500 MHz NMR - Kepler

Training Guide

The 500 has a liquid nitrogen cooled Prodigy probe installed. This three channel probe can be tuned for a variety of NMR active nuclei, including ^{19}F (on the same channel as ^{1}H), ^{31}P and ^{11}B. It has a variable temperature range of ambient to 80C.

Please note: all users of the 500 must be trained by a NMR Facility Staff Member

before they can use the instrument.

1. Log into the 500 computer with your account.

2. Click the colorful Centos icon in the lower left corner and select Run Command. In the Run window that pops up near the upper center of the screen, type **topspin**. Select Run topspin. This will open the Topspin software that controls the instrument.

3. **Insert your sample.** There are a couple different ways to insert your sample, and both involve turning on the eject air FIRST. You can type **ej** on the command line OR click the LIFT button on the BSMS Display.

*If you do not see the BSMS display, type **bsmsdisp** on the command line.*

Make sure you remove the dummy sample from the magnet and the spinner, and then properly set your sample in the spinner. Do not forget to use the depth gauge.

Insert your sample by typing **ij** on the command line OR by clicking the LIFT button again. You will hear the air turn off and you can close the BSMS display.
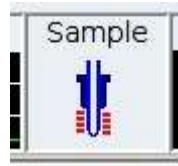

This means your sample is down and the instrument is able to detect it. If you see a question mark, it means there is no sample in the magnet or, for some reason, the instrument cannot detect it. If you have not set your sample correctly in the spinner with the depth gauge, it may not be able to detect it.

4. **Create a dataset.** You can create a dataset by typing **edc** on the command line OR by clicking the Create Dataset button.
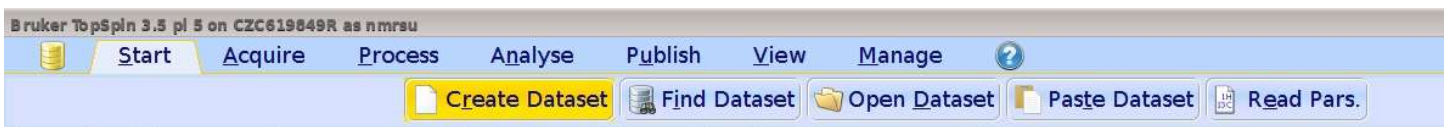
Give your sample a name (spaces are not recommended, use _ instead). Experiment number and processing number can both be set to 1. Pick your solvent from the dropdown menu and make sure you have the directory set to your account.
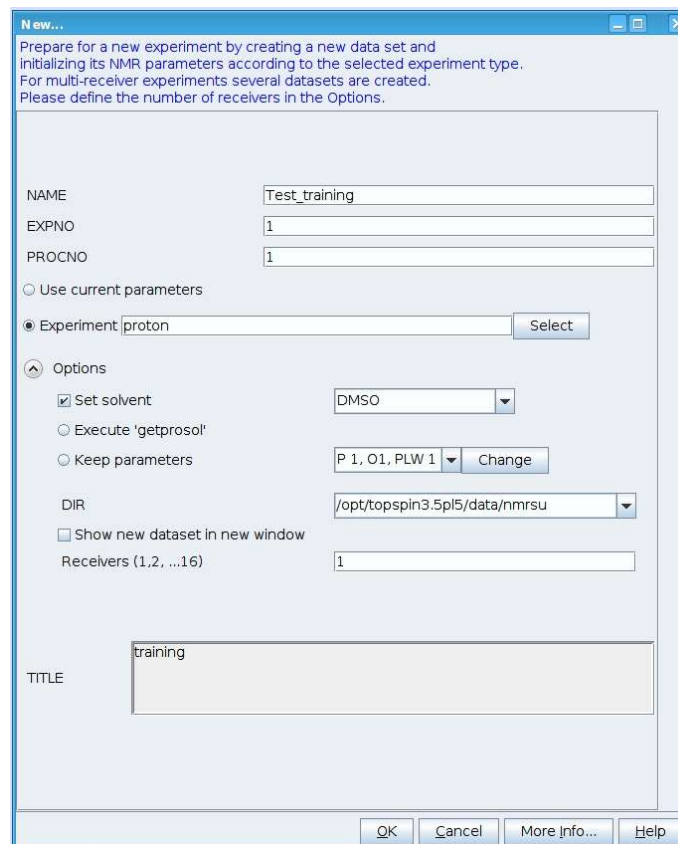
If you click the Select button at the end of the Experiment box, you will get a window with an abbreviated list of experiments. Pick the one you want and then click *Set selected item in editor* in the bottom right corner.
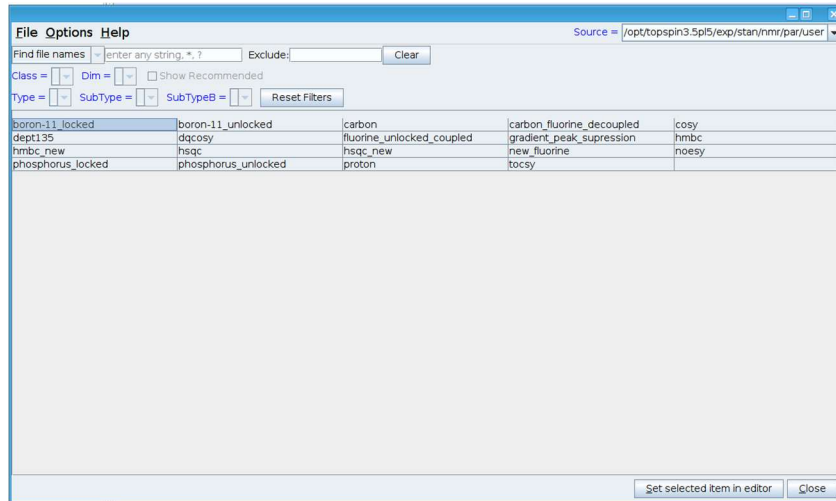
Add a title if you would like, and once you are happy, click OK. It's a good idea to type **ii** on the command line at this point.

5. **Lock on your sample.** You can type **lock** on the command line OR click the Lock button in the Acquire tab and select your solvent. Wait for the autolock to finish.

6. **Tune.** You can type **atma** on the command line OR click the Tune button. You may see the wobb curve flash across the screen and the dip should be centering on 500 if you have selected ^{1}H parameters.


7. **Shim your sample.** You can type **topshim** on the command line **OR** click the Shim button. Wait for Topshim to finish and relock.

*If topshim fails and complains about not enough time or not enough points, you can type **topshim durmax=30**. If the shims are still ugly and topshim fails again, try reloading the standard shim file by typing **rsh standard.shim**, and running topshim again.*

8. **Set the gain.** You can type **rga** on the command line OR click the Gain button.

9. **Change parameters.** If you type **ns** on the command line and hit enter, a window will appear with the number of scans that will be taken. You can adjust this number, adding more scans if necessary. If you are running a ^{1}H, remember to pick 4, 8, 16, 32, 64, 128, 256, or 512 scans. If you want to double the signal to noise in your spectrum, you need to run 4xs as many scans.
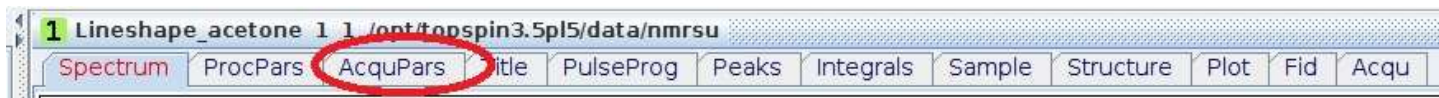
You can check other parameters by clicking the AcquPars tab in the Spectrum window area.

10. **Start the acquisition.** You can type **zg** on the command line OR click the **Go** button.

11. Your data should be automatically saved at the end of the acquisition. If not or if you'd like to save it again, click the little disk icon on the left.

12. Don't forget to remove your sample and insert the dummy when finished. Exit Topspin by typing Exit on the command line. Log off the computer and sign the User book.

Please report any issues you have with the instrument to a NMR staff member.

We can't help you or fix an instrument problem if we don't know about it.