

# TOPSPIN User Guide

revised 6-01-06

## Part I: Acquiring the NMR Spectrum



1. Double-click on the Topspin icon to start the software (if it's not open already).
2. Type "**lockdisp**" to open the lock window.
3. To remove and insert a new sample:
  - a. Press the {Lift On/Off} button on the BSMS unit to eject the sample.
  - b. Remove the sample and spinner from the magnet.
  - c. Wipe down your sample tube with a clean chemwipe.
  - d. Insert your sample into the spinner, being careful not to touch the spinner with your hands. The spinner easily picks up dirt and oils from your hands, which end up inside the NMR.
  - e. Check the sample depth in the spinner using the depth gauge.
  - f. Insert the sample into the top of the magnet.
  - g. Press the {Lift On/Off} button on the BSMS unit to insert the sample.
4. Setting the Solvent and Locking:
  - a. Type "**lock**" and select your solvent.
  - b. If the sample doesn't lock, type "**rfshim**" to be sure the reference ( $\text{CDCl}_3$ ) shims are loaded, then type "**lock**" again and reselect your solvent.
5. Shimming:
  - a. Manually adjust Z1 and Z2 by pressing the corresponding button on the BSMS unit and turning the wheel to maximize the lock level.
    - i. If the lock goes off-screen, press {Lock Gain}, lower the gain until the lock level is in the top two boxes, then go back to shimming.
  - b. Press {Standby} on the BSMS when done.
  - c. If you need to retrieve a shim set other than  $\text{CDCl}_3$ , type "**rsh**" and the list of available shim sets will appear. Click on the shim set you wish to use. They are named for the probehead and solvent (example: *QNP-CDCl3*).
6. Setting up a New File for Acquisition:

- a. Type “**new**” to set up your new experiment.

*ICON*

- b. Change the name of the file.
- c. Click on [OK] to create the file.
- d. To set up a Proton observe, type “**1h**”
- e. To set up Carbon observe, type “**13c**”.

7. Acquiring Data

- a. Type “**rga**” to automatically adjust the instrument receiver gain.
- b. Type “**ns**” to set the number of scans (16 is typical for 1H, 128-512 for 13C).
- c. Type “**zg**” to start the acquisition.

8. Reading the Data

- a. Type “**tr**” to read the FID while it is acquiring.
- b. Type “**efp**” to FT the data and see a spectrum.
- c. Type “**apk**” to autophase the spectrum.
- d. If you want to stop acquisition before it is done acquiring (ie before ns number of scans), type “**halt**”.
- e. **NOTE:** You must repeat the commands **tr efp apk** every time you want to read data or when the acquisition is complete!

9. If you wish to start over with a new sample:

- a. Type “**rsp**” to open the temp file again.
- b. Go back to Step 5 above to remove your old sample, insert a new one, lock, shim, setup a new file and acquire new data.

10. When you are done acquiring data:

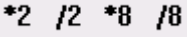






- a. Type “**rsp**” to open the temp file again.
- b. Follow Step 5 above to remove your sample and insert the reference sample.
- c. Type “**rfshim**” to recall the reference shims.
- d. Lock to CDCl<sub>3</sub> by typing “**lock cdcl3**”.
- e. Type “**exit**” to exit Topspin.
- f. Sign in the logbook.

## Part II: Basic Processing and Plotting

### 1. Opening Files and FTing Data


- a. Click on File -> Open (*icon*) and find your file name.
- b. Click OK. If multiple experiments were run with that filename, you may have to select an EXPNO.
- c. Type “**efp**” to FT your data.

### 2. Zooming In / Zooming Out




- a.  Increase/decrease vertical scale by factor of either 2 or 8.
- b.  Press LMB down while dragging mouse up/down to inc/dec vertical scale manually.
- c.  Scales to tallest peak.
- d.  Scales out full sweep width.
- e.  Moves spectrum upfield/downfield.
- f.  Moves spectrum up/down.
- g.  Switches scale between Hz and ppm.

### 3. Zooming In / Out Using the Mouse

### 4. Manual Phasing

- a. Click on  to enter phase mode.
- b. The buttons above your spectrum should look like this:

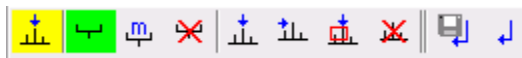




- c. Click and hold the LMB on the  button to perform zero-order phasing.
- d. Click and hold the LMB on the  button to perform first-order phasing.
- e. Click on  to save and return when you are done phasing.

### 5. Calibrating the Spectrum



- a. Click on .





- b. Place your cursor in the upper left hand corner of the spectrum.
- c. Click and drag LMB down to the lower right hand corner of the spectrum.
- d. The maximum and minimum are automatically set based on the region you select.
- e. To delete your peak picking regions, click .
- f. Click on  to save and return.

#### 8. Manual Peak Picking

- a. Click on  to manually select peaks. A red cursor will appear.
- b. Click the LMB on each peak you want to pick.
- c. Click  to save and return.

#### 9. Plotting

- a. Type “**xwinplot**” to open the plotting software.
- b. A default layout of the 1-D spectrum appears.
- c. To adjust the horizontal scale, move the crosshair into the spectrum area.
  1. Click the right mouse button.
  2. Select ‘Edit’.
  3. Change the y-axis to be whatever range you need (ie 10 – 0 ppm)
  4. Click Close when you are done.
- d. To adjust the vertical scale, move the crosshair into the spectrum area.
  1. Click the right mouse button.
  2. Select ‘1D/2D-Edit’.
  3. Use the buttons to adjust the vertical scale of the spectrum.
  4. Click on Close when it is OK.
- e. Click on ‘File’.
- f. Click on ‘Print’.