National/Regional NMR Resources @UConn

1985
• Gregory P. Mullen NMR Structural Biology Facility

2015
• National Center for Biomolecular NMR Data Processing and Analysis

2019
• Biological Magnetic Resonance Data Bank (BMRB)

2021
• Network for Advanced NMR (NAN)
What’s NMR used for?

At UCH we use it to

• Understand the molecular basis of biology and disease
• Characterize potential drug targets (proteins)
• Find compounds that interact with targets

Prof. Bing Hao
Spore germinant factors, NSP3: Bacillus, Covid-19

Jeff Hoch
NSP3, p16, PfPMT: Covid-19, Cancer, Aging, Malaria

Prof. Dmitry Korzhnev
PCNA: Cancer

Prof. Irina Bezsonova
USP7: Cancer, Neurodegeneration
Quo vadis?

- Structure-based drug discovery
- Biologics (e.g. mAB) process monitoring
- Metabolic profiling
- Diagnostics
- Food industry

Instructional Workshops

Monday October 18, 2021 (all times in EST)

- **4:30 – 7:30 PM: Wine Tasting by NMR**

  Presented by: Lloyd Sumner (Univ Missouri), Adam Schuyler (UConn Health), David Wishart (Univ Alberta), and Robert Powers (Univ Nebraska)

  We request that you register for a free NMRbox account to maximize your involvement and register for the Event "MANA Conference" on the NMRbox website. You should register BEFORE the workshop to enable access workshop data and software. The "Wine Tasting by NMR" workshop is supported by the NMRbox platform. If you want to follow along with the tutorial and access the workshop data and software, you must sign-up for a free NMRbox account (if you don’t already have one) and register for the MANA event on the NMRbox website.

Using a proprietary metabolite profiling platform and customized machine learning algorithms, Olaris can identify individual molecular profiles so detailed that the guess work in how to treat a patient’s disease is removed. By collaborating with patients, clinicians, hospitals, payers and biopharma Olaris generates data with high clinical utility. This data enables healthcare providers and their patients to pursue the most effective treatments.

Additionally, the comprehensive Olaris profiles can help pharmaceutical companies take novel approaches to develop targeted medicines, adding value and efficiency to our health-care system.
1.2 GHz NMR spectrum of urine
Ultra-High Field NMR GHz-Class Sites
World Map of Systems delivered and on order (October 2021)

America’s
1.0 GHz 1
1.1 GHz 3
1.2 GHz 1

Europe & IL
1.0 GHz 5
1.2 GHz 10

APAC
1.2 GHz 1
Network for Advanced NMR (NAN)

- 1.1 GHz
  - St. Jude Children’s Research Hospital (private)
- 1.2 GHz
  - OSU, expected 2023

[Map showing connections between various institutions with NSF logo]
Expanding NAN

Sites to be determined

- NSF STC or TIP
- $100M would provide 5 x 1.1 GHz instruments (including at UConn) and 5 years of operational costs across 7 sites

Name needed for umbrella organization

UConn Means NMR
Space: The next frontier

Older magnets are not shielded, requiring more space.
Two of our instruments have shielded magnets, but two are not shielded.
Replacement cost: ~$3M

Dry space: the NMRbox, BMRB, and NAN teams are dispersed.
Lab space: we are running out of space for benchtop instruments and people. New faculty recruitment is hampered.

Computer space: we are running out of space in our High Performance Computer facility. Computational needs for NMRbox and NAN are both expected to grow substantially.
Reproducibility

Confirmation in science relies on *reproducibility*

- Studies by Pharma have found 70% or more of published studies are *not reproducible*
- Barriers to reproducibility include missing data, software, and descriptions of processing and analysis workflows
- Funding agencies and congress are all increasingly concerned with reproducibility
FAIRness
Fosters reproducibility

Findable

Accessible
Originally articulated for data, FAIR principles can be applied to any knowledge asset: Software, Instruments, Protocols

Interoperable

Re-usable
NAN facilitates reproducibility

- FAIRness for instruments, data, protocols
- Connect 26 NMR spectrometers to the UConn archive for automatic and secure data archiving
- Harvest information about samples ("metadata") at the time the experiment is performed
- "Browse" instruments, data, protocols by metadata
- Simplify deposition of data to public data repositories (e.g. BMRB)