

Introduction to the NMR Facility

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Howdy

Welcome to the Chemistry NMR Facility at Texas A&M University. Our facility includes 9 NMR spectrometers, an EPR, a helium recovery facility, and 3 full-time staff positions. Although this facility is physically housed within the Chemistry Department, we provide services to the entire TAMU community and beyond. We do ask everyone to conduct themselves in a safe and mindful manner.

Safety Notices

- Never, for any reason, are you to bring a person with a pacemaker close to a magnet.
- Avoid bringing ferromagnetic materials anywhere near a magnet. This includes most tools and office supplies.
- Be wary of bringing electronics close to a magnet, we are not responsible for their loss.
- Do not use the instrument for any purpose other than those for which it has been designed and set up.
- Do not bring food or drink into the lab.
- Some instruments have additional safety requirements, be familiar with and observe them.

Rules and Etiquette

There are some solid rules, and good practices.

- Never, for any reason, allow anyone else to use your login information. Violating this rule can have severe repercussions at the university level for all involved.
- Do not make a reservation for anyone else or that you do not plan to keep, and delete a reservation if circumstances prevent you from keeping it as planned.
- Never take someone else's sample out of the sample changer.
- Your experiments are expected to be completed within your reserved time.
- You may use the instrument without a reservation, but if someone has made a reservation during a time slot: that person has priority and you must surrender the instrument to that person.
- When your immediate use for the instrument is done you should either log out or change user. Never power down the computer.

System Introduction

The TAMU chemistry department systems are detailed below. Please note that each system is described for the configuration you are most likely to find, but other options may be utilized – check first.

1. Avance Neo 400MHz Broadband Systems in Room 1318 (Tango and Waltz)

These systems are capable of running (almost) any choice of nucleus, and are equipped with 60 position sample changers and automatic tuning. These systems run in Icon-NMR as first-come, first-served and so are not on the reservation system. **All initial NMR training is done on these systems. An open call training class is held every Tuesday morning at 0900hrs in room 1318.**

2. Inova 500MHz H/F/P/C System in Room 1221

This system has a quad probe that allows experiments with one high-band (H/F) and one low-band (P/C) nuclei to be done. Contact the staff for access to the initial training videos, and then to arrange taking a quiz. Once the quiz has been passed, an in-person training session will be scheduled.

3. VnmrS 500MHz H/F/P/C System in Reed-McDonald Room 415

This system has four channels, and a probe that can use them all. In other words, experiments with any combination of H/F/P/C may be done on this system. Training on this system requires proficiency with the Inova 500MHz. Then you may contact the staff for access to the initial training videos, arrange to take a quiz, and then schedule an in-person training.

4. Avance III 400MHz Broadband System in ILSB Room 1163

This system is capable of running (almost) any choice of nucleus, and is equipped with a 60 position sample changer and automatic tuning. This system runs in Icon-NMR as first-come, first-served and so is not on the reservation system. Accounts for this system are only made for ILSB users, but **training for this system is done with the training on Tango and Waltz (see above).**

5. Avance 500MHz Cryoprobe System in Room 1238

This system is equipped with a H/C/N cryoprobe, and is meant for longer acquisitions of low concentration samples. It is equipped with a 24 position sample changer and automatic tuning. Training for this system must be scheduled with the staff, initial training is done for the Icon-NMR mode with additional training available for manual mode.

6. VnmrS 500MHz Broadband System in Room 1327

This system is equipped with a H/F{X} probe, and is intended for very long acquisitions and special applications. Training for this system is available to users that are proficient with the VnmrS 500MHz in Reed-McDonald. Contact the staff to arrange training.

7. Avance Neo 400MHz Solid-State System in Room 1324

This system runs solid-state experiments only. It is on the iLab reservation system, contact Vladimir Bakhmoutov (1323 Chemistry, 979-845-8993, bakhmoutov@tamu.edu) to schedule time. Training on this system is more of an apprenticeship: it has to be. If you are going to be a significant, consistent user and would like to run the system yourself – contact Vladimir.

8. VnmrS 300MHz System in Room 2211E

This system is solely used by the organic labs. It is running VnmrJ 4.2A software in a Walkup mode. This system is not available for research work, and training is held only as part of the lab courses.

9. EPR in Room 1133

This system alternates between room temperature and cryogenic temperature work from week-to-week. The system is scheduled using iLab using separate calendars for each temperature. Training needs to be scheduled with the staff, and you must be proficient with room temperature operation before doing cryogenic work.

Reservations

Faces

Faces is a web-based scheduling service that makes it possible for authorized clients to reserve resources on a first-come, first-served basis. Faces Scheduling System software is designed to facilitate the scheduling of scientific instruments and other resources in a research environment, and serves as a web accessible sign-up sheet. It was developed by William York and Saeed Roushanzamir at the Complex Carbohydrate Research Center at the University of Georgia.¹

The Faces website is <https://faces.ccrcc.uga.edu> and our group is TAMU_CHEM_NMR. You will be sent an email with your user name and initial password. Please see the Faces Primer document in our Training Center (<https://nmr.chem.tamu.edu/TrainingCenter.php>) for more details, including specific time allotments and rules for each system. All NMR instruments that require a reservation are scheduled through Faces, but you will only see those systems for which you have been trained.

iLab

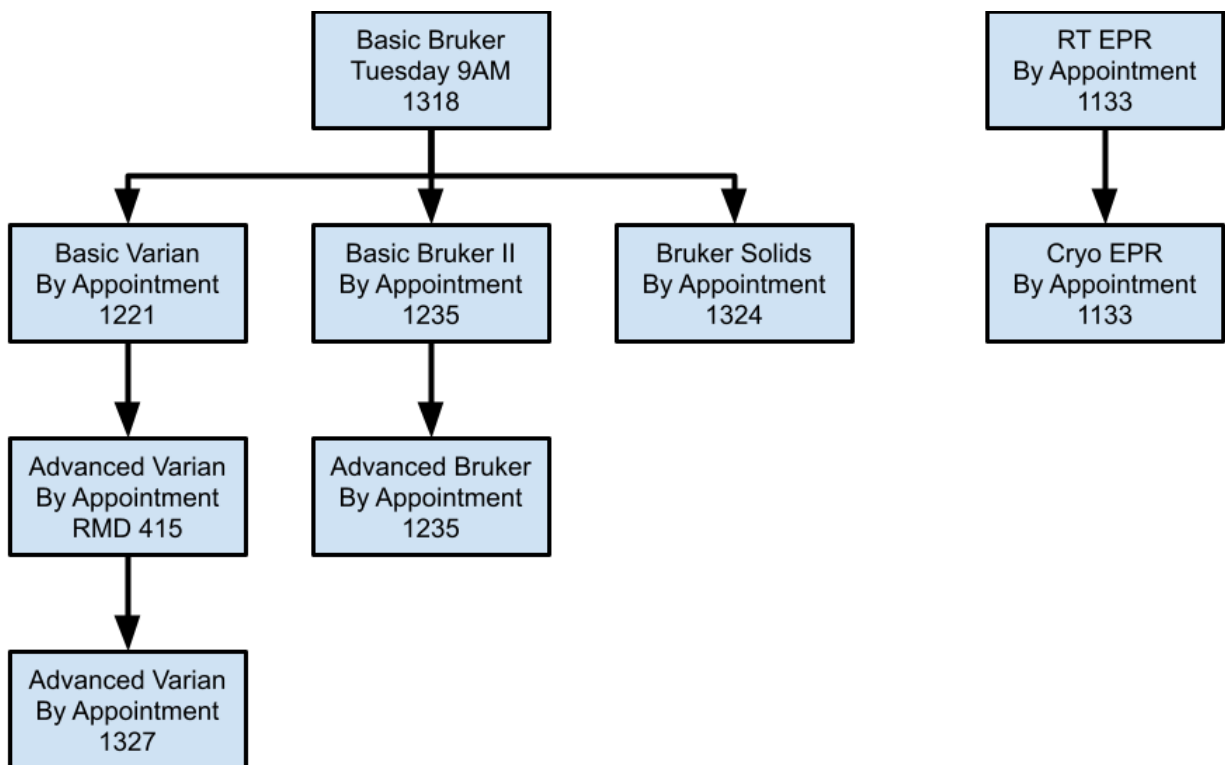
The solid-state NMR and EPR are reserved using the iLab system (https://tamu.corefacilities.org/service_center/show_external/4728). All solid-state NMR reservations must be approved by the staff. The EPR has two calendars as weeks alternate between room temperature and cryo temperature experiments. All cryo temperature EPR reservations must be approved by the staff.

Training

In the systems' introductions (above) a brief description for being trained on the instrument is given. In a more facility-wide view-point, the training on our systems is done in an order that adds incrementally to the understanding required to use the system correctly. The training pathway itself is more clearly represented by a flowchart (see below).

¹ Taken from <https://faces.ccrcc.uga.edu/ccrcfaces/faq0.php>

Flowchart



Variable temperature training for each system (if appropriate) is a separate training on that system and is arranged by appointment.