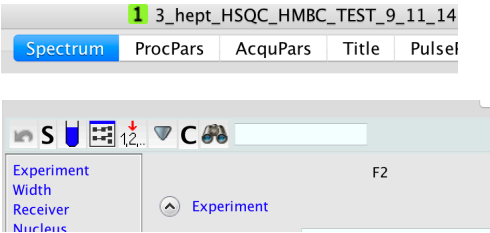


1. Log into the workstation. Click the start menu, choose Bruker NMR Software, then choose the version of Topspin at the bottom of the list which will be the latest patch level. NOTE: On Zeus and Ares, there is only one version, TS 1.3PL10.
2. The first time you log in it will ask you if you agree to the license agreement. You must select 'yes' to proceed. It is useful to set some preferences now. At the top of the Topspin window, select 'manage', then 'preferences'. Check the first and last box in the 'administration items'. Scroll to the bottom and click 'apply'. 3 Lines up from the 'apply' button, click 'change' for 'status bar preferences'. Check all the boxes down through 'lock signal' and then 'sample state'. Click 'apply'. Exit Topspin by typing 'exit' [enter] in the command box. Re-enter the software after 15 seconds and your preferences should have taken effect.

3. Type 'edc' [enter] in the command box at the bottom of the screen. A new window will pop up asking you for a folder name, experiment number (EXPNO), process number (PROCNO), directory for data storage (DIR), solvent (select your solvent from the list), and Experiment (select from list). The newer version of this box is shown to the right. When you hit the 'Select' button to choose an experiment, go to the top right of the new pop up window and change the source, to the /user folder which contains the typical experiments we use in the department. Typical ^1H and ^{13}C experiments are PROTON_BROWN and C13CPD_BROWN. Zeus and Ares have a slightly different box that includes the data path which is /opt/topspin and a user box which is your username. For the newer software, once you have picked your experiment, YOU MUST CLICK THE 'OPTIONS' tab and designate the path to the data as shown above (this path is written down on each cheat sheet next to each spectrometer keyboard). Click 'ok' when you are finished.

4. Place your NMR tube in the blue or tan spinner and set the appropriate depth with the gauge located at each spectrometer. Type 'ej' [enter] and exchange your sample with the one in the magnet. THERE SHOULD ALWAYS BE A TUBE IN THE MAGNET. IF NO TUBE COMES UP, COME FIND RUSS. Type 'ij' [enter] to lower your sample into the magnet. Type 'lock' [enter] in the command window and select your solvent and OK. Below where you enter the commands in the TS window you will see text pop up telling you that lock is finished. Once locked, you will need to shim on the sample. For Artemis and Cronus, just type 'topshim' enter and wait for it to finish. NOTE: If you plan to run any 2-D experiments, it is imperative to optimize the lock by typing 'loopadj' [enter]. However, this command only works if the lock gain value, after locking is <117. You can manually lower this value by opening the digital bsms panel ('bsmsdisp' [enter]) for Cronus/Artemis, or using the external bsms panel for Zeus/Ares. Once in the digital bsms panel, click the lock tab, then 'lock gain' and lower it down to below 117 bearing in mind that the vertical position of the lock signal on the screen needs to be returned to the position it was after locking (~70% of the way toward the top of the lock window). You can increase the lock power to achieve this position. Similarly, you will find 'lock gain' and 'lock power' buttons on the bsms panel beside the monitor on Zeus/Ares. When lock gain is below 117, you can use the 'loopadj' command.

5. On Zeus and Ares, open the lock display by typing 'lockdisp'. You should see an orange box next to the green 1 in the top right of the screen, click it to open the lock display. While watching the lock signal's vertical position on the screen, begin adjusting the z and z2 shims on the BSMS panel to the right of workstation keyboard. Push the 'z' button on the bsms panel and turn the knob in either direction while monitoring the lock signal. Improvements in shimming are evidenced by the horizontal lock signal line moving vertically upward toward the top of the screen. When the horizontal line reaches the top of the screen you need to press the lock gain button and reduce the value until the line is back near the 70% level of the screen size. Continue to maximize the signal moving back and forth between z and z2. Adjust lock gain or lock power (push buttons) to keep the horizontal line in the display window. This whole process should take no more than 3-5 minutes. If after you have shimmed, you still cannot attain a good lineshape (expand around the solvent peak in your spectrum to check the lineshape, it should be Lorentzian), you can try recalling a recent shim file by typing rsh [enter] and select the most recent shim file (usually is lineshape_most_recent). After doing this, repeat the z and z2 adjustment.

6. You can either type 'eda' [enter], or just click on the little tab that says AcquPars. This is where you can adjust the number of scans (ns), sweep width (SW), center of spectrum (o1p), and acquisition time (AQ). You should have already specified the solvent in the 'edc' window. But if you want to double check, scroll to the bottom of the AcquPars window and you will see the solvent selection option. You will notice a little blue button that looks like a test tube at the top left of the eda window. Left mouse click on this, it is the 'getprosol' button which calls in the correct pulse widths/power levels for the probe in the spectrometer. Alternatively, you could just type 'getprosol' in the command window at the bottom of the screen. Click the 'Spectrum' tab when you are finished.
 

The screenshot shows two windows from the software. The top window is titled '3_hept_HSQC_HMBC_TEST_9_11_14' and has tabs for 'Spectrum', 'ProcPars', 'AcquPars', 'Title', and 'Pulse'. The 'AcquPars' tab is active. The bottom window is titled 'Experiment' and has a 'Nucleus' dropdown menu. A blue button with a test tube icon is visible in the top left corner of the 'Experiment' window.

7. If you are running anything but a ^1H detected experiment, type 'atma' [enter] to automatically tune the probe to the nucleus you are hoping to detect. Type 'rga' [enter] to optimize the receiver gain for your sample. Finally, type zz to begin your experiment. The default setting is 1 scan for ^1H so you can ensure you are shimmed well enough before acquiring multiple scans. If you are running a longer X-observe experiment, you can type 'tr' [enter], followed by 'efp' [enter], to process the scans you have thus far acquired. NOTE: efp applies the default line broadening of 0.3Hz. If you are looking for coupling smaller than this, just type 'fp' to process the FID. The 'apk' command will autophase the spectrum. The 'abs n' command will perform a baseline correction.