

A few rules of the NMR lab

Basic / General

1. **If an NMR tube breaks, throw the glass away in room 37** (and the solvent away in the waste bottle near the sink in room 35). There is a broom in room 35 that you may use
2. **If an NMR tube breaks in the probe, or something else goes badly wrong, let Robin (or Rick or Weihua, or anyone on the advisory committee) know as soon as possible** (x6219, robin.stein@mcgill.ca)
3. **Do not leave any NMR tubes standing in their spinners in NMR tube racks.** It is likely that they will break
4. **Only use marker on the top 2" (5 cm) of the NMR tubes.** (We always wash blue and red ink from the inside of the spinners when we clean them. This ink eventually makes it down into the NMR probe and shows up in your spectrum as artifacts or poor shimming)
5. In the non-autosampler instruments, **leave an NMR sample in the instrument when you are finished** (usually, this will be an empty NMR tube)
6. **Do not wear gloves** in the NMR rooms
7. **Do not use tubes where the cap does not fit properly** (this is unsafe not only for you, but for other people who may remove your tube from the spinner and dislodge the cap, exposing the glass)
8. **Wipe your NMR tubes with Kimwipes** (not paper towels) before putting them in the sample changer or magnet
9. **Do not adjust the depth gauges**—Varian gauges should be set between 67 and 70 mm, and Bruker ones should be set to 2 cm
10. **Log out** (click "Logout" or "Change user") **when you are finished**, so that the next person does not accidentally run their samples under your login

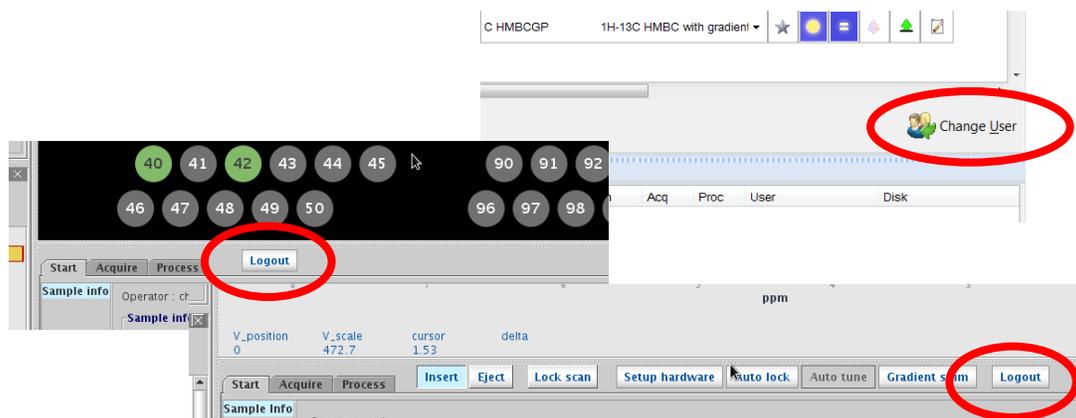


Figure 1. Change User (Bruker) and Logout (Varian) buttons. If you cannot see the Logout button on the Varian, go to the Start panel.

Bruker AVIIIHD 500

1. Pay attention to the **sample position number** you are dealing with. It is easy to get confused!



Figure 2. Note that positions 5 and 8 are occupied: positions 6 and 7 are empty.

2. Only remove samples that are either **complete** (**yellow** in the sample position diagram) or that are shown in **green** in the diagram (meaning that the current day's automation run has no information about them-probably, they ran previously). **Never remove samples that are pink, meaning that they are still in the queue!**

When you remove samples, put them in the *same number position* in rack 1 as the position you removed them from. Samples already in rack 1 go in rack 2; samples already in rack 2 go in rack 3; samples in rack 3 go to unnumbered spots in the front. Keep the same numbers in racks 1-3! For more information, see

<http://nmr.chem.mcgill.ca/Documents/RemoveSample500Autosampler.pdf>.

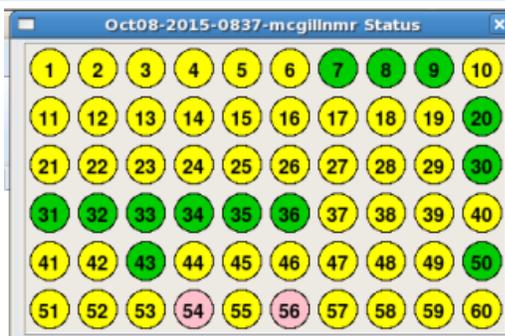


Figure 3. In this diagram, positions 54 and 56 are queued. The other positions can be removed from the sample changer.



3. Do **not** put your sample in the same position as is currently in the magnet

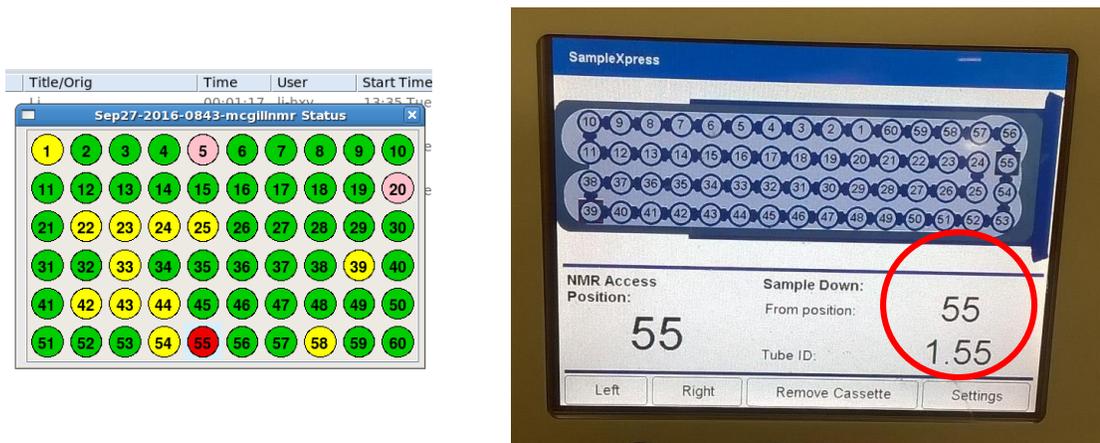


Figure 4. Do **not** put a sample in position 55 in this example. Note that the “Sample down” position (right side of sample changer screen) is the important one, not the “NMR Access Position”, if they are different. Do not put a sample in the “Sample Down” position.

Varian Mercury 300

1. **8" tubes only** (no 7", no J. Young, no badly chipped 8" tubes that are no longer 8" long)
2. **No pink or light turquoise-blue caps** (these are reserved for Chem 362/392 labs)
3. **Do not put your sample in the same position as the sample that is in the magnet.** This position is marked in blue on the computer screen and it is indicated in the bottom left of the computer screen, even when no one is logged in!

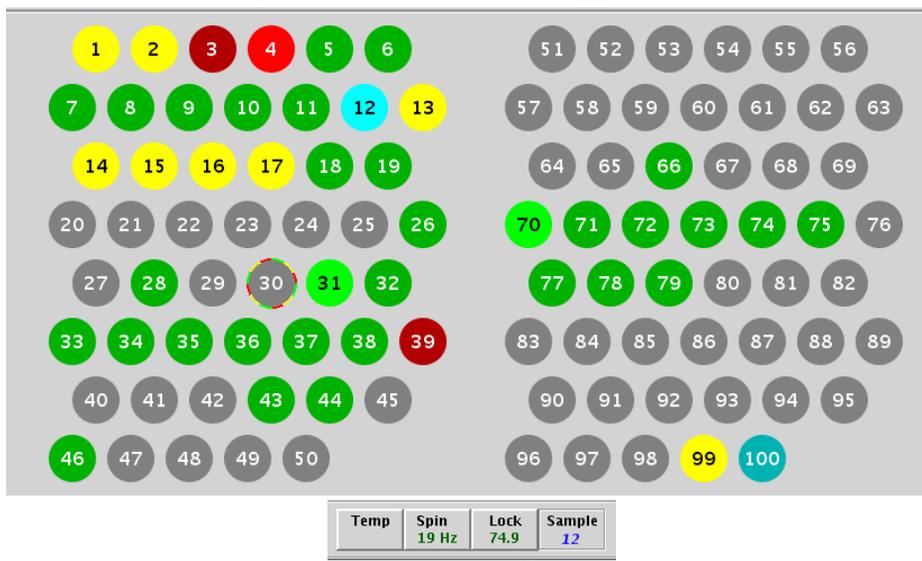


Figure 5. In this example, position 12 is currently in the magnet. Do not put your sample in that position!

4. Only **remove samples that are either complete** (green in the sample position diagram) **or** that are shown in **gray** in the diagram (meaning that the current day's automation

run has no information about them-probably, they ran during a previous day). Put the sample that you removed into the same number position in the racks on the table. If that position is already occupied, move the sample in the rack into a non-numbered spot and place the sample from the sample changer into the same number position in the rack as it came from in the sample changer.

Varian VNMRS 500

1. **Use Clear as soon as you log in**, if you don't use a study queue, so that data gets saved properly
2. You must **tune the probe** if you do ^{13}C and/or 2D experiments. This has two effects: it gives you the best possible signal-to-noise ratio, and it protects the instrument from damage.
3. If you change the temperature, **reset the temperature to 25 °C** when you are finished

Varian Mercury 400

1. **Use Clear as soon as you log in**, if you don't use a study queue
2. **Do not ever use a spinner from the QANUC 500** (if a second spinner is needed, take one from the Mercury 300)