

New User Checklist – Bruker

Prepare your sample

- A typical sample is 5-150 mM (see Quick Reference for recommended concentrations and how to estimate your concentration).
- The solvent height should be 4 cm (0.55 mL).
- Use a pure, dry, deuterated solvent.
- Avoid heterogeneous solutions (suspended solids, bubbles, emulsions, etc.)

Log in to TopSpin - Icon Automation

- Click the *Change User* button if the login window is hidden.
- Use your chemistry computer account.
- If you can't log in, double check that your password hasn't expired.

Place your sample in the sample changer

- Carefully place your sample in a turbine and wipe both your sample and the shaft of the turbine with a KimWipe.
- Use the depth gauge to position your sample correctly (the white stopper should be set at 2.0 cm – be sure to check this and *do not* move it from this position).
- Find an empty position to place your sample.
- If all the positions are full,
 - check the automation page and find a position labeled *Available* or where every spectrum is labeled *Finished*;
 - carefully remove the sample and place it in the large beaker (be very careful when handling other users' samples!)

Setup your study

- Double-click the position corresponding to where you put your sample (or highlight it and click *Add*).
- Enter a name for this data (this will be the name of the directory that's created in your NMR folder).
- Choose the correct solvent in the drop-down menu.
- (optional) Enter any descriptive text in the *Title* box and an email address if you want to receive notifications when your spectra finish.
- Choose the desired protocol from the drop-down menu.
- Customize this by clicking on the equals sign button.
- Use the *Add* button to add additional lines if more than one protocol is desired.

Submit your study

- Highlight all your protocols (or just the top line where the sample number is displayed) and choose *Submit*.

Finish

- Log out of Automation by clicking the *Change User* button.
- Retrieve your sample from the sample changer once it's finished.

New User Checklist – Varian

Prepare your sample

- A typical sample is 5-150 mM (see Quick Reference for recommended concentrations and how to estimate your concentration).
- The solvent height should be 5 cm (0.67 mL).
- Use a pure, dry, deuterated solvent.
- Avoid heterogeneous solutions (suspended solids, bubbles, emulsions, etc.)

Log in to VnmrJ

- Use your chemistry computer account.
- If you can't log in, double check that your password hasn't expired.

Place your sample in the magnet

- Eject the sample currently in the magnet.
- Carefully remove the sample from the turbine and place it in the sample rack.
- Carefully place your sample in the turbine and wipe both your sample and the shaft of the turbine with a KimWipe.
- Use the depth gauge to position your sample correctly.
- Insert your sample in the magnet.

Setup your study

- (optional) Load the standard shims using the button above the main display.
- Choose *New Study*.
- Enter a name for this data (this will be the name of the directory that's created in your NMR folder).
- Choose the correct solvent in the drop-down menu.
- (optional) Enter any descriptive text in the comment box and an email address if you plan to email yourself processed data.
- Add any NMR protocols to the study that you want to collect.
- Customize these by double-clicking on the protocol name in the study. You may need to choose the *default* page to see useful parameters like # of scans and chemical shift windows.
- (optional) Submit only a Proton, check the quality and concentration, and then use the *continue* button to continue the study, adding more protocols, etc.

Submit your study

- If you get red error messages related to acquisition in process or study already in queue, etc., you can usually fix this using the *Automation* menu, *Background* sub-menu, *New Background Run*.
- If that gives an error (usually about automation already in progress), you can choose *Resume* first, and then *Abort Acquisition*, and then *New Background Run* (all in the *Automation – Background* menu)

Finish

- Eject your sample and put the dummy sample back in the turbine.
- Insert the dummy sample in the magnet.
- Log out of VnmrJ