



**Volume 1**  
**June 17, 2024**

***“The best kept  
secret at UGA”***

## What’s New in the CCRC NMR Facility?

The Complex Carbohydrate Research Center NMR Facility may be the best kept secret at the University of Georgia. “But wait”, you are thinking, “I know about the NMR facility and have even used it.” This Newsletter is designed to let you discover the many things—some old and many new—that you might not know. These might even help you in your research. Each issue will feature a different capability that you might want to add to your research tool chest. We will also update you on the latest facility news.

### Did you know...

**Did you know that the CCRC NMR facility now has the most sensitive  $^{13}\text{C}$  probe in the world?** I didn't think so.

Through an NIH R01 grant and partnerships with the National High Magnetic Field Laboratory and Bruker, we have developed a new  $^{13}\text{C}$  high-temperature superconducting probe for our 21.1 T (aka 900, aka "lunar lander").

Most people who use NMR will measure  $^1\text{H}$  (proton) spectra. There is good reason for this, because protons are abundant and a great NMR nucleus with high sensitivity. So, what's wrong with that? Nothing if your sample is pretty simple and doesn't have a lot of overlapping signals. But for samples such as complex carbohydrates, there is a lot of overlap in  $^1\text{H}$  NMR spectra and it can be hard to figure out what is going on, even with 2D NMR.

### **$^{13}\text{C}$ NMR: great for complex carbohydrates**

$^{13}\text{C}$  NMR is great for overlapping samples like complex carbohydrates. Whereas  $^1\text{H}$  NMR has a chemical shift range of about 10 ppm,  $^{13}\text{C}$  has a range of about 200 ppm! That is a lot of room to put more signals before there is overlap. Also, there are experiments using  $^{13}\text{C}$  detection that greatly simplify the identification of unknown organic molecules. One of the best is called INADEQUATE [Don't you love some of our acronyms? This was coined by Ray Freeman and stands for Incredible Natural Abundance DoubleQUAntum Transfer Experiment.] An INADEQUATE spectrum provides the complete carbon backbone assignment of a molecule.

### **$^{13}\text{C}$ NMR: excellent for compound ID**

Why don't more people use  $^{13}\text{C}$  NMR? Mostly, because it is relatively insensitive compared with  $^1\text{H}$  NMR. And the great INADEQUATE experiment is the most challenging at natural abundance (1.1 %  $^{13}\text{C}$ ), because it requires two adjacent  $^{13}\text{C}$  atoms, which has a probability of  $(0.011)^2 = \frac{1}{8264}!!$

Our new  $^{13}\text{C}$  HTS probe has outstanding sensitivity. When compared to a good room temperature broadband probe (which is what most people have used if they have done  $^{13}\text{C}$  NMR), our new probe is about 15 x more sensitive. This translates to either 15 x less material required or a whopping 225 x less time needed to record the same spectrum compared to a broadband probe. We have 2 other outstanding  $^{13}\text{C}$  cryoprobes in our facility, and the new probe is about 2 x more sensitive than the best commercial probe.

Please contact us if you want to see how this probe can help you in your research.

## CCRC NMR Facility News

You might have heard about the NSF-funded Network for Advanced NMR (NAN). We will provide more detail about how the many ways that NAN will enhance your NMR research in later newsletters, but the big-ticket item in NAN is the new 1.1 GHz NMR for UGA.

This will be one of the first 1.1 GHz systems in the US. Our NAN partner at UW-Madison has their 1.1 GHz system running now for solid state applications and St. Jude's has another one for internal use. The CCRC NMR Facility 1.1 GHz will be the first in the US for a user facility that is dedicated to solution NMR (metabolomics, glycomics, structural biology).

Our system will arrive at the CCRC lower parking lot on June 24 and will be craned into the facility on June 25! It will be exciting for us and chaotic for anyone who parks at the CCRC, so pay attention to notices about the restrictions in lower lot parking around that time. There will be some good photo ops in the NMR Overlook room, so feel free to stop by to watch some of the action.

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