# TopSpin 3.5pl5 Acquisition Instructions

Revision – July 2016 for AVIII 600 MHz (NMR-Sage)

These are basic instructions setting up NMR experiments. Note: all commands are case sensitive! For more details contact the NMR manager. Never attempt an unfamiliar experiment without help!

1. Log in the computer (NMR-Sage) with your chemistry domain account.
2. Double click on the TopSpin 3.2 icon to launch the program.

***CREATE DATA SET***

3. Type **new** to create a filename for your new experiment.
4. OPTIONS – select parameter set and click 'getprosol'.
5. Enter a filename for your sample ('NAME'). *Important:* Ideally your NMR data should be stored on one of the NMR network drives (found my clicking on My Computer). Please include ASC-osuname.# when creating directories. For example: X:\data\ASC-osuname.##\nmr.

***INSERT SAMPLE & SPIN***

6. Type **sx #** with the # corresponding to the position in the SampleCase. Your sample must be in a spinner and cannot be taller than nine (9) inches. (J-Young tubes may need shortened).
7. Spin the sample by right-clicking on the sample icon and selecting Toggle spin (ro). You may also spin the sample using the **bsmsdisp** spin button. The sample is spinning when the sample icon looks like: 


***LOCK, TUNE, AND SHIM***

8. Open the lock display by typing the command **lockdisp** or click  **.**
9. Read in the standard shim file: **rsh BBFO.shim**.
10. Type **lock** or click  and choose your solvent from the list. Wait until finished.
11. Type **atma** to tune the probe. If you selected your NMR experiment when creating a **new** file, the instrument is set up properly. If you need to change experiments, type **rpar** and select your experiment from the user parameter list. *Important:* Type **getprosol** to set the power levels and pulse widths, otherwise there will not be an NMR signal.
12. Type **topshim** to shim.

***ACQUIRE SPECTRUM***

13. Set the receiver gain and start the acquisition with the command **rga**;**zg**. The acquisition progress automatically will appear.
14. To save and view the data during the middle of the acquisition, enter **tr** to transfer your data to disk (optional).
15. Enter **efp** to process your saved data.

***PROCESS SPECTRUM***

16. To phase, enter **apk**. You may need to manually phase the spectrum.
17. To correct the baseline, type **abs n**. This will flatten the baseline which may result in more accurate integrals. Remember that the regular PROTON parameter set is NOT a quantitative experiment.
18. Calibrate, integrate, and peak peak as usual.
19. To print, type **plot0** and use the plot editor as usual. You will not be able to make a .pdf. Use the plot tab in order to create a document for .pdf.

***FINSIHING UP***

20. Type **new** to begin a new experiment on this sample or:
21. To eject, type **sx ej**.
22. Remove your sample, exit TopSpin 3.2, and log off the computer.

***ICON NMR (OPTIONAL)***

23. Open TopSpin and type **icon** on the command line. Select the Automation option.
24. Click the START button at the top to start your 'run'.
25. Select the sample number and fill out the experiment parameters as usual.
26. Submit all experiments.
27. When finished, click the STOP button at the top and close IconNMR.
28. During the 'run', you may return to Topspin (use the Windows button on the keyboard) and monitor the acquisition process. The data is automatically stored to both the local drive and to the NMR-Sage drive.