

500 MHz User Guide

Login to computer

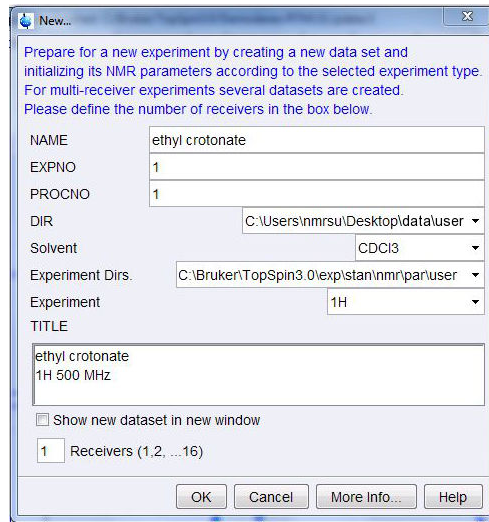
- On the Windows Welcome screen, select your group's login.
- TOPSPIN should launch automatically after you login. If TOPSPIN does not launch automatically, use the icon on the desktop to start the program.

Loading a sample

- Check your solvent height. For best shimming homogeneity, the sample height should be 5cm.
- Wipe the exterior of the tube clean using a Kimwipe.
- Type “**ej**” to turn the lift on.
- Place your sample into the spinner. Do not use pieces of paper or Kimwipe to secure a loose sample!
- Use the depth gauge to adjust the spinner height on the tube.
- Carefully place your sample into the bore. Make sure air flow is on before releasing sample!
- Type “**ij**” to turn off the lift.
- Type “**ro on**” to turn on sample spinning, if desired.



Experiment Set-Up

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



- Give your experiment a name and experiment number.
- *IMPORTANT*** Topspin 3.0 no longer has a separate field for user name. Instead, you must specify your user name in the directory path. To make sure that your experiments are stored in your personal directory, you must enter your user name in the DIR field between “data/” and “/nmr”



- Choose the correct solvent and experiment parameters from the list. Enter the title for your experiment. Press OK when finished.
- Enter the command “**rsh temp**” to read the shim presets file.
- Open the lock display using the “open lock display”  button on the toolbar or by double-clicking on the miniature lock display in the status bar.
- Call the auto-locking routine by pressing the “lock” button  in the toolbar of the lock window. Choose the correct solvent from the list when prompted.*
- Enter the command “**atma**” to automatically tune and match the probe.*

- Enter the command “**topshim**” to automatically optimize the shimming.*
- Enter the command “**rga**” to automatically receiver gain adjust the instrument.
- Enter the command “**ns**” to set the desired number of scans.

* 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; once during the setup of the initial proton experiment and once during the setup of the first experiment using the carbon channel (13C, DEPT135, HMQC, or HMBC).


Acquisition and Processing

- Enter the command “**zg**” (zg means zero and go). The spectrometer will start to acquire the spectrum. The time remaining for the experiment will be displayed in the status bar
- 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

- Click on the “Process” tab in the menu bar.








- Locate the solvent peak in the spectrum.
- Expand the solvent peak so that the center can be easily identified.
- Click the “Calib Axis” button  Calib. Axis on the toolbar.
- Left-click on the center of the solvent peak. Enter the correct reference value for your solvent.

Integration

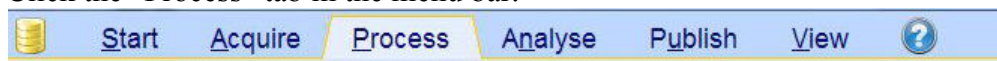
- Click the “Process” tab in the menu bar.





- Click the integral button in the toolbar. 
- Delete the automatically-generated integrals. First select all integrals  and then delete the selected integrals .
- Click on the integral region button  to manually define integral regions. Drag the cursor over a peak to integrate that region.
- To calibrate the integral values, right click the integral region 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 “Process” tab in the menu bar.



- Click the peak picking button  Pick Peaks 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.