

# TOPSPIN 2 User Guide

## Login to computer

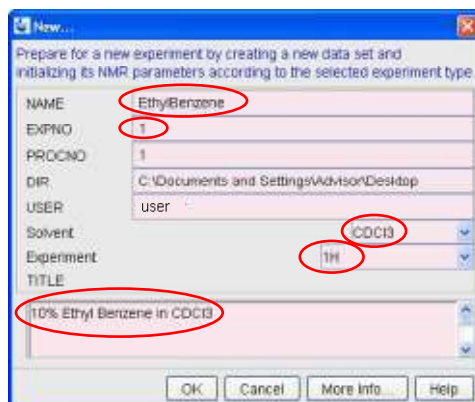
- On the Windows Welcome screen, click on the name of your advisor/group.
- TOPSPIN should launch automatically after you login. If TOPSPIN does not launch automatically, double-click the "Topspin 2.1" icon on the desktop to start the program.



## Preparing and inserting a sample

- The height of the solvent in the NMR tube should be about 5 cm.
- Use only good quality NMR tubes. Do not use cracked NMR tubes or tubes that don't fit well in the spinner. Do not use Kimwipes to hold a loose tube in the spinner.
- Clean the outside of the tube using a Kimwipe.
- Type "ej" to turn the lift air on. Take the previous sample out of the magnet.
- Place your sample into the spinner, and use the depth gauge to adjust the spinner height on the tube.
- Carefully place your sample onto the magnet bore. **Make sure air flow is on before releasing sample!**
- Type "ij" to turn the lift off and lower the sample.
- Type "ro on" to start sample spinning.

## Experiment Set-Up

- Type “new” in the pink command line. The dialog below will appear.




- Complete the fields circled above:
  - NAME – the name of your sample
  - EXPNO – 1 for the first experiment you run on the sample, 2 for the second, etc.
  - SOLVENT – the deuterated solvent used in your sample
  - EXPERIMENT – the type of experiment you wish to run on the sample (1H, 13C, DEPT135, etc.)
  - TITLE – the text to appear on the spectrum printout
- Read in the shimming presets by typing “**rsh temp**” at the command line. The command ‘rsh’ means “read shim file”.
- Click the “open lock display”  button on the toolbar. The Lock Display window will open.
- Click the lock  button in the toolbar of the lock window.\*
- Type “**atma**” to automatically tune and match the probe.\*
- Type “**topshim**” to start the automatic shimming routine.\*
- Type “**rga**” to automatically receiver gain aadjust the instrument.
- Type “**ns**” to set the desired number of scans.

*\* Note: The “lock” and “topshim” steps only need to be performed once per sample. The “atma” step should be performed once for each nucleus to be observed; first during the setup of the initial proton experiment and again during the setup of the first carbon or other X nucleus (11B, 19F, etc.) experiment.*






### Acquisition and Processing

- Type “**zg**” (zg means zero and go). The instrument will start to acquire the spectrum.
- When acquisition is finished, enter “**ef**” to Fourier transform the FID.
- Enter “**apk**” for automatic phase correction.
- Enter “**abs**” for automatic baseline selection and correction.


### Spectrum Calibration

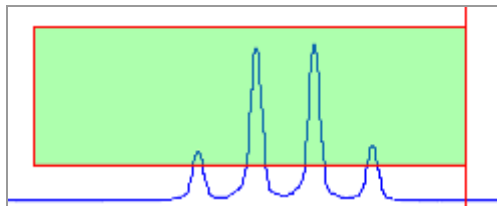
- Find the solvent peak in the spectrum.
- Expand the solvent peak so that the center can be easily identified.
- Click the calibration button  on the toolbar.
- Left-click on the center of the solvent peak. Enter the standard chemical shift of this peak.

### Integration

- Enter the integration mode by clicking on the integral button  in the toolbar.
- Delete any existing integrals. First click  to select all integrals, then click  to delete the selected integrals.
- Click on the integral region button  to begin defining new integrals. Drag the cursor over a peak to integrate that region.
- To calibrate the integration values, right click the peak you wish to use as a reference and choose “Calibrate”.
- Click the save and return button  when you are done defining integrals.

### Peak Picking

- Click the peak picking button  on the toolbar.
- Drag the cursor over the tip of a peak to select it. The green box only needs to enclose the tip of the peak; dragging to the box to the baseline may cause noise to be identified as peaks.



- Click the save and return button  when you are done picking peaks.

### Plotting

- Type “plot” to open the plotter.
- Instructions for the plotter software are available on the NMR Facility website: <http://www.chem.pitt.edu/facilities/nmr-spectroscopy-0>