

Magnetic Resonance Center: Notes and Rules

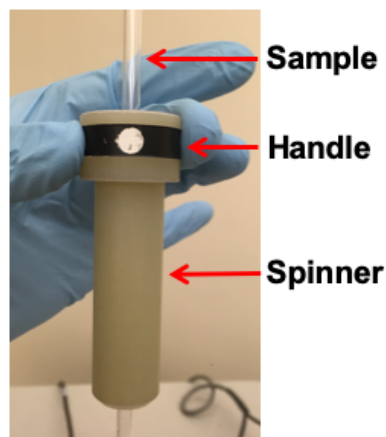
Spectrometer Sign Up Rules:

1. You must sign up for iLab to be able to make reservations on the spectrometers. Once your PI (who gets an email when you sign up for iLab online) has accepted you as a member of his/her lab, **you need to let me know**, so that I can grant you access to the NMR calendars.
2. **The “day queue” for the Varian/Agilent 500 (*Tomoya*) extends until midnight**; therefore only 20-minutes per user is allowed from **8 am to midnight** on this spectrometer—the day queue is from **8 am to 10 pm** on *William*, (cold probe) **and 8 am to 8 pm** on *Boylan* (600 MHz) and *Shoshana* (Prodigy). The 400MHz system *Meagan*, is reserved exclusively for the Hoveyda lab.
3. As it stands, claiming additional NMR time after your allotted 20 minutes end is allowed, **if there are no users waiting to access the spectrometer**. However, pre-planned back-to-back NMR reservations by two or more users are strongly discouraged, particularly if they occur during "high-traffic" times (e.g. ~3 to 6 pm on weekdays, give or take). On the rare occasions that this absolutely must happen, the overall time should be **limited to 1 hour, with a 30-minute waiting period** for any potential repeats—this is simply to be fair to all users.
4. To avoid any unintended time reservation errors, we strongly suggest that all "long" experiments (e.g., ¹³C NMR of large molecules) be performed overnight, following the NMR lab rules. If it is a rare "one-time" request, please speak to the Director for permission before setting up the experiment.
5. Reservations on any of the NMR spectrometers may be done **ONLY one day in advance** (meaning just past midnight on the previous day). Early reservations may be deleted—you can reclaim the slot at the proper time of course.
6. Do not sign up for multiple spectrometers for overnight use unless time on the second spectrometer **has not been claimed by 8 pm that same night**. In special cases (publication crunch, fast-degrading samples etc.), as always, please come discuss potential spectrometer bookings with the Director.
7. Saturdays are considered a regular week day in the NMR lab, but you are allowed to make longer (no time limit) reservations on *William*, *Shoshana* or *Boylan* on Sundays. So theoretically, you may book one of these to run long experiments all day on Sunday, until 8 am Monday morning (**Tomoya operates according to the usual rules even on Sunday**). However, please be cognizant of other users when making these longer reservations, and talk to each other in emergencies.

Safety:

1. Sample Loading:

- Remember to first insert your sample into the sample holder (a.k.a. “spinner,” \$560 each, so please do not drop!), and then load it into the magnet. **Do NOT drop your sample tube, or the empty spinner into the magnet!**
- After switching the eject air ON, **make sure you hear the sound of gas** exiting the upper barrel before loading your sample. If you do not hear the loud gush of air, please inform us immediately, and **DO NOT INSERT** your sample!
- Hold the spinner from the top, and please avoid touching the lower part, since it helps keep the upper barrel and sample holder in the probe clean (we do **NOT** spin samples).



2. Spectrometer and Lab Safety:

- Make sure your experiment is **stopped** before logging out: **DO NOT leave the system pulsing without a sample in the magnet!**
- Please make use of all the steps on the ladder, and **do NOT touch or put any weight on the magnets!**
- Keep the lab quiet (respect for all) and clean—**no food or drinks in the lab.**

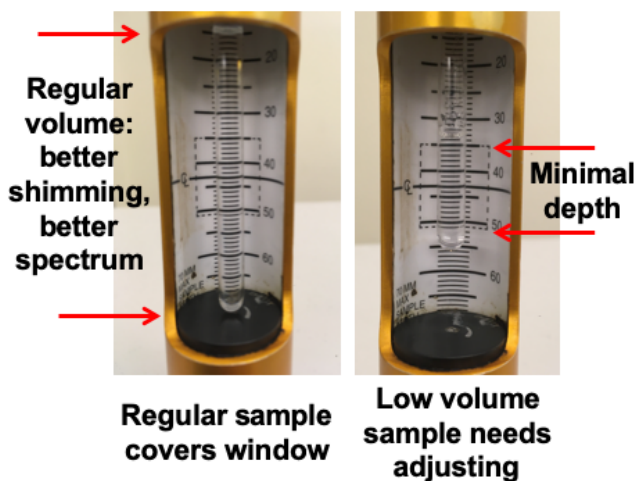
3. Accidents:

- If you make any mistakes in the lab, **please let us know immediately.** Mistakes happen, but we need to be aware of them as soon as possible, to avoid compounding any potential issues.
- **Do NOT unplug ANY accessories in the NMR lab! Do not restart any of the computers!** Please inform us if there is an issue, and leave a note explaining the situation (on the desk) for the next user.
- Please let us know if there is any situation that seems out of the ordinary e.g. low air pressure, frozen software etc. Please **DO NOT** attempt to “fix” any problems with the spectrometers on your own: **this is a liability issue.**
- Please do your best to avoid the MRC if you are tired. This is usually when you make absent-minded yet catastrophic errors (e.g. dropping a sample into the magnet without the eject air on).
- If you accidentally break your sample outside the magnet, we will help you clean it up. However, please be very careful to not break a sample *inside* the magnet (**by dropping it without the eject air**), because it would put the spectrometer out of order for a significant period of time.

Pre-Acquisition Acquisition Guidelines:

1. Sample Preparation:

- Sample volume of **600 μl** (for a regular 5 mm NMR tube) is strongly encouraged for optimal shimming.
- If volume is less: **do NOT use Shoshana**! For the other systems, center the sample along the box in the depth gauge, as shown in the figure.
- Deuterated solvents (D_2O , CDCl_3 etc.) are required to “lock” the sample.

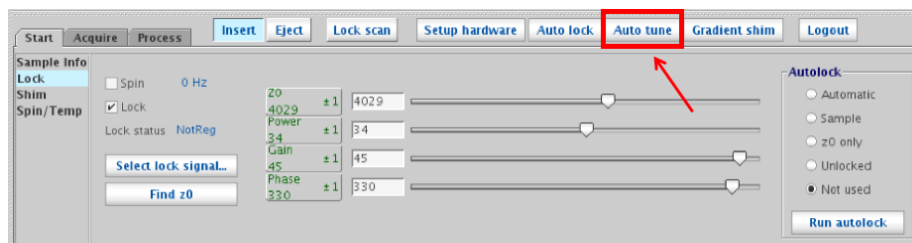


2. Tuning the Spectrometers:

- Make sure you have selected the desired experiment (^1H , ^{13}C , ^{31}P etc.) which can be chosen from the dropdown Experiment Menu (see below).



- Tuning your sample can now be done in one click (shown in the figure below).



- If you are acquiring data for very similar samples in the same solvent (e.g. a number of ^1H NMR spectra for small molecules in chloroform), you do NOT have to tune after every sample change. You should, however, shim at each step (automated gradient shimming works best).
- If you run a ^{19}F spectrum, please retune the system back to ^1H before you leave (open a new ^1H experiment, and click “Auto Tune” **before ejecting the sample.**)
- **Your level of access to the iLab calendars will depend on your training i.e. you may be limited to just the Varian/Agilent but not the Bruker systems.**

3. Solutions to Common iLab Issues:

- If your screen blacks out in the middle of a session, first “pause” and then “restart” your session on kiosk. If this does not help, please contact the Director.
- Please return on time to save your overnight experiments; it is best to make a new iLab reservation to do this. Alternatively, please leave a detailed note for the next user so that s/he can save your data for you.

4. File Transfers and Processing:

- All saved files can be accessed via the BC network and transferred onto your personal devices. Any **SFTP** app of your choice (Fetch, Cyberduck, Filezilla etc.) can be used to transfer your files. **Please use your own lab printers for hard copies.** Feel free to contact us if you need assistance. The spectrometer names (starting from the EPR-end of the lab) for file transfers are as follows:
 - The Bruker 500 with cold probe (**William**)
 - The Varian/Agilent 500 MHz (**Tomoya**)
 - The 400 MHz system (**Meagan**, only used by the Hoveyda lab)
 - The Bruker Prodigy 500 MHz (**Shoshana**)
 - The Varian/Agilent 600 MHz (**Boylan**)
- BC has a license for the Mestrenova software, so it is free to access within the BC network. Your lab mates should be able to advise you on the installation and usage (with many YouTube videos!) as well our TC Howard White.
- Remember to never use spaces when naming your saved data.
- You can use the command line or GUI on VJ (or Topspin): please **do not overwhelm the software with multiple simultaneous commands.** i.e. wait for one command to be executed before giving the next command.

5. Rules for Miscellaneous Time Reservations:

- **If we are at lower capacity for any reason (e.g. Covid) please refer to the ramp-up plans posted online** for a more detailed description of the rules and regulations pertaining to facility access during the specific ramp-up periods (25% capacity, 50% capacity etc.)
- Please contact the MRC staff for consultations to set up any experiments that may require more careful fine-tuning of the hardware and/or software, or those that may take a longer time e.g. VT experiments, kinetics, 2D ROESY etc.
- Always contact the MRC staff via email to set up EPR reservations.

Etiquette Rules:

1. Please adhere to all the reservation rules outlined above (or in the ramp-up plans during lower capacity operations), and follow all general safety protocols outlined at BC (by our Operations Manager and Safety Officer, Dr. Ian Parr). If you have any questions, feel free to email the MRC Director.
2. Please treat your fellow researchers with respect when using the facility i.e. minimize disruptive behavior and excessive noise, collect your data and leave the lab, making sure the spectrometer is ready for the next user.
3. **Please do not destroy any common items e.g. keyboards, mice, computers.**
4. Please feel free to use the saran wrap on the keyboards if you want to be extra careful (e.g. avoiding the spread of Covid.)
5. We expect mutually respectful conversations in the event of any disputes. Please be kind to each other, and respectful of the MRC staff—thank you!

WE RESERVE THE RIGHT TO CHANGE ANY OF THESE POLICIES AT ANY TIME AS WE SEE FIT.