

Bruker NEO 400/500 MHz Standard Operating Procedure

Bruker Avance Neo NMR spectrometers (operating at 400 and 500 MHz) are two channel broadband instruments equipped with an iProbe, AutoTune assembly and variable temperature unit. They also have a SampleCase (sample changer assembly).

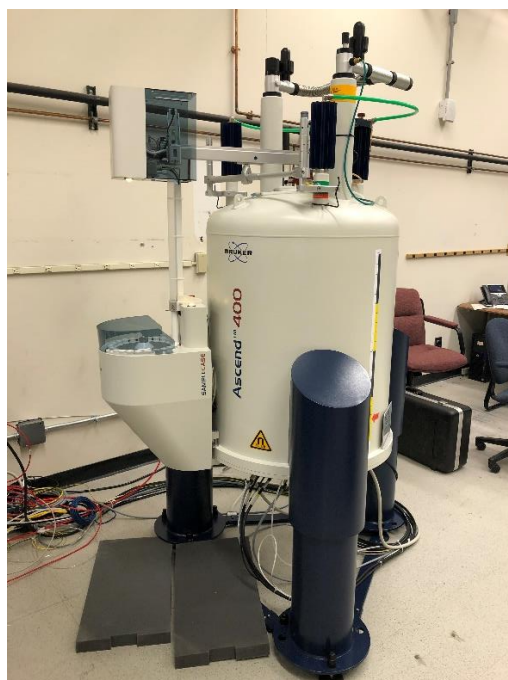
This SOP is for using the Bruker automation software IconNMR.

You will access the instrument using your Research Adviser's group account.

You will store your data in your sub directory under your group account.

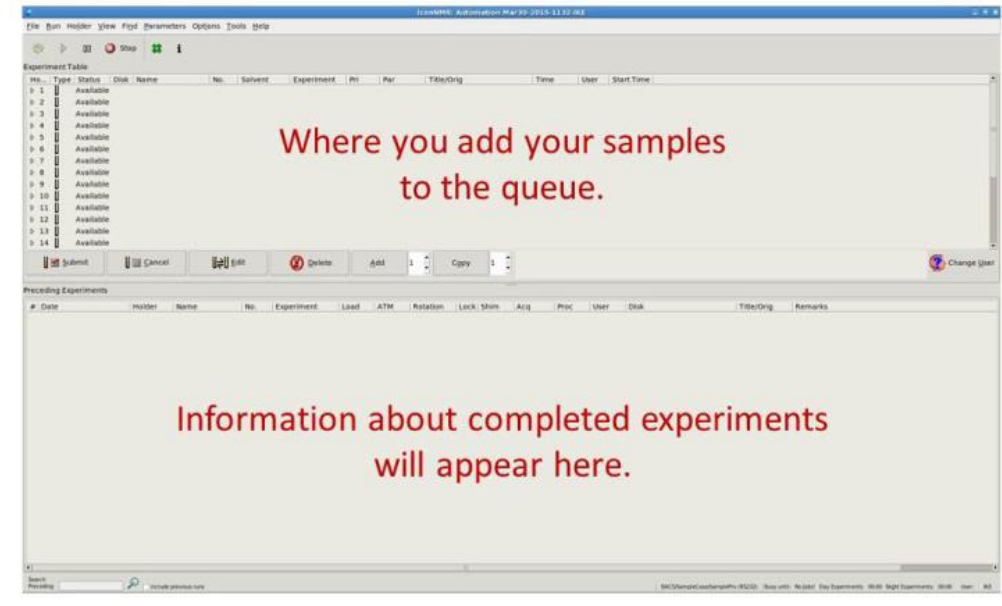
Some things to note before running samples on the Bruker NEO 400/500 MHz instruments

- Do not use spinners or depth gauges from the Varian instruments for samples to be run on the Bruker instruments or vice versa
- There is no sample in the instrument when it is not in use (unlike the Varian instruments)
- Never place an empty spinner in the autosampler case without a sample in it
- Sample slot 8 in the autosampler is unavailable and is for calibration samples ***only***. Do not attempt to run a sample in that slot.
- All sample operations should be done using the auto sampler. Sample cannot be inserted/ejected manually.
- The Bruker Neo spectrometers Auto- Lock/Shim/Tune every sample. There is no need to Lock/Shim/Tune manually.



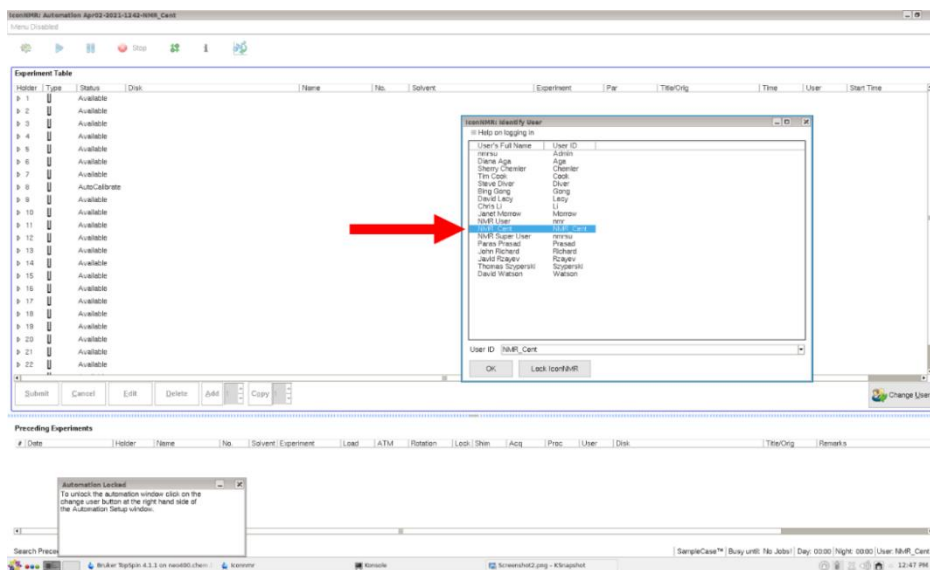
If you need help contact Dr. Sukumaran (dks@buffalo.edu)

IconNMR Interface

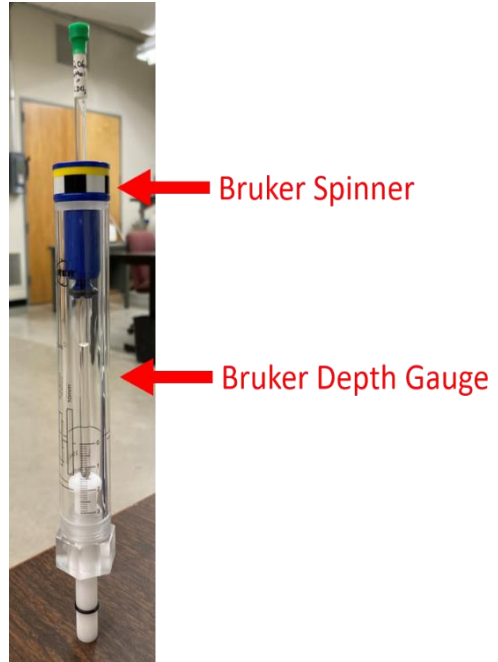


Running an Experiment

1. When you arrive, IconNMR screen should appear with its Automation window as shown below. **Never exit out of this window.** Click on "**change user**" in the bottom right, if the user list does not show up (this will logout the previous user, allowing you to login)
2. Double-click on your professor's name and login using your group's password.

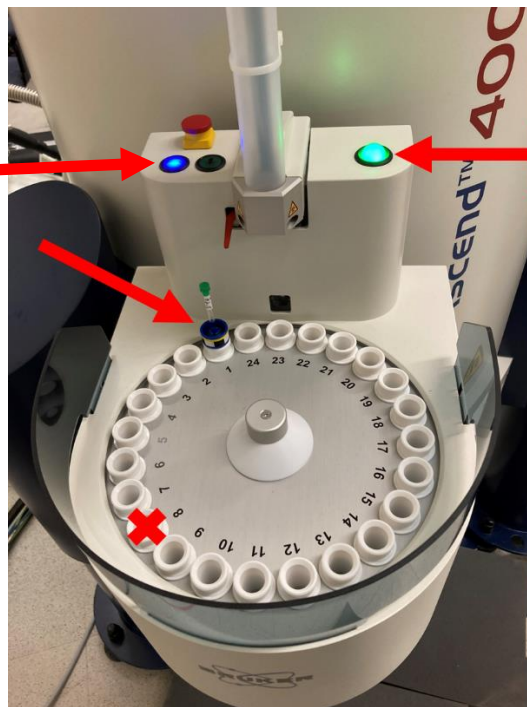


3. Put sample into a Bruker spinner and adjust height using the Bruker depth gauge. Maximum Height from the top of the spinner to the top of the tube **should not exceed 9.5 cm.**



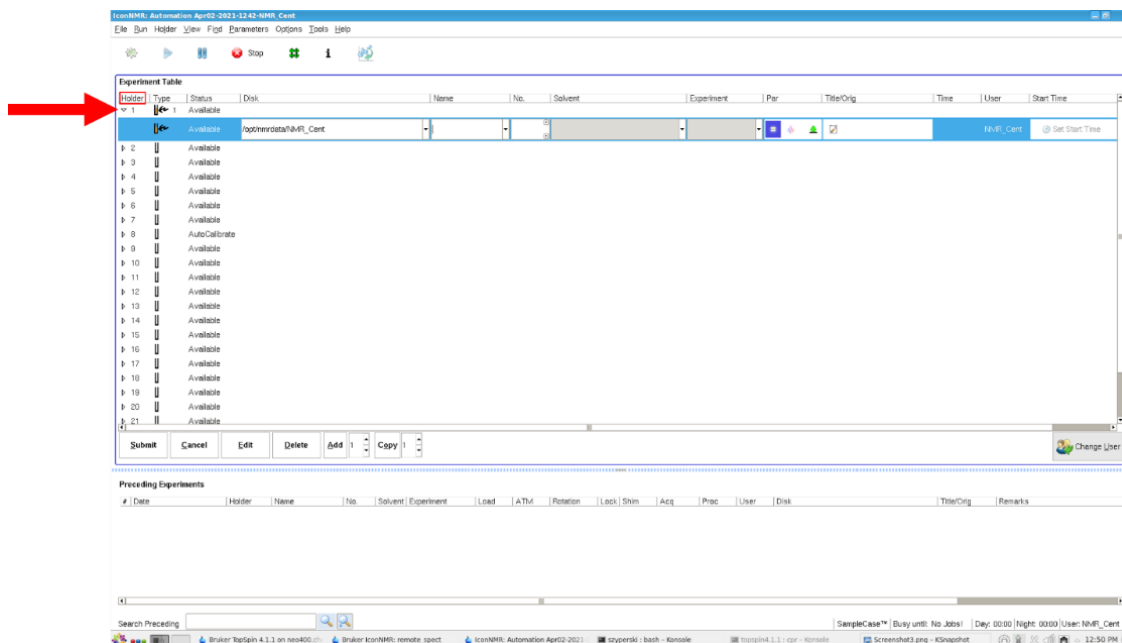
4. Place sample(s) into the autosampler and note the sample slot location(s) (NOTE: do not use holder 8).

Blue: Use this button to advance the carousel



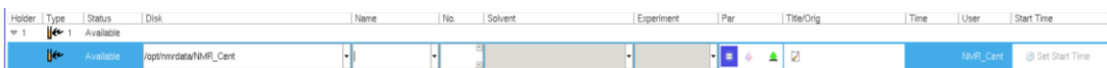
Green = no sample in instrument
Yellow = sample in instrument

- Double-click on the holder number your sample is in. This will open a dropdown window.



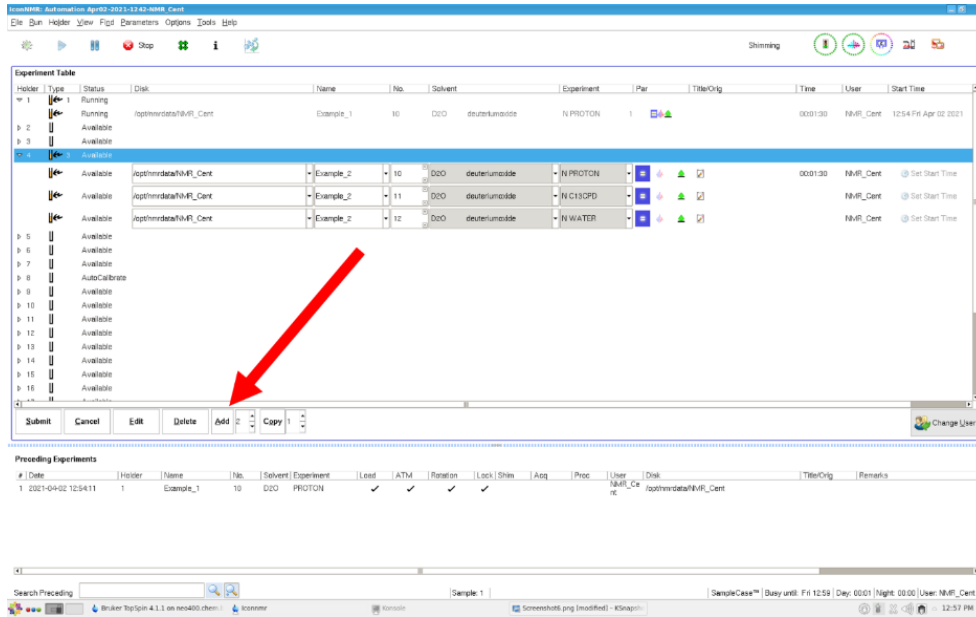
If you have a question about what a button does, you can hover your mouse over the button without pressing it, and it will tell you what it does.

- Enter all the information for each sample by either typing in the information or selecting it from a dropdown box

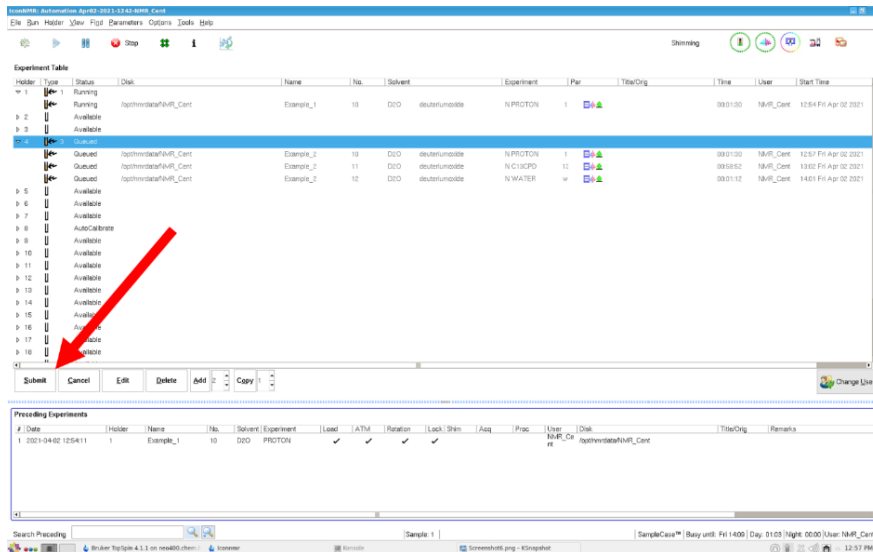


- Disk: The directory where the data will be saved (use the drop down to navigate to your directory within your group directory)
- Name: sample name – date file will be saved under this name in the directory (use a single word name, if necessary use underscore (_) to link words)
- No.: experiment number for that sample (will be filled automatically)
- Solvent: solvent for the sample (from the pull down)
- Experiment: experiment you wish to run (from the pull down)
- Par: parameters for the experiment. Double-click on the '=' symbol to change parameters from the displayed list
- Title/Orig: enter your email (@buffalo.edu) and a descriptive title for the sample

- If you wish to run multiple experiments on the same sample highlight the holder number. At the bottom of the window, click **“add”**, and fill-in the just the experiment you want run, any change in paraments and title. Repeat step 7 for each additional experiment you wish to run for that sample.



- Once all information is filled in, highlight each holder number of your sample(s) you wish and hit **“submit”** at the bottom left. For a single holder/sample running multiple experiments, select that holder and hit **“submit”** – all experiments queued under that holder will be run in that order.

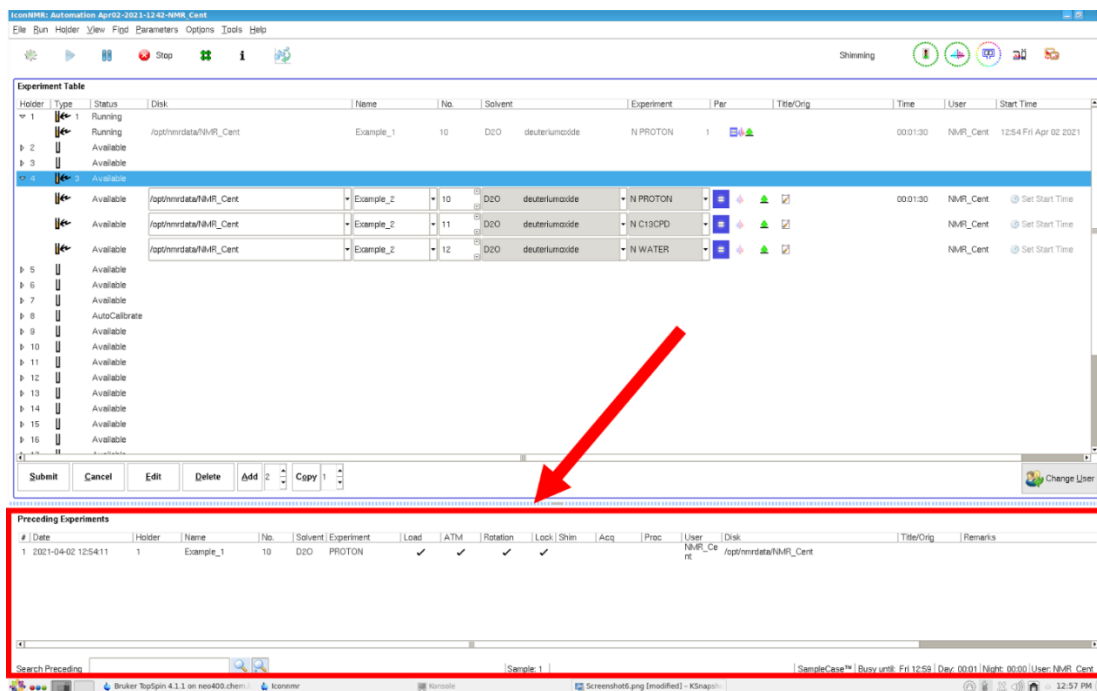


- Before you leave, click “**change user**” in the bottom right to log out. Once you do so, no other user can edit or change your sample’s information
- When you come down to pick up your sample(s), remove each sample from the SampleCase and place the spinners on the table. **Caution:** do NOT remove your sample while the carousel is moving, and do NOT reach across the center where the sensor is located. In case you need to rotate your sample spinner, press the **Blue button** on the sample case once for every slot.

Do Not press either the Green Button or the Red switch

Data Processing

Completed experiments can be seen in the bottom window “Preceding Experiments” on the IconNMR screen



To inspect your spectra, simply double-click on your completed experiment in the Preceding Experiments list. If data acquisition and processing is complete, you will see a checkmark under Acq and Proc by your experiment. At this point you can double-click to view your spectrum in Topspin.

A copy of the raw data (in zip format) and a copy of the processed spectrum (in PDF format) will be emailed to an email indicated in the experiment setup step (step 7) as soon as data collection is complete. You are expected to return to the instrument at that point to collect your sample.

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