

# Installing and Using Bruker TopSpin

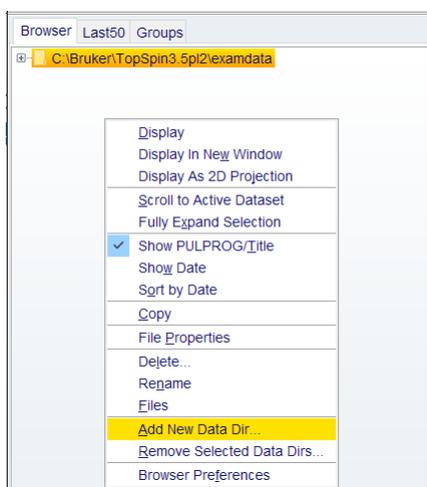
## Installation

1. Make an account with Bruker at <https://www.bruker.com/about-us/register.html> (follow prompts to create and confirm your account)
2. Download TopSpin 4 from <https://www.bruker.com/service/support-upgrades/software-downloads/nmr.html>. (Note: if you have a 32-bit Windows computer, download TopSpin 3 from <https://www.bruker.com/service/support-upgrades/software-downloads/nmr.html>)
3. Double-click on the downloaded (or unzipped file) and follow the prompts to install it. Accept defaults. Choose the password **mcgill** when prompted. Note that installation can take up to half an hour.
4. Start TopSpin.
5. To get a license:
  - a. choose “Request a free Academic license” when prompted; follow the instructions to get your 25-character CodeMeter license ticket
  - b. back in TopSpin, choose Install License Ticket. Follow the prompts. If you run into trouble, try Firefox in Windows or Safari on Mac; go to site <http://licensecentral-bbio.bruker.de/index.php>
  - c. finally, quit TopSpin with Exit and restart it
6. If you are using Windows, run Expinstall and accept all defaults
7. Go to the Settings in TopSpin (upper right) and enable “Auto-open last dataset when restarting TopSpin”. Open the second set of icons by clicking on the double-arrow at the right of the other icons

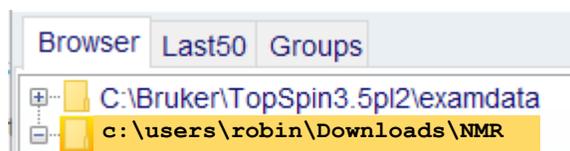
## Opening Data in TopSpin

### Setting up TopSpin

- Start TopSpin
- On the left, in the data browser, right-click and choose Add New Data Dir...



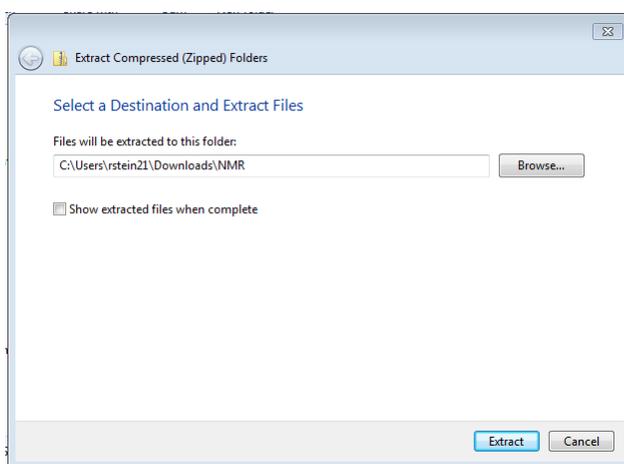
- On a Mac, add the directory /Home/<username>/Downloads/NMR; on a PC, add c:\users\<username>\Downloads\NMR



## Unzipping data

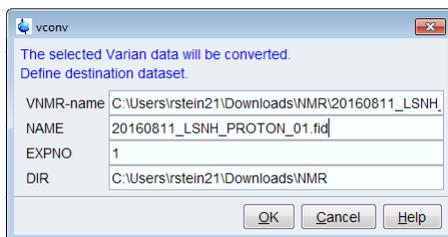
The data you receive from the Varian spectrometer will be zipped up.

- On the Mac: when you save it from your email, it will be automatically unzipped. I recommend that you save it to a folder called NMR in your Downloads folder
- On a PC, you must unzip it manually. Save the zip file to your Downloads folder. Right-click on the data file, and choose Extract All... When prompted for the location, delete the final directory and change it to NMR



## Getting Varian data into TopSpin

On PCs, type `vconv` to open Varian data. Browse to the directory and click OK. You will be asked to choose a name (the default is the Varian name), a directory (use `c:\users\\Downloads\NMR` for a PC, and `/Users/<username>/Downloads/NMR` on a Mac), and an expno (best is just to choose 1).



On Macs, type `getvarian` to open Varian data (this requires a routine you can get from the facility manager). Follow the prompts, including browsing to the dataset.

If data doesn't get processed automatically, click on Process / Proc. Spectrum.



## Some Notes on Using Topspin

### Zooming in

Click and drag to zoom in; double-click to see the whole spectrum. There is an icon to return to the previous view.

If you open a 2D dataset, it may look very wrong (peaks appearing twice, reflected about a horizontal diagonal, oddly-shaped peaks, etc.). If that is the case, try typing `varian2da` or `varian2db`. These routines, which are available from the facility manager, set up processing parameters correctly for different phase-sensitive 2D experiments (HSQC, DQCOSY, etc.).

### Basic processing

#### *Baseline correction and $t_1$ noise reduction*

Type `abs n` for a 1D dataset and `abs2` followed by `abs1` for a 2D dataset (direct and indirect dimensions).

To reduce the appearance of  $t_1$  noise (vertical noise bands) in 2D spectra, type `t1away` (request this routine from the facility manager).

#### *Peak-picking and integration*

Type `ppf` for automatic peak picking (or go to Process / Pick Peaks and click on the little arrow to bring up this option). Click on Process / Pick Peaks to pick peaks manually. The first icon in the spectrum window will allow you to select peaks by drawing a box over them. Another icon will allow you to pick specific individual peaks. Right-clicking on a peak will give you an option to delete it. When you are done, click on the floppy-disk-with-arrow icon to save your work.

Type `abs` to integrate automatically (and also baseline correct – `abs n` will baseline correct without integrating). The first icon in the spectrum window will let you click and drag over a region to define an integral. Another icon will let you split an integral. Right-click to calibrate the integrals. When you are done, click on the floppy-disk-with-arrow icon to save your work.

### Multiple display mode

Use the multiple display icon to go into Multiple Display Mode. In this mode, you can look at multiple spectra. Every spectrum you open will display on top of the starting spectrum. If you start with a 2D spectrum, you can view both 1D and 2D spectra. Use the list of spectra in the bottom left to select a particular spectrum; use the icons in the multiple display window to scale just that spectrum independently of the others.

Use multiple display mode to load a collection of spectra if you want to plot them together.

### Plotting

Use the Plot flowbar to output the current view. Or, click on the Plot tab to use the currently defined plot layout—the arrangement of items on the page. If you want to plot multiple spectra that you have loaded in multiple display mode, use the small arrow in the plot portfolio (bottom left) to load them. Click outside of the plot region to be able to insert new elements (spectra, shapes, etc.). Select an element on the plot to customize it. Use the options on the left panel for customization, and save your layout when you are finished so that you can reuse it.