS micelles through solution NMR. Despite the challenge, we propose a structure of ZIKV NS2B based on NMR experimental data, which was consistent with the molecular dynamics data and with the described in the literature. Our work will be important to improve understanding of the role of NS2B in viral replication and for prospection of inhibitors against ZIKV.

**POSTER 046**
**No nosey NOE: Analysis of 1H R1ρ relaxation dispersion in presence of dipolar coupling**
Presenting Author: Rubin Dasgupta

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1H R1ρ relaxation dispersion experiments allow the characterisation of biomacromolecules undergoing conformational exchange between a highly populated ground state (GS) and higher energy excited states (ES), which are invisible to conventional structure elucidation methods. However, cross-relaxation due to nearby protons can hamper the analysis of exchange parameters, and it can be mistaken for an additional ES. A systematic study of how the cross-relaxation contributes to 1H R1ρ in nucleic acid is presented using a DNA model system. A theoretical description is given for the effects of cross-relaxation on the 1H R1ρ experiment and its properties are discussed. This numerical model might allow reliable fitting of 1H R1ρ data in presence of cross-relaxation hence facilitating the investigation of ES in biomacromolecules.

**POSTER 047**
**Structural Dynamics Study of Thermophilic Proteins by NMR - TTHA0849 of Thermus thermophilus**
Presenting Author: Karen Stephanie dos Santos

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TTHA0849 presents a PR-10 fold that forms a hydrophobic cavity. This work aims to characterize the structural dynamics of TTHA0849 in its free and bound state and compare it with the mesophilic counterparts (Bet v 1, among others) that shares the same fold and the ability to bind hydrophobic compounds. We used intrinsic fluorescence, circular dichroism, and NMR to evaluate the structure, dynamics, and interaction with hydrophobic compounds. TTHA0849 recombinant protein was obtained and purified by chromatography, and our data showed it has high thermal stability and chemical resistance. Furthermore, we have evidence of complex formation with compounds. The backbone assignment is almost complete (93 %), and relaxation parameters (R1, R2, and hetNOE) were collected in different temperatures and are being analyzed.

**POSTER 048**
**Visualizing Proteins in Mammalian Cells by 19F NMR Spectroscopy**
Presenting Author: Wenkai Zhu

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In-cell NMR spectroscopy is a powerful tool to investigate the behavior of biologically important molecules in physiologically relevant environments. We studied proteins delivered into mammalian cells by electroporation and showed that interactions with cellular components frequently broaden resonances in 1H-15N HSQC spectra beyond detection. This contrasts findings from 19F spectroscopy, where resonances for selectively fluorinated proteins are readily observed. In addition, we show that 19F paramagnetic relaxation enhancements (19F PREs) can provide valuable distance information for structure characterization in physiological contexts. The in-cell 19F PRE-derived distances are in good agreement with in-cell 19F ENDOR measurements on the same paramagnetic proteins, thus providing an effective means to obtain accurate distances in the cellular milieu.

**POSTER 049**
**Hsp104 Chaperone Induces "Off-pathway" Oligomerization of Aβ-42 Monomers**
Presenting Author: Shreya Ghosh

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Hsp104 is a unique disaggregase chaperone found in yeast, yet has been shown to function synergistically with mammalian chaperones, without displaying any overt toxicity and in turn, conferring increased stress tolerance. Additionally, Hsp104 is also the sole known chaperone to disaggregate mature amyloid fibrils. While the ability of Hsp104 to prevent and disaggregate fibrils is common knowledge, yet the pathway, mechanism, and kinetics associated with the activity still remains unanswered. To this end, I have used a

combination of NMR along with imaging techniques of EM and AFM and showed that Hsp104 aids in the formation of "off-pathway" Aβ-42 oligomers that cannot materialize further into fibrils.

**POSTER 050**
**Drug-like Small Molecules That Inhibit Expression of the Oncogenic MicroRNA-21**
Presenting Author: Bhawna Chaubey

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The discovery of drug-like small molecules which bind specifically to the precursor of the oncogenic and pro-inflammatory microRNA-21 with mid-nanomolar affinity is reported. The small molecules target a local structure at the Dicer cleavage site and induce distinctive structural changes in the RNA which correlate with specific inhibition of miRNA processing. The most potent one reduces cellular proliferation and miR-21 levels in cancer cell lines without inhibiting kinases or classical receptors. Structurally conservative single nucleotide substitutions eliminate the conformational change induced by the small molecules, which is not observed in other miRNA precursors. These molecules are highly ligand-efficient (MW330) displaying specific biochemical and cellular activity, thereby providing an avenue towards therapeutic development in multiple diseases where miR-21 is abnormally expressed.

**POSTER 051**
**Partial Assignments of Tunicate βγ-crystallin Structure**
Presenting Author: Mina Mozafari

Complete Author List:
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Tunicate Ciona intestinalis (Ci-βγ-crystallin) is a model to study evolution of vertebrates as it has an evolutionary position between the microbial crystallins and the vertebrate lens proteins. The single-domain βγ-crystallin of the tunicate Ci-βγ-crystallin represents the single-domain ancestor of the vertebrate βγ-crystallin. It has been shown that the tunicate Ci-βγ-crystallin has a high affinity to bind to Ca2+ and that this binding greatly stabilizes the protein both thermally and chemically. However, human γS-crystallin doesn't bind to Ca2+ but it stays stable. NMR spectroscopy is used to study the structure and properties of Ci-βγ-crystallin to better understand the stability and evolutionary progression from ancestral to human lens βγ-crystallins.

**POSTER 052**
**Probing Biodegradation Mechanism and Kinetics of Stimuli-Responsive Microcapsules Utilizing 1H NMR Spectroscopy**
Presenting Author: Uyen Thi Do

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In this study, the stimuli-responsive microcapsules were fabricated using gelatin, alginate, and hyaluronic acid as wall materials; additionally, enzyme-induced decomposition mechanisms were proposed by observing spectral changes in 1H NMR analyses. The synthesized microcapsules are spherical, tunable in size, with high encapsulation efficiency, and neutral pH-induced cutaneous release of hydrophobic core from microcapsules was recorded. Examination of the short-term and long-term degradation kinetics reveals that the determination of the degradation rate constant of the major components in the capsule is feasible and suggests two types of 4-stage degradation mechanisms that are enzyme-specific. These findings suggest that capsule decomposition can be thoroughly investigated using 1H NMR spectroscopy to provide a practical strategy for monitoring degradation properties in developing new biodegradable materials.

**POSTER 053**
**An Investigation on Microbial Degradation of Biodegradable Microcapsules Using 1H-NMR for Innovative Eco-friendly Material Development**
Presenting Author: Yeeun Park

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Biodegradable microcapsule based on natural polymer is considered a replacing material of microplastics without causing environmental pollution. However, in the case of measuring biodegradability of these particles, there is disadvantage that it takes quite a long time. In this study, we discuss the investigation of pre-screening that confirms the degradation of natural polymer-based microcapsules by microorganisms using 1H-NMR. Experiments confirmed that the spectrum of a sample containing microcapsules and microbes became sharp than that of only microcapsules. Also, the new peak that didn't appear in the 1H-NMR spectrum of only microcapsules and microorganisms was also observed. Through this, the possibility of biodegradation pre-screening technology that can be executed on an NMR-based lab-scale was conformed.

**POSTER 054**
**NMR chemical shift assignments of the SCoV-2-delta element 3_s2m utilizing multidimensional NMR**
Presenting Author: Tobias Matzel

Complete Author List:
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The SCoV-2 genome consist of a 30.000 nt (+) strand RNA which not only encodes for the viral proteins but also shows highly structured 5' and 3' untranslated regions. One of these regulatory RNA elements is the stem loop II motive 3_s2m, which is highly conserved between distantly related viruses although its function is still unclear.
Utilizing a 4D-HMQC-NOESY-HMQC experiment and different 13C filtered NOESY spectra chemical shifts were assigned for over 90% of the relevant NMR resonances. The 4D was used to assign NOEs between aromatic (H6/H8) and sugar H1' protons, which enabled us to assign 98% of the C6, C8 and C1' resonances. We then assigned C2' C5' sugar resonances using selective labelling in combination with 13C-filtered NOESYs.

**POSTER 055**
**Structural and Dynamical Investigation of Small Proteins**
Presenting Author: Dennis J Pyper

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Small proteins have been ignored in the past, because detection and identification of the coding DNA posed significant problems. Modern transcriptomics technologies have made it possible to identify increasingly more sORFs. They were found in all domains of life and it was shown that they have a variety of purposes. We apply NMR to obtain the structures and dynamics of small proteins in their apo state as well as with ligands. Furthermore, NMR enables us to identify the folding state of small proteins, which include folded, partially folded, molten globule or an unstructured state. As part of an academic collaboration we investigated 37 small proteins (14 - 78 amino acids). For three small proteins we calculated high-resolved solution NMR structures.

**POSTER 056**
**Insightful 1H-NMR Studies of Physical Properties and Solubilization in Polymeric composites for Advanced Industrial Applications**
Presenting Author: Jiwon Kim

Complete Author List:
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NMR spectroscopy can provide vital information on the design and formulation improvements of polymeric composites, which can be effectively used in cosmetics and medical applications. Here, industrially practical NMR approaches are introduced that analyze the fundamental reason of phospholipid solubilization by specific surfactants, and the comparison of physicochemical properties in nanoliposome according to the packing structure. As a first project, we explored that 1,2-hexandiol prevents crystallization of phospholipids by performing a 1H-NMR-based titration experiment to investigate the phenomenon that phospholipids are selectively solubilized only on 1,2-hexandiol. Subsequently, the pliability of nanoliposome with hexagonal (C16) and orthorhombic (C22) packing structures was compared by measuring T2 relaxation according to the temperature, and hexagonal packing samples were found to be more flexible.

**POSTER 057**
**Intrinsically Disordered Motifs Regulate the Interaction between the p47 Adaptor and the p97 AAA+ ATPases revealed by methyl-TROSY NMR**
Presenting Author: Rui Huang

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VCP/p97, an enzyme critical to proteostasis, is regulated through interactions with protein adaptors targeting it to specific cellular tasks. One such adaptor, p47, forms a complex with p97 to direct lipid membrane remodelling. We use methyl-TROSY NMR to characterize the structural dynamics of p47 and p47–p97 complexes and discovered that disordered regions in p47 are critical in directing intra-p47 and p47–p97 interactions via several previously unidentified linear motifs. One of these motifs, named SHPN, regulates p47 binding to p97 in a manner that depends on the nucleotide state of p97. NMR and electron cryo-EM data have been used as restraints in molecular dynamics trajectories to develop structural ensembles for p47–p97 complexes in ADP- and ATP-bound conformations.

**POSTER 058**
**Analysis of Sidechain Dynamics using Slow-Relaxing Methyl Quadruple-Quantum Coherences**
Presenting Author: Christopher A. Waudby

Complete Author List:
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We present an experiment for to measure the relaxation rates of two quadruple-quantum transitions in $^{13}CH_3$-labelled methyl groups. These coherences are protected against relaxation by intra-methyl dipolar interactions and so have unexpectedly long lifetimes within perdeuterated biomacromolecules. These coherences have high sensitivity to chemical exchange and therefore provide ideal probes of dynamic processes. We show analysis of magnetic field-dependent zero-, double- and quadruple-quantum Hahn echo relaxation rates provides a robust indication of chemical exchange and can determine relative magnitudes of proton and carbon chemical shift differences. We also report new CPMG relaxation dispersion experiments that exploit quadruple-quantum coherences to provide increased sensitivity and improved precision in parameter estimates, particularly for $^{1}H$ chemical shift differences.

**POSTER 059**
**NMR Characterization of the C-terminal Domain of the Streptococcus Mutans Adhesin P1**
Presenting Author: Emily-Qingqing Peng

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Streptococcus mutans is the virulent bacterium primarily responsible for dental cavities. Prior work indicates that the naturally occurring C-terminal truncation product (C123, 51kDa) of the cell surface-localized adhesin P1 plays an important role in the formation of functional amyloids. We are characterizing C123 in its soluble and amyloid forms by solution NMR and DNP-enhanced solid-state NMR, respectively. Using AlphaFold, we developed constructs for both C123 and the individual C3 domain (17.5 kD) that exhibit

superior NMR resolution compared to earlier constructs used for microbiology and X-ray diffraction experiments. This enabled us to improve solution NMR assignments for comparison to our ssNMR studies of the structural transition to amyloid.

**POSTER 060**
**Development of an NMR Method for Selective Detection of Protein Acetylation**
Presenting Author: Kyungryun Lee

Complete Author List:
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Acetylation regulates protein functions involved in cellular processes including gene expression, protein-protein interactions, and enzymatic reactions. Therefore, determination of protein acetylation is important to predict protein behaviors in cells. In this work, we developed an NMR pulse sequence, Ac-FIND (Acetylation-FIltered and aNd eDited), based on the isotope filtering and editing technique to selectively detect protein acetylation. Ac-FIND was able to detect signals arising from acetylated moieties of both chemically acetylated α-synuclein and ubiquitin. Furthermore, a single signal corresponding to intracellular N-terminal acetylation was observed by Ac-FIND when non-acetylated $^{13}C/^{15}N$ labeled α-synuclein was introduced into live HEK293 cells. The results presented here demonstrate the usefulness of NMR method for detecting specific protein modifications in vitro as well as in live cells.

**POSTER 061**
**A Study of the PopZ Binding Partners Mechanism**
Presenting Author: Logan M Brown

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Intrinsically disordered proteins (IDPs) are found in all life forms, serving essential functions throughout the cell cycle. Despite the importance of this class of protein, surprisingly little is known about how they function. One example of these IDPs is PopZ which plays an important role in the cell cycle of Caulobacter crescentus, where it is responsible for gathering essential proteins to the cell poles during cell division. Currently, there are 10 known binding partners for PopZ each with vastly different structures and functions. We aim to elucidate the mechanism for this protein-protein interaction with two of its binding partners that will enhance our understanding of how the shared hub-binding site is so promiscuous yet maintain specificity to protein binding targets.

**POSTER 062**
**Statistical Approaches for Robust Analyses of 15N Spin Relaxation Measurements**
Presenting Author: Bruce Johnson

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Inferences about the dynamics of biological macromolecules requires specification of appropriate theoretical models for NMR spin relaxation in solution. Here we describe two approaches to model selection and their integration into a user-friendly GUI based software application. We illustrate the two approaches with an application to nitrogen-15 relaxation measurements on the bZip transcription factor domain of the Saccharomyces cerevisiae protein GCN4. Nitrogen-15 relaxation data at four static magnetic fields allowed bootstrap aggregation. The first approach utilizes
bootstrap aggregation, or bagging, to mitigate the effects of model-selection error in fitting variants of the model-free formalism. The second approach utilizes regularization to select model parameters that minimize overfitting. These two approaches are integrated into our RING NMR Dynamics application.

**POSTER 063**
**Structural characterization of an Antifreeze Protein, ApAFP752**
Presenting Author: Krisztina Varga

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Antifreeze proteins are found in a wide range of cold adapted organisms, and they contribute to their freeze resistance. Antifreeze proteins adsorb to the ice surface and inhibit the growth of ice crystals. The goal of this project is to investigate the mechanism by which antifreeze proteins protect against the damage typically inflicted by the cold, including the underlying molecular mechanism of ice-binding. Here we are presenting structural and functional characterization of an antifreeze protein, ApAFP752 from the desert beetle Anatolica polita utilizing nuclear magnetic resonance (NMR) spectroscopy and other biophysical methods. Current work focuses on the application of this protein in cryopreservation protocols, and on engineering a version of the antifreeze protein with enhanced activity.

**POSTER 064**
**Surface Accessibility of Intrinsically Disordered Protein Residues Probed by 2D Time-Resolved Photo-CIDNP Experiments**
Presenting Author: Jonghyuk Im

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Surface accessibility data can provide crucial information in determining the correct conformational ensemble of intrinsically disordered proteins. Photochemically induced dynamic nuclear polarization (photo-CIDNP) takes place upon a transient interaction between a photo-excited dye and a surface-exposed aromatic residue. Herein, we made technical advancements to investigate the surface accessibility of alpha-synuclein (α-Syn) using time-resolved photo-CIDNP (TR-CIDNP). High-energy laser pulses were transferred to NMR samples via an optical fiber by implementing a pulse stretcher. 2D TR-CIDNP spectra were acquired at ultrahigh resolution while maintaining sample integrity under multiple laser irradiations. Simultaneous application of laser and rf pulses enabled quantitative analysis of TR-CIDNP. Surface accessibility of four tyrosine residues and conformational change of α-Syn induced by divalent cations was accurately investigated by photo-CIDNP.

**POSTER 065**
**Probing the Dynamics of Cataract-Related Human γS-crystallin Deamidation Variants**
Presenting Author: Megan Rocha

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The human eye lens is a transparent tissue despite being filled at an impressive 400 mg/mL with a class of extremely-long lived proteins called crystallins. As crystallins age, they accumulate solubility damaging post-translation modifications, such as deamidation, until a tipping point is reached and cataract-related light scattering aggregates are formed. Our lab has shown that progressive deamidation of human γS-crystallin (HγS) increases the protein's susceptibility to oxidation with minimal structural perturbation. I hypothesize that distorted protein dynamics are the underlying cause of oxidation susceptibility in HγS deamidation variants. The fast dynamics of four HγS deamidation variants were determined by NMR spectroscopy. My data reveals that residues critical for HγS stability have significantly altered protein dynamics.

**POSTER 066**
**Dynamic Basis for dA-dGTP and dA-d8OGTP Misincorporation via Hoogsteen Base Pairs**
Presenting Author: Stephanie Gu

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Replicative errors contribute to genetic diversity for evolution but can lead to genomic instability. Here, we show DNA dynamics determines the frequency of misincorporating the A-G mismatch and altered dynamics explains the frequency of 8-oxoguanine misincorporation. NMR measurements revealed Aanti-Ganti (pop. >91%) forms sparsely-populated and short-lived Aanti+-Gsyn (pop. ~ 2%, kex ~ 137 s-1) and Asyn-Ganti (pop. ~ 6%, kex ~ 2200 s-1) Hoogsteen conformations. 8OG redistributed the ensemble rendering Aanti-8OGsyn dominant. A kinetic model where Aanti+-Gsyn is misincorporated quantitatively predicted dA-dGTP misincorporation by

human polymerase β, its pH dependence, and 8OG impact. Thus, 8OG increases replicative errors relative to G because guanine oxidation redistributes the ensemble in favor of Aanti-8OGsyn which exists transiently and in low-abundance in A-G.

**POSTER 067**
**Identifying and Overcoming Artifacts in 1H-based Saturation Transfer NOE NMR Experiments**
Presenting Author: Lucio Frydman

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Magnetization transfer experiments are versatile NMR tools providing site-specific information about organic and bio-molecules, as driven by polarization being transmitted by chemical exchanges or by cross-relaxation processes. We have recently discussed how saturation magnetization transfer (SMT) experiments could leverage repeated repolarizations arising from exchanges between labile and water protons, to enhance connectivities revealed via the nuclear Overhauser effect (NOE). Repeated experience with SMT has shown that a number of artifacts may arise in these experiments, which may confound the information being sought, in particular when seeking small NOEs among closely spaced resonances. Herein these phenomena are experimentally demonstrated, theoretically analyzed, and resolved with a number of proposals.

**POSTER 068**
**Interaction studies of DNA G-quadruplex and Zuo1 protein complexes by NMR spectroscopy**
Presenting Author: Ines Burkhart

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We investigate here the protein Zuo1, an eukaryote-specific J-protein from S. cerevisiae. Zuo1 was identified as a novel G4 binding protein in vitro and vivo and is able to influence the conformational equilibrium of G4s. Our findings suggest that the C-terminal domain is mainly responsible for G4 interactions. We investigated the complex formation of 15N-labelled Zuo1 with human and yeast derived G4-DNAs. Besides NMR spectroscopy we use CD spectroscopy and ITC to unravel the binding properties of the complex. Our results show that Zuo1 binds semi-stabilized G4 structures with stronger affinity than highly stabilized forms. We investigated two different sequences with various ionic conditions. Our data support the idea that Zuo1 discriminates between G4s with different thermodynamic stabilities.

**POSTER 069**
**Dissecting the Conformation-Dependent Substrate Specificity of Vitronectin**
Presenting Author: Kyungsoo Shin

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Vitronectin is a major serum protein capable of binding to many groups of molecules to modulate physiological and pathological processes. Vitronectin is often recruited to insoluble deposits associated with age-related diseases, but the biophysical mechanism behind this remains elusive. Previously, we determined the structure of vitronectin's largest domain (i.e., hemopexin-like domain). This four-bladed β-propeller domain is topologically complex with electrostatic protrusions and hydrophobic grooves for many potential molecular interactions. Using NMR, we identify the binding sites of various molecules observed in disease-related insoluble deposits. We demonstrate structural plasticity and how it regulates substrate specificity using biophysical and biochemical approaches, providing insight into how vitronectin conformational flexibility may be utilized to control its molecular interplay for disease progression.

**POSTER 070**
**Cost-Efficient Stable Isotope Labeling of Proteins Overexpressed in Mammalian Cells**
Presenting Author: Ravinder Elupula

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We have developed culture media containing stable isotope-labeled amino acids (15N and 13C15N) for mammalian HEK293T and insect Sf9 cells. The culture media are based on stable isotope-labeled protein hydrolysates from fermented Cupriavidus necator. The media were optimized to achieve high isotope incorporation and protein yields. For this purpose, the cells were adapted to low serum culture media. In addition, labeled biomass-derived hydrolysates, labeled yeast autolysates and lipid extracts were explored as media ingredients. Overexpressed eGFP yields in the new media were comparable with cells cultured in standard DMEM/F12 media. Based on pH, osmolality, glucose concentration and turbidity the media are stable for at least 8 weeks when stored at 4°C.

**POSTER 071**
**Histone H4 Tail Conformation in Nucleosomes Studied by Paramagnetic NMR**
Presenting Author: Wenjun Sun

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The packaging of DNA into chromatin plays a critical role in genome function. The fundamental repeat unit of chromatin, the nucleosome, consists of ~147 bp DNA and a histone protein octamer containing two copies each of histones H2A. H2B, H3 and H4. Dynamically disordered H4 N-terminal tails are key components in chromatin regulation. Here we investigate the conformational ensemble of these H4 tail domains in nucleosomes by paramagnetic relaxation enhancement (PRE) solution NMR spectroscopy and recombinant nucleosomes reconstituted with 15N-enriched H4 and labeled with paramagnetic tags at multiple histone H3 sites located on the nucleosome surface. The experimental PRE data are interpreted in conjunction with MD simulations, which indicate that H4 tails engage in a fuzzy interaction with nucleosomal DNA.

**POSTER 072**
**Dynamic properties and functional roles of sizable intrinsically disordered linkers in villin/dematin family of cytoskeleton regulators in plants and humans.**
Presenting Author: Serge L. Smirnov

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Dedicated actin-regulating proteins incessantly remodel non-covalent actin filaments of the cytoskeleton according to the changing environmental conditions. Villin, dematin and other related actin regulators have folded and sizable intrinsically disordered regions (IDRs) in their polypeptides. Plant villins have IDRs of 150-190 residues which connect two folded segments. Our data indicate that some of these IDRs are capable of specific F-actin binding thus providing novel actin binding sites. Dematin has a massive IDR (315 amino acids) which is capable of regulatory binding with the only folded domain in the protein. The poster presents NMR applications for deciphering dynamics and binding interfaces in the IDRs in plant villin and human dematin as well as NMR characterization of functional features in these proteins.

**POSTER 073**
**Chemical shift assignment of 43x2kDa TrpB from Pyrococcus furiosus**
Presenting Author: Hanna Kavaleuskaya

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The tryptophan synthase complex is an allosteric enzyme catalyzing the last two steps in the biosynthesis of the L-tryptophan in bacteria, plants, and fungi. The two reactions are kept in phase by allosteric interactions between the two subunits. Due to the size limit for solution-state NMR, the beta subunit TrpB has remained poorly characterized. To study the system of TrpB, we used combination of solution and solid-state NMR of a wild type PfTrpBwt and standalone PfTrpB2B9 from Pyrococcus furiosus. Backbone walk experiments, as well as 4D-SOFAST-HMQC-NOESY-HMQC were recorded for TrpB2B9. We were able to obtain 50% of assignment. This approach will allow us to analyze the mechanisms of allosteric communication in multi-subunit proteins on a milli- to micro-second timescale.

**POSTER 074**
**Structure Elucidation of RNA Aptamers Bound to Derivative Hoechst Dyes**
Presenting Author: Natasha Evans

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RNA aptamers are oligonucleotides that can specifically bind to small target molecules with high affinity and are typically selected through a process known as Systematic Evolution of Ligands by Exponential Enrichment. A 2008 study by Sando et al. identified an RNA aptamer that binds to a Hoechst dye derivative with tert-butyl (tBu) substituents. The goal of this research is to elucidate the structure of the tBu Hoechst-RNA complex using a combination of nuclear magnetic spectroscopy and computational modelling experiments. Preliminary results suggest that the RNA aptamer forms a stem-loop structure, with a central bulge region to accommodate for the bulky tBu groups. Determining the structure of this complex will allow for its potential use as an aptamer-based biosensor building block.

**POSTER 075**
**Tackling a tripartite glycan conundrum: Flexibility/Sparse structural data/Signal resolution**
Presenting Author: Marcos

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We face common, and often interconnected, challenges in the NMR structural studies of glycans, namely: 1) Discrimination of distinct conformations amongst a conformation-rich landscape; 2) Limited structural data for more reliable molecular modeling; 3) Spectral overlap, especially for homopolymers. We are tackling these issues by improving sensitivity and spectral resolution, though both cannot be simultaneously achieved. We show that labile 1H signals can help alleviate two of these challenges, increase structural data and provide a path to discriminate potentially "biologically active" conformations; therefore, improving the quality of both, the acquired data and the derived structural models. We also present our ongoing efforts to enhance the spectral resolution to enable the structural studies of larger homo- and hetero-oligosaccharides.

**POSTER 076**
**Structural and Dynamical Investigation of the Histidine Triad in GMCSF**
Presenting Author: Jennifer Cui

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GMCSF is a cytokine that displays promiscuous binding with ligands dependent on pH. A cluster of three histidine residues appear to be central to changes in structure and subsequent binding interactions. In order to understand the structure, stability, and motions contributed by each of the histidine residues composing the histidine triad, we have mutated each one to either Arg, Tyr or Asn. We have determined changes in structure and dynamics which allow us to rank importance of position and chemical properties of each histidine to the overall behaviour of GMCSF.

**POSTER 077**
**Structural Characterization of Phosphoethanolamine Methyltransferase from P. falciparum Using Solution NMR Spectroscopy and MD Simulations**
Presenting Author: Alexandra Pozhidaeva

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Recent emergence of drug-resistant malarial Plasmodium emphasizes the need for development of new treatments. Phosphatidylcholine, a major phospholipid of P. falciparum membranes, is synthesized through a pathway in which phosphoethanolamine methyltransferase (PfPMT) converts phosphoethanolamine to phosphocholine. This pathway is absent in mammals making the enzyme an attractive therapeutic target. Crystal structures of the PfPMT single S-adenosylmethionione-dependent catalytic domain with its substrates/inhibitors have been determined. Yet, the structure of the apo protein has never been crystalized suggesting conformational dynamics. Here, we characterize apo PfPMT and gain insight into the mechanism of its inhibition by amodiaquine using solution NMR methods in combination with molecular dynamics simulations. This work provides a basis for future efforts to develop new potent anti-malarial compounds.

**POSTER 078**
**Determination of the Structural and Dynamical Properties of the crucial periplasmic chaperone SurA**
Presenting Author: Filippo Castegnaro

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Survival protein A (SurA) is a crucial ATP-independent holdase chaperone residing in the periplasmic space of Gram negative bacteria and is essential for the cell viability in stationary phase. It plays a central role in the biogenesis of different outer membrane proteins (OMPs), transporting them from the inner to the outer membrane avoiding their misfolding and aggregation. Despite the general knowledge about SurA-function, the detailed mechanisms of how SurA transports its Omp cargo as well as how it transfers the unfolded OMPs to the BamA downstream remains elusive. To gain more knowledge about this important periplasmic chaperone and its role in OMPs biogenesis, we are studying the structure and dynamic properties of SurA at atomic level using solution NMR techniques.

**POSTER 079**
**NMR Investigation of Cyclic-di-GMP Riboswitch Folding Pathway**
Presenting Author: Ji-Yeon Shin

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Riboswitch is a structural RNA motif located at the 5'- end of bacterial mRNA, consisting of aptamer domain and expression platform. The aptamer domain binds a ligand, and the expression platform is responsible for gene expression by switching its conformation. Among the numerous types of riboswitches, this study investigates the folding pathway of the c-di-GMP riboswitch through NMR experiments. The conformational changes of its 3 states (free, apo and holo) under different conditions of $Mg^{2+}$, salt and c-di-GMP at the level of secondary and tertiary structure were determined through analysis of NMR spectra. Further NMR and ITC experiments with site-specific RNA mutations confirm the importance of tertiary interactions for the structural stability of RNA.

**POSTER 080**
**A Study on the Target DNA Recognition of the Human Transcription Factor Meis1**
Presenting Author: Seo-Ree Choi

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Myeloid ecotropic viral integration site-1 (Meis1) is a human transcription factor and plays an important role in myeloid leukemia. Meis1 contains a three amino acids loop extension (TALE) homeobox domain (HD) and specifically binds to a common DNA sequence, 5' – TGACA - 3'. In this study, we performed NMR experiments on the complexes of TALE-HD of human Meis1 (Meis1-HD) with a decamer DNA duplex containing its consensus sequence. We prepared the mutant DNA duplexes containing a single base-pair substitution as well as double or triple substitution mutants and compared the Meis1-HD-DNA interactions using HSQC titrations. This study provides key structural features of the Meis-HD-DNA complex and the information about the molecular mechanism of target DNA recognition of the MEIS1.

**POSTER 081**
**Structural Investigation of Human U6 snRNA Recognition by The Spliceosome Recycling Factor SART3**
Presenting Author: Kyeong-Mi Bang

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Human SART3 is a multifunctional protein involved in the pre-mRNA splicing, including assembly and recycling of the U4/U6 snRNP. SART3 contains two RRMs at the C-terminus, whereas the homologous yeast Prp24 employs four RRMs for specific U6 snRNA recognition. We investigated the tertiary interaction between RRMs and U6 snRNA using biochemical assays and NMR methods. We report monomeric SART3 binds tightly to the asymmetric bulge of U6 snRNA, demonstrating that two RRMs sufficient to bind the U6 snRNA. SART3 RRMs adopt a tandem βαββαβ motif, and they bind to the bulge region of U6 snRNA via a conserved electropositive surface and aromatic residues. Also, we confirm that 5'-end regions of bulge of U6 snRNA interact with SART3 RRMs.

**POSTER 082**
**NMR Hydrogen Exchange study of wild type and mutant MIR390a**
Presenting Author: Ho-seong, Jin

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In plants, primary transcripts with miRNA foldbacks are processed by the RNase-III like enzyme DICER-LIKE1 complexed with HYPONASTIC LEAVES1 and SERRATE to generate miR/miR* duplex. The levels of mature miR390 influence the leaf number prior to flowering in the life cycle of plants. The G-to-A point mutation that was calculated to stabilize a relatively nonpaired region near the base of the miR390a foldback, resulting in misprocessing of the miR390/miR390* duplex. To understand the molecular mechanism of biogenesis of primary miR390a to mature miR390, an NMR hydrogen exchange study was performed using model RNAs mimicking the cleavage site of wild-type (WT) and bulge-stabilizing mutant pri-miR390a constructs.

**POSTER 083**
**Towards Understanding Protein Quality Control of Integral Membrane Proteins by the Bacterial Metalloprotease FtsH**
Presenting Author: Hannah Fremlen

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FtsH is an essential zinc-dependent integral membrane protease residing in the Escherichia coli (E. coli) inner membrane responsible for degradation of unfolded or aggregated proteins as a part of the protein quality control machinery. As a member of the AAA+ protein family, FtsH requires several cycles of ATP to unfold and translocate substrates for subsequent cleavage. Both the ATPase domain and the protease domain reside on a single polypeptide chain in the cytosolic region and assembles into a homohexamer with a ring-like structure. Despite its vital role in E. coli, still very little is known about this membrane protein. To gain further insight into the detailed structure and dynamic properties of FtsH, solution NMR is used as the main method.

**POSTER 084**
**Structural Elucidation of the PH Domain of Akt-like Kinase in Trypanosoma cruzi: A New Target for Treatment of Chagas Disease**
Presenting Author: Karina A. Stadler

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Chagas disease is caused by the protozoan parasite Trypanosoma cruzi. The disease is endemic to Latin America but current treatment options are inefficient and cause severe side effects. Although Akt-like kinase (TcAkt) represents a promising drug target, its structure and mechanism of action are still not resolved. Human Akt is stated to be activated by phosphoinositide (PIP) binding, enabling the pleckstrin homology (PH) domain to dislodge from the kinase domain. The structure and binding studies of the N-terminal TcAkt PH domain reveal PIP-induced structural changes, highly associated with kinase activation. Our findings reveal unique insights into the structure and functionality of the so far scarcely understood TcAkt, thereby forming the basis for the development of efficient drugs against Chagas disease.

**POSTER 085**
**How to find needles in a haystack: an STTD on-cell NMR method to boost interaction studies**
Presenting Author: Tamás Milán Nagy

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Saturation Transfer Difference (STD) NMR experiments have been used routinely to characterize protein-ligand interactions. However, care has to be taken when studying complex systems with on-cell STD methods; interference should be avoided with any non-specific interactions of small or high molecular weight components present in cells.
The triple difference STD (STTD) strategy proposed here can eliminate the contribution of any undesired specific and non-specific interactions, and so the resulting spectrum reveals the direct binding between the protein and ligand of interest. Experimental findings are demonstrated on different biological samples. First, the binding between rapamycin and the TRPM8 menthol receptor is investigated in atomic detail, then interactions between endomorphin-2 and mu-opioid receptor (MOR) mutants are presented.

**POSTER 086**
**Structural Basis of Substrate Recognition and Allosteric Activation of the Pro-apoptotic Mitochondrial HtrA2 Protease**
Presenting Author: Emelie Aspholm

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HtrA2 is a mitochondrial serine protease of the HtrA family found in all kingdoms of life. Residing in the inner mitochondrial membrane it exerts a role in protein quality control and acts as a proapoptotic factor when released into the cytosol, cleaving inhibitor of apoptosis (IAP) proteins such as XIAP. HtrA2 has been implicated in Parkinson's and Alzheimer's disease and in several different cancer types, making it an important target of study. We have used advanced solution NMR spectroscopy methods together with biophysical and biochemical characterization to show how HtrA2 is allosterically activated via its PDZ domain. Further, we show that divalent metal ions can modulate the activity of HtrA2, refining the model of HtrA2 regulation in the apoptotic pathway.

**POSTER 087**
**Structural studies of AgA by solution NMR**
Presenting Author: Maria Luiza Caldas Nogueira

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Dental caries is one of the most prevalent infectious diseases. It has a high impact on an individual's quality of life and its healthcare-associated costs. S. mutans is the primary pathogen that causes dental caries resulting from biofilm formation. Biofilms are composed of polysaccharides, proteins, and eDNAs. S. mutans has four known amyloidogenic proteins: SMU_63c, Adhesin P1, WapA, and cnm. WapA is cleaved by sortase Aga. WapA binds collagen I, and fibronectin, and promotes dendritic cell maturation. It is a vaccine candidate against S. mutans caused teeth caries. Despite its importance, the AgA structure is still not available. Here we use solution NMR to perform structural studies of the AgA.

**POSTER 088**
**Using NMR to enable the discovery of small molecules stabilizing the interaction between 14-3-3 and Estrogen receptor α**
Presenting Author: Adam Lewis

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The 14-3-3 adapter protein binds an array of client proteins. The biological consequence of 14-3-3 binding depends on the client in question but can affect cellular localization, activity, stability, trafficking or complex formation. It was demonstrated that phosphorylation of Estrogen receptor α (ERα) at T594 favors binding of 14-3-3, thereby inhibiting receptor dimerization and transcriptional activity. We initiated an effort to identify small molecules that enhance the 14-3-3:ERα interaction. Primary screening hits were validated using two NMR-based assays: a 19F-CPMG-1D reporter assay and a 1H,15N-2D-TROSY-HSQC assay. The 19F reporter assay confirmed complex stabilization while 2D NMR confirmed binding. These efforts allowed prioritization of hits for X-ray confirmation and medicinal chemistry optimization.

**POSTER 089**
**Human Znf706: A Tiny G-quadruplex-Binding Protein**
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The cellular function and structure of a large percentage of proteins containing disorder remains enigmatic. We identified that a tiny human protein Znf706 that is characterized by a high degree of charge and partial disorder binds to G-quadruplexes, an emerging cellular component whose biological roles need to be better defined. NMR studies combined with other biophysical, biochemical, and cellular approach revealed that Znf706 preferentially binds to G-quadruplex with sub-micromolar to nanomolar affinity. 19F NMR revealed Znf706's preference to bind parallel G-quadruplexes, and NMR backbone assignments of Znf706 enabled us to identify G-quadruplexes binding to its dynamic and disordered N-terminal domain. Znf706 and well-characterized G-quadruplexes serve as biophysically amenable models to help in the understanding of protein and G-quadruplex interactions.

**POSTER 090**
**Elucidating Biomacromolecular Interactions with DIrect Saturation COmpensated (DISCO) NMR**
Presenting Author: Darcy C. Burns

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Interactions between protein and macromolecules are imperative to biomaterials development. When exogenous materials are introduced to biological fluids they are rapidly bound by native protein. The nature of these binding interactions determines the fate of the candidate materials. Despite their importance, the causal link between polymeric biomaterials composition and their protein binding mechanisms are poorly understood. This is partly driven by the lack of tools to investigate the underlying solution-state binding interactions at atomic resolution. We developed Direct Saturation Compensated NMR to help address this shortfall. DISCO is a refinement of the saturation transfer difference (STD) and double difference (STDD) techniques that correct for R.F. irradiation spillover artifacts and was used to probe binding interactions in different mucin-polymer bioconjugates.

**POSTER 091**
**Ligands and Fast Dynamics in the Neurotensin GPCR: Extracting Parameters from High Noise Triple Quantum Relaxation Data.**
Presenting Author: Scott Anthony Robson

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*Scott Robson (Indiana University); Fabian Bumbak (Monash University); Joshua J. Ziarek (Indiana University)*

G protein-coupled receptors (GPCRs) convey ligand-based signals from outside to inside the cell through changes within the GPCR itself. The signaling information that can be passed is multifaceted and dynamic changes within the receptor seem to play a role in how signals are transmitted. We have used 3Q/SQ methyl relaxation experiments to monitor fast dynamics of methionine sidechains in the presence of various ligands for the Neurotensin receptor. These experiments are insensitive and low solubility of GPCR/micelle samples means data collection and analysis is challenging. We have adopted Bayesian parameter estimation to extract order parameters by simultaneously fitting models for 3Q and SQ relaxation rather than the traditional 3Q/SQ ratio method. This approach is more robust given high noise.

**POSTER 092**
**Pulsed Saturation in Hyper-CEST NMR for Hosts with Different Exchange Kinetics**
Presenting Author: David Hernandez

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HyperCEST NMR with exchanging hyperpolarized 129Xe and molecular hosts reveals the presence of such molecules at picomolar detection limits. The combination of applied RF saturation and the Xe exchange kinetics is critical to achieve optimum signal contrast while avoiding unwanted RF heating. Here, we study the HyperCEST responses of two types of Xe hosts for BP and dSNOB saturation. Depolarization of Xe with a short residence time in hosts with desirable faster exchange benefits from the shaped pulses. However, the full potential of such agents can only be realized when strong saturation is applied where the dSNOB pulses are slightly outperformed by the BP scheme. With a growing family of HyperCEST reporters, the optimum saturation scheme should be chosen carefully.

**POSTER 093**
**Probing Glycan-Galectin Interactions with State-Of-The-Art Multinuclear NMR and Computational Methods**
Presenting Author: István Timári

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The inhibition of glycan-galectin interactions represents a promising perspective towards developing therapeutics controlling cancer development. We have investigated the binding of multiple human Galectin-3 (hGal-3) inhibitors, specifically that of di(β-D-galactopyranosyl)selenide (SeDG), and di(β-D-galactopyranosyl)diselenide (DSeDG) analog. The binding affinities of these derivatives to hGal-3 were determined by 1H-15N HSQC and competition STD experiments. We have demonstrated that the enhanced detection sensitivity inherent in our original 1H-77Se CPMG-HSQMBC method got a further significant boost by using 77Se-enriched ligands,

such as [77Se]DG. Our work opens perspectives for utilizing isotopically enriched selenoglycosides for rapid monitoring of lectin-binding of selenated as well as non-selenated ligands. The synthesis, NMR and computational study of novel glycomimetics targeting of hGal-3 protein are on the way in our group.

**POSTER 094**
**Using Intermolecular Paramagnetic Relaxation Enhancements to Constrain Dynein/Dynactin Interactions**
Presenting Author: Nikolaus M. Loening

Complete Author List:
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Cytoplasmic dyneins are multiprotein complexes that carry out retrograde transport in cells. In mammalian dynein, processive motion is only observed when dynein interacts with another protein complex, dynactin. The main site of interaction between dynein and dynactin is the N-terminal portion of dynein intermediate chain (N-IC) and the coiled-coil 1B (CC1B) region of the p150Glued subunit of dynactin. Despite evidence for this interaction from binding studies, the exact location of where these proteins bind remains elusive due to the dynamic nature of the interaction and the presence of intrinsically-disordered regions in IC. By using intermolecular paramagnetic relaxation enhancements (PREs) we have been able to constrain the location of IC binding on p150Glued.

**POSTER 095**
**Utilizing SAR by NMR and CADD-based Screening Methods to Develop Novel CDTb-RBD2 Drug Inhibitors**
Presenting Author: Mary Cook

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C. diff is an oft-reoccurring and hard-to-treat gut infection, especially in strains containing binary toxin (CDT), which possesses an ART toxin component (CDTa) and a pore-forming/delivery subunit (CDTb). CDTb assembles into symmetric and asymmetric di-heptameric states, both of which possess surface-accessible receptor binding domains (RBD1 & RBD2). RBD2 has been shown to be critical for CDT toxicity, making it the target for NMR-based drug discovery studies. Utilizing "SAR by NMR", 2D [1H, 15N]-HSQCs were collected from a small molecule fragment screen, looking for perturbations that indicated binding effects - and therefore possible binding sites. These sites were confirmed with SILCS, which was then used (with other CADD methods) to generate a compound list for the next round of NMR-based screening.

**POSTER 096**
**Specificity-enhancing Mutations Remodel Dynamic Allostery in CRISPR-Cas9**
Presenting Author: Erin Skeens

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CRISPR-Cas9 is an innovative genome editing tool with broad applications in bioengineering. However, the occurrence of off-target effects has limited its use as a precision therapeutic for human disease. Efforts to engineer variants of Streptococcus pyogenes Cas9 for increased specificity have revealed that Rec3, a subdomain of the recognition lobe, is an important functional handle for specificity, as many variants contain the majority of their specificity-conferring mutations within Rec3. The mechanisms by which mutations in Rec3 contribute to the specificity of Cas9, especially considering their distance from the catalytic sites, is not well understood. We employed solution NMR spectroscopy and MD simulations to characterize the structural and dynamic effects of high-specificity mutations on Rec3 and more broadly, Cas9

**POSTER 097**
**Development of a high-resolution NMR technique to measure diffusion of proteins at near-physiological conditions**
Presenting Author: Jongchan Lee

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*Jongchan Lee (Seoul National University); Jung Ho Lee (Seoul National University); Sho Hee Park (Seoul National Univerisity)*

Measuring the translational diffusion of proteins can provide useful information about their size, shape, and surrounding environments. NMR technique, called diffusion NMR or diffusion-ordered spectroscopy (DOSY), is widely used to study the diffusion of molecules. In this study, we have proposed a method that separates the nuclei used for diffusion measurement (alpha protons, 1Hα) and those used for detection (1H/15N and 13C'/15N correlations). This effort improved the resolution of diffusion measurements on polypeptides in a mixture of biomolecules, thereby permitting the investigation of coexisting species under near-physiological conditions.

**POSTER 098**
**A Potassium Ion-Dependent Structural Switch in the G-rich Region of a Long-Noncoding RNA**
Presenting Author: Jasna Brcic

Complete Author List:
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Long-noncoding RNA REG1CP was shown to promote cancer cell proliferation and tumorigenicity by activating the REG3A gene in colorectal cancer. The mechanism involves REG1CP binding and recruiting helicase FANCJ to the REG3A locus. A guanine-rich (G-rich) sequence within REG1CP was proposed to fold into a non-canonical structure called G-quadruplex (G4) which is recognized by FANCJ. We show by NMR that a G-rich oligoribonucleotide from REG1CP forms two structures, a hairpin (HP) and a G4, that coexist in slow exchange in K+ solution and provide insight into their folding topologies, interconversion, and how they interact with FANCJ-peptides. Our structural study suggests that conformational switching between G4 and HP structures within REG1CP could modulate REG1CP and FANCJ interaction implicated in colon cancer.

**POSTER 099**
**NMRFAM User Program**
Presenting Author: Katherine Henzler-Wildman

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The NMRFAM user program provides access to 10 NMR spectrometers (500 MHz – 900 MHz) equipped for a variety of solution and solid-state NMR experiments, with three more spectrometers scheduled for installation this year (including 1.1 GHz). Our scientists provide advice and assistance in experimental design, data acquisition and processing for studies of molecular structure, dynamics and interactions. We have experience with a range of sample types, including soluble and membrane proteins, fibrils, RNA, small molecules, and metabolomics. We offer training in experimental design, data acquisition, data processing and analysis for solution and solid-state NMR of proteins and RNA.

**POSTER 100**
**Backbone Conformational Equilibrium Correlates with Enzyme Activity in Mismatched DNA**
Presenting Author: Gary Meints

Complete Author List:
*M. N. Westwood (Michigan); A. Pilarski (Missouri State University); C. Johnson (Missouri State University); Gary Meints (Missouri State University)*

A mystery remains regarding how repair enzymes such as thymine DNA glycosylase (TDG) identify a canonical DNA base in the incorrect pairing context. We have previously used 31P NMR to investigate the energetics of DNA backbone BI-BII interconversion and the effect of a mismatch or lesion compared to canonical DNA. We found perturbations to the free energy (~1 kcal/mol) and enthalpy (2-5 kcal/mol) of activation for the BI-BII interconversion localized to the phosphates flanking the mismatch. We found correlations of our DNA phosphate backbone equilibrium (Keq) to enzyme kinetics or binding parameters of several enzymes, suggesting the backbone equilibrium may play a role in mismatch recognition and/or conformational rearrangement and energetics during nucleotide flipping or other aspects of enzyme interrogation.

**POSTER 101**
**Structural and functional characterization of SARS-CoV-2 Nucleocapsid linker reveal RNA binding and regions of self-association**
Presenting Author: Hannah Stuwe

Complete Author List:
*Hannah Stuwe (Oregon State University); Patrick Reardon (Oregon State University); Zhen Yu (Oregon State University); Kaitlyn Hughes (Oregon State University); Sahana Shah (Oregon State University); Elisar Barbar (Oregon State University)*

The nucleocapsid protein (N) of SARS-CoV-2 is essential for virus replication, genome packaging, and maturation. N is comprised of N-terminal and C-terminal folded domains that are separated by a disordered, Ser,Arg-rich, linker and flanked by disordered tails. We have analyzed the linker region using NMR spectroscopy and other biophysical techniques. Our results show that the linker region binds viral RNA and that this binding is modulated by phosphorylation and naturally occurring mutations. Further, we have assigned an alpha-helical region in the linker and shown that this region undergoes concentration dependent self-association. These data show that the linker region can contribute to functions normally associated with the folded domains and suggests it could regulate protein-protein interactions and RNA-protein interactions.

**POSTER 102**
**Structural determinants of the versatile functions of RNA complexes in the SARS-CoV-2 Nucleocapsid**
Presenting Author: Patrick N. Reardon

Complete Author List:
*Patrick Reardon (Oregon State University); Aidan B. Estelle (Oregon State University); Zhen Yu (Oregon State University); Kaitlyn Hughes (Oregon State University); Elisar J. Barbar (Oregon State University)*

The nucleocapsid (N) protein of the SARS-CoV-2 coronavirus binds to viral RNA, condensing it inside the virion, facilitating viral transcription in infected cells, and phase separating with RNA to form liquid condensates. However, the structural determinants of these interactions are not clear. To identify the role of RNA structure in mediating these interactions, we characterize the binding between the folded domains of N and short model RNA segments. We demonstrate that the N-terminal domain (NTD) binds preferentially to single-stranded RNA. We identify a second, weak RNA-binding face on the NTD and another on the C-terminal domain that are critical for phase separation. We propose a model of how variations in N-RNA binding can promote binding, phase separation, or virion formation.

**POSTER 103**
**Targeting Receptor Binding Domain 1 (RBD1) From Clostridioides difficile Binary Toxin (CDT) With Drug-Like Fragments**
Presenting Author: Spiridon E Sevdalis

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Hypervirulent cases of Clostridioides difficile (C. difficile) infection express C. difficile binary toxin (CDT). CDT is comprised of a catalytic A subunit (CDTa) and seven cell binding/translocase B subunits (CDTb). CDTb's receptor binding domains (RBDs) were revealed to be important for CDT toxicity. A novel calcium-binding site was discovered in RBD1, facilitating the formation of a stable conformation in the presence of calcium. As RBD1's fold facilitates CDT activity, development of inhibitors specific to RBD1 was initiated. Screening of RBD1 in the presence of 1000 chemical fragments was monitored by tracking residue CSPs from 2D [1H, 15N]-HSQC spectra. These NMR data informed Site Identification by Ligand Competitive Saturation (SILCS) simulations to generate larger, drug-like compounds specific for RBD1.

**POSTER 104**
**Biophysical Characterization of Novel Plexin–GTPase Interactions**
Presenting Author: Chinmayi Prasanna

Complete Author List:
*Chinmayi Prasanna (Case Western Reserve University); Maria Iannucci (Case Western Reserve University); Matthias Buck (Case Western Reserve University)*

Plexin receptors play a crucial role in neuronal development, particularly in axon guidance, cytoskeletal re-arrangement, and signal transduction. In earlier work, Buck lab discovered a unique Rho GTPase binding domain (RBD) in plexins. The Rho-family regulatory GTPases interact with RBD carrying out plexin regulation in the intracellular environment. In addition to this region, another part of the plexin intracellular region appears to interact tightly with certain Rho GTPases. The structural mechanism of the effects of Rho GTPases on plexin signaling still remains elusive. In this study, we use various plexin constructs to probe interaction with Rho GTPases using–microscale thermophoresis (MST), nuclear magnetic resonance (NMR) spectroscopy, and AlphaFold 2 (AF2) based predictions and obtain structural and sequence-specific insights.

**POSTER 105**
**Backbone Conformational Equilibrium Correlates with Enzyme Activity in Mismatched DNA**
Presenting Author: Gary Meints

Complete Author List:
*M. N. Westwood (Michigan); A. Pilarski (Missouri State University); C. Johnson (Missouri State University); Gary Meints (Missouri State University)*

A mystery remains regarding how repair enzymes such as thymine DNA glycosylase (TDG) identify a canonical DNA base in the incorrect pairing context. We have previously used 31P NMR to investigate the energetics of DNA backbone BI-BII interconversion and the effect of a mismatch or lesion compared to canonical DNA. We found perturbations to the free energy (~1 kcal/mol) and enthalpy (2-5 kcal/mol) of activation for the BI-BII interconversion localized to the phosphates flanking the mismatch. We found correlations of our DNA phosphate backbone equilibrium (Keq) to enzyme kinetics or binding parameters of several enzymes, suggesting the backbone equilibrium may play a role in mismatch recognition and/or conformational rearrangement and energetics during nucleotide flipping or other aspects of enzyme interrogation.

**POSTER 106**
**Thermodynamic and kinetic characterization of non-conventional hydrogen bonding in Lewis antigens**
Presenting Author: Jeahoo Kwon

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The Lewis antigens are a well-known family, whose structures were thought to be conformationally inflexible, until recently. Herein, we provide evidence for conformational flexibility between hydrogen bonded conformations and non-hydrogen bonded for 10 Lewis antigens and two of their rhamnose analogs. We also characterize the thermodynamics and kinetics of the H-bonds in these molecules, using an alternative method to simultaneously fit a series of temperature-dependent fast-exchange NMR spectra. We determined that the H-bonded conformation is favored by approximately 1 kcal/mol over the non-H-bonded conformation. Additionally, comparison of temperature-dependent 13C linewidths in various Lewis antigens and the two rhamnose analogs, reveals H-bonds between the carbonyl oxygen of the N-Acetyl groups of N-Acetylglucosamine and the OH2 group of galactose/fucose.

**POSTER 107**
**Progress Towards Characterizing a Solution Phase NMR Oligomer of Peptides Derived from Aβ**
Presenting Author: Jason Zhu

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The Aβ peptide assembles into oligomers and fibrils that are central to the pathology of Alzheimer's disease (AD). Despite mounting evidence suggesting that oligomeric species are neurotoxic, there are few high-resolution models of Aβ oligomer assembly in aqueous solution. To address the need for models of cytotoxic oligomers, I synthesized peptides derived from the amyloidogenic fragments from the central and C-terminal regions of Aβ and evaluated their assembly using 1H NMR, TOCSY, NOESY, DOSY, and other NMR techniques. The amyloidogenic peptides adopt β-hairpin conformations, are soluble at millimolar concentrations, and show concentration dependent oligomerization. These studies provide insight into how Aβ oligomerizes in aqueous solution.

**POSTER 108**
**Investigating the Structural Change of Ci-$\beta\gamma$-Crystallin at Various Calcium Concentrations**
Presenting Author: Matthew Jimenez

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Tunicate (Ci-$\beta\gamma$-crystallin) is from a vertebrate $\beta\gamma$-crystallin lineage before the evolution of the lens. The $\beta\gamma$-crystallin superfamily contains both the vertebrate eye lens and the microbial calcium binding proteins. The vertebrate $\beta$- and $\gamma$- crystallins are structural proteins that make up the refractive tissue of the lens while the microbial $\beta\gamma$-crystallin proteins bind to divalent cations. Tunicate contains both properties. Studying the calcium binding affinity on tunicate through various concentrations will describe the evolution process of $\beta\gamma$-crystallins and the role of calcium binding stability. This is done through titrating different protein to calcium concentration ratios on tunicate then taking HSQC's to determine the calcium binding sites and the structural changes that tunicate undergoes through various ratios of calcium.

**POSTER 109**
**Structural Insights into Selective Complexation of Rare Earth Elements by Peptide Surfactants Revealed by NMR Spectroscopy**
Presenting Author: Surabh KT

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Rare earth elements (REEs) are crucial components in numerous modern technologies. However, current REE separation processes are challenging, energy-intensive, and detrimental to the environment. Recently, we developed an eco-friendly REE separation process at the air-water interface using a peptide surfactant (LBT1LLA) derived from $Ca^{2+}$ binding loops in calmodulin. The peptide surfactants bind trivalent $REE^{3+}$ cations with high affinity and show selective complexation along the lanthanide series, enabling subsequent recovery and isolation. Here, we elucidate the 3D molecular structures of bound and unbound LBT1LLA using multidimensional solution-state biomolecular NMR to better understand ion coordination in the binding loop. In addition, we identify specific residues that perturb $REE^{3+}$ selectivity, yielding insights into design principles for targeted REE complexation.

**POSTER 110**
**Structure and Chaperone Activity of Human Heat Shock Protein B8**
Presenting Author: Daniel C. Farb

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Aggregation of certain globular proteins has been implicated with neurodegenerative diseases such as ALS and dementia. HspB8 (Heat shock protein B8), an ATP-independent chaperone protein, binds misfolded proteins and thereby prevents their pathological aggregation. To fully understand the chaperone activity of HspB8, a high-resolution structure of the chaperone is needed. Size-exclusion chromatography and MALDI-TOF mass spectrometry have confirmed that HspB8 occurs in a monomeric and dimeric state in solution, therefore solution NMR is a suitable tool for this. Solution NMR relaxation measurements and chemical shift perturbations will report on the structural transformation in the head and tail domains of HspB8 upon interaction with misfolded proteins. Here, we present our initial characterization of HspB8 and assess sample conditions for NMR measurements.

**POSTER 111**
**HIV-1 p17 Interactions with Heparan Sulfate**
Presenting Author: Kari Pederson

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Glycosaminoglycans (GAGs) are expressed ubiquitously on mammalian cell surfaces and interact with a wide variety of biological molecules to modulate processes, including immune response, regulation of cell growth and blood-stream clotting. Disruption of GAG-binding has the potential to prevent infection by viruses, such as HIV-1, and to reduce inflammation caused by autoimmune disorders. Within HIV-1, three proteins are known to bind to the sugars present on the surfaces of human cells. One of these, p17, is the focus of this study. Here we investigate the sequence specificity of the heparan sulfate-p17 interaction using microarray screening and NMR titration. HIV-1 p17 demonstrates a preference for binding to 2-O-sulfated heparan sulfate, which may present a target for future drug development.

**POSTER 112**
**Phosphopeptide Binding Modulates Arrestin 2 Isoleucine Conformational Dynamics**
Presenting Author: Tucker Shriver

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Arrestins underpin critical signaling pathways in the body, yet the structural mechanism of their activation remains unclear. Crystal structure data of bound and unbound structures of Arrestin 2 reveal the presence of a 20 degree interdomain twist between portions of the protein upon binding. Previous work by Shiraishi et al (2021) determined that multiple methyl NMR peaks occur for single isoleucine residues, suggesting the presence of slow conformational exchange. This work shows that this exchange is sensitive to the presence of the fully phosphorylated Vasopressin-2 receptor c-terminal peptide (V2Rpp) and that the Ile residues experience similar global thermodynamic and conformational changes upon V2Rpp binding. Such behavior suggests that these isoleucine methyls may be sensitive probes of Arrestin 2 activation.

**POSTER 113**
**Pre-Homonuclear Decoupling: NMR Measurements of Intrinsically Disordered Proteins at Ultrahigh Resolution**
Presenting Author: Sohyun Jung

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Intrinsically disordered proteins (IDPs) carry out important functions in cells and are related to the pathogenesis of many neurodegenerative diseases. To analyze IDPs, it is necessary to resolve different NMR signals generating from IDP residues. In this work, we present a new homonuclear decoupling scheme called Pre-Homonuclear Decoupling (PHD). The PHD method does not apply radiofrequency pulses and pulsed field gradients during the FID period, but is rather based on the in-phase/antiphase (IPAP) principle. We applied PHD to HSQC/TROSY and observed 3-fold narrower 1HN line widths compared with the control experiments. The PHD scheme provided narrow 1HN line widths with minimal artifacts for high-resolution analysis of IDPs.

**ECLECTICA IN MAGNETIC RESONANCE** (Posters 114 – 121)

**POSTER 114**
**Electric-field-induced orientation of molecules in solution**
Presenting Author: Ulrich Scheler

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In-situ application of a strong electric field induces orientation of molecules bearing an electric dipole moment in aqueous solution. In proton-only experiments the resulting residual dipolar coupling is detected in a J-resolved experiment. For a small molecule ß-alanine a weak order parameter is observed. A peptide of 10 residues exhibiting a dipole moment of 200 D shows a residual dipolar coupling that can be described by a Gaussian broadening of the dipolar lineshape and is scaling with the applied electric field. The electric field is applied synchronously to the NMR experiment and can thus be applied selectively for certain periods of the experiment.

**POSTER 115**
**Artificial Intelligence (AI)-based Lanthanide Sensing Utilizing $^{19}$F-Paramagnetic Guest Exchange Saturation Transfer ($^{19}$F-ParaGEST) Fingerprinting**
Presenting Author: Amnon Bar-Shir

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Highly-selective non-fluorescent analytical tools are required to monitor complex media lanthanide traces. Here, we combine our lanthanide-based $^{19}$F paramagnetic guest exchange saturation transfer (**$^{19}$F-paraGEST**) approach with magnetic resonance fingerprinting (**MRF**) to show an **AI-driven NMR-based lanthanide sensing platform**.
For this, a Bloch-McConnell-equations-based library of $^{19}$F-paraGEST effects was generated for Ln-α-CD (host) - fluorinated guest pairs and trained an AI-based system to reveal lanthanides' identity and concentration in an unknown solution. Using an optimized MRF acquisition protocol, the platform was examined on combinations of Ln-α-CDs, where the AI-MRF system recognized up to three lanthanides and their concentrations.
We envision **$^{19}$F-paraGEST MRF**, currently developed for nine lanthanides, will allow fast and selective sensing of lanthanides in wastes for future green chemistry applications.

**POSTER 116**
**On the Effects of Quadrupolar Relaxation in Earth's Field NMR Spectra**
Presenting Author: Adam Robert Altenhof

Complete Author List:
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NMR conducted at earth's field is not sensitive to the chemical shift interactions and yields only J-coupled spectra (JCS). These experiments offer several benefits over those at high field; however, several aspects of JCS have not been explored, such as the effects of relaxation from quadrupolar heteronuclei. Coupling from 14N to 19F or 1H is common in small organic compounds and can have a significant impact on the JCS depending on the magnitude of T1(14N) and T2(14N). Herein, I will describe a study on fluoropyridine samples with unique fluorine substitution that demonstrates the effects of 14N relaxation on JCS. SPINACH simulations are used to model the magnitudes and signs of all J-couplings for fluoropyridines and to determine T1(14N) and T2(14N).

**POSTER 117**
**Stereochemical Effects on Chemical Exchange Measured with Homonuclear J-coupling Spectroscopy**
Presenting Author: Stephen Devience

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We demonstrate stereochemical effects on proton exchange between a chiral solvent and chiral solute. We used homonuclear J-coupling spectroscopy with the Synchronized Echo pulse sequence at 6.5 mT to measure proton exchange between the chiral solvent ethyl L-lactate and both achiral and chiral solutes. Spectra of ethyl L-lactate mixed with water show that proton exchange modulates the intensity of spectral dips. Ethyl L-lactate spectra in the presence of either L- or D-mandelic acid showed no difference. However, spectra of ethyl L-lactate mixed with the ester methyl L- or D-mandelate showed that the D enantiomer exhibited faster exchange. We hypothesize that differences in the geometry of collisions and/or hydrogen bonding with L vs. D entantiomers strongly affect the rate of exchange.

**POSTER 118**
**Is CEST Possible at Ultralow Fields? 1H-14N Scalar Relaxation as an Alternative to Saturation Pulses**
Presenting Author: David E. Korenchan

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Ultralow-field MRI would benefit from access to molecular information, but the absence of measurable chemical shifts poses a major challenge. We propose to sensitize proton signal to amide and/or amine chemical exchange by inducing the depolarization of proton spins via scalar coupling to nitrogen-14, producing an effect analogous to proton radiofrequency saturation in chemical exchange saturation transfer (CEST) MRI. We demonstrate with high-field NMR spectroscopy of a highly concentrated urea sample that we can induce amide proton scalar relaxation by Hartmann-Hahn matching, and we show that the resulting signal depletion decreases the water proton pool via chemical exchange. Future work will adapt this technique to ultralow-field MRI scanners to provide chemical exchange contrast on low-cost MRI scanners.

**POSTER 119**
**Boosting 19F-NMR Sensitivity via Spectral Focusing for Target Environmental Analysis**
Presenting Author: Flavio Vinicius Crizostomo Kock

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In this work, a new NMR approach that uses single and multiple focusing to select discrete signals and/or chemical shift windows is introduced. In summary, the target 19F signals are first isolated by a gradient spin echo, and then focused by a train of shaped pulses during acquisition, with real time compensation for off-resonance phase decoherence. The user can choose whether to target one species (for example a multiplet from a single compound) or a window (for example all (CF2)n groups, to gauge long chain content in a mixture) depending on the goal of the study. Detection limits are improved by one order of magnitude for simple well dissolved systems and approaching 2 orders of magnitude for complex polymeric systems.

**POSTER 120**
**Solid State NMR Analysis of Chemical Agent Degradation on Composite Beads**
Presenting Author: David J. McGarvey, Ph.D.

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Using High-Resolution Magic Angle Spinning (HR-MAS) techniques, the reactions of chemical agents on composite beads were investigated. The composite beads consist of an active component that is integrated into a polymer matrix. The non-destructive nature of the NMR experiment allowed for the determination of the kinetics of the degradation, and a half-life of the agent on the matrix was determined. Both structural and quantitative information can be obtained simultaneously, so the identity of the breakdown products could be determined, as well as the rate of formation of each over time.
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**POSTER 121**
**Water-Proton T2 Relaxation in Tree Leaves Using Nuclear Magnetic Resonance at Hypogeomagnetic Fields**
Presenting Author: Anne Fabricant

Complete Author List:
*Anne Fabricant (Helmholtz Institute, University of Mainz); Dmitry Budker (Helmholtz Institute, JGU Mainz and UC Berkeley); Danila Barskiy (Johannes Gutenberg University Mainz)*

In our labs, we are developing a portfolio of experiments which employ magnetic-sensing techniques from physics and chemistry to investigate vital processes in living plants. Here we report on a relaxometry setup within the framework of zero-to-ultralow-field nuclear magnetic resonance (ZULF NMR) applied to the study of water dynamics in intact ex vivo green leaves.

**HYPERPOLARIZATION METHODOLOGIES** (Posters 122 – 168)

**POSTER 122**
**Towards Tabletop Recyclable Hyperpolarization with a Compact Freeze, Melt, and Flow DNP Polarizer**
Presenting Author: Charlotte Bocquelet

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*Charlotte Bocquelet (CRMN); Quentin Stern (UCBL); Huu-Nghia Le (CP2M); Laurent Veyre (CP2M); Chloe Thieuleux (CP2M); Roberto Melzi (Bruker Italia); Daniel Banks (Bruker Biospin); James Kempf (Bruker Biospin); Sami Jannin (CRMN)*

Hyperpolarization methods provide a way to greatly improve the inherently low sensitivity of NMR. Dissolution Dynamic Nuclear Polarization (d-DNP) was introduced more than twenty years ago, and now provides a 10'000-fold gain in sensitivity on a routine basis. However, the experiment is in a single-shot manner, therefore mostly incompatible with NMR spectroscopy, ruling out for example phase cycling and multidimensional sequences. Our ambition is to turn dissolution DNP into a new version that will be widely compatible with NMR spectroscopy by replenishing hyperpolarization with a compact closed-loop freeze, melt, and flow system. Here I will present the design and performances of the polarizer, with some preliminary results regarding the flow.

**POSTER 123**
**13C Radio Amplification By Stimulated Emission of Radiation (RASER) of Hyperpolarized Pyruvate**
Presenting Author: Shiraz Nantogma

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We demonstrate 13C RASER from tautomeric mixture of HP allyl [1-13C]pyruvate (ketal and hemiketal forms) prepared by hydrogenation of propargyl [1-13C]pyruvate with parahydrogen. 13C RASER pyruvate signals are produced from sample concentrations as low as 125 mM using commercial detector with Q of 32. We also show that although the substrate undergoes fast exchange (compared to the time scale of the experiment) between its ketal and hemiketal forms, the 13C RASER signal from one species does not "bleed" to less concentrated species that cannot enter RASER emission on its own. This work paves the way for 13C molecular imaging of HP pyruvate on conventional MRI scanners that lack 13C excitation electronics.

**POSTER 124**
**Hyperpolarized 13C NMR of Biofluid Samples at Natural Abundance by Dissolution Dynamic Nuclear Polarization**
Presenting Author: Victor Ribay

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Dissolution dynamic nuclear polarization (d-DNP) has recently shown promises for applications to 13C NMR metabolomics at natural abundance, however, previous studies have been restricted to metabolite extracts. Here we report, for the first time, the suitability of 13C d-DNP to provide rich information on a biofluid (urine). Single-scan 13C spectra recorded after d-DNP exhibit dozens of metabolite signals at natural abundance with a high resolution and repeatability. Moreover, accurate absolute concentrations can be retrieved relying on a standard addition workflow. These preliminary results showcase the ability of d-DNP to provide highly resolved and hyperpolarized spectra of biofluids, thus opening promising application perspectives for both untargeted and targeted metabolomics.

**POSTER 125**
**Across cities dDNP: design and performance of a compact He bath cryostat with NMR capability to transport hyperpolarized samples**
Presenting Author: Andrea Capozzi

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Hyperpolarization via dissolution Dynamic Nuclear Polarization (dDNP) has the potential to revolutionize diagnostic radiology. Nevertheless, the methodology struggles to enter everyday clinical practice. One of the reasons why broad consensus among clinicians is still missing lies in the technical complexity that characterizes hyperpolarization via dDNP. Differently from PET, hyperpolarized (HP) MR contrast agents cannot be transported and have to be prepared on-site.
We developed a robust methodology to change this paradigm. We herein present our latest updates on transportable hyperpolarization technology. Combining non-persistend UV-induced radicals and purpose build hardware, we demonstrated the first "across-cities-dDNP" experiments. We hyperpolarized glucose in Copenhagen, transported it for 320 km, and performed HP-MRI at Aarhus University Hospital in a rat model.

**POSTER 126**
**Overhauser Effect or Thermal Mixing or Something New**
Presenting Author: Yifan Quan

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We propose a new mechanism for DNP that is different from OE, SE, CE and TM. We denote the mechanism as Resonant Mixing (RM). We believe that this mechanism is responsible for the observed dispersive shaped DNP field profile for trityl samples near the EPR center. This new effect is purely due to the mixing of states by the microwave field together with the hyperfine coupling. The theory is furthermore applied to treat the OE, providing an analytical solution. When the ZQ and DQ cross relaxations are different we obtain an absorptive shaped DNP field profile near the EPR center, i.e. OE, while when they are the same, we obtain a dispersive shaped DNP field profile, i.e. RM.

**POSTER 127**
**Magic Angle Spinning EPR at 14 T**
Presenting Author: Ilia Kaminker

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Dynamic Nuclear Polarization (DNP) is revolutionizing solid-state NMR spectroscopy by allowing for over a hundredfold signal enhancements. Most contemporary DNP experiments are performed under magic angle spinning (MAS), and considerable experimental and theoretical effort has been dedicated to describing electron-nuclear polarization transfer, being the most crucial part of DNP, under these conditions. While this polarization transfer has been extensively studied using EPR under static-DNP conditions, yielding valuable mechanistic insights, this process was never experimentally investigated using EPR under MAS. Here we describe the first EPR experiments performed on spinning samples at 14 T and 390 GHz. This development paves the way for experimental observation of polarization transfer under the relevant conditions, serving to better understand DNP and facilitate further developments.

**POSTER 128**
**Efficient Polarization Re-distribution in Hyperpolarized Propane Produced Via Pairwise Parahydrogen Addition**
Presenting Author: Nuwandi M. Ariyasingha

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Polarization redistribution between nascent parahydrogen-derived protons with other protons is studied in hyperpolarized propane using Parahydrogen Induced Polarization. We have synthesized site-selective isotopically labeled 3-D-propylene for our studies. The deuterium presence in HP propane breaks the magnetic equivalence of methyl protons, which resonate at different frequencies. Pairwise parahydrogen addition to 3-D-propylene leads to 1,2-addition of parahydrogen, which we confirm by detecting corresponding PASADENA spectra, when synthesis is performed in the weakly-coupled regime at 14 T. Next, we employ ALTADENA (strongly-coupled) regime for pairwise addition to confirm that parahydrogen-derived HP protons can spontaneous polarize the –CDH2 protons, which did not originate from parahydrogen. These findings improve our understanding about hyperpolarized symmetric small hydrocarbons.

**POSTER 129**
**Relaxation Dynamics of Nuclear Long-Lived Spin States in Parahydrogen Hyperpolarized Butanes**
Presenting Author: Anna Samoilenko

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We present a systematic relaxation dynamics study of hyperpolarized butane as a potential candidate for inhalable hyperpolarized contrast agent in human lung imaging. HP butane was prepared via pairwise parahydrogen addition using 1-butene and 2-butene and detected at high-filed and low-field for comparison. Heterogeneous pairwise parahydrogen addition to butene provides a simple and robust approach for creating HP butane in the gas phase with high signal enhancements (PH~1% at 1.4 T) in comparison with widely studied HP propane using Rh/TiO2 catalyst. Moreover, the lifetimes of HP butane in both high-field (3.5±0.1s at 3.7 atm) and low-field (5.8±0.1s at 3.7 atm) are greater compared to that of HP propane making HP butane an excellent candidate for human pulmonary imaging and beyond.

**POSTER 130**
**Reversible NMR Hyperpolarization of 15N in Unmodified Amino Acids Unraveled at High Magnetic Field**
Presenting Author: Ewoud Vaneeckhaute

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Amino acids (AA's) and ammonia are unique metabolic markers, exerting essential roles in the nitrogen metabolism and cell regulation across plants and humans. Parahydrogen, the singlet spin isomer of molecular hydrogen, stands out as an exceptionally competitive hyperpolarization agent to boost their signal intensity in NMR. Production of hyperpolarization fueled by p-H<sub>2</sub> relies on transition metal catalysis, rather than on physical principles, thus inducing chemically selectivity towards specific molecular targets, traditionally excluding unmodified AA's from its repertoire. Here, we present an elegant all-high-field approach to reversibly hyperpolarize <sup>15</sup>N heteronuclei in free and catalyst-bound pristine alanine and ammonia while at the same time providing swift straightforward access to the molecular structure of the active hyperpolarization catalyst complexes.

**POSTER 131**
**Multi-dimensional Mapping of SABRE-SHEATH 13C Hyperpolarization of [1-13C]pyruvate**
Presenting Author: Isaiah Adelabu

Complete Author List:
*Isaiah Adelabu (Wayne State University); Shiraz Nantogma (Wayne State University); Thomas Theis (North Carolina State University); Boyd Goodson (Southern Illinois University); Eduard Chekmenev (Wayne State University)*

NMR hyperpolarization boosts sensitivity of MRI by 4-6 orders of magnitude, therefore, enabling real-time metabolic imaging. HP [1-13C]pyruvate is the leading 13C HP contrast agent because of its central role in metabolic activities with elevated uptake in cancers and other diseases. Rapid hyperpolarization of [1-13C]pyruvate via SABRE technique has enabled polarization values of up to 15%. Here, we report on simultaneous pH and temperature mapping of SABRE hyperpolarization process of [1-13C]pyruvate demonstrating complex trends that are readily understood through 2D mapping. We find that temperature and pH modulate C-13 polarization as well as the exchange rates and chemistry of SABRE process, therefore, enabling new approaches to improve the efficiency of SABRE-SHEATH polarization process of [1-13C]pyruvate.

**POSTER 132**
**Benchtop N-15 NMR Spectroscopy (1 T) of in situ Hyperpolarized Molecules with Natural Isotopic Abundance**
Presenting Author: Danila Barskiy

Complete Author List:
*Raphael Kircher (Johannes Gutenberg University Mainz); Jingyan Xu (Johannes Gutenberg University Mainz); Danila Barskiy (Johannes Gutenberg University Mainz)*

Analytical applications of benchtop NMR spectrometers could be expanded if robust hyperpolarization techniques were available for generating high degrees of
proton and heteronuclear spin polarization at natural isotopic abundance and without the need for sample shuttling. By using SABRE (Signal Amplification By Reversible Exchange) and optimized pulse sequences, we demonstrate NMR signals from biomolecules at mM concentrations in situ at 1 tesla (Figure 1). Since nuclear polarizations achieved in this way can exceed ten percent and measurements can be repeated multiple times, the sensitivity of benchtop-NMR detection is sufficient for measuring molecules at natural abundance of 15N nuclei. The presented methodology may find utility for the analysis of low-concentration chemicals using benchtop NMR spectroscopy with the aid of affordable hyperpolarization.

**POSTER 133**
**Biomolecular Applications of Low-Field NMR using SABRE Hyperpolarization**
Presenting Author: Christian Hilty

Complete Author List:
*Pierce Pham (Texas A&M University); Ratnamala Mandal (Texas A&M University); Olga Korzh (Texas A&M University)*

Nuclear spin hyperpolarization changes the sensitivity equation in NMR by uncoupling spin polarization from the magnetic field. Thus, low-field detection under biologically relevant conditions becomes possible. Here, we demonstrate the use of SABRE hyperpolarization for the detection of biomolecular interactions, whereby polarization is generated and signals are detected at milli-Tesla magnetic fields and below. This mode of detection not only presents an opportunity for simplification and cost savings in routine NMR experiments such as for ligand screening, but also significantly expands the magnetic field range accessible for the measurement of molecular dynamics and related parameters.

**POSTER 134**
**The Virtues of Stopping Dynamic Nuclear Polarization**
Presenting Author: Sami Jannin

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In dissolution dynamic nuclear polarization experiments, the near unity polarization of unpaired electron spins is transferred to surrounding nuclear spins via microwave irradiation. By intermittently stopping DNP by simply gating the microwaves, one can restore the near-unity electron spin polarization within a fraction of a second. As the electron polarization gets back towards unity, the electron flip-flop probability vanishes, which has a dramatic effect on transverse nuclear relaxation and on nuclear spin diffusion. I will present here the virtues of intermittently stopping DNP by simple microwave gating, which enables us to perform more efficient cross-polarization, detect EPR line shapes without EPR instrumentation, measure electron spin-lattice relaxation, and microwave saturation time constants, and study nuclear spin diffusion of invisible nuclear spins.

**POSTER 135**
**Hyperpolarization of Dopamine and its Application using Home-Built Parahydrogen Instrument**
Presenting Author: Quy Son Luu

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Dopamine is not only associated with Parkinson's, Alzheimer's, and schizophrenia diseases but also a precursor to polydopamine (PDA) formation. The PDA is a well-known mussel-inspired adhesive for multifunctional surface modification. Here, we built the bubbling system with high pressure (3 - 5 atm) and controlled the bubbling time via infrared (IR) remote control with an Arduino. In addition, we study the tracking of dopamine and the mechanism of PDA formation through the 1H and 13C nuclear magnetic resonance (NMR)-based signal amplification by reversible exchange (SABRE) and SABRE in shield enables alignment transfer to heteronuclei (SABRE-SHEATH) technique.

**POSTER 136**
**Hyperpolarized 29Si Magnetic Resonance Spectroscopy of Selectively Radical-Embedded Silica and α-Quartz Nanoparticles**
Presenting Author: Thi Quynh Nguyen

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Silica nanoparticles exhibit favorable characteristics for development as 29Si MRI probe. To mitigate the inherently low sensitivity of 29Si MRI, Dynamic Nuclear Polarization (DNP) technique can be applied to greatly amplify the NMR signals. Here, the 29Si DNP hyperpolarization of silica nanoparticles with selectively radical embedding in core, shell, and entire particles, are discussed. These particles can self-polarize without external radical addition and owing to the distribution of radicals homogeneously inside the particles, significant enhanced 29Si hyperpolarization signal is achieved. However, the signal lifetime is relatively short due to the paramagnetic effect of embedded radicals, thus amorphous silica is converted to crystalline α-quartz structure to extend the T1 relaxation time and open the opportunity for in vivo 29Si MRI application.

**POSTER 137**
**NMR at microTesla Fields for Hyperpolarization Applications**
Presenting Author: Laurynas Dagys

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The obstacle of low sensitivity in NMR may be alleviated by enhancing typically weak signals by orders of magnitude with use of hyperpolarization techniques. In this work we present Para-Hydrogen Induced Polarization (PHIP) as an efficient and convenient method for versatile production of hyperpolarized targets. The method can be performed at different magnetic fields each providing different benefits, but we direct the focus to microTesla fields as a regime that provides design freedom in aspects such as scalability and robustness. We discuss how relaxation influences polarization transfer techniques and demonstrate that variety of methods can be conveniently applied at microTesla fields. These developments display the potential for widespread application of hyperpolarization using PHIP on many target molecules.

**POSTER 138**
**Hyperpolarized solution-state NMR spectroscopy via intermolecular NOE with parahydrogen-polarized source molecules**
Presenting Author: Anna Parker

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In the past year we have published and presented work showing significant solution-state NMR enhancement by using overwhelming source magnetization to cross relax with small target molecules in solution. This work was originally demonstrated using optically-polarized naphthalene 1H spins and shown to give enhancements up to 2600 (over 60 MHz), 50 (400 MHz), and 40 (600 MHz). In the current work we show our efforts to translate this idea to a parahydrogen-polarized source molecule to enable a more accessible, high throughput method. Primarily, we have observed that conversion of singlet-state polarization to usable magnetization under normal experimental conditions is physically limited and is linked to the dipolar field effect. We will discuss such obstacles and recent advancements in this presentation.

**POSTER 139**
**Utilizing N@C60 as a Polarizing Agent: Electron-Decoupled MAS DNP**
Presenting Author: Nicholas Alaniva

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Nitrogen endofullerene (N@C60) is a well-protected unpaired electron source that features extremely narrow electron resonances and long relaxation times. Here, frequency-chirped microwaves are used to decouple electron- and 13C-spins in magic-angle spinning (160 parts-per-million) N@C60:C60 powder, improving DNP-enhanced 13C NMR signal intensity by 12% for 7 s polarization, and 5% for 30 s polarization. This extension of electron decoupled MAS DNP beyond previously employed trityl radicals is a step toward utilizing N@C60 as a controllable electron-spin source for magic-angle spinning magnetic resonance experiments.

**POSTER 140**
**Proton-only Detection of Hyperpolarized 13C2-pyruvate by S2M and R pulses**
Presenting Author: Iuliia Mandzhieva

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Hyperpolarized NMR has been developed to create high degrees of nuclear spin polarization approaching order unity compared to a polarization of ∼10−5 at thermal equilibrium.
Pyruvate is the most promising HP MRI substrate agent because it plays a central role in vital metabolic pathways and could be used as a biomarker for various diseases. However, HP MRI detection requires specialized 13C capabilities, including installing expensive coils and the entire RF hardware chain of amplifiers for pulses and TR switches and spectrometers.
The combination of SABRE-SHEATH and S2M/S2M composite/R pulses create an opportunity for proton-only HP MRI with existing MRI scanners and may be particularly attractively when used with low-field MRI machines establishing an affordable molecular imaging platform.

**POSTER 141**
**Catalyst and Methanol Free Injection of SABRE Hyperpolarized [1-13C]Pyruvate Detected In Vivo**
Presenting Author: Keilian John MacCulloch

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First catalyst and methanol free solution of hyperpolarized pyruvate detected in vivo employing the Para-Hydrogen Induced Polarization (PHIP) modality known as Signal Amplification By Reversible Exchange (SABRE). SABRE is a simple, inexpensive, and fast hyperpolarization modality that directly hyperpolarizes pyruvate near room temperature. In this work, highly polarized [1-13C]pyruvate was generated in an ethanol/water mixture and then filtered through a C18 cartridge for catalyst removal prior to injection into a healthy Wistar rat. The hyperpolarized pyruvate signal was monitored in vivo with a dynamic pulse sequence in a 1.5 T MRI.

**POSTER 142**
**Enabling the Broad Class of Alpha-Keto Acids as SABRE Hyperpolarization Targets and Exploring Their Polarization Dynamics**
Presenting Author: Stephen McBride

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In this work, we expand the scope of SABRE substrates by employing SABRE-SHEATH and temperature cycling to hyperpolarize six different α-keto acids: [1-13C]pyruvate (PYV), α-ketoglutarate (AKG), oxaloacetic acid (OAA), phenylglyoxylic acid (PGA), phenylpyruvate (PPYV), and 2-oxobutyrate (2-OB). Additionally, we obtained T1 relaxation and polarization buildup measurements to develop a theoretical model to characterize SABRE polarization relaxation and buildup dynamics. In conclusion, several new α-keto acids were added to the SABRE substrate scope, and a mathematical model for the SABRE dynamics was refined to explain the hyperpolarization build-up and decay dynamics.

**POSTER 143**
**Improving SABRE Polarization Through Three-Dimensional Magnetic Field Manipulation**
Presenting Author: Shannon L Eriksson

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X SABRE is a rapidly developing heteronuclear hyperpolarization modality where μT magnetic fields along the leading axis are commonly used to facilitate population transfer between spin states of interest. Because the necessary fields are small, it is trivial to rapidly change the magnetic field in three dimensions, a degree of freedom that has yet to be explored. Here, we introduce pulse sequences developed using conventional magnetic resonance techniques like decoupling, as well as an arbitrary shaped pulse optimized using an evolutionary strategy. These pulse sequences protect singlet spin order in existing pulsed SABRE SHEATH techniques, facilitate direct measurement of the initial coherent dynamics in this complex system, and improve magnetization yields up to 7-fold and singlet yields up to 4-fold.

**POSTER 144**
**Optimizing Parahydrogen-Enhanced 1H MRI Using a Clinical "Point-of-Care" Low-Field Scanner.**
Presenting Author: Nadiya Iqbal

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When combined with hyperpolarization, low-field (LF) MRI has the potential to address many limitations presented by conventional MRI. We report on our continuing efforts to explore the potential for integrating a clinical low-field (64 mT) point-of-care MRI scanner with parahydrogen-based hyperpolarization. To increase the scanning speed, we have investigated imaging of SABRE-hyperpolarized substrates using a batch-mode approach where SABRE is performed in the fringe field, followed by rapid sample transfer to the scanner's head coil, boosting the signal to allow high-resolution images to be obtained in under 15 s. We are currently working on building a continuous flow system to enable uninterrupted SABRE 1H MRI to better enable optimization, as well as efforts to perform low-field MRI with HP propane gas.

**POSTER 145**
**Data-constrained Determination of Applied Flip Angles to Improve Hyperpolarized 13C MR Kinetic Modeling in the Presence of Large B1 Variations Encountered in Abdominal Imaging**
Presenting Author: Tanner Nickles

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A major challenge in the clinical translation of [1-13C]pyruvate hyperpolarized (HP) 13C MRI in human abdominal studies is B1 inhomogeneities across the large FOV that could confound metabolite-specific imaging methods. Given variations in B1, the exact applied flip angle in all voxels across the abdomen is often unknown, leading to errors in the quantification of metabolite conversion-rates. To overcome this limitation in abdominal studies, kinetic modeling within a numerical simulation regime was successfully used to determine the actual flip angle in the presence of variations in B1 without explicitly knowing it. In this study, the estimated flip angle approximated ground truth and <7% kPL bias was determined at both high and low metabolite conversion-rates.

**POSTER 146**
**DNP Study of Crude Oil Suggests Several Competing DNP Mechanisms**
Presenting Author: Timothy Keller

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The radical content in crude oil gives rise to several DNP mechanisms, most notably the Overhauser effect and solid effect. In this work, we provide evidence for a 3rd DNP mechanism in crude oil, the cross effect.
In recent work, we have performed high resolution DNP at low fields in liquids. This resolution has allowed us to distinguish the aliphatic and aromatic protons in the 1H NMR spectrum of crude oil.
We find that aromatic protons of crude oil exhibit larger enhancements than the aliphatic protons. At high microwave powers, we observe a decrease in the enhancement for many samples. We attribute this to an "over-saturation" effect which provides evidence for the cross effect DNP mechanism.

**POSTER 147**
**Advances in SABRE hyperpolarization, including RASER detection, and first in-vivo demonstrations**
Presenting Author: Thomas Theis

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Parahydrogen induced polarization (PHIP) is cherished for its relative simplicity and ease. Here we report on the most recent progress with hydrogenative and non-hydrogenative PHIP (aka SABRE). We report on three major advances, which include (a) SABRE-SHEATH (SABRE in Shield Enables Alignment Transfer to Heteronuclei) hyperpolarization of carbon-13 in many different alpha-keto acids, thereby significantly broadening the substrate scope (b) the first carbon-13 Radiofrequency Amplification By Stimulated Emission of Radiation (RASER) measurements exhibiting striking non-linear "quantum" detection thresholds and (c) the first in-vivo molecular imaging after SABRE-SHEATH hyperpolarization of [1-13C]pyruvate showing the detection of metabolic conversion of pyruvate to lactate, carbonate pyruvate-hydrate and alanine.

**POSTER 148**
**Improved TinyPol Radicals for High-Field and Fast MAS DNP NMR**
Presenting Author: Moreno Lelli

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Here we present the development of new water-soluble di-nitroxides biradicals, analogous to TinyPol, but with optimized molecular geometry, promoting high electron-electron (e-e) magnetic interaction, and incorporating also recent concepts such as the stereo-controlled conformation and efficient radical-solvent interaction.
These new systems show excellent performances, especially at high magnetic fields and fast MAS.
In particular, M-TinyPol(OH)4 shows enhancements up to about 200 even at 65 kHz of MAS frequency and 18.8 T. These systems provide high overall sensitivity that places them at the highest values among the polarizing agents developed in aqueous media at 18.8 T. The role of the structural improvements will be discussed, also with the aid of simulations.

**POSTER 149**
**Investigation of LC-Photo-CIDNP Magnetic-Field Dependence of Molecules bearing a Quasi-Isolated Spin Pair via a Rapid Shuttle Field-Cycling Device**
Presenting Author: Siyu Li

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Low-concentration photo-chemically induced dynamic nuclear polarization (LC-photo-CIDNP) is an emerging optically enhanced technique that leads to significant NMR sensitivity enhancements in solution. LC-photo-CIDNP requires solvent-exposed aromatic moieties, e.g., tryptophan and tyrosine. This study investigates the magnetic-field dependence of the 13C LC-photo-CIDNP of a Trp isotopolog (Trp-alpha-13C-beta,beta,2,4,5,6,7-d7) bearing a quasi-isolated 1Halpha-13Calpha spin pair. We employed a new rapid-shuttle field cycling device with in-situ side illumination and fast field-transition times. This setup enables rapidly shuttling NMR samples and maintaining excellent resonance lineshapes. Analysis of the magnetic-field dependence of LC-photo-CIDNP of Trp-alpha-13C-beta,beta,2,4,5,6,7-d7) led to identifying remarkable enhancement factors of ca. 1,000 at low illumination fields (ca. 50 MHz, 1.18T). This approach bears promise for the future detection of larger biomolecules (e.g., proteins).

**POSTER 150**
**PHIP 13C Radiofrequency Amplification by Stimulated Emission of Radiation (RASER)**
Presenting Author: Christopher Nelson

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Hyperpolarized Magnetic Resonance Imaging (HP MRI) is hailed as a next-generation molecular imaging modality. Because 13C resonate at ~4 times lower frequencies compared to protons, excitation of 13C spins is hardly possible with conventional clinical MRI scanners. In this work, we demonstrate a 13C RASER, detected without an excitation pulse, in HP ethyl [1-13C] acetate prepared via pairwise addition of parahydrogen to vinyl [1-13C] acetate and polarization transfer from the protons to the carbon-13 via magnetic field cycling. RASER signals were detected using a non-cryogenic 1.4T NMR spectrometer. RASER signals were observed for several minutes from a single sample, achieving 21mHz NMR linewidths. Our work demonstrates the feasibility of 13C RASER creation using a bolus of HP ethyl-[1-13C] acetate.

**POSTER 151**
**15N SABRE-SHEATH and NMR/MS/DFT Characterization of Amino-Metronidazole, a Metabolic Product of the Antibiotic and Prospective Hypoxia Contrast Agent Metronidazole**
Presenting Author: Ishani Senanayake

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The antibiotic metronidazole (MNZ) has gained interest as a potential MRI contrast agent for imaging hypoxia. SABRE-SHEATH can provide efficient hyperpolarization of 15N3-MNZ, but the envisioned MRI approach requires that MNZ will rapidly undergo structural changes in hypoxic environments with significant 15N frequency differences manifested in its downstream metabolic products. We have conducted computational (DFT) studies to predict 15N chemical shifts of different relevant species, as well as performed NMR studies of amino-MNZ (despite anticipated stability concerns). Direct hyperpolarization of naturally abundant 15N spins in amino-MNZ via SABRE-SHEATH (enhancement ~18,000), along with long-duration 1H-decoupled 15N NMR experiments, allowed comparison with both 15N3-MNZ and naturally abundant MNZ, showing significant 15N shift differences that showed good agreement with DFT predictions.

**POSTER 152**
**Dissolution DNP on hydrophobic molecules using organic solvents opens new perspectives for the study of complex organic mixtures**
Presenting Author: Chloé Gioiosa

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Dissolution DNP has proven to be a very powerful hyperpolarization technique enabling exceptional increase in sensitivity in liquid state NMR. Over the last two decades, numerous applications of dDNP have emerged in fields of research such as metabolomics, biochemistry or imaging on rather aqueous matrices. It is however yet to be widely developed in fields such as the energy industry where hydrophobic matrices need to be probed. Here, we present our first d-DNP results on 13C labelled benzaldehyde prepared in a toluene glassing matrix, hyperpolarized through cross-polarization on a Bruker prototype DNP polarizer, and rapidly dissolved with isopropanol and injected in a 14T spectrometer. These first experiments allowed us to reach signal enhancement over 70 000 with 11% 13C polarization.

**POSTER 153**
**SABRE Hyperpolarization of Cytosine and other Nucleobases**
Presenting Author: Max Gemeinhardt

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A number of DNA nucleobases were polarized by an efficient and comparatively low-cost methodology, signal amplification by reversible exchange (SABRE) and its heteronuclear extension, SABRE in Shield Enables Alignment Transfer to Heteronuclei (SABRE-SHEATH). For example, SABRE hyperpolarization of natural abundance 3-methyladenine yielded 15N signal enhancement of ~3,300 at 9.4 T. The same methodology afforded 15N and 13C signal enhancements of doubly labeled cytosine of up to ~240-fold and ~50-fold, respectively. The hyperpolarization-enhanced spectra of the different nucleobases can provide insight into the presence of different tautomers and their respective ability to support SABRE processes. In turn, this information can potentially help to select and successfully hyperpolarize novel biologically relevant molecular targets for various envisioned applications.

**POSTER 154**
**Fast Nanomolar Detection and Fragment Screening on a Benchtop NMR Spectrometer Boosted by Photo-Induced Hyperpolarization**
Presenting Author: Gabriela Stadler

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The sensitivity limitation of NMR spectroscopy can be overcome by photo-chemically induced dynamic nuclear polarization (CIDNP). The expansion of the method's chemical space is shown with the design of a 212-compound fragment library and its screening against PIN1 at 600 MHz. With single-scan experiments of a few seconds using low micromolar concentrations, we reach an unprecedented screening rate of 1500 samples per day with our new flowthrough system. Moreover, photo-CIDNP spectra are acquired within 3 minutes on a cryogen-free 80 MHz benchtop spectrometer, which is demonstrated by a miniscreen with 28 fragments. We reached a detection limit of 100 nM in only 3 minutes on the benchtop spectrometer, while without hyperpolarization no signal was detected after days of continuous measurement.

**POSTER 155**
**The Emergence of Efficient DNP in Trityl-Based Multiradicals at Sub-Nanometer Electron-Electron Distances**
Presenting Author: Raj Chaklashiya

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Multi-Electron Dynamic Nuclear Polarization (ME-DNP) has enormous potential for quantum sensing of nuclei through enhancement of NMR signal, but its current implementations are through radical clustering, a stochastic process that is difficult to control. A fine-tuned multiple-electron geometry with strong and asymmetric coupling would provide precise control over quantum coherences and polarization transfer for optimal ME-DNP. Here we share both our experimental and theoretical results on how to achieve controllable 1H ME-DNP in a designed electron geometry: a trityl-based tetra-radical. Our findings give us the design parameters necessary for electron geometries to achieve controllable ME-DNP for quantum sensing.

**POSTER 156**
**SABRE Hyperpolarization with up to 200 bar Parahydrogen in Standard and Quickly Removable Solvents**
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In this work, we report on SABRE hyperpolarization up to 200 bar in standard and quickly removable solvents. We employ a recently introduced low-cost, versatile high-pressure setup, which enables spectroscopy measurements with a compact NMR magnet. With this setup, we achieved 2% SABRE polarization at a substrate concentration of 60 mmol/l, equal to a molar polarization of 1.2 mmol/l. Additionally, SABRE hyperpolarization in liquefied ethane and compressed CO2 at 200 bar was demonstrated. Eliminating standard SABRE organic solvents such as methanol in hyperpolarization techniques is a prerequisite for molecular medical research.

**POSTER 157**
**Hyperpolarized Liquid-State 13C NMR Signals from 1H Dissolution-Dynamic Nuclear Polarization via INEPT Transfer**
Presenting Author: James Tolchard

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The low sensitivity of NMR spectroscopy and imaging can be boosted by factors approaching ~10000x with hyperpolarization methodologies, such as dissolution-dynamic nuclear polarization. In small molecules, 13C-spins are typically polarized either directly, which is slow and yields low polarizations, or indirectly by pulse sequences such as cross-polarization, which is efficient but often unavailable. Here, we present the hyperpolarization of 1H-spins, which polarize rapidly and to a higher extent, before dissolution and a subsequent refocussed INEPT transfer to 13C polarization. Importantly, we exploit the minimal transfer time between our polarizing instrument and spectrometer (~1.7s) to overcome short 1H relaxation times. We will present our hardware setup, 13C polarization recoverable from solid-state 1H hyperpolarization, and simulations aiding the interpretation of 13C lineshapes.

**POSTER 158**
**Hyperpolarization of 15N Betaine**
Presenting Author: Magnus Karlsson

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NMR signals can be enhanced by several orders of magnitude with hyperpolarization techniques. A limitation of hyperpolarization is the lifetime of the signal; The signal created by hyperpolarization will decay towards the thermal level with the T1 of the nucleus. Hence, hyperpolarization molecules with long T1 nuclei are much preferred. Quaternary ammonium compounds can have long 15N relaxation time constants with several examples in the > 5 minutes range. Here we present results from experiments with one such compound: 15N labeled betaine.

**POSTER 159**
**The Steady-State PHIP RASER: Generating a Continuous NMR Signal**
Presenting Author: Jing Yang

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RASERs (Radio Amplification by Stimulated Emission of Radiation) allow to measure high-precision NMR spectra as well as study nonlinear phenomena. To operate a RASER, a population inversion is required, which can generated by hyperpolarization methods. With parahydrogen fueled RASERs, various new use-cases were unveiled in the recent years, all based on RASERs with multiple frequencies. However, parahydrogen fueled RASERs operating at high magnetic fields are burdened by the parahydrogen pumping itself.
In this work, we report on a steady-state multimode RASERs operating in different regimes pumped by hyperpolarized ethyl acetate. We demonstrate operating regimes dominated by five different scenarios depending on the population inversion: a starting RASER, the "normal NMR" two-mode RASER, frequency combs, period doublings, and chaos.

**POSTER 160**
**Ultra-low Temperature Overhauser Dynamic Nuclear Polarization**
Presenting Author: Scott A. Southern

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Overhauser DNP is possible in insulating solids when dynamics can result in the modulation of hyperfine couplings. We discovered that the methyl functionalization of the Blatter radical could activate the Overhauser Effect (OE), resulting from the methyl group dynamics modulating the hyperfine coupling to its protons, providing a mechanism for intramolecular cross-relaxation.
We predicted the free energy barrier for methyl rotation to define an approximate rovibrational wavefunction describing the dynamics, enabling us to predict the temperature dependence of the cross-relaxation.
Ultra-low temperature MAS-DNP experiments were used to study the mechanism of methyl-driven OE DNP. We observed increasing OE performance with decreasing temperature for $CH_3$ and $CD_3$ radicals, suggesting that at very low temperatures, librations are the dominant source of cross-relaxation.

**POSTER 161**
**Clustering of P1 centers, and by proxy NV centers, observed by DNP and EPR**
Presenting Author: Santiago Bussandri

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Through a collaborative study, we have found that P1 centers are clustering in more significant ways than previously anticipated using DNP profile measurements and EPR methods at room temperature and high field. Understanding the spatial distribution of P1 centers is critical because it directly reflects on the distribution of NV centers, which are essential tools for quantum information sensing. By decomposing the 7T DNP profile, we were able to identify different electronic spin populations and their respective EPR and DNP properties. ELDOR spectroscopy measurements and 13C DNP build-up experiments demonstrated the presence of a broad clustered species, in two common types of diamonds used widely in the community. These findings provide valuable insights for the development of advanced quantum technologies.

**POSTER 162**
**Following Expected and Unexpected Molecular Interactions of Cucurbit[6]uril in a Molecular Relay with HyperCEST NMR**
Presenting Author: Leif Schröder

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Cucurbit[6]uril (CB6) and cucurbit[7]uril (CB7) are macrocyclic hosts that bind to different ends of the two-faced guest (TFG) AMADA-Put. Their cavities and portals can also be occupied by other competing guests and the details of the TFG transition from CB6 to CB7 were not yet fully known. Here, we investigate this transition using Xe-129 as a hyperpolarized monoatomic guest that is very sensitive to perturbations of the accessibility of CB6. We analyze anticipated and unexpected changes in saturation transfer responses for HyperCEST z-spectra that give insights into the rearrangements at the CB6 cavity. These insights should be included into the overall promiscuous binding behavior of CBs in various applications.

**POSTER 163**
**Optimization of laser-induced OH• Radical Generation in Water**
Presenting Author: Leon M. Geiger

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The use of radicals to transfer spin polarization to nuclei is an important technique to increase the signal intensity of NMR measurements. The classical methods require several tens of minutes and therefore suffer from the degradation of radical concentration during the generation process when spin-traps like DMPO are used. By using high-power pulsed laser systems, we can generate more radicals in a shorter timescale compared to the UV-generation method. Additional advantages are that only water is required to form OH• instead of hydrogen peroxide, and there is potential to locally generate radicals for in situ applications. From the EPR spectroscopy, the amount of bonded OH• radicals were calculated. Together with the number of spins, the DMPO capture efficiency was determined.

**POSTER 164**
**Sustainable and cost-effective MAS DNP at 30 K with cryogenic sample exchange**
Presenting Author: Gaël DE PAËPE

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We present a home built setup to perform sustainable and cost-effective fast Helium MAS DNP at 30 K with cryogenic sample exchange capability. Using cAsymPol-POK, a newly introduced polarizing agent for DNP, we report large signal-to-noise improvement for proton-dense methyl-containing organic powdered samples that are difficult to polarize at 100 K (currently the lowest temperature accessible in most DNP labs).

**POSTER 165**
**Hyperpolarized glucose for non-invasive In-Cell measurements of glycolytic bottlenecks**
Presenting Author: Pernille Rose Jensen

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The control and response of metabolic networks is still incompletely understood, even in highly studied model organisms. Without counterpart experimental data, computational mechanistic models remain hard to probe for their predictive value in vivo. Direct real-time measurements of metabolic flux can be obtained in cellular systems with 13C NMR using dissolution upon dynamic nuclear polarization in the solid state (dDNP-NMR). Here, we show recent strides in improving dDNP-NMR assays to include detection of the metabolites from upper part of the glycolysis, which have been shown as key steps in control of glycolytic flux.

**POSTER 166**
**Overhauser DNP in Supercritical Ethane at High Magnetic Field**
Presenting Author: thierry dubroca

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DNP in liquids is challenging, particularly at high magnetic fields, where resolution is needed to solve scientific questions. We present here a large sample volume pressure cell combined with a double resonance (13C-1H) liquid DNP probe capable of delivering significant microwave power at the sample operating at 150-600MHz (i.e.14.1T). This newly developed cell is applied to perform scalar Overhauser DNP with 13CCl4 and 13CHCl3 in supercritical ethane. The low viscosity fluid promotes short correlation times which increase the DNP efficiency. Efforts are on the way to increase the pressure range of the cell to accommodate a wide variety of supercritical fluids with the ultimate goal of being able to perform 1H ODNP at high magnetic fields.

**POSTER 167**
**DNP-Enhanced NMR Analyses of Surface Group Interactions & Distributions on Colloidal Silica Particles**
Presenting Author: Matthew Lertola

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The surface functionalization of colloidal silica particles is a key determining factor of their macroscopic properties, including colloidal stability. Solid-state NMR is an important tool for understanding silica surface chemistry at the atomic level, which requires surface-selective techniques with enhanced sensitivity, especially for dilute loadings of covalently grafted organic groups. Here, we use solid-state DNP NMR methods to establish the surface distributions of two types of organic groups on silica nanoparticles. In particular, solid-state 2D DNP-enhanced 13C{1H} heteronuclear correlation (HETCOR) NMR analyses of freeze-dried silica nanoparticles reveal differences in the extents of commingling of surface organic groups between samples, which explain differences in their respective stabilities as colloidal suspensions.

**POSTER 168**
**Investigation of DNP Mechanisms**
Presenting Author: Ravi Shankar Palani

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Dynamic Nuclear Polarization (DNP) overcomes the issue of low sensitivity that Nuclear Magnetic Resonance (NMR) suffers from. The mechanism at play is determined by a host of factors including, but not limited to, the nature of the radical and microwave irradiation frequency. In this work, we discuss methods to investigate finer details of the underlying DNP mechanism and the polarization pathway in BDPA family of radicals and trityls. In BDPA our investigation led to designing Phe-d5-BDPA that specifically attenuates the DQ cross-relaxation pathway, improving enhancment by 50%. In trityls, we discuss the plausibility of thermal-mixing and characterize the mechanism under different conditions. We also investigate the competition between simultaneously active DNP mechanisms with multitone microwave irradiation and observe interesting spin-physics.

**INSTRUMENTATION** (Posters 169 – 193)

**POSTER 169**
**Stripline Lenz lens add-on with one order of magnitude signal enhancement**
Presenting Author: Jianyi Liang

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A Lenz lens is an electrically passive metallic radiofrequency interposer placed between a sample and a tuned or untuned nuclear magnetic resonance (NMR) detector. Its utility is to focus the B1 field of the detector onto a smaller sample space. Here we explore a novel embodiment of the Lenz lens, which acts as a non-resonant stripline interposer, i.e., the B 1 -field acts along the longitudinal volume of a sample container, such as a capillary or other microfluidic channel that is coincident with the axis of the stripline. The results show an enhancement up to one order of magnitude for a broadband application, i.e. from 130MHz to 500MHz.

**POSTER 170**
**Automation in solid state NMR**
Presenting Author: Jochem Struppe

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Herein we show a new strategy for automated experiment setup by using radio frequency reference fields, provided in lookup tables to automatically calculate rf pulses for excitation or recoupling, spinlock fields during cross polarization or decoupling fields for homo- or heteronuclear spin decoupling. This approach permits controlling the maximum decoupling field through simple field parameters, available in lookup tables, instead of abstract, machine oriented rf-power values. Often, these fields are synchronized with or have specific relationships to the magic angle spinning frequency. The approach permits easy experiment setup for any CPMAS experiment, whether it is a simple basic CPMAS experiment or a more complicated NMR experiments like any high-frequency MAS experiments with rotation rates of 111 kHz and above.

**POSTER 171**
**Cryogen-free 9.4 T Solid state MAS NMR system**
Presenting Author: Eugeny Kryukov

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The ongoing crisis with liquid helium supply is getting more severe. We offer dry superconducting magnets based on cryogen-free cold heads that can replace the conventional magnets up to of 750 MHz 1H frequency. Our magnets are not only free from liquid cryogens, they are very compact and allow for probe insertion from the bottom or from the top of the magnet. The field value can be easily changed and made stable in an hour after the field ramp. This feature makes it possible to use the same magnet at many fixed fields or in a field sweep mode.
All of the above features were experimentally demonstrated on our in house 9.4 T MAS NMR system.

**POSTER 172**
**Spin Echoes, Adiabatic Pulses, With Fantastic Sensitivity: Can Your Probe Do This?**
Presenting Author: Paul Ellis

Complete Author List:
*Paul Ellis (Doty Scientific); Daniel Arcos (Doty Scientific); F David Doty (Doty Scientific)*

We have examined the performance of a standard Doty 4 mm MAS probe utilizing adiabatic (WURST) pulses. The performance of the probe demonstrated an excellent bandwidth and sensitivity. To accomplish these objectives, we have used two spin echo methods. The details of these methods are outlined within this presentation. We applied the spin echoes to three different samples, 119Sn in the form of SnO, 79Br as KBr, and 25Mg as Mg(O2CH)2•2H2O. The latter two samples are quadrupolar in nature with spins of 3/2 and 5/2, respectively. All the samples were at natural abundance for the spin systems of interest.

**POSTER 173**
**Advances in Spherical Rotor DNP**
Presenting Author: Lauren Price

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Spherical rotors have many advantages for MAS DNP but the current 3D printed plastic stators are unable to withstand the cryogenic temperatures required. Here we introduce a probe assembly designed for spherical rotors at cryogenic temperatures. This system was used to successfully perform the first MAS DNP using spherical rotors. Using 9.5 mm spherical rotors, a maximum DNP enhancement of 256 on a sample of 20 mM AMUPol, 4 M 13C 15N Urea in 60/30/10 d-8 glycerol/D2O/H2O was obtained. The sample was spinning at a frequency of 2 kHz and a temperature of 107 K. This system is also being scaled for 6 mm spherical rotors which will increase spinning frequency to above 5 kHz.

**POSTER 174**
**NMR Spectroscopy of Nanomole Amount Samples on a Homebuilt 2.1 Tesla NMR Magnet Using a Microsolenoid**
Presenting Author: Sander Baas

Complete Author List:
*Sander Baas (WUR); Aldrik Velders (WUR, UCLM)*

The past decades have brought increasingly strong magnetic fields to NMR, in order to improve resolution and sensitivity, with the current highest commercial field strength of 28.2 Tesla.. In recent years however, there has been a renewed interest in NMR at fields of several Tesla, making use of more affordable permanent magnets to produce the B0 field. We present a compact, cheap, homebuilt 2.1 Tesla NdFeB permanent magnet system for NMR spectroscopy. Sample handling occurs via a capillary-based microfluidic probe, with a microsolenoid transceiver coil. Currently the magnet system is operated in non-shimmed mode, with a movable probe stage for sample positioning. Coupled with hyperpolarization, samples amounts in the lower nanomole range (mM concentration) can be detected within a minute

**POSTER 175**
**Advanced Integration of Batch-Mode Clinical-Scale SEOP Xenon-129 Generation-3 Hyperpolarizer**
Presenting Author: Clementinah Oladun

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Hyperpolarized 129Xe gas is a revolutionary MRI contrast agent that has been recently FDA approved for clinical use. Hyperpolarized 129Xe is produced via spin-exchange optical pumping. Our clinical-scale batch-mode generation-3 SEOP hyperpolarizer employs batch-mode production, as well as in-situ polarimetry of Rb electron and 129Xe nuclear spin polarization. Here, we demonstrate next-generation advanced automation and systems integration embodied by our 129Xe hyperpolarizer. NMR and NIR polarimetry are performed in real time in a fully automated fashion using an ARM-based SMT32 microcontroller and a purpose-built low-field NMR spectrometer and a NIR spectrometer without any other devices. The resulting real-time 129Xe nuclear- and Rb electron polarization values are employed for auto-calibration and HP 129Xe production quality monitoring.

**POSTER 176**
**Ball-Shift Automation to Achieve Reproducible Mapping of Transceiver Coils**
Presenting Author: Jose Luis Uribe

Complete Author List:
*Jose Uribe (UC Irvine); Matthew Derek Jimenez (UC Irvine)*

Achieving homogenous radiofrequency (rf) magnetic fields in solid-state NMR transceiver coils is essential for maximizing sensitivity during experimentation. Manual methods to measure coil homogeneity successfully and accurately have been a time-consuming and error-prone task, specifically with assessing spatial accuracy. An automated method that uses inexpensive and open-source equipment to create a modular, yet specialized tool, is presented, the Auto-Ball Shift (ABS). This mechanical apparatus is fully controlled by an Arduino UNO; designating pins, controlling direction, rotation speed, etc. The addition of an A4988 microstepper allows for precise fine

increments as low as 0.05mm. An automatized data collection scheme that uses Python scripting is used. This makes for a hands-free method which returns parsed rf coil data ready for mapping.

**POSTER 177**
**Room-Temperature Overhauser DNP with Microwave Powers of Just 100's of Milliwatts at 7 T**
Presenting Author: Alexander A. Nevzorov

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*Alexander Nevzorov (North Carolina State University); Antonin Marek (North Carolina State University); Gabriel Arias (North Cariolina State University); Sergey Milikisiyants (North Carolina State University); Alex I. Smirnov (North Caroilna State University)*

Currently, performing DNP at >200 GHz involves expensive gyrotrons. We demonstrate that all-dielectric photonic band-gap resonators (PBGR) make it possible to use compact, frequency-agile solid-state mm-wave sources with output powers of <400 mW to achieve appreciable solid and Overhauser DNP effects. We report on room-temperature Overhauser DNP gains of about 50 for 1M PhP3 and 100mM BDPA co-dissolved in d-toluene. Anodic Aluminum Oxide nanopores were employed as holders for creating thin, flat liquid samples to enhance the resonator performance. The results demonstrate the ability of a tuned resonator to effectively concentrate mm-waves for both liquid and solid samples. A dramatic increase in the PBGR Q-factor up to >1,000 can be achieved by utilizing full-defect photonic crystals. Supported by NIH 1R01GM130821.

**POSTER 178**
**Development of a Novel 13C HTS Probe at 21.1 T**
Presenting Author: Arthur S Edison

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Direct observation of 13C has many advantages in biological solution NMR spectroscopy. The primary limitation is the relatively low sensitivity of 13C compared to 1H. We report a new 13C HTS probe at 21.1 T with a novel 3-mm x 6.2-mm rectangular tube geometry. The volume of the rectangular sample tube is about 425 uL, allowing us to develop applications that were previously impractical with a smaller volume probe. We also have the option of using a 3-mm standard cylindrical tube with a reduced volume. The overall mass sensitivity is between about 2-3 times greater than a commercial 5-mm TXO cryogenic probe on the same instrument, depending on the sample. Data from urine and other biological samples will be shown.

**POSTER 179**
**Improving Low (<100 mT) and Ultra-low (<10 mT) Field RF Fidelity with Active Transmit/Receive Switches and Q-Switching for Quantitative Magnetic Resonance**
Presenting Author: Karl Stupic

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Low and Ultra-low magnetic field technology has seen expanded use in recent years for deployment as point-of-care systems for healthcare. As these systems continue to find further applications, issues such as phase stability and RF pulse fidelity at low RF frequencies is important to consider for quantitative results. Presented here are active switches utilized for both transmit/receive switches as well as for Q switching with the needed stability. These active switching systems are necessary as common passive switch designs such as crossed diodes can present phase instability due to low power requirements at low RF frequencies. Additionally, quality factor (Q) of RF coils plays a large role in pulse shape at low frequencies leading to added uncertainty in quantitative measurements.

**POSTER 180**
**A Portable and Low-Cost MRI System Using an Impedance-Mismatched Front-End and SoC-Based Controller**
Presenting Author: Soumyajit Mandal

Complete Author List:
*David Ariando (University of Florida); Soumyajit Mandal (Case Western Reserve University)*

In low-field NMR applications, such as emerging portable MRI devices, the benefit of impedance matching are not apparent, since reflections become insignificant at low frequencies (<10 MHz). However, the use of matched probes and transceivers is still standard practice at low frequencies (100 kHz-10 MHz), except for the use of audio transceivers at extremely low frequencies (<100 kHz). This work provides an alternative by using tuned but impedance-mismatched circuits for both signal transmission and reception and highlighting its benefits for portable MRI. A compact battery-powered pulsed-mode gradient driver is also described. The B0 field is generated by a low-cost Halbach array assembled from Ferrite magnets and 3D-printed holder. The system controller is an SoC-FPGA supporting autonomous measurement operations.

**POSTER 181**
**Single-sided magnetic resonance sensor as a pre-clinical platform for analysis of complex tissue phantoms**
Presenting Author: Sydney Sherman

Complete Author List:
*Sydney Sherman (MIT); Alexa Zammit (MIT); Amena Khatun (MIT); Michael Cima (MIT)*

Tissue microstructure can be indicative of pathology. The purpose of this work is to construct a portable permanent magnet array and RF coil sensor capable of acquiring signal from muscle tissue in clinical settings and differentiating microstructural differences. We have developed a portable, single-sided magnetic resonance sensor. The homogeneous region, B0 = 0.2T, is 12-15mm above the surface of the RF coil which allows for the clinical assessment of muscle tissue. Multi-compartment muscle and fat tissue phantoms were fabricated to have varying microstructural properties. A CPMG pulse sequence is used to acquire T2 relaxation metrics and diffusion weighted T2 signal. Microstructural differences in droplet size and distribution of phantoms does not affect T2 relaxometry data, but does affect diffusion-weighted T2.

**POSTER 182**
**The Network for Advanced NMR: The Knowledgebase Progress**
Presenting Author: Songlin Wang

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The mission of NAN, the Network for Advanced NMR, is to provide state-of-the-art NMR instrumentation to investigators in the US and abroad to advance relevant areas of science. The development of the NMR Knowledgebase (KB) in the areas of solution structural biology, metabolomics, biological solid-state NMR, and materials solid-state NMR is a part of the NAN mission, which includes writing standard protocols, standardizing regularly used pulse sequences, acquiring example datasets, and providing data processing templates. Here we present solid-state NMR KB content development to highlight key components of the KB and its application in the areas of biological and materials NMR.

**POSTER 183**
**Development of Simplified Oxygenated System for in Vivo Solution State NMR**
Presenting Author: Peter Costa

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The development of flow systems is critical for maintaining aquatic organisms for environmental toxicology, thus allowing for exposure studies in their native and unaltered state for in vivo solution state NMR. Current approaches use flow lines that have the potential to burst and clog, require large volumes of media, and multiple expensive HPLC pumps. The proposed "bubble pump" provides several unique advantages such as no clogging, small and constant solution volume, and no need for pumps or fluid lines in and out of the probe. The flow system is designed for in vivo solution state NMR experiments, for both large and smaller diameter probes with potential applications in toxicity and metabolomics-based research.

**POSTER 184**
**Exploring the Potential of Broadband Complementary Metal Oxide Semiconductor Micro-Coil Nuclear Magnetic Resonance for Environmental Research**
Presenting Author: Daniel Lysak

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With sensitivity being the Achilles' heel of nuclear magnetic resonance (NMR), the superior mass sensitivity offered by micro-coils can be an excellent choice for tiny, mass limited samples such as eggs and small organisms. Here, the potential of broadband complementary metal oxide semiconductor (CMOS) based micro-coils for environmental research is investigated. Numerous heteronuclei such as 7Li, 11B, 13C, 19F, 23Na, 31P and 81Br were detectable and 13C and 19F were used to study two realistic environmental samples: a sprouting broccoli seed and a single Daphnia magna egg. The D. magna egg was exposed to hexafluorobenzene, and the contaminant was monitored within the egg by 19F NMR. Overall, broadband CMOS microcoils are shown to have significant potential for environmental research.

**POSTER 185**
**Simplifying triple resonance experiment for high quality NMR spectra with Multi Frequency Drive System**
Presenting Author: Hiroaki Sasakawa

Complete Author List:
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Organic compounds with phosphorus and boron nuclei often exhibit spectral complexity and reduced sensitivity in NMR analysis due to J couplings between hydrogen and carbon with these nuclei. We developed a triple resonance system called Multi Frequency Drive System (MFDS) to address this issue, enabling triple resonance experiments with a standard 2-channel NMR system. Using a JEOL JNM-ECZL600G spectrometer equipped with the ROYALPROBE™ P+, we conducted various solution NMR measurements. We present examples of signal enhancement and spectrum simplification achieved by triple resonance measurements of 1H, 31P, and 11B collected with a 2-channel NMR instrument.

**POSTER 186**
**Development and applications of a 1.01 GHz (23.7 T) NMR system**
Presenting Author: Yoshitaka Ishii

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We discuss development of an ultra-compact 1.01 GHz NMR magnet, and its preliminary NMR applications. The new ultra-compact 1GHz NMR magnet utilizes high-temperature superconducting (HTS) coils made of bismuth-based cuprates besides conventional low-temperature superconducting coils. Because of the high current density of the HTS coil, the magnet weighs only 1.6 tons and its footprint is the smallest among the existing 1 GHz NMR systems. The cryogenic refrigerator mounted on the magnet eliminates needs of regular liquid-helium refilling. We have successfully collected multi-dimensional solution NMR and solid-state NMR data for proteins at a 1H frequency of 1.01 GHz. The quality of the NMR data and other research progress from the ongoing project to develop 1.3 GHz NMR will be also discussed.

**POSTER 187**
**SABRE Hyperpolarization and In Situ 1H NMR Signal Detection via Large Custom-Made Solenoid Coils**
Presenting Author: Roman V. Shchepin

Complete Author List:
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Hyperpolarization techniques require equipment with starting "price tag" of thousands of dollars in case of parahydrogen-based methodology (e.g. SABRE) and often exceeding millions in case of d-DNP, creating a substantial entrance barrier for many researchers. To tackle this issue, we develop a custom coil winding machine, which allowed us to prepare a number of solenoid magnet coils with high degree of magnetic field homogeneity. One of the solenoid coils was used (8 mT static field) in a 1H SABRE experiment, allowing signal detection at both external 1.4T magnetic field (tabletop NMR) as well as in situ when it is attached to low-field NMR spectrometer bringing the total cost of parahydrogen setup within few thousands of dollars!

**POSTER 188**
**Control of Bruker NMR Spectrometers from Python with KovriginNMR**
Presenting Author: Evgenii Kovrigin

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*Evgenii Kovrigin (University of Notre Dame)*

An object-oriented Python software package, KovriginNMR, has been designed to enable Bruker spectrometer control from Topspin Python interface. KovriginNMR is intended to help NMR users construct workflows incorporating multiple samples, experiments, as well as variable-temperature operation. A user is able to automate as much or as little of their workflow as desired, and the software may be started from user's own account (no need for NMR superuser privileges). KovriginNMR automatically logs events taking place during its operation and includes time stamps, sample and experiment names, data paths, thus assisting accurate record-keeping. The KovriginNMR Workflows module supports development of complex experimental routines involving multiple samples and experiments while the KovriginNMR VT module enables automated NMR measurements in a broad temperature range.

**POSTER 189**
**Cryogen Reclamation System for NMR Magnets**
Presenting Author: Takuya Matsumoto

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NMR magnets are usually cooled by two kinds of cryogens, ie.liquid helium and liquid nitrogen. The boil-off rates of the cryogen in general NMR magnets are typically around 20 cc/h for liquid helium and 200 cc/h for liquid nitrogen. We have developed new cryogen reclamation system that can greatly suppress the evaporation both of liquid helium and liquid nitrogen.
The system was tested with an NMR magnet, and it was confirmed that the noise generated by system vibration was at a level that would not interfere with NMR measurements. It has also confirmed that the magnet maintained stable zero boil-off status for more than 6 months.

**POSTER 190**
**Fabricated Coplanar Waveguide Integrated with Microfluidics for Use in Nitrogen-Vacancy (NV) NMR**
Presenting Author: Emma Huckestein

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Nitrogen-Vacancy (NV) centers have emerged as promising quantum sensors of local magnetic environments due to their spin-state dependent fluorescence, optical addressability, and room temperature behavior. In recent years, many pioneering works have demonstrated NV-based NMR, but have confined their experiments to bias fields less than 0.1 T due to engineering challenges associated with microwave delivery. In this work, we fabricate a coplanar waveguide with integrated microfluidics that homogeneously delivers microwaves with frequencies up to 6 GHz and with 15 – 30 MHz power.

**POSTER 191**
**A Practical Approach to Passive Shimming of NMR Magnets**
Presenting Author: Ilya Litvak

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Shim systems supplied with commercial NMR magnets are designed to meet homogeneity specifications for particular applications. On the other hand, for home-built, custom, or otherwise out-of-spec magnets, inhomogeneity may be beyond the range of the active shims. Ferromagnetic passive shims take very little space and are field-deployable, thus being an attractive option.
We will share approach to designing ferromagnetic shims using a low-tech method. Our calculations were performed using Excel spread sheet; steel foil pieces were cut to size by hand and attached using consumer grade adhesive tape. The method can be used with little prior experience. The technique was tested while designing ferromagnetic shims for the 1500 MHz Series-Connected Hybrid (SCH) magnet at the National High Magnetic Field Laboratory.

**POSTER 192**
**A Miniature Magnetic Field Sensor Utilizing Integrated NMR RF Transceiver**
Presenting Author: Guang Yang

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Imperfections in gradient spatial constancy can affect MRI image quality.
To address this issue, we present a small magnetic field sensor designed for monitoring magnetic fields during imaging. The sensor includes a CMOS RF transceiver IC and a small NMR probe with a water sample, which are inserted into the MRI bore, and a controller with an FPGA module, PLL, and ADC that stays outside the bore and connects to the transceiver IC via power and SPI cables.
The field sensor prototype successfully captured FID using a 0.51-T permanent magnet.

**POSTER 193**
**The LLWG: A Low-loss, Low-cost, Small-diameter THz Waveguide for MAS-DNP in NB Magnets**
Presenting Author: F David Doty

Complete Author List:
*F David Doty (DOTY Scientific Inc); Glenn N. Doty (DOTY Scientific Inc); John Staab (DOTY Scientific Inc); Paul Ellis (DOTY Scientific Inc)*

A novel waveguide for the 70-1500 GHz range will be presented that achieves loss more than two orders of magnitude below that of fundamental-mode waveguides at 400 GHz, comparable to that of corrugated waveguides of similar size, but is possibly two orders of magnitude more manufacturable at small diameters. The novel Laminate-Lined Waveguide (LLWG) is being integrated into a NB MAS probe for DNP that includes a high-mode THz cavity compatible with MAS and is expected to permit routine low-cost operation below 15 K. The goal is to enable MAS-DNP in NB high-field magnets using solid-state sources.

**METABOLOMICS** (Posters 194 – 209)

**POSTER 194**
**Using NMR to Characterize Mitochondrial PolgD257A Mutator Mouse for Mitochondrial Diseases and Toxicity**
Presenting Author: Qiuwei Xu

Complete Author List:
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Mitochondrial dysfunction is often a cause of many human diseases. PolgD257A impairs DNA replication "proofreading" and leads to progressive accumulation of mutation in mitochondrial DNA. The PolgD257A mouse provides an animal model for mitochondrial neuronal disease target validation. We have applied NMR metabolomics to identify metabolites and pathways related to mitochondrial dysfunction. Our internal library of over 700 endogenous metabolites provides an opportunity of quick chemical identification and shifts our focus on biochemical interpretation. In this presentation, we will show our recent work of metabolomics profiling of PolgD256A mutator mouse model and analysis of pathways under which significant changes were observed in mitochondria, glycolysis, and many other endogenous metabolites.

**POSTER 195**
**13C NMR Spectroscopic Tracking of the Biochemical Changes in the Leloir and Glycolytic Pathways under Hypoxia in Liver Cancer**
Presenting Author: Daniel Anable

Complete Author List:
*Daniel Anable (University of Texas at Dallas); Lloyd Lumata (University of Texas at Dallas)*

The Leloir pathway is the main metabolic pathway for the catabolism of the glucose epimer galactose [1,2]. The Leloir pathway involves 4 major enzymes in which glucose-1-phosphate is produced from galactose: 1, galactokinase; 2, galactokinase 1-phosphate uridyl transferase; 3, UDP-galactose 4-epimerase; 4, UDP-glucose pyrophosphate [1,2]. This pathway primarily occurs in the liver and serves as an alternate energy source for liver cells through conversion into glucose-6-phosphate and the glycolytic pathway. In this study, the metabolism of D-galactose was investigated using 13C NMR spectroscopy in liver cancer vis-à-vis the glycolytic pathway (glucose metabolism) in light of the Warburg effect under normoxic and hypoxic conditions.

**POSTER 196**
**Pluronic F-127 as a gel matrix for in-cell NMR**
Presenting Author: Cale Thornton

Complete Author List:
*Cale Thornton (Boise State University); Nicole Elizabeth Aughtry (Boise State University); Wesley Joseph Hirons (Boise State University); Lisa R. Warner (Boise State University)*

In-cell NMR is a technique that can be used to analyze metabolic pathways in a wide variety of cells in vivo. However, cells larger than ~2 micrometers in diameter, tend to settle to the bottom of the NMR tube over the course of hours, no longer centered in the coil. This limits application of in-cell NMR to smaller cells, shorter experiment time, or specialty tubes. One approach to mitigate this problem is to suspend cells in a gelatinous medium. Pluronic F-127 is a biocompatible thermosensitive hydrogel that has potential as a gel matrix for in-cell NMR and has previously been used to study magnetically aligned Pf1 phage. Here, we examine Pluronic F-127 as a gel matrix for in-cell NMR experiments.

**POSTER 197**
**Revisiting Sample Preparation Protocols in Metabolomics**
Presenting Author: Saraa Al Jawad

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Sample preparation is a critical step in metabolomics, and standardization across labs is important for reproducible results. The current best practices in sample preparation for both urine and serum/plasma were optimized for room-temperature NMR probes and use phosphate buffers. Kelly (2002) has shown that phosphate buffers reduce the sensitivity of cryoprobes by about 2/3. This problem is even worse in urine, which has an overall salt concentration of >200 mM before any buffer is added. We previously found that DMSO minimizes the effects of salt and may improve sensitivity at high fields and with cryoprobes. We will present improved sensitivity in urine DMSO samples using a 5-mm cryoprobe at 600 MHz. At higher fields, the benefit should be even greater.

**POSTER 198**
**Tracking the Influence of Transition and Lanthanide Metals on the Glycolytic Pathway of Neuroblastoma Cells Using 13C NMR**
Presenting Author: Cody Larsen

Complete Author List:
*Cody Larsen (University of Texas at Dallas); Lloyd Lumata (UT Dallas)*

Despite their toxicity, lanthanides are a common starting material for developing contrast imaging agents to enhance the signal intensities of magnetic resonance imaging. Consequently, this work seeks to investigate the effects that lanthanide and paramagnetic transition metal ions have upon glucose metabolism and lactate production via the glycolytic pathway of cultured neuroblastoma cancer cells. The metabolic pathways were studied using 13C NMR spectroscopy by monitoring the conversion of glucose to lactate over 48 hours using a Bruker 600 MHz NMR spectrometer. Preliminary results indicating inhibition and excitation of certain lactate products will be presented, along with other experimental results.

**POSTER 199**
**Hydrogen-Deuterium Addition and Exchange in N-Ethylmaleimide Reaction with Glutathione**
Presenting Author: Daniel Raftery

Complete Author List:
*Daniel Raftery (University of Washington); Vadim Pascua (University of Washington); Fausto Carnevale Neto (University of Washintgon); G. A. Nagana Gowda (University of Washington)*

Glutathione is an ubiquitous thiol compound abundantly present in virtually every living cell. It is a powerful antioxidant critically required to protect cells from oxidative damage and free radical injury. It is very challenging to analyze glutathione in its native form from biological samples since the active form spontaneously becomes oxidized. To address this challenge, we developed a simple chemical derivatization method using N-ethylmaleimide (NEM) for the analysis of the notoriously unstable reduced glutathione antioxidant and its oxidized form. The chemical derivatization exhibited several intriguing phenomena including the generation of 12 different hydrogen-deuterium isotopomers of NEM-glutathione. The findings broaden the scope of metabolite profiling and impact areas of metabolomics, small molecule synthesis, and bioconjugation chemistry.

**POSTER 200**
**13C NMR Study of the Effect of Sodium Dichloroacetate (DCA) in Glucose Metabolism of Cultured Colorectal Cancer Cells**
Presenting Author: Emmanuel Ameh

Complete Author List:
*Emmanuel Ameh (The University of Texas at Dallas); Lloyd Lumata (University of Texas at Dallas)*

In this study, the effects of dichloroacetate on the metabolism in cultured colorectal cancer cells have been studied via 13C NMR spectroscopy. Cancer cells utilize glucose at a higher rate under the glycolytic pathway for ATP production as compared to normal cells. In particular, this study used carbon-13 NMR spectroscopy to track the glucose metabolism in the presence of dichloroacetate at different concentrations in cultured Colo-205 and LoVo colorectal cancer cell lines. The details of these results will be presented. This study is supported in part by the Welch Foundation grant AT-2111-20220331, the UT Dallas CoBRA and SPIRE seed grants, US Department of Defense CDMRP grants W81XWH-21-1-0176, W81XWH-22-1-0105, W81XWH-19-1-0741, HT9425-23-1-0062, and W81XWH-22-1-0003.

**POSTER 201**
**Tracking the effects of LDH and hexokinase inhibitors on glucose metabolism in cancer cells using NMR**
Presenting Author: Asiye Asaadzade

Complete Author List:
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Sodium oxamate is an inhibitor of lactate dehydrogenase (LDH), specifically LDH-A, an important enzyme that is active in cell and is responsible for catalyzing the reversible conversion of pyruvate to lactate.1 On the other hand, 2-deoxy-glucose (2DG) is a glucose analog that acts as hexokinase inhibitor suppressing glycolysis in tumor cells.2 In this work, we have investigated via carbon-13 nuclear magnetic resonance (NMR) spectroscopy the metabolic effect of varying concentration of sodium oxamate and 2DG administered separately on [1-13C] glucose metabolism in a variety of cultured cancers cell including renal cell carcinoma (786-O), hepatocellular carcinoma (HepG2), and glioblastoma (SfXL) cells.

**POSTER 202**
**2D 1H-13C Experiments for Targeted Analysis of Structural Sub-classes in-vivo**
Presenting Author: William Wynne Wolff

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In-vivo NMR is a powerful tool for tracking the biochemical responses of organisms in response to environmental stress but has been limited by poor resolution as a result of the extreme inhomogeneity of living organisms, and in the chemical complexity of an organism. Targeted pulse programs can support environmental studies, but often discard information that might be useful in understanding the mode of action of environmental stressors. To address these challenges, we introduce two new targeted pulse sequences: an in phase anti-phase (IPAP) HSQC to separate amides and acids alongside a conventional HSQC, and a 2D HCCH-TOCSY to obtain additional correlations whilst maintaining high resolution in a narrow band.

**POSTER 203**
**Exploration of Materials for Planar and Three-Dimensional Microcoil Production**
Presenting Author: Vincent Moxley-Paquette

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5-axis CNC micromilling is an excellent prototyping tool for microcoil technology, allowing for custom made microcoils with built-in sample wells tailored to specific mass-limited samples. Although Cu-laminated Teflon was previously the material of choice for developing microcoils with this method, creating microcoils on other materials (including Acrylic, which cannot withstand the heat required for soldering) was not thoroughly explored. In addition, due to the limitations of 5-axis milling, machining more complex 3D volume microcoils (saddle coils and solenoids) required the use of a high-precision Elara 4-axis CNC milling machine. In this presentation, the performance of microstrips machined from number of Cu-laminated dielectrics will be compared, with the materials providing the best lineshape/SNR used to make microsolenoid and microsaddle coils.

**POSTER 204**
**Mixing it Up with NMR: Low-Field NMR Undergraduate Mixture Analysis Experiments using Real-World Samples**
Presenting Author: Katrina Steiner

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The current gaps in NMR education can largely be attributed to three barriers: 1) the lack of access to expensive high-field NMR facilities, 2) the highly specialized and complex nature of operating high-field instruments, and 3) the lack of readily available teaching materials. Benchtop NMR aids in addressing the first two barriers, while the two undergraduate experiments presented here address the third. The poster will introduce two benchtop laboratory experiments that involve the mixture analysis of real-world samples. The first uses 1D 1H NMR techniques to identify unique spectral fingerprints in three different cocktails. The second is more advanced and applies 1D, 2D, and specialized experiments to pattern match and identify the ingredients in the popular energy drink Red Bull.

**POSTER 205**
**Low-Field, but Not Low Quality: 1D Simplification, Selective Detection, and Heteronuclear 2D Experiments for Improving Low-Field Environmental NMR**
Presenting Author: Katelyn Downey

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NMR spectroscopy could be an effective environmental research tool, but high-field NMR is financially and physically inaccessible. Alternatively, low-field NMR is accessible but is also less sensitive and suffers from spectral overlap. Therefore, this work investigates experiment types (1D spectral simplification, selective, and heteronuclear 2D experiments) that can help overcome sensitivity and overlap challenges in low-field analysis of environmental samples. Notable findings include that JRES is more sensitive but less effective than PSYCHE at removing homonuclear coupling. Both GEMSTONE and DREAMTIME are efficient selective experiments, but GEMSTONE is simpler to operate, whereas DREAMTIME can perform multiple selection. Ultimately, low-field NMR spectroscopy has untapped potential in environmental research, and further optimization may make it a viable tool in future applications.

**POSTER 206**
**Exploring Proton-only Experiments and Filters for In Vivo Samples: Potential and Limitations**
Presenting Author: Kiera Ronda

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In order to understand the environmental impacts of anthropogenic activities, it is essential to assess the impacts of contaminants on living organisms. Therefore, environmental metabolomics has become an increasingly important area of research. In vivo Nuclear Magnetic Resonance spectroscopy is ideally suited to analyze the complex systems observed in living organisms. However, limitations associated with spectral overlap and overwhelming water signals make these studies difficult. Two-dimensional experiments can simplify the analysis, but often require 13C labeled organisms, which are more costly and less applicable to natural systems than their non-labeled counterparts. Thus, this work will examine the practicality of 1H filters and different suppression techniques in the analysis of non-labeled organisms as a complementary tool to increasingly expensive 13C enrichment.

**POSTER 207**
**NMR compatible Bioreactor without Background Signal**
Presenting Author: Julia B. Schulte-Hermann

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Studying metabolic pathways or profiles of bacteria through NMR provides exciting opportunities in different fields, including medicine, environmental science, and biology. Since NMR is non-invasive and non-destructive, it allows long term monitoring of chemical processes without having to interrupt and extract samples, or even destroy the samples in the process. Therefore, time-course metabolic measurements of the same sample is possible.
In this work, we present an NMR compatible, rapid manufactured bioreactor for incubation of Escherichia coli. It is compatible with a 10 mm coil of a standard high field NMR spectrometer and can be inserted directly into the detection area. This bioreactor ensures the vitality of the organisms and provides a suitable bio- and magnetic field-compatible environment.

**POSTER 208**
**NMR Methods for Determining Lipid Turnover via Stable Isotope Resolved Metabolomics**
Presenting Author: Penghui Lin

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Here we report a quick and easy way to estimate the incorporation of 13C into different subunits of complex lipids by NMR using cellular phosphatidylcholine lipids (PCs) as internal standard in stable isotope tracer experiments. The ratios of peak intensities of other species to that of PC methyl groups in both the proton and the HSQC spectrum could be used for enrichment calculation. This method provides a simple tool for generating an overview of 13C incorporation into lipid molecules, which can be utilized as a standalone approach or to compliment targeted mass spectrometry-based lipidomics workflows. Further, with the detection limit as low as 2%, it provides very valuable information other techniques cannot easily generate.

**POSTER 209**
**Development of MR Brain Phantoms to Improve Understanding of In-vivo Molecular Dynamics**
Presenting Author: Mira Menon

Complete Author List:
*James Collins (University of Florida); Joanna Long (University of Florida); Mira Menon (University of Florida)*

To determine the quantitative accuracy and reliability of applying existing MR techniques in vivo for measuring metabolites concentrations, as well as to assist with the development of new methods for their quantitation, high quality phantoms that mimic the in vivo composition of metabolites and their local environment are required. A phantom based on multilamellar vesicles (MLVs) composed of lipids extracted from porcine brains were used to evaluate how each thickening agent affects small molecule metabolite linewidths and motion. To assess the various phantoms, T1, T2, T2* and diffusion measurements were made using optimally shimmed sample preparations. Comparisons are made with ex-vivo brain tissue samples at the same field strength, and potentially reveal details about metabolite local environment in brain tissue.

**MRI MRS** (Posters 210 – 226)

**POSTER 210**
**Dual Signal Ultrasensitive Magnetic Resonance Probe for Precise Drug Delivery Monitoring**
Presenting Author: Chenlu Yuan

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We synthesized an ultrasensitive 129Xe NMR probe with dual signals. It is a hollow nanoparticle composed of water-soluble CB[6]. It has two different hydrophobic cavities. Two 129Xe NMR signals with different chemical shifts can appear in a single detection, just like a mobile phone with dual SIM cards, which can interact with the electromagnetic waves from multiple "operators" transmitting towers with different frequencies at the same time. Therefore, it will not easily "lose contact" in complex environments, effectively avoiding the occurrence of false positive and false negative in complex biological environment detection, improving the accuracy and sensitivity of single detection, and has broad application prospects.

**POSTER 211**
**Diffusion Tensor Imaging With Three Types Of Correction To Reveal Physiological And Morphological Differences in The Liver**
Presenting Author: Artur T. Krzyżak

Complete Author List:
*Weronika Mazur (AGH University of Science and Technology); Artur Krzyak (AGH University)*

In pursuance of the liver parametrization based on the diffusive properties, diffusion tensor imaging (DTI) was proposed as a superior technique. DTI data were corrected for noise (increasing number of excitations), systematic errors (using B-matrix spatial distribution, BSD) and geometrical distortions (applying the affine registration relying on a 3D algorithm from a python library for the analysis of MR diffusion imaging). Diffusion tensors were calculated using four approaches, each encompassing different b-values sets. DTI metrics obtained after three types corrections evinced the largest reflection of the liver physiology and morphology. Based on the preliminary results with the age division, it can be suspected that distinguishing the perfusion- and diffusion-dominated signals, morphological and physiological differences in the livers are DTI-sensitive.

**POSTER 212**
**The CaRAP, HISuc Hypotheses: Significant Advances at the Limits of 3T Proton MR Spectroscopy.**
Presenting Author: Ralph E Hurd

Complete Author List:
*Ralph Hurd (Stanford); Meng Gu (Stanford); Daniel Spielman (Stanford)*

The neurological stress resulting from cardiac bypass can be followed by dynamic single voxel spectroscopy. Dynamic changes are reported in a CBP piglet model. Glutamine changes led to the Circulatory-arrest Recovery Ammonia Problem hypothesis. Results predicted a significant bolus of ammonia reaching the brain on re-perfusion, confirmed by blood ammonia assays. High Hypoxic-Ischemic Succinate has been established as a marker for elevated ROS and damage during re-perfusion. Succinate elevation was observed during circulatory arrest. In addition to discoveries with high potential clinical consequence, the model itself provides the controlled feedback and validation needed for the improvement of MR spectroscopy. In this presentation we show how the MR spectroscopy protocol has evolved over the past 3 years.

**POSTER 213**
**Using MRI to Study High Pressure Nutrient Infusion**
Presenting Author: Julia Kerr

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*Julia Kerr (Lawrence Livermore National Laboratory); Daniel M. Gruber (University of California, Davis); Matthew P. Augustine (University of California, Davis)*

High pressure assisted infusion of nutrients into food is in situ monitored with magnetic resonance imaging (MRI). The model food used here is peeled apple flesh. The nuclear spin relaxation properties of the water surrounding the apple flesh are enhanced by adding paramagnetic manganese cations for MRI relaxation contrast during pressurization. This work tracks the efficiency of pressure induced nutrient infusion in situ, demonstrating that pressure gating and ramping offer no nutrient mass transport advantage over operation at constant pressure and that the presence of a peel expectedly disrupts solute transport into the fruit. High pressure assisted infusion, with all pressurization schemes studied here, yields nearly 100-fold faster infusion times than at ambient pressure.

**POSTER 214**
**Association of MR-based functional and physical phenotyping with body impedance analysis**
Presenting Author: Chetna Banga

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With growing demand for precision medicine, phenotyping is gaining much attention. This study has evaluated MR-based resting–state functional activity and body composition,and correlated with body impedance analysis in healthy volunteers (n=40). Resting state fMRI and mDIXON-Quant sequence for fat evaluation in abdomen and thigh were carried out at 3T. Body impedance analyzer was used to calculate body fat percentage, visceral fat area and mass, subcutaneous and segmental fat mass in different body regions i.e bilateral limbs (arms and legs) and trunk and visceral fat level. Volunteers were categorized into two different groups on the basis of their BMI values- < 25 kg/m2 (Group I) and > 25 kg/m2 (Group II). This study brings out the potential of MR in phenotying

**POSTER 215**
**Monitoring The Molecular Status of Pinwheel [2]Rotaxanes Using 19F-NMR/MRI: A Mechanistic Study**
Presenting Author: Zhongxing Jiang

Complete Author List:
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Here, we have assessed the potential of 19F NMR and 19F MRI to monitor the molecular dynamics of [2]rotaxanes and provide insight into mechanical bonds (MB) and mechanical movements (MM). We developed novel 2-blade pinwheel [2]rotaxanes, containing symmetrical fluorine atoms on the wheel and axle to yield sensitive 19F NMR/MRI reporters of molecular dynamics. 1H/19F NMR studies revealed that the relaxation rates of the reporters strongly depend on the MB&MM. Solid-state 19F NMR measurements further demonstrated that the wheel in [2]rotaxanes exhibits a longer rotational correlation time and undergoes slower rotational motion than the macrocycle. The formation of MB in [2]rotaxanes leads to significant modulations of rotational correlation time and thus the relaxation rates of the fluorine atoms.

**POSTER 216**
**Impact of Selected Polysaccharide Model Systems on the Relaxivity of Dissociated Gd-Ions from Gadolinium-based Contrast Agents (GBCAs)**
Presenting Author: Patrick Werner

Complete Author List:
*Patrick Werner (German Cancer Research Center (DKFZ)); Matthias Taupitz (Charite); Leif Schrder (German Cancer Research Center (DKFZ))*

The use of GBCAs in medical imaging is widespread, but recent studies have raised concerns about the potential long-term retention of released Gd3+ ions. The mechanisms underlying this retention are not yet fully understood, but interactions with polysaccharides like glycosaminoglycans may play a critical role. We here demonstrate that the molecular weight of the polysaccharide in the microenvironment appears to impact the water accessibility of bound Gd3+, which in turn affects the observable r1 values in MRI scans. This means that the embedding of Gd in tissues may not always result in hyperintense signals in MRI scans as reported. Further research is necessary to understand the molecular interactions involved in Gd retention and relaxometry can provide important insights.

**POSTER 217**
**Single-Sided NMR for Hydrogel Characterization**
Presenting Author: Daniel Gruber

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Hydrogels - hydrophilic polymers that maintain integrity when hydrated - have been synthesized to be responsive to external stimuli, such as temperature and pH and have found a wide variety of uses. Knowledge of their physical properties is crucial for effective design and integration. We describe a contactless technique to measure hydrogel swelling and swelling rate using the NMR-MOUSE and an inversion recovery-leveraged pulse sequence, resulting in spatial precision below 100 µm and temporal precision below 10 minutes per data point. A dephasing delay pulse sequence reveals diffusion and tortuosity, giving insight into physical structure. This is demonstrated with pH-sensitive "smart" hydrogel as a simple example elucidating changes resulting from different formulation and preparation strategies, as well as conditioning.

**POSTER 218**
**MRS in Neurosciences – Recent advances in In-vivo spectroscopy methods and applications at the Stanford Center for Cognitive and Neurobiological Imaging**
Presenting Author: Laima Baltusis

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The interest of measuring metabolic changes via MRS techniques and combining that information with functional MRI measurements continues to grow. The Stanford Center for Cognitive and Neurobiological Imaging (CNI) spectroscopy program has become a best practice through a community effort of spectroscopy expertise from CNI staff, MRI scientists, and an expanding user community each supporting spectroscopy research projects conducted at CNI.
We will present new recent developments and results of focal MRSI using the semi-LASER sequence in challenging and less well studied areas of the human brain such as the basal ganglia regions where complex functions related to movement, cognition, and emotion are carried out and where single voxel data is of generally lower quality.

**POSTER 219**
**Lipid Nanoparticles Enhanced with Gadolinium Chelating Lipids as New, Potential Contrast Agents in Magnetic Resonance Imaging**
Presenting Author: Karolina Gębicka

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The aim of the research was to develop new MRI contrast agents based on GMO (glyceryl monooleate) lipid nanoparticles loaded with two types of Gd-chelating lipids: DTPA-BSA (Gd) and DPPE-DTPA (Gd). The effect of these two types of high-molecular-weight Gd-chelating lipids on the structure of fabricated GMO-based lipid nanoparticles and their physicochemical properties, such as particle size, long-term colloidal stability and morphology were studied. The substantial results include MRI contrast properties studied by means of relaxation times measurements and MR imaging efficiency.
Results indicate that developed GMO/DTPA-BSA-Gd and GMO/DPPE-DTPA-Gd nanoparticles have the potential for efficient MR contrast agent, and further, considering their unique properties, for the development of multifunctional systems combining diagnostics and therapy in a single system.

**POSTER 220**
**Imaging Protein-Ligand Interactions via 19F-MRI**
Presenting Author: Dilara Faderl

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Ligands interact with proteins non-covalently, influencing the population distribution of conformational states, and thus modulate the function of the protein. Magnetic Resonance Imaging provides a window through which it is possible to characterize these molecular interactions.
As a model system for monitoring binding, we have used 4-trifluoromethyl)benzamidine (TFBA) and trypsin as the ligand and target protein, respectively. In presence of increasing trypsin concentrations, the 19F-MR signal changes of TFBA reflected the change in T2 upon binding. By adding in a dose-dependent manner an 19F MR-invisible competitor ligand, benzamidine (BA), we observed a corresponding recovery of the TFBA 19F signal intensity. By comparing 19F-T2-weighted MR images of TFBA in the presence of different BA concentrations, the TFBA-trypsin interaction could be characterized.

**POSTER 221**
**Ultra-High Resolution fMRI in Awake Mice at 14T**
Presenting Author: David Hike

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This study utilizes implantable RF coils as a novel head fixation mechanism in awake mouse functional magnetic resonance imaging. The implantable RF coils provide significantly higher SNR for fMRI studies and the head fixation method limits motion-induced artifacts considerably. SNR comparisons were done at 9.4T and 14T with a commercial coil as control at 9.4T. All fMRI studies were done at 14T using the implantable coils. Current whisker stimulation data shows strong barrel cortex activation with additional activation seen in the retrosplenial area, ventral posteromedial nucleus, and upper limb somatosensory cortex. Future work can utilize this setup to record real-time pupillometry and whisking movement for use as regressors, providing a behavior-driven mapping tool to study other animal models.

**POSTER 222**
**NMR Characterization of Unfrozen Brine Vein Distribution and Structure in Frozen Systems**
Presenting Author: Peng Lei

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Due to the freezing point depression, in frozen systems, unfrozen water persists between the interface of ice crystals and/or particles. This water forms a liquid vein network (LVN) in dynamic and complex frozen systems. By investigating the development of the distribution and structure of the LVNs, the process of ice recrystallization can be studied in frozen systems using magnetic resonance tools such as MRI, relaxation and self-diffusion measurements. The distribution and structure of the LVN are studied as a function of temperature, salinity, particle size and ice binding protein. These results help to understand problems as broad as how frost heave happens in cold regions or how to better preserve frozen food or cryopreserve cells.

**POSTER 223**
**An innovative approach for the design of a 20 mT, 90 cm bore, Bitter-type electromagnet for earth field MRI.**
Presenting Author: Gianni Ferrante

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We present an innovative project of a Bitter-type electromagnet featuring 20mTesla B0 and 90cm inner bore, designed as magnetic polarization coil for a 'pre-polarized Earth-Field MRI' system.
The Bitter electromagnet offers an excellent homogeneity over 60 cm sphere and presents a very simple mechanical assembly.
The pre-polarized earth field MRI system is developed within the PRIMOGAIA, Horizon2020 project, funded by the European community. The main objective of the whole project is to develop a suitable technology 'to search for new contrasts linked to molecular events for the very early diagnosis of pathologies.
Details and spec of the magnet system are shown in the poster.

**POSTER 224**
**Are we ready for in vivo Sodium(23Na+)-based functional MRI (SOBA-fMRI) under 14T?**
Presenting Author: Yuanyuan Jiang

Complete Author List:
*Xin Yu (MGH); Yuanyuan Jiang (MGH)*

Conventional fMRI methods map brain function based on the hemodynamic responses of vessels coupled to neuronal activity. How to directly measure neuronal activity through the NMR signal is an ongoing challenge of neuroimaging. In particular, to identify the "true fMRI" signal directly linked to the neuronal activity—e.g., the action potential (AP) or local field potential (LFP) mediated by transmembrane ion movement—x nuclei-NMR has the potential for improved mapping specificity compared to proton-based hemodynamic fMRI. Here, we applied a reshuffled k-t space FLASH sequence to directly map the Sodium-based (23Na) (SOBA) fMRI signal changes in rat brains with 0.4x0.4x2mm spatial resolution and 10ms TR. In contrast to positive BOLD fMRI signals, we detected negative SOBA signals in the activated barrel cortex.

**POSTER 225**
**Multi-nuclear MRI and MRS Using 0.35 T Clinical MRI Scanner**
Presenting Author: Md Raduanul H. Chowdhury

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Hyperpolarized 129Xe, propane and [1-13C]ketoisocaproate are potential hyperpolarized contrast agents for their utility in lung imaging and molecular imaging of cancer. We use low-field (0.35 T) MRI scanner to demonstrate the pilot feasibility of multi-nuclear imaging in phantoms imaging and spectroscopy using these HP contrast agents. For HP 129Xe, we used a natively supported 129Xe GRE sequence to demonstrate ultra-fast slice-selective 2D GRE MRI with 64x64 imaging matrix with in-phantom SNR of 180. For HP propane, we demonstrate a sub-second 2D GRE scan with 64x64 imaging matrix and SNR of 210. Moreover, a post-mortem injection

of hyperpolarized [1-13C]ketoisocaproate allowed dynamic MRS scan in a freshly euthanized mouse demonstrating the delivery of 9% polarization (starting polarization is 12% inside the polarizer).

**POSTER 226**
**Comparing Diffusion Measurement Protocol of Polyvinylpyrrolidone (PVP) Solutions Across Three MR Systems**
Presenting Author: Cassandra M Stoffer

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The apparent diffusion coefficient (ADC) of water is an important biomarker in tissue health that can be measured using NMR and MRI techniques. Aqueous solutions of polyvinylpyrrolidone (PVP) with well-defined ADC values are used in MRI calibration objects (phantoms) to ensure the accuracy of data across imaging systems. In this work, PVP solutions are prepared using solute from various manufacturers with various molecular weights. A molecular weight survey is conducted by measuring the ADC values of prepared solutions across 3 systems: 128MHz (3 T) NMR, 128 MHz (3 T) MRI, and 2.4MHz (56 mT) unilateral NMR. We compare diffusion measurement protocol across these systems and develop PVP solutions that better mimic human tissue for use in MRI phantoms.

**ORGANIC INORGANIC AND HYBRID MATERIALS** (Posters 227 – 253)

**POSTER 227**
**29Si and 1H NMR structural study of Chrysocolla, an amorphous copper containing silicate: Application to archeological copper metallurgy.**
Presenting Author: Claire Roiland

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*Sibylle Manya (ENSCR); Valentina Figueroa Larre (UCN); Benoit Mille (C2RMF); Jean-Baptiste d'Espinose de Lacaillerie (ESPCI); Thierry Bataille (ISCR - ENSCR); Gwendal Kervern (CRM2); Laurent Le Polls (ISCR - ENSCR); Claire Roiland (ISCR - UMR 6226 CNRS UR1)*

A unique archeologic site located at Ujina-Collahuasi (Tarapacá, Chile) gives many clues to understand the functioning of the pre-hispanic furnaces to reduce ores to metal, especially in copper metallurgy. The main copper ore used appears to be Chrysocolla, a natural amorphous paramagnetic mineral with a proposed formula unit Cu2H2 (Si2O5)(OH)4·nH2O. In this work, we highlighted the necessity to employ adiabatic pulses to ensure a full excitation of the paramagnetic component. This is crucial to perfectly record broad lineshape and thus, to probe correlations between silicium and proton in this mineral. All those results allow us a good understanding of the Chrysocolla structure necessary to go further on the understanding of its thermal degradation during the metallurgy process.

**POSTER 228**
**Solution State NMR-Guided Purification of Carbon Quantum Dots**
Presenting Author: Cody Soper

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Carbon-based quantum dots have gained popularity over the last decade due to their low cost, scalable green production, biocompatibility, and favorable optoelectronic properties. Following bottom-up synthesis, the resulting product is often a mixture of carbon dots and partially-reacted precursor molecules with similar fluorescent signatures as the carbon dots. As such, these impurities are difficult to identify using fluorescent spectroscopy, and are too small to detect utilizing electron microscopy. Here, we present our initial results using solution-state 1H and 13C NMR to guide the purification of carbon dot mixtures via dialysis and size exclusion chromatography. Preliminary findings demonstrate that 1H and 13C NMR spectra of samples at different stages of purification show spectral signatures that are lacking in fluorescence spectroscopy.

**POSTER 229**
**Dynamic Nuclear Polarization for Perovskite Photovoltaics**
Presenting Author: Aditya Mishra

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Solid-state NMR has been used widely within the perovskite community to study cation incorporation, phase segregation, halide mixing, disorder, and dynamics. However, insensitivity prevents the study of application-relevant thin films, especially for surface coatings and additives. Firstly, we will show how tailoring the organic cation's relaxation properties helped us design impregnation dynamic nuclear polarization (DNP) experiments that achieve unprecedented bulk signal enhancements for hybrid perovskites. Secondly, we will show the possibility of DNP for three-dimensional inorganic perovskites doped with high-spin metal ions. The achieved sensitivity enhancements can be explained in terms of the dopant concentration, relaxation times, microwave absorption, and spin-diffusion. These DNP methods will pave the way to establishing structure-activity relationships in these materials for photovoltaic applications.

**POSTER 230**
**Molecular Fingerprint of Wetland Soil Elucidated by Solid-State NMR and DNP**
Presenting Author: Tuo Wang

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Wetland soil is important for carbon storage but it has been threatened by sea level rise. We employed DNP methods to collect high-resolution 2D 13C/1H-13C correlation solid-state NMR spectra on unlabeled soil collected from a brackish island in Louisiana. The island is only 55 km from New Orleans but has been rapidly shrinking over the past five years and finally disappeared in 2021. We identified a highly preserved lignocellulosic core in the surface soil layer and plants grown on top of it. Extending to a 2-m depth allowed us to examine the molecular changes of soil over an 11-century period. The composition and properties of the soil are influenced by many geological and historical factors as well as human activities.

**POSTER 231**
**Impacts of Electrolyte Speciation on Ion Binding Environments in Aluminum-Quinone Batteries Elucidated by Dipolar-Mediated and Multiple-Quantum Solid-State NMR Methods**
Presenting Author: Leo W Gordon

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Organic materials are earth-abundant, sustainable cathode alternatives for aluminum-metal batteries, however the electrolytes necessary to reversibly electrochemically plate and strip aluminum at room temperature contain a variety of polyatomic ions, leading to nuanced and complex charge storage mechanisms. Here, we determine electrolyte speciations with liquid-state NMR, and leverage multidimensional solid-state dipolar-recoupling NMR methods alongside multiple-quantum techniques to determine the nature and binding environments of solid aluminum-organic discharge products in three electrolytes. Complexed aluminum species are identified by their $^{27}$Al-$^{1}$H dipolar interactions, and quadrupolar parameters determined by $^{27}$Al{$^{27}$Al} MQ-MAS are linked with computationally-derived quantities to understand the physical characteristics of these bound ions. DFT calculated desolvation pathways were also validated by experimental measurements to conclusively reveal the ionic charge storage mechanism.

**POSTER 232**
**Understanding the Solvation Structure of Li-Ion Battery Electrolytes Using DFT-Based Computation and 1H NMR Spectroscopy**
Presenting Author: Julia Im

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Molecular dynamics simulations, density functional theory calculations, and 1H NMR spectroscopy were applied to understand the Li-ion electrolyte system, lithium bis(trifluoromethanesulfonyl)imide(LiTFSI) in tetraglyme(G4). By combining the computational and experimental methodologies, we show that the various solvation structures, dominated by the coordination between the tetraglyme solvent and lithium cation, directly influence the chemical shift separation of resonances in the 1H NMR spectra of the solvent. Thus, the 1H NMR spectra can be used to predict the fraction of tetraglyme involved in the solvation process, with a quantitative agreement with predictions from MD simulation snapshots. Overall, our results demonstrate the reliability of a hybrid computational and experimental methodology to understand the solvation structure and hence transport mechanism of the LiTFSI-G4 electrolyte system.

**POSTER 233**
**Scalable nanoporous networks for carbon capture via solid-state NMR spectroscopy**
Presenting Author: Haiyan Mao

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Carbon capture and sequestration reduce carbon dioxide emissions and is critical in accomplishing carbon neutrality targets. We demonstrate new sustainable, solid-state, polyamine-appended, cyanuric acid–stabilized melamine nanoporous networks (MNNs) via dynamic combinatorial chemistry (DCC) at the kilogram scale toward effective and high-capacity carbon dioxide capture. Polyamine-appended MNNs reaction mechanisms with carbon dioxide were elucidated with double-level DCC where two-dimensional heteronuclear chemical shift correlation nuclear magnetic resonance spectroscopy was performed to demonstrate the interatomic interactions. The coordination of polyamine and cyanuric acid modification endows MNNs with high adsorption capacity, fast adsorption time, low price, and extraordinary stability to cycling by flue gas. This work creates a general industrialization method toward carbon dioxide capture via DCC atomic-level design strategies.

**POSTER 234**
**Paramagnetic Solid-State NMR: Direct Observation of the 55Mn Nuclei in Manganese Oxides for Batteries**
Presenting Author: Anne Mirich

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Using traditional pulse sequences, direct observation of the transition metals (TM) in the cathode framework does not work. However, under certain conditions, the electrons spin pair to give S=0. By taking advantage of the spin pairing behavior in an extended lattice system, solid state NMR experiments were able to collect 55Mn spectra in an MnO2 solid. The amount of spin pairing was determined using SQUID experiments. Select ssNMR spectra were modeled using hybrid DFT calculations. Results showed that the total number of electron spins is less than what would be predicted, supporting the electron spin pairing theory.

**POSTER 235**
**Structural Analysis of Nitrogen-Containing Hydrothermal Carbon by NMR**
Presenting Author: Zhaoxi Zheng

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Molecular level detail is required for any attempt at rational design of N-hydrochar. 13C-glucose and 15N-glycine, model precursors that mimic major food waste components, were used to synthesize N-hydrochar characterized by NMR. Nonlabeled N-hydrochar synthesized from food waste was also studied and added for comparison. Quantitative composition analysis of labeled N-hydrochar was carried out both on 13C and 15N. Spectral editing showed >55% of carbons are not bonded to hydrogen, and >52% of carbons are aromatic. Rotational-echo double-resonance (REDOR) shows each nitrogen is bonded to two carbons in glucose and one carbon in glycine, and >65% of those carbons are not protonated. 15N NMR combined with 2D 13C-15N heteronuclear single quantum (HSQC) identified a wealth of possible forms of nitrogen.

**POSTER 236**
**Mechanistic Insights into Processive Polyethylene Hydrogenolysis: An in-situ NMR Study**
Presenting Author: Tommy Yunpu Zhao

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Chemical polymer upcycling by processive catalysts is a promising plastic waste remediation strategy, with the capability of producing selective, high-value products from waste plastics with minimal energy input. We employed in situ MAS NMR to study the underlying mechanism of processive polyethylene (PE) hydrogenolysis by mSiO2/Pt/SiO2 catalysts. We found that most PE-Pt interactions do not lead to C-C bond cleavage but rather release the polymer back into the melt. The hydrogenolysis to H/D exchange ratio increased with increasing shell thickness, indicating that longer pores inhibit the premature release of polymer thus afford higher extent of processivity. Coarse-grained molecular dynamics simulations were able to reproduce the trends observed in the experiments and further correlate pore geometry to processivity.

**POSTER 237**
**Increased sodium mobility in sodium carbonphosphonitride thermosets from plasticization seen through Na-23 longitudinal relaxation behavior**
Presenting Author: Christopher A. Klug

Complete Author List:
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Reacting phosphorus cyanide with lithium dicyanamide affords a conductive, thermosettable resin; however, the conductivity of the thermally cured resin at room temperature is too low to be practical for solid-state electrolyte applications. By exchanging out lithium with sodium and adding a plasticizer, the cured resin's conductivity is dramatically improved. Here, we characterize the cured resin's sodium variant with and without the plasticizer using solid-state NMR. Sodium-23 spectra contain a sharp peak and a broad band, suggesting two different types of Na-23 environments. Variable temperature spin-lattice relaxation measurements reveal broad band Na-23 relax faster for the plasticizer-containing sample, signifying an increase in sodium mobility achieved through plasticizer introduction. Kinetic parameters extracted from the relaxation rates will be presented.

**POSTER 238**
**Structural verification and in-situ measurements of ZIF-67 in an electrochemical supercapacitor cell**
Presenting Author: Mark O. Bovee

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Metal-organic frameworks (MOFs) are attractive as supercapacitor electrode materials because their high porosity promotes electrolyte-electrode interactions, boosting the system's capacitance. Previous work by our group characterized ZIF-67, a MOF displaying promise as an electrode material, using high resolution MAS NMR. These measurements revealed NMR can sense "guest" molecules in the pores. Here, we continue our study of ZIF-67 by measuring ZIF-8, a structural analog that replaces ZIF-67's paramagnetic Co2+ centers with diamagnetic Zn2+. Comparing the materials' 13C spectra provides further verification to our structural analysis of ZIF-67. Additionally, we present preliminary in-situ measurements of a supercapacitor cell that incorporates ZIF-67 as the positively charged electrode. Proton spectra of the electrolyte reveal features that change as a function of applied voltage.

**POSTER 239**
**Probing the Ultrastructure of Oakwood Lignocellulose by Quantitative Solid-State NMR Analysis**
Presenting Author: Zhenhuan Sun

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The lignocellulose ultrastructure of 13C-enriched young oakwood was analyzed using quantitative 13C NMR and spin diffusion. Proximities and domain sizes of 4 major components: lignin, acetylated hemicellulose, noncrystalline and crystalline cellulose, were probed using 2D 13C-13C exchange NMR. Spin diffusion out of crystalline cellulose documented 2.5±0.4 nm diameter crystal cores, corresponding to 3.5±1.5 nm thick cellulose microfibrils. The experimental data were matched by numerical simulation of spin diffusion in a quantitative model with a macrofibril of (6nm)2 cross-sectional area consisting of four cellulose microfibrils surrounded by hemicellulose and lignin. The macrofibril diameter was further validated by local equilibration in 1D 13C spin diffusion NMR and independently in a CHHC experiment with 13C-detected 1H spin diffusion after selective cellulose suppression.

**POSTER 240**
**Distinguishing Degradation Products in Carbon Capture Polymers with ROCSA and Machine Learning**
Presenting Author: Maxwell Marple

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Aminopolymers are promising sorbent materials for direct air capture applications that can be regenerated by exposure to elevated temperatures and steam. However, during regeneration the aminopolymer is susceptible to degradation that limits usable lifetime. Amine reactions with CO2 are complex and depend on temperature, humidity, and CO2 concentration, forming a wide variety of carbonyl-type environments. This complexity makes detecting degradation products difficult with standard solid-state NMR techniques. We use a 2D chemical shift anisotropy correlation measurement, ROCSA, to distinguish between chemisorbed and degraded products based on their 13C CSA parameters. To aid interpretation, we developed a machine learning model that classifies the type of carbonyl site based on its CSA values trained on over 100 crystal structures from DFT calculations.

**POSTER 241**
**Direct Probing of Neighboring Sodium for Bridging Oxygen Atoms in Sodium Silicate Glasses with Solid-state NMR Spectroscopy**
Presenting Author: Jeongjae Lee

Complete Author List:
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Sodium, silicon, and oxygen, constituting the majority of Earth's crust and mantle in forms of silicate minerals and melts, also find common use in many commercial glasses such as amorphous soda-lime glass. In this study, we show that the sodium distribution in amorphous sodium silicate glasses is likely to be more homogeneous than previously expected from the accepted modified random network (MRN) model. NMR correlation spectroscopy between the oxygen and sodium species in form of 17O→23Na triple quantum heteronuclear correlation experiments between quadrupolar nuclei unambiguously demonstrate the existence of sodium atoms in the immediate vicinity of bridging oxygen (Si–O–Si species), a feature unexpected from the MRN model.

**POSTER 242**
**Investigating the Role of Solid Acid Catalyst in Depolymerization of Polyolefins using SSNMR**
Presenting Author: Jinlei Cui

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Chemical recycling with catalysts can break the polymers into smaller monomers, which can then be reformed into high-quality materials. Fluorinated alumina oxide (F-Al2O3) is a catalyst that can improve the depolymerization of polyolefin, and its effectiveness is related to the proximity between the polymer and the catalyst's surface. In this study, the copolymer(ethylene-co-dodecene) was introduced into two distinct catalysts: fluorinated F-Al2O3 and Al2O3. Under a spinning rate of 10 kHz, 13C{27Al} TRAPDOR was

utilized with dynamic nuclear polarization (DNP) under 100k at 9.4T. The data indicated that F-Al2O3 exhibits a substantially faster dephasing compared to Al2O3, suggesting that the copolymer is in closer proximity to the former's surface.

**POSTER 243**
**Understanding Oxidative Degradation Mechanisms of Ethyl and Propyl Amines**
Presenting Author: Hannah Eshelman

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Polyethyleneimine (PEI) is a promising candidate for direct air capture (DAC) due to low volatility, low cost, and high selectivity and adsorption capacity for CO2. However, oxidative degradation of amine-containing adsorbents is a concern for DAC processes due to the abundance of oxygen in the air and temperature swings used for adsorbent regeneration. Solution state NMR was used to study a variety of aminooligomers containing either ethyl or propyl spacers and taking on either a branched or linear configuration to represent fragments of PEI. Corresponding 1H, 13C, 1H-1H COSY, and 1H-13C HSQC NMR of aminooligomers throughout their degradation was used to identify products and help determine the most stable configuration for new amine-containing DAC adsorbents.

**POSTER 244**
**Strategies for Oxygen-17 and Calcium-43 NMR studies of biomaterials: isotopic labeling, (ultra)-high field NMR and DNP**
Presenting Author: Danielle Laurencin

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Oxygen and calcium are highly abundant elements in living organisms. They are notably found within mineralized tissues like bone and teeth, and in pathological calcifications like kidney stones. Thus, to help understand the structure of these materials, 17O and 43Ca NMR appear as valuable probes, due to the high sensitivity of the NMR parameters of these nuclei to their local environment. Yet, both isotopes are very challenging. Here, some of our recent work aiming at using 17O and 43Ca NMR to investigate the structure of synthetic biomaterials will be presented.

**POSTER 245**
**Investigating the structure of synthetic opioid precursors with single crystal X-ray diffraction and multi-nuclear solid-state NMR spectroscopy**
Presenting Author: Harris E. Mason

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With the current synthetic opioid epidemic raging in the U.S., there is a significant need to understand the structure and chemistry of fentanyl, its analogues, and its precursors. The compound N-phenyl-4-piperidinone, referred to as NPP, is a critical precursor in the "Siegfried method" for the synthesis of the synthetic opioid fentanyl and its analogues. This material can serve as a "safe" alternative to fentanyl for structural studies. Here, we present the results of a systematic multinuclear solid-state NMR and single crystal X-ray diffraction (SC-XRD) study of the NPP crystal structure as a function of the coordinating anion strength.

**POSTER 246**
**Understanding the Electrochemical Discharge Mechanism in Li-CFx Batteries from the Atomic to Macroscopic Scales by Solid-State NMR Spectroscopy**
Presenting Author: Loleth Robinson

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NASA is vetting ultra-high-energy-density Li-CFx batteries for its mission concept to Europa, a moon of Jupiter with liquid water underneath its icy surface. The main challenges associated with this mission are battery aging during the long journey to Jupiter and high gamma radiation. These factors can have significant negative impacts on battery materials and electrochemical performance. As such, much remains to be understood about the electrochemical discharge processes at a molecular level and how the local compositions, structures and interfaces of the electrode materials change at different states-of-charge. Here, we combine quantitative and multi-dimensional, dipolar-mediated NMR measurements, coupled with electrochemical impedance spectroscopy, to enable elucidation of molecular-level environments and quantification of the electrode composition as a function of state-of-charge.

**POSTER 247**
**Understanding Speciation in Ionic Liquid Analogue Electrolytes for Rechargeable Al Batteries**
Presenting Author: Jonah Wang

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Rechargeable aluminum metal batteries are attractive due to aluminum's earth abundance, high theoretical capacity, low cost, and inherent safety. Ionic liquid analogue (ILA) electrolytes have been investigated as lower cost and less corrosive alternatives to state-of-the-art chloroaluminate ionic liquid electrolytes. However, much remains to be understood regarding how the types and populations of electrolyte species affect their physical and electrochemical properties. In this work, we use quantitative 1D 27Al and 1H single-pulse NMR measurements, as well as 2D 27Al{27Al} EXSY NMR experiments, to reveal molecular-level environments, populations, and dynamics present in Lewis acidic AlCl3-urea-[EMIm]Cl electrolyte mixtures of varying compositions. The results reveal insights into how electrolyte speciation and dynamics relate to its electrochemical properties.

**POSTER 248**
**Quantification monitoring of drug loading in metal-organic layers by 129Xe MRI**
Presenting Author: Xin Zhou

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Metal-organic framework layers (MOLs) are two-dimensional nanosheets of metal-organic frameworks (MOFs). Compared with the three-dimensional MOF materials, MOL may provide more surface area for 129Xe exchange due to its ultra-thin sheet structure. This specific capability makes MOL to be a potential 129Xe MRI contrast agent with improved availability. The porous ultra-thin structure and high specific surface area make MOL as a multifunctional drug-carrying cage. After DOX molecules occupied the surface and pores area of MOL, the chemical microenvironment and exchange process between MOL and 129Xe atoms is affected depending on aperture occupancy rate dominated by DOX-loading concentration. A 129Xe MRI method is provided for the quantification monitoring of drug loading concentration.

**POSTER 249**
**Indirect detection of solid-state platinum species by {1H}195Pt PE-RESPDOR NMR**
Presenting Author: Anna Pischer

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Nanoscale platinum is commonly used as a heterogeneous catalyst to facilitate chemical reactions that are the foundation for many industrially important energy and chemical manufacturing applications. Characterizing the electronic and bonding environments of solid-state platinum species by 195Pt NMR provides insights into their atomic-level compositions and structures. Historically, direct detection and resolution of 195Pt NMR signals have been limited due to their extremely broad lineshapes and the low Pt contents of industrially relevant materials. Nevertheless, indirect detection of 195Pt through a sensitive dipolar-coupled nucleus, such as 1H, enables solid-state 195Pt NMR spectra to be acquired with improved sensitivity. Results will be presented on the use of 1H{195Pt} PE-RESPDOR NMR and related techniques to analyze platinum species dispersed on heterogeneous catalysts.

**POSTER 250**
**Fast Field Cycling NMR applied to polymers: tacticity and molecular weight**
Presenting Author: Donald Bouchard

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In this study, we want to show the power of the Fast Field Cycling [1,2] NMR relaxometry (FFC) technique by addressing the assessment of one of the key properties of polymers, the tacticity,
We present a case study on the most widely used and well-known industrial polymer: the polypropylene. The "Tacticity" has important implications on its physical and mechanical properties. In this study, we investigate the potential of the FFC technique to discriminate commercially available isotactic polypropylene (PP) from atactic PP.

**POSTER 251**
**Proton NMR to Evaluate Changes in Activity of Water in High Concentrated Aqueous Zinc Battery Electrolyte**
Presenting Author: Alexis Scida

Complete Author List:
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Aqueous-based battery systems have been highly studied due to their inherent increase in safety; however, they face major issues regarding limitations in the electrochemical stability window and parasitic hydrogen evolution reaction (HER). Strategies, including increasing salt concentration, and the addition of co-solvents can help decrease free water molecules' reactivity, and form protective interface layers, thereby limiting unwanted side reactions. Herein, proton NMR and T1 spin-lattice relaxation are utilized to corroborate the changes in the chemical environment associated with water in a unique highly concentrated, multi-salt electrolyte for zinc-ion batteries. Changes in chemical shifts denote a decrease in acidity and polarization, whereas a reduction in relaxation time is evident in changes in long-range order of water.

**POSTER 252**
**Unusual Crystal Chemistry in High-rate Battery Electrodes via 23Na NMR and DFT**
Presenting Author: Kent Griffith

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*Kent Griffith (UC San Diego)*

In this work, we focus on multinuclear solid-state NMR characterization to explore the relationship between composition, crystal structure, and defect chemistry in a series of complex sodium and lithium niobium oxides. The role of defects on electrochemical transport properties in these new high-rate electrode or solid electrolyte materials will be discussed. Starting with average structure models from X-ray and neutron diffraction, we then turn to a local structure perspective from NMR that is more sensitive to defects and disorder. One- and two-dimensional 6,7Li and 23Na NMR spectra provide insights on mobile cation positions and dynamics as well as alkali sublattice vacancies. (Ir)reversible changes upon cycling are identified. DFT calculations and numerical simulations support the spectral assignments in these complex oxides.

**POSTER 253**
**2D J- and Dipolar-mediated Correlation NMR Techniques for Structural Characterization of Dilute Heteroatom Sites in Zeolite Catalysts**
Presenting Author: Michael B Schmithorst

Complete Author List:
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Aluminosilicate zeolites are crystalline, nanoporous materials used as catalysts in a variety of applications, including environmental emission control. NMR is well suited to the characterization of the local environments of 29Si and crucial 27Al atoms in the zeolite framework, however, their relative distributions are challenging to establish due to their non-stoichiometric compositions, low natural abundance of 29Si, non-periodic ordering and quadrupolar nature of 27Al, and inhomogeneous broadening of NMR signals. We demonstrate that the combined use of low-temperature J- and dipolar-mediated 2D 27Al-29Si HMQC and 2D 29Si-29Si INADEQUATE correlation NMR techniques provide detailed and complementary new understanding of dilute structural features of zeolite frameworks, which correlate with their macroscopic catalyst reaction properties.

**SMALL MOLECULES NATURAL PRODUCTS** (Posters 254 -271)

**POSTER 254**
**Fast dynamics of difluprednate in micelles or swollen-micelles revealed by 19F NMR spin relaxation rates**
Presenting Author: Kang Chen

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Molecular rotational dynamics was determined at a nanosecond time scale for lipophilic drug molecule difluprednate encapsulated in viscous micelles. Fast drug molecule motion suggested inter-molecular interaction governed rotational dynamics over the viscosity in the Stokes-Einstein–Debye equation. Using this study as an exemplar, we propose that quantitative NMR is generally applicable in studying soft-core emulsion solutions.

**POSTER 255**
**"Dark" phosphate no longer dark?**
Presenting Author: Jiaqi Lu

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Phosphate is the most abundant anion in the human body as integral structural components of cell membranes and bones. When bound with calcium, phosphates are hypothesized to form cluster. However, the underlying assembly mechanism of phosphate species and other factors that lead to bone formation processes are not well understood. We have found evidence that phosphate species including orthophosphates, pyrophosphates and adenosine phosphates associate into dynamic assemblies in dilute solutions that are spectroscopically 'dark', and that the aggregation propensity increases with rising temperature. Recently, we found pH also played an important role in affecting the phosphate aggregation in 'dark state', and chemical exchange saturation transfer (CEST) was employed in this study to provide new spectroscopic evidence for phosphate aggregation.

**POSTER 256**
**NMR Relaxation and Solution Dynamics of Four-/Five-coordinate Co(II) Complexes**
Presenting Author: Matthew P. Grindle

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The physical properties of systems employed in solid state are derived from inherent properties of the molecules and the constraints on the molecule that effect crystallization. We use NMR to measure the characteristics of two related compounds in solution at 207-347K. Solution NMR relaxation rates are measured to provide electronic dynamics information which relates to magnetic relaxation in the solid state. Data is presented on two similar five-coordinate complexes (TpPh,MeCo(guaiacol) and TpPh,MeCo(thioguaiacol) (TpPh,Me = tris-3-phenyl-5-methyl-1-pyrazolylborate)). They differ by the substitution of one atom (S for O) coordinated to the central metal. Both complexes show approximate TBP geometry in crystalline form. In solution, TpPh,MeCo(thioguaiacol) is stable under all conditions, while TpPh,MeCo(guaiacol) is dynamic, converting between four- and five-coordination at higher temperatures.

**POSTER 257**
**$^{19}$F-centered NMR Spectroscopy for the Analysis of Complex Mixtures**

Presenting Author: Nicholle Bell

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We present NMR methodology that uses $^{19}$F as a 'spy' for the structure determination of mono-fluorinated compounds in complex mixtures. This $^{19}$F-centred NMR analysis consists of a complementary set of broadband, phase-sensitive NMR experiments that utilize the substantial sensitivity of $^{19}$F and its far reaching heteronuclear couplings to obtain $^{1}$H, $^{13}$C and $^{19}$F chemical shifts, values of $J_{HF}$, $J_{HH}$, and $J_{FC}$ coupling constants and the sizes of $^{13}$C induced $^{19}$F isotopic shifts – parameters that underpin the structure elucidation process. This new methodology is illustrated on solving the structures of disinfectant by-products produced by chloramination of a single mono-fluorinated phenolic compound.

**POSTER 258**
**NMR metabolomics based chemosensory differentiation of anti-obese phytocompounds**
Presenting Author: Ankita Singh

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Obesity is a global epidemic. Recent research on phytochemicals and plants with nutritional and medicinal values has gained interest in obesity management. In this study, NMR metabolomics was used to differentiate 22 phytochemicals and 38 medicinal plants in pungent and non-pungent groups. Anti-lipase assays were conducted to study their anti-obesity properties. Multivariate analysis of NMR data demonstrated the potential of proton NMR metabolomics in identifying and differentiating medicinal plants and their active phytochemicals with anti-obesity properties which was confirmed with anti-lipase assays and alkaloid analysis.

**POSTER 259**
**Identifying Individual Molecules in a Small Molecular Mixture via Unsupervised Analysis**
Presenting Author: Madhur Srivastava

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Resolving small molecule mixtures by NMR spectroscopy has been of great interest for a long time for its precision, reproducibility, and efficiency. However, spectral analyses for such mixtures are often highly challenging due to overlapping resonance lines and limited chemical shift windows. The existing experimental and theoretical methods to produce shift NMR spectra in dealing with the problem have limited applicability owing to sensitivity issues, inconsistency, and/or the requirement of prior knowledge. We resolved the problem by decoupling multiplet structures in NMR spectra by the wavelet packet transform (WPT) technique, followed by a scheme to deploy the method in predicting the composition of the corresponding molecular mixtures from their 1H NMR spectra in an automated fashion.

**POSTER 260**
**31P NMR Spectroscopy Parameters for Structural Analysis**
Presenting Author: Markéta Tichotová

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Phosphorus is a biogenic element and a crucial component in modern organic synthesis. However, a stereogenic centre on the phosphorus atom causes formation of two enantiomers. These are difficult to separate, and stereoselective synthesis is usually challenging. The determination of the absolute configuration is also often hindered. Therefore, an NMR method able to assign the stereochemistry on phosphorus would be a solution.
In this work, we examine 31P NMR parameters for the structural analysis of model compounds. We complement experimental NMR data with quantum-chemical calculations. Furthermore, we present a new route for profound conformational sampling using artificial intelligence. 31P-13C J-coupling analysis unequivocally assigned the relative configuration, while 31P-based RDC analysis requires further investigation. We tested a new molecular-dynamics-based method, MDOC.

**POSTER 261**
**$^{15}$N-Mediated J-Couplings in Conformational Analysis of $^{15}$N-Glycomimetics**
Presenting Author: Radek Pohl

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In this contribution, we would like to present a joint NMR & DFT study dealing with $^{15}$N-labeled glycomimetics – compounds structurally resembling natural carbohydrates with a $^{15}$N label in the position that is close to the location of the conformational change. The labeling provides extra NMR parameters, especially *J*-couplings that are sensitive to the conformation. The $^{15}$N labeling enables exploring (a) aminomethyl group rotation, (b) aglycone conformation, or (c) N-disaccharide conformation. The approach combines molecular dynamics simulations, DFT calculations of NMR parameters, and fitting the calculated *J* couplings with experimental values. The results of the study reveal redundant $^{15}$N-mediated *J*-couplings sensitive to conformational changes and show that the approach can predict conformers of such $^{15}$N-glycomimetics in solution.

**POSTER 262**
**Something from Nothing: Automated Compound Sparing NMR**
Presenting Author: Francisco Silva

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clear Magnetic Resonance (NMR) Spectroscopy has played a key role in Pharmaceutical R& D as a gold standard in structure identity; however, the amount of material tends to be in the low milligrams. In our previous Direct-to-Weigh (DTW) NMR workflow, laborious NMR sample preparation was used where samples were manually weighed out from a standard vial and remaining valuable material was used in various screening cascades. The spent vial was then discarded with unweighable material. Here in a new Automated Compound Sparing (ACS) NMR, the spent unweighable vials were utilized as the source of NMR sample. A high recovery vial on a modified liquid handler, tasked with solvation and transfer, enabled automation of NMR sample preparation. A comparison of the

**POSTER 263**
**NMR and Machine Learning Study of Crude Oil Stability**
Presenting Author: Vilko Smrecki

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The stability of crude oils and their components is one of the biggest challenges in petroleum industry, as there is no single method to determine stability of all fractions. To explore possibilities to predict crude oil stability, statistical multi-way analysis (MWA) and machine learning (ML) methods were coupled with DOSY NMR spectroscopy and compared with various parameters affecting crude oil stability. An extensive ML multivariate linear regression was performed to model crude oil stability in terms of various measured properties, such as aromaticity, API gravity, percentage of aliphatic chains, asphaltene content and relative diffusivities. The correlations obtained for mixtures as complex as crude oil were exceptionally good, proving that this new and robust model can accurately predict crude oil stability.

**POSTER 264**
**Changes in components of T2 relaxation in chicken breast meat after slaughtering**
Presenting Author: Hong Zhuang

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Changes in T2 relaxation in chicken breast fillets (pectoralis major) were investigated during the conversion of muscle to meat and postmortem storage. Fillets were removed from bones within 5 min after bleeding and placed in ice. T2 relaxation in muscle was measured using Bruker LF-NMR 90II over the postmortem period (from 0.5 to 168 h). Results from distributed analysis show four components with relaxation times of 5, 42, 148, and 378 ms, respectively, at the early postmortem phase (< 24 h), but only three components were noted at the end of storage. Relative content of 42-ms component increased and 378-ms component decreased during the conversion of muscle to meat. Findings reveal that T2 components change both quantitatively and qualitatively postmortem.

**POSTER 265**
**Revision of Improbable Natural Products: The Benefit of Combined Usage of Chemical Knowledge with Computer Assisted Structure Elucidation (CASE) and DFT**
Presenting Author: Mikhail Elyashberg

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New natural products are still reported at a high rate. Their structures are usually elucidated using 1D and 2D NMR data, as well as high resolution MS spectra. However, it is not uncommon to see erroneous structures reported. In this poster we discuss the potential ways to uncover incorrect structures, as well as report a robust way to revise them, using a combination of CASE and DFT calculation. This is an attractive alternative to total synthesis, made possible by the evolution of software packages for CASE and DFT in recent years. Specific examples will be illustrated.

**POSTER 266**
**Unequivocal Identification of Two-bond Heteronuclear Correlations by i-HMBC to Facilitate the Elucidation of Complex Natural Product Structures at Nanomole Scale**
Presenting Author: Mikhail Reibarkh

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HMBC is an essential experiment for determining multiple-bond heteronuclear correlations in organic molecules, including natural products, yet its major limitation is differentiating two-bond from longer-range correlations. Previous approaches to overcome this suffer drawbacks such as restricted utility and poor sensitivity. Here we present a sensitive and universal i-HMBC (isotope shift detection HMBC) methodology to identify two-bond HMBC correlations using isotope shifts. Experimental utility was demonstrated at the nanomole scale with only a few hours of acquisition time for structure elucidation of several complex proton-deficient natural products, which were otherwise too challenging for conventional 2D NMR experiments. i-HMBC overcomes the key limitation of HMBC without significant reduction in sensitivity and thus could replace the latter as an essential structure elucidation experiment.

**POSTER 267**
**Quantifying Hidden Fluorine in Aqueous Film-Forming Foams via 19F NMR**
Presenting Author: Esteban Hernandez

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Aqueous film-forming foams (AFFFs) are mixtures used in extinguishing high-hazard flammable liquid fires. These mixtures have historically contained long chain per- and polyfluoroalkyl substances (PFAS), which have been a topic of interest due to being linked with a variety of health problems. The use of AFFFs in both military (MilSpec) and commercial (non-MilSpec) applications has led to PFAS being found in high concentrations near population centers. Current analytical methods to quantify PFAS in AFFFs are often complicated, time-consuming, and expensive. As the concern of PFAS contamination grows, rapid and inexpensive methods are needed to quantify total fluorine in environmental mixtures. This work focuses on the use of 19F qNMR as a means to quickly and reliably deduce total fluorine concentration.

**POSTER 268**
**Internuclear Distance Measurements between 1H and 14N in Multi-Component Rigid Solids at Fast MAS**
Presenting Author: Yutaro Ogaeri

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1H-14N internuclear distances are readily and accurately measured using the symmetry-based phase modulated resonance-echo saturation-pulse double-resonance (PM-S-RESPDOR) method in rigid solids. Analytical equation of the fraction curve easily provides 1H-14N couplings. However, this treatment is only applicable when NH proton resonance is well separated from the other proton peaks, which is not necessarily satisfied even at fast MAS >60kHz, especially in multi-component systems. To overcome this problem, T-HMQC filtering is applied to suppress the 1H signals other than NH proton prior to the PM-S-RESPDOR experiments. The method is well demonstrated on two components acetaminophen-oxalic acid (APAP-OXA) systems.

**POSTER 269**
**P-chirogenic Compounds Analyzed by 31P NMR Parameters**
Presenting Author: Anna Hruzíková

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P-chirogenic molecules with another stereogenic center are present as a mixture of two diastereomers. Their separation and crystallization for determination of stereochemistry is challenging by X-ray diffraction. NMR spectra of 31P isotope can be easily recorded on commonly used NMR probes due to 100% natural abundance, spin ½ and high sensitivity. In this work, we search for new approaches employing 31P NMR parameters in structural analysis complemented by quantum-chemical calculations. At first, we used conformational sampling of studied DSIs to generate all potential conformers. The low-energy conformers were found by DFT calculations. Subsequently, we investigated the possibility of using 31P J-couplings and residual dipolar couplings (RDCs) to assign relative configuration on phosphorus.

**POSTER 270**
**31P Derivatization and NMR Detection Strategies for Tannin Analysis**
Presenting Author: Luke Fulton

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*Luke Fulton (University of North Carolina Chapel Hill); Marc ter Horst (UNC Chapel Hill)*

Tannins are biomolecules that present as mixtures of highly similar structures which poses a challenge for both general characterization and content determination. Three quantitation strategies were compared: PULCON, deconvolution, and 2D qNMR. PULCON does not have a reference compound alongside the tannin to simultaneously serve as a chemical monitor. For deconvolution, the extent of overlap contributes to less accuracy than typically associated with internal standard methods. 1H and 31P correlations observed through 2D NMR exhibited more overlap in the aliphatic region than was expected. Due to the lack of aromatic proton correlations, we investigated phenol as an alternative reference compound, an option not available to 1D methods.

**POSTER 271**
**Eliminating Ambiguity in Small Molecule Structural Characterizations with J-Couplings and Computational Methods**
Presenting Author: James Harper

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Certain J-couplings provide structural information (e.g. the Karplus relationship relating three-bond 1H/1H couplings (3JHH) to dihedral angle). However, finding other general rules has been challenging. The development of accurate computational methods for computing J-couplings provides an alternative path that involves building all feasible structures then comparing computed and experimental values. This process encompasses one, two and three bond couplings to identify unknown structures with high confidence. This poster describes measurements of 1JCC in two partially characterized natural products and provides information to finalize these characterizations. A second study provides complete structural characterization of a novel natural product using only 1JCC data and 81 candidate structures. Work evaluating the merit of 2JCH and 3JCH values in structural studies is also described.

**THEORY COMPUTATION AND DATA PROCESSING IN NMR** (Posters 272 – 302)

**POSTER 272**
**Can Three-Site Relaxation-Exchange Maps be Asymmetric?**
Presenting Author: Bernhard Bluemich

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Asymmetric relaxation maps in three-site exchange report circular flow between the relaxation sites. This disagrees with detailed balance according to which the exchange between any pair of sites must be balanced in thermodynamic equilibrium. Confined vacancy diffusion by random jumps on a 2D checkerboard grid and confined gas diffusion were modelled to explore the impact of topological constraints on diffusion. Both models produce density variations across the pore. Moreover, in equilibrium diffusion up to 1% of the molecules appear to move in circular paths near the walls. This motion may result from pore resonance corresponding to diffusion eigenmodes. If confirmed by experiment, then detailed balance of multi-site exchange does not necessarily apply when the exchange is impacted by topological constraints.

**POSTER 273**
**Acquisitions with random shim values enhance AI-driven NMR shimming**
Presenting Author: Moritz Becker

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Shimming is still a time-consuming and cumbersome burden preceding most NMR experiments. Meanwhile, artificial intelligence is a promising approach to speed up and improve signal-based shimming algorithms. We present multiple enhancements for the applicability of AI-driven shimming, focusing on reference sample peaks for benchtop magnets. Our improvements include randomized dataset collection, upscaling from linear shims to an additional higher-order shim, and a novel flexible neural network architecture. We utilize a temporal history combining previous spectra and random shim offsets to explore the shim space, before applying predictive shimming steps guided by our neural network. The application reduces the linewidth from ~ 4 Hz to below 1 Hz, within less than 10 acquisitions, and helps avoid local minima of traditional algorithms.

**POSTER 274**
**REDEN: Multi-Fitting NMR Peaks Deconvolution-based Peak Picking Software**
Presenting Author: Abigail Chiu

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In NMR analysis, the accurate detection of signals, known as "peak picking," is essential for subsequent procedures. To address the issue of lower intensity peaks being obscured by more intense peaks, we present REDEN, a software that effectively identifies peaks in both 2D and 3D NMR spectra. Our integrated, cross-platform and open-source software can be accessed independently or as part of the Poky suite. It utilizes four fitting algorithms to deconvolute specified regions of an NMR spectrum, allowing for precise identification of all peaks. REDEN also provides options for fine-tuning and troubleshooting through Basic and Advanced modes. The advanced mode offers a wealth of data and fine-tuning capabilities, including 3D and contour plots of intermediate processing steps.

**POSTER 275**
**Post-acquisition correction of NMR spectra distorted by dynamic and static field inhomogeneity of cryogen-free magnets**
Presenting Author: Alexander Karabanov

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We describe analytical and numerical mathematical methods for post-acquisition correction of NMR spectra distorted by static and dynamic magnetic field inhomogeneity, typical for cryogen-free magnets. For the dynamic inhomogeneity, we apply a variant of the reference deconvolution method. For the static inhomogeneity, we apply the method of a delayed Fourier acquisition time. We verify our approach by post-processing experimental NMR spectra of liquid water and ethanol samples and obtain good results in both static and dynamic cases. This work complements our previous work on instrumental suppression of the cold head distortions. The results presented contribute to the general field of processing NMR spectra and serve towards a more extensive use of cryogen-free magnets in
high-resolution NMR spectroscopy.

**POSTER 276**
**Automated Chemical Shift Assignments of MAS Solid-State NMR Spectra of Complex Protein Systems by ssPINE/ssPINE-POKY**
Presenting Author: Andrea Estefania Lopez Giraldo

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We have developed a software package called ssPINE that automates the process of recognizing, categorizing, and assigning signals from various types of multidimensional ssNMR spectra of proteins. Additionally, we have developed a graphical user interface called ssPINE-POKY, which is a plugin integrated with the POKY suite. This interface allows users to easily submit ssPINE jobs, visualize, verify, download, and browse results. The combined package supports automated peak assignments and facilitates three-dimensional structure calculations. The ssPINE web server is available as a free alpha version accessed through a web submission form.

**POSTER 277**
**The Free Energy Landscape of Flexible Molecules studied using MD Simulations with Tensorial Orientational Constraints**
Presenting Author: Ulrich Sternberg

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Dipolar interactions are often measured as RDC tensors encoding orientations of molecules or molecular groups with respect to the external magnetic field. Used as constraints in MD simulations, the RDC tensors initiate molecular re-orientations and rotations of molecular groups. Such MDOC simulations can be augmented by scalar NMR parameters as 3J-couplings and NOE distances. They generate trajectories of molecules at ambient temperatures that are controlled by the energy and the entropy terms of the system. MDOC simulations demonstrated their power in elucidating chiral configurations, NMR parameter assignments and conformer distributions even for highly flexible molecules. In well studied molecules like strychnine new conformers were found that appear only with rising entropy.

**POSTER 278**
**Towards an Unlimited Number of Analytical Solutions for the Bloch Equations**
Presenting Author: Christian Bonhomme

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In this presentation, we tackle the problem of finding new analytical solutions for the Bloch equations, distinct from the celebrated Rabi and Rosen-Zener models. The solutions are obtained by combining the newly developed Path-Sum approach and reverse-engineering of the system of coupled linear differential equations. An unlimited number of analytical solutions is obtained consequently.

**POSTER 279**
**The POKY Suite for Biomolecular Solution and Solid-State NMR Spectroscopy**
Presenting Author: Woonghee Lee

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POKY is a professional-grade software suite for NMR-based structural biology and drug design. It offers advanced algorithms and modern technologies, including artificial intelligence and machine learning, to maximize user experience and productivity. POKY supports a wide range of NMR data and experiments, and can be easily integrated with other tools and databases. It is suitable for researchers and developers working in structural biology and drug design, and supports recent advances in the field, including 13C-detected solution NMR for intrinsically disordered proteins and 1H/13C/19F detected solid-state NMR for large, insoluble, and membrane proteins. POKY is freely available at https://poky.clas.ucdenver.edu and includes web servers and plugins for automated assignments and structure calculation.

**POSTER 280**
**Broadband Adiabatic Inversion Cross-Polarization: Theory and Applications**
Presenting Author: James J. Kimball

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Large anisotropic interactions make it challenging to acquire uniform ultra-wideline (UW) solid-state NMR spectra with high S/N ratios. Conventional CP experiments are well known to aid in signal enhancement; however, they typically operate over limited bandwidths. The broadband adiabatic-inversion cross-polarization (BRAIN-CP) sequence, which utilizes WURST pulses for polarization transfer, has been shown to compensate for these bandwidth limitations; however, to date, comprehensive experimental and theoretical investigations have only been conducted for static spectra of spin-1/2 and spin-1 nuclei. In this work, we demonstrate significant broadband CP enhancements for both static UW NMR spectra of half-integer quadrupolar nuclei and MAS spectra of spin-1/2 nuclei. Analytical and numerical simulations, along with applications to extremely unreceptive nuclei (99Ru and 103Rh), are presented.

**POSTER 281**
**EM simulation-based detector modeling and pulse compensation for parallel NMR experiments**
Presenting Author: Mengjia He

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In parallel NMR probes, radio frequency interference becomes a significant problem due to the coil's inductive coupling and matching network's enhancement, especially among the open coil system without excellent electrical isolation\cite{kupceParallel2021b}. This issue may cause pulse sequence coupling and signal transfer between multiple homonuclear channels. Based on the electromagnetic simulation, we present a theoretical framework to evaluate the coupling effects, calibrate the parallel pulse sequences with compensated cooperative pulse and split the composited FIDs from multiple channels. These results would help walk close to the capacity limit of designing parallel NMR probe in fixed magnet system.

**POSTER 282**
**Zero- to Ultra-low field NMR: Probing the Selection Rules of Angular Momentum**
Presenting Author: Adam Ortmeier

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Zero- to Ultra-low Field (ZULF) NMR is an emerging tool that can be used as a cheap alternative to conventional high-field NMR for a fraction of the cost without forfeiting sensitivity to molecular structure. Another remarkable aspect of ZULF NMR is that it creates spaces where the J-coupling Hamiltonian is the predominant interaction of the system. In this system, at ultra-low field, the coupled basis's energy states are close enough together where we can probe them. This gives us a unique opportunity to look at the selection rules of angular momentum. Where, depending on the axis of detection relative to the axis of a weak perturbing magnetic field, we observe different ZULF NMR spectra.

**POSTER 283**
**Robust Automated Backbone Triple Resonance NMR Assignments of Proteins Using Bayesian-Based Simulated Annealing**
Presenting Author: Anthony C Bishop

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Assignment of individual resonances of nuclear magnetic resonance (NMR) spectra to specific atoms within a protein remains a labor-intensive and often challenging task. Here we present a new algorithm BARASA for the automated assignment of backbone triple resonance spectra of proteins. The algorithm utilizes a Bayesian statistical analysis of predicted and observed chemical shifts in combination with simulated annealing to search for an optimal solution. The algorithm is tested against systems ranging in size to over 450 amino acids including examples of intrinsically disordered proteins (IDPs). BARASA is robust, accommodates incomplete and incorrect information, is sufficiently fast to allow for real-time evaluation of data acquisition, and outperforms currently employed algorithms – especially in cases of sparse data.

**POSTER 284**
**NMR Metabolite Quantification by Neural Networks Using Explainable AI Approach**
Presenting Author: Hayden Johnson

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Neural networks show promise for improving speed and automation of data processing for quantitative NMR analysis; however, neural networks are commonly thought of as a black-box approach – potentially discouraging usage in research. We examine this issue in a metabolomics context by generating a dataset from simulated metabolite signals, training a multi-layered perceptron for metabolite quantification, and using the integrated gradients method to facilitate interpretation of our model. Using integrated gradients, we obtain scores attributing model predictions to input features to gain insight into how spectral intensity at each chemical shift contributes to model-estimated concentrations. Results show the model recognizes target metabolite signals in a mixture spectrum and determine concentrations by assessing relative peak intensities, much like a human spectroscopist.

**POSTER 285**
**NUScon: New Tools for Evaluating and Optimizing Data Processing on Nonuniformly Sampled NMR**
Presenting Author: Adam Schuyler

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NUScon (nuscon.org) was founded as a community-driven contest with open challenges for reconstructing spectra from nonuniformly sampled (NUS) experiments. The original NUScon evaluation workflow starts with uniformly sampled NMR data, injects synthetic peaks, subsamples to produce NUS challenge data, reconstructs the spectrum with contestant scripts, and tests how the resulting spectra recover the injected peaks. We present here new modules to expand the scope of NUScon to evaluate sampling schemes and peak pickers. The NUScon software enables anyone to easily explore the modular tasks and evaluate how they impact spectral quality, thereby improving how we design and process NMR experiments. The NUScon software is delivered on the NMRbox platform (nmrbox.org), so any of its 250+ software packages can be utilized.

**POSTER 286**
**Fastcoords for Structural Biology Surveys in NMRbox**
Presenting Author: Hamid R. Eghbalnia

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Computation plays a critical role in nuclear magnetic resonance spectroscopy (NMR) applications in structural biology, and more broadly, all applications of structural biology. Many advancements have been enabled by access to data archives such as the Protein Data Bank (PDB), the Biological Magnetic Resonance Data Bank, and the AlphaFold Structural Database (ASB). Here we describe fastcoords, a software package that builds on the computational resources available on NMRbox (NMRbox.org) to simplify and accelerate search and analysis of structural data in archives such as the PDB and ASB, as well as federation of data from different resources. We demonstrate the significant gains in computational speed by performing search and processing operations on approximately 500 thousand AlphaFold protein structures.

**POSTER 287**
**Molecular Dynamics Approach in Modeling NMR Lineshape of non-Markovian Fluids**
Presenting Author: Mohamad Niknam

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Direct measurements of non-Markovian self-diffusion behavior are, to our knowledge, not currently possible with existing methods. In this work, we look at non-Markovian dynamics of diffusing spins with Molecular Dynamics simulations, present two methods for the prediction of NMR lineshape, and compare the results to the experimental observations. In the second part, we study the relationship between the lineshape and temperature, wall separation, and interaction with the wall.

**POSTER 288**
**Quadrupolar NMR Crystallography – Crystal Structure Prediction (QNMRX-CSP)**
Presenting Author: Robert Schurko

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A new Quadrupolar NMR Crystallography Crystal Structure Prediction (QNMRX-CSP) protocol will be presented, which uses experimentally measured and theoretically determined 35Cl electric field gradient (EFG) tensor parameters for the prediction, refinement, and validation of crystal structures of organic HCl salts, including pharmaceutical compounds. The protocol comprises three modules, which feature methods for molecular fragment selection, crystal packing with Monte-Carlo simulated annealing, and plane-wave DFT calculations (of EFG parameters and for structural refinement). Aspects including benchmarking, blind predictions of unknown structures, determinations of uncertainties of atomic positions, and possible applications using other quadrupolar nuclei (e.g., 14N, 17O, and 23Na) will be discussed.

**POSTER 289**
**ChemisTwin: A Novel Online Platform for electronic Reference Materials for NMR applications**
Presenting Author: Albert Farre Perez

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ChemisTwin is a digital portal which will contain an extensive database of electronic reference materials (eRM) acting as digital twins of the physical reference materials. These eRM are produced from physical certified reference materials (CRM) and the eRM is based on a digital package of datasets that defines a physical material. The use eRMs in the platform allows customers to perform the identity verification and content determination of their analytes of interest by uploading the raw data from the corresponding instrument. This solution allows the customer to automatically compare their sample with the eRM and provides a detailed report. This product provides our customers with a readily available, more sustainable, significantly less involved, and more error-proof solution.

**POSTER 290**
**Flow Encoding Established by Optimal Control RF Pulse**
Presenting Author: Mehrdad Alinaghian Jouzdani

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Flow encoding MRI is traditionally achieved by applying bipolar gradients. In this study, we show that velocity can be encoded into phase during the excitation time. First, a mathematical model is designed. Then, optimal control (OC) theory is used to design the required flow encoding RF pulse. Also, GRAPE algorithm is employed to minimize the cost function in the OC problem, and a constraint is added to make the RF pulse slice selective. This method enables one to achieve shorter echo times hence enhance signal-to-noise ratio. Furthermore, a non-linear relation can be made which improves phase-SNR of regions with lower flow rates, for example close to vessel walls.

**POSTER 291**
**Network for Advanced NMR Data Handling**
Presenting Author: Chris Bontempi

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The Network for Advanced NMR (NAN) provides many resources for simplifying and democratizing the use of high-field NMR. Data Transport automatically transmits acquisition data (VNMRJ/OpenVJMR and TopSpin) to a central repository. A sophisticated Data Browser allows users to browse and manage the repository contents and seamlessly integrates with NMRBox, BMRB and Globus. The Knowledge Bases allow users of all levels to conduct new experiments and better understand the process, while allowing experts to share their vast experience with the community. Resource Connector allows users to see the spectrometers and other resources available for their use. Dashboards ease administrative tasks and provide visibility into all aspects of the facilities and the system. NAN aims to be essential to any NMR lab.

**POSTER 292**
**Structure-Based Resonance Assignment Strategy for Sparsely Labeled Proteins**
Presenting Author: James H. Prestegard

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Recent advances in computational prediction of protein structure offer new opportunities for NMR characterization of ligand binding, protein-protein interaction and dynamics. However, assignment of NMR resonances reporting on these phenomena is a prerequisite. Traditional triple resonance assignment often requires expression in bacterial hosts, precluding work on proteins requiring extensive post-translational modification (glycoproteins) or folding chaperones, and for large proteins extensive overlap of resonances from uniform labeling can limit resolution. Here, we illustrate a sparse-labeling strategy applicable to mammalian cell expression along with a software tool (ASSIGN_SLP) for sequence specific assignment of resonances. New additions to the tool, including the use of data dependent on paramagnetic tags and the use of accelerated molecular dynamics to account for internal motion are discussed.

**POSTER 293**
**The BMRB archive of Protein, Nucleic Acid and Metabolite NMR Data**
Presenting Author: Kumaran Baskaran

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Biological Magnetic Resonance data Bank (BMRB: https://bmrb.io) serves the biomolecular NMR community by maintaining a curated archive of primary and derived data and metadata linked to scientific investigations under the "FAIR Principles" (Findable, Accessible, Interoperable, and Reusable). The goal of BMRB is to empower scientists in their analysis of the structure, dynamics, and chemistry of biomolecular systems and to support further developments in the field of biomolecular NMR spectroscopy. BMRB is a member and a core archive of the Worldwide Protein Data Bank (wwPDB: https://www.wwpdb.org). As of February 2023, BMRB holds over 11 million chemical shifts from 15729 macromolecule entries and a library of carefully curated NMR spectroscopic data of over 1000 small molecules.

**POSTER 294**
**Towards Shorter Composite Refocusing and Inversion Pulses for NMR**
Presenting Author: Stephen Wimperis

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Novel composite 180° pulses are designed for NMR and MRI. Rather than being constructed from 180° pulses, the new sequences are constructed from 90° pulses, with the aim of finding shorter sequences overall. The primary focus is on composite pulses that are dual compensated – broadband with respect to both rf inhomogeneity and resonance offset – and have antisymmetric phase schemes, hence forming spin echoes without phase errors. In particular, new dual-compensated refocusing pulses are presented that are constructed from ten 90° pulses, whereas the existing equivalents effectively consist of eighteen 90° pulses. The use of 90° pulses creates a number of theoretical difficulties for the design process and these are tackled here using average Hamiltonian theory and numerical searching.

**POSTER 295**
**A Flexible and Automated Approach to NMR Spectral Assignment using Full Bayesian Inference**
Presenting Author: Joseph Courtney

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Assigning NMR spectra can be challenging, especially for complex systems like Intrinsically Disordered Proteins (IDPs) and high-molecular weight complexes. Existing algorithms like Probabilistic Interaction Network of Evidence (PINE) are fast and accurate for solution-state spectra of small globular proteins but becomes less useful for larger and more complex molecules. To address this challenge, we have developed a flexible approach to NMR spectral assignment using full Bayesian inference based on probabilistic programming. Our approach is more general and flexible, enabling the inclusion of additional prior knowledge and new experimental schemes. Utilizing probabilistic programming enables the evaluation of a wide range of hypothetical structures and assignments, providing a powerful tool for NMR analysis.

**POSTER 296**
**SelEx – a fast and easily setup 1D exchange NMR spectroscopy experiment**
Presenting Author: Markus Rotzinger

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Observing chemical exchange in a variety of media is a challenge occasionally associated with isotope exchange to monitor dynamic processes. One frequently used method is EXchange SpectroscopY (EXSY) which gives information about chemical exchange processes on a variety of timescales. EXSY requires the acquisition of time-consuming two-dimensional spectra. In this work we provide a faster alternative, via an experiment which uses spatial encoding to extract similar information in a 1D experiment. Therein, all protons are observed at once, but in different slices of the detection volume. The experiment can be carried out in a single scan to identify exchanging sites in a 1D spectrum.

**POSTER 297**
**Quantum optimal control module of Spinach library**
Presenting Author: Ilya Kuprov

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In magnetic resonance, optimal control theory is used to generate pulses and pulse sequences that achieve instrumentally difficult objectives (for example, uniform 13C excitation in a 1.2 GHz magnet) with high precision under stringent time and radiofrequency/microwave power constraints. At the moment, the most popular framework is GRAPE (gradient ascent pulse engineering, 10.1016/j.jmr.2004.11.004).
This poster reports our recent mathematical and software engineering work on the various extensions and refinements of the GRAPE framework, and on its implementation as a module of Spinach library. Recently implemented functionality includes: fidelity Hessians and regularised Newton-Raphson optimisation, generalised curvilinear waveform parametrisation, prefix and suffix pulse sequences, multi-target and subspace control, keyhole states and subspaces, cooperative pulses and phase cycles, and piecewise-linear control sequences.

**POSTER 298**
**Sensitivity of Nonuniform Sampling Experiments**
Presenting Author: Yulia Pustovalova

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All common techniques for spectral reconstruction of multidimensional NMR experiments employing nonuniform sampling (NUS) are nonlinear. Low-intensity signals are often lost during spectrum reconstruction. Increasing the number of transients can improve sensitivity at the expense of lower NUS coverage. However, there is a trade-off between the number of sampled points and transients for time-limited experiments. The standard metric for uniformly sampled data, signal-to-noise ratio, is unreliable for NUS spectra reconstruction. So, here we use intrinsic receiver operating characteristic (IROC) analysis to explore the nonlinearities caused by NUS reconstruction algorithms, NUS sampling and noise level. We find evidence for noise-dependent phase transitions reminiscent of the Donoho-Tanner phase transition for nonuniform sampling coverage.

**POSTER 299**
**Improved Signal Detection in Magnetic Resonance with Pseudorandom Phase Encoding**
Presenting Author: Michael W. Malone

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Magnetic resonance based signal detection can be greatly complicated by radio frequency (RF) interference, especially when frequency components of the interference are close to the target signal. By pseudorandomly varying the phase of a magnetic resonance signal, however, a "fingerprint" can be encoded in the target signal that distinguishes it from the RF interference. We describe a modification to the Carr-Purcell Meiboom-Gill sequence and show how it allows us to reject strong interference even at our target signal frequency. This has the potential to improve fieldable deployments of magnetic resonance systems for substance detection.

**POSTER 300**
**A New Generation of NMR Data Processing Software for a New Generation of Chemists**
Presenting Author: Alex Waked

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To close the skills gap reported in chemical sciences graduates, students need educational experiences that mimic their future careers. However, logistical and financial barriers often make such work difficult to replicate in an academic environment. In particular, NMR and other analytical data processing software have historically been difficult to implement in chemical education. In response, we present the first commercially available browser-based NMR and hyphenated chromatography/MS processing application—Spectrus JS. Designed to address the barriers presented by its predecessors, it provides a convenient and cost-effective way to deploy and access NMR and analytical data processing tools in academic environments, helping educators better equip the next generation of chemists.

**POSTER 301**
**Analyzing the use of \textit{in situ} Receiver Operator Characteristic to Evaluate Nonuniform Sample Reconstructions**
Presenting Author: D. Levi Craft

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Nonuniform sampling (NUS) has allowed spectroscopists to tailor their experiments to reduce data collection time and improve spectral quality. The Nonuniform Sampling and Reconstruction Contest (NUScon) has released a workflow for evaluating spectral reconstructions. We extend this workflow to include a new evaluation metric using \textit{in situ} receiver operating characteristic (IROC). This study evaluates how to interpret the results of an IROC analysis alongside the standard approach of computing a point-spread-function and calculating its peak-to-side-lobe ratio, a known standard for approximating the relative intensity of signals to artifacts introduced into a reconstructed spectrum. This study presents tools for assessing spectral quality and optimizing ML-based techniques, which served to jump start a spectroscopist's workflow.

**POSTER 302**
**Nutation-Based Longitudinal Sensing Protocols for High-Field NMR With Nitrogen Vacancy Centers in Diamond**
Presenting Author: Declan Daly

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Nitrogen vacancy (NV) centers in diamond allow for accessible NMR experiments on samples of just a few picoliters. NV-NMR has been unable to work in the high-field regime due to the challenge of making NV's sensitive to high frequency Larmor signals. We investigate the experimental viability of NV-NMR at high field with a new experimental protocol called DRACAERIS (Double Rewind ACquisition Amplitude Encoded Radio Induced Signal). We will discuss how finite pulse lengths and spin-spin couplings affect the resulting NMR spectra and identify reasonable experimental parameters. Additionally, we will highlight recent progress towards the experimental realization of DRACAERIS NMR.

**LATE**

**POSTER 303**
**Contrasting lanthanide and actinide complexation by polyoxometalates via solution-state NMR**
Presenting Author: Christopher Colla

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Deciphering the solution chemistry and speciation of actinides is inherently difficult due to radioactivity, rarity, and cost constraints, especially for transplutonium elements. In this context, the development of new chelating platforms for actinides and associated spectroscopic techniques is particularly important. In this study, we investigate a relatively overlooked class of chelators for actinide binding, namely the polyoxometalates (POMs). We provide the first NMR measurements on americium-POM and curium-POM complexes, using 1D 31P NMR, variable temperature NMR, and spin-lattice relaxation time (T1) experiments. Reaction constants, reaction enthalpy, and reaction entropy were extrapolated from the NMR data. The proposed POM-NMR approach allows for the study of trivalent f-elements even using microgram amounts and in phosphate-containing solutions where they are typically insoluble.