

Using the Bruker Avance 300 with TopSpin 2.0

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Getting Started:

1. Double click on the TOPSPIN 2.0 icon on the desktop
2. Go to the Spectrometer menu → Icon-NMR → Automation
3. Sign into Getzler_lab
4. Password: polymer

Getting Started When TOPSPIN is Already Open:

1. Click the change user icon and sign into Getzler_lab
2. Check to see if any samples are queued by going to the Holder menu → delete completed
3. Open a file by clicking Browser/N:/ **Getzler_lab** /Your file

Entering Your Sample Into the Queue:














1. Double click on the number containing your sample
2. Pick a format (this designates file name)
3. Select the solvent used
4. Select experiment → [e.g. N Proton 1H 16 Scans (5 clicks down on the side bar)]
5. Type name, compound name, ID number, and the solvent
6. Click submit

Troubleshooting: If the sample does not start, go to the menu Run → New Run


Note: The error “solvent none is specified” is OK. Just ignore it.

Opening and Formatting a Spectrum:

1. To work on the spectrum of a sample you just ran double click where it says finished on the automation screen and the spectrum should appear

2. If under the spectrum tab it says data available but no spectrum appears go to the processing menu→Fourier transform and then go back to the processing menu→phase correction, this should bring up the spectrum
3. If you did the Fourier transform to get your spectrum to appear skip steps 4 through 9
4. click on the manual peak picking icon 
5. Right click and select delete all regions
6. Click the return and save icon 
7. Click the integral icon  directly to the right of 
8. Click on each integral on the spectrum and choose delete current integral
9. Click the save and return icon 
10. Check where your solvent's residual peak should be on the chart hanging on the wall near the door (DMSO, for example, should be at 2.5 ppm)
11. Check where water and acetone should be located in your particular solvent
12. You can zoom in on an area by left click and dragging across the desired area
13. Click the spectrum calibration icon 
14. Select the center of the solvent peak and type the correct place when prompted
15. Select the integration icon  to integrate the individual peaks
16. The small peaks you see about 20 hertz away from the peak are called spinning side bands (the peak position is defined as the center of the doublet)
17. You do not need to integrate the solvent, water, or acetone peaks (Ex: In DMSO water will have a peak around 3.3 ppm and acetone will be found around 2.09 ppm)
18. The  icon toggles between using a function like integration and being able to zoom in to better see the peaks
19. You can reset to the original size after zooming by using the  icon
20. The  icon is used to change the height of the peaks
21. The  icon can be used to reset the peaks to their original height
22. Then use the  icon to select the peaks (just the tops in small green boxes)
23. Right click and delete all regions
24. Save and return 

Using TOPSPIN Plot Editor

1. The easiest way to open a file in the plot editor is to select print (while the file is open in TOPSPIN 2.0) and select open in TOPSPIN plot editor
2. To open layout select File→Open layout→N:→Data→Getzler_lab→Layouts
3. If you have made changes in TopSpin (*e.g.* changed integrations, picked new peaks, acquired a new spectrum) and want to put that data in, go to Topspin→get current data set
4. Once your spectrum is correctly formatted choose the  icon and click and drag to open up a smaller version of your spectrum within your spectrum
5. Right click on the smaller spectrum and select 1D/2D edit, which should bring up a box with options to make the spectrum wider or more narrow so you can magnify important parts of the spectrum for later reference