NMR center news - 2/3/2022

1. CTSI grants for NMR usage are now available to ND labs

We have great news to share: we obtained a **CTSI Designated Core** status.

How is it useful for you?

It is now possible to obtain a grant from Indiana CTSI to pay for your use of NMR instruments. The condition is that your project must (potentially) benefit medicine in some way in a future. Think: free NMR time for your research!

How to obtain the money?

PIs may write a short proposal and get up to $10,000 from CTSI to cover NMR usage. Postdocs may write their own application and get $5000 for their own NMR usage.

Details from CTSI website

CTSI “PILOT FUNDING FOR RESEARCH USE OF CORE FACILITIES”, deadline in March; $10,000 for two years; https://indianactsi.org/wp-content/uploads/Guidelines-Spring-2021.pdf

CTSI Postdoc Challenge Grant Funding to Use CTSI Designated Core Facilities, deadline in February; $5,000 for one year. https://indianactsi.org/wp-content/uploads/Postdoc-Challenge-RFA-2021.pdf

2. Organic Structure Elucidation at MRRC

New software: MNova Structure Elucidation

We purchased a network license for MNova Structure Elucidation plugin! This is a software to help you semi-automatically solve structures of small and medium-sized organic compounds. It is available to anyone with Notre Dame NetID on campus or through VPN. We are preparing a set of tutorials to help you learn the software. Stay tuned!

How much compound do I need for structure elucidation?

You can work with samples as dilute as 5 mM. To give you a sense of how much material it is: for a molecule of 650 Da molecular weight, you only need 1 mg to make a sample in a Shigemi tube (0.3 ml). You can collect all necessary data within about 24 hours on a Bruker 800 with a room-temperature TXI probe and solve the structure within a few days.

3. Cryogenic and room-temperature probes at Bruker 800

One bit of sad news in this newsletter: our Cryoprobe on Bruker 800 developed problems with cold preamplifiers and is out of service for now. We are working with Bruker on its repair but the advanced age of the probe (17 years) may make unsuccessful.

The good news is that **Bruker 800** with a room-temperature **TXI** probe is still **the best deal for proton detection in a 100-mile radius**. If compared to Bruker 500 in McCourtney, the TXI probe on Bruker 800 allows to collect data almost 8 times faster with the same signal quality (signal-to-noise ratio). In addition, 800 MHz magnet gives nearly double resolution relatively to 500. The sample requirements for structure elucidation (above) are given for the room-temperature TXI probe currently installed at Bruker 800.

For detection of carbon, sensitivities of Bruker 800 (with BBO probe), Varian 600, and McCourtney 500 are similar. However, for structure elucidation projects, Bruker 800 with a BBO probe is essential because increased spectral resolution allows to resolve closely spaced peaks of stereoisomers with greater confidence thus aiding and speeding up signal assignment.

With any questions or comments, please, email us at nmr@nd.edu