

Kennesaw State University Nuclear Magnetic Resonance facility users guide

Before using any of the equipment in KSU's NMR facility, you must read and sign this document. DocuSign is preferred for faculty and staff.

I have read the following users guide and confirm that I will adhere to facility policies.

Signed: _____ Name: _____ Date: _____

Principle investigator: _____ Dept. affiliation: _____

To schedule training or discuss capabilities and/or projects with Dr. Leeper please book his time in his calendar with the following link: <https://thomas-leeper.youcanbook.me>

Facility instrumentation: Knowledge of the facility capabilities will be useful for determining which instruments will suit your needs. Multiple instrument upgrades have happened recently so even experienced users should consult this guide and familiarize yourself with new features.

300 MHz instrument – This system was updated with a refurbished magnet and new console, probe, and workstation. This system can function similar to the 400 MHz system for routine samples, albeit without a sample changer. New and improved functionality includes: a new broadband tunable 2-channel probe capable of collecting ^1H , ^{19}F , ^{13}C , ^{15}N , and ^{31}P in directly detected spectra; two channel capabilities enable decoupling and/or double resonance spectroscopy e.g. HSQC between ^1H and a broadband nucleus; a new windows PC workstation, automated tuning and matching; gradient shimming; and access to IconNMR. This system is intended for routine research samples and for teaching. Access is scheduled via Faces.

400 MHz instrument – This system is unchanged from prior capabilities and includes: 24 tube SampleCase automated sample insertion, a broadband tunable 2-channel probe capable of collecting ^1H , ^{19}F , ^{13}C , ^{15}N , and ^{31}P directly detected spectra; two channel capabilities enable decoupling and/or double resonance spectroscopy e.g. HSQC between ^1H and a broadband nucleus; temperature stabilization via BCU or liquid nitrogen for variable temperature NMR; automated tuning and matching; gradient shimming; and access to IconNMR. This system is intended for routine and advanced research samples. Access is scheduled via Faces.

600 MHz instrument – This new high-field system provides the following capabilities: SampleJet automation (5 x 96 samples or 30 conventional tubes); triple resonance ^1H , ^{13}C , ^{15}N cryoprobe with very high sensitivity; three channels for simultaneous decoupling of ^{15}N and ^{13}C or triple resonance spectroscopy; automated tune/match; gradient shimming; temperature stabilization via BCU; Linux workstation, and non-uniform sampling for reduced experiment time in multidimensional experiments; This system is intended for advanced research samples, such as polymers and biomolecules. Access is scheduled via Faces and may require assistance from Dr. Leeper.

Training: All users of the KSU NMR facility must be trained for safe and efficient NMR use. For users already familiar with the 400 MHz and/or with familiarity with the prior 300 MHz system, this would

only be a brief update (~ 15 to 20 minutes). *All users who want to use the new 300 MHz system need to have this brief update.* For users wishing to become trained on the 600 or for users new to the facility, Dr. Leeper offers *ad hoc* training, preferably in groups of 2 to 3 (see the following link to book training time: <https://thomas-leeper.youcanbook.me>).

Types of tubes: All three systems can accommodate a variety of 7 inch long 5 mm diameter NMR tubes but Wilmad or Bruker make the best tubes. Most tubes have a rating such that they are only intended to be used for fields of that rating or lower. Thus, tubes rated for the 300 MHz NMR would have poorer performance on the 400 or 600 instrument and are not recommended. *For users wishing to purchase tubes compatible with all three instruments it is recommended to buy a pack of **Bruker Z172600** tubes (100 unracked tubes with bar coded caps for ~\$240 = \$2.40 per tube).* Details for purchasing racks of 96 tubes for the 600 MHz instrument can be provided for high throughput work.

Scheduling: NMR time will be booked at: <https://faces.ccrcc.uga.edu> with Group *KSU_CHEM*. Users must obtain a Faces login and password from Dr. Leeper if they have never done so before. *Unscheduled walkup use of the 300 is no longer be permitted.* It is strongly recommended that users for the 300 and 400 limit blocks to one hour and those who wish to book longer blocks should do so for nights and weekends. After each experiment is completed users must sign the logbook using a regular ballpoint pen (not sharpie or pencil) to confirm that the spectrometer remains in working order and is ready for the next user; each spectrometer has its own paper logbook.

Tidiness: It is expected that users will clean up after themselves. Samples left in tube racks for more than a week may be collected and disposed of at Dr. Leeper's discretion. Please do not leave KimWipes, glassware, or papers littering the workstation desks.

Data storage and removal: Please make every effort to organize datasets into folders following a regular scheme. Data hygiene is very important. Flash drives must be free of malware or viruses or we will have to reinstate the flash drive ban. All computers have optical drives and a stack of writable CDs and DVDs are available in the vestibule. The 300 is not typically going to be on the network but can be temporarily networked by request. NMR data on the spectrometer computers is not intended for long-term storage; drives fail so it is strongly recommended that you transfer your data offsite for processing. Bruker offers free processing software here: <https://www.bruker.com/service/support-upgrades/software-downloads/nmr/free-topspin-processing/nmr-topspin-license-for-academia.html>

Printing: Two printers are available; one for 300 and 400 and one for the 600. Neither are networked and are intended to be used appropriately and only for printing spectra for notebooks or class use. Printouts left in the printer will be reused as scrap paper.

Publications: In the acknowledgement section for publications resulting from work performed in the KSU NMR facility, please provide the following statement: *"The authors would like to acknowledge Kennesaw State University Academic Affairs for support of the NMR facility, which made possible the research necessary for the completion of in this project."*

Special pandemic-related instructions: Masks must be worn by unvaccinated users while in public areas of the KSU campus, including the NMR lab. In addition, please make every effort to social distance and to wipe down keyboards and work surfaces with the sanitizing wipes provided.