Instructions for Bruker Topspin NMR Acquisition and Processing

- Log on and initiate your session in OpenInstrument using your JHED ID and password
- Open Topspin software from the icon on the desktop
- Prepare sample for insertion into magnet by putting your tube into the sample spinner and adjusting the height with the depth gauge

Initial Steps

Command	Description	Guide Icon	GUI Icon
ej	• eject the standard or previous sample with the ej command • exchange your sample for the standard sample on the column of air		
ij	• type ij to lower your sample		
aqguide	• from the spectrometer pull down menu at the top, open the data acquisition flow chart or use the command aqguide		

Follow the Icons in the Guide

Command	Description	Guide Icon	GUI Icon
new or edc	• create a new experiment, fill in the fields of the dialogue box • experiment name, experiment number, processing number (does not have to match expt #), and your user ID • *do not use slashes, colons, or pipes in the experiment name* • directory should be **U:** • choose solvent from the drop-down menu • choose a directory for parameter sets from the drop-down menu. • Use …/par/user/ for routine experiments • choose an experiment, e.g. proton or c13cpd • enter a title that will appear at the top of your spectrum • click OK to close the dialogue box		
lock <solvent>	• locks the spectrometer to the deuterium signal in your solvent • choose the appropriate solvent from the drop-down list		
probe match/tune atma or atmm	• matches the internal reflectance to a 50Ω impedance and tunes to the correct frequency for your solvent and nucleus (if doing broad band work)		
ro	• rotate or spin sample at 20 Hz		
topshim topshim gui	• shimming improves the homogeneity of the field • choose topshim and then press start in the pop-up window		
ased eda	• acquisition parameters for the pulse sequence being run • edit acquisition parameters, all acquisition parameters are shown		
getprosol	• reads in parameters from table specific for the probe and solvent		
rga	• sets receiver gain automatically		

zg	• start acquisition		
tr	• saves the data of the current number of scans while the experiment is still running • this allows the data to be processed while the data is still acquiring		
halt	• stops the acquisition run and saves the data		
stop	• stops the acquisition without saving any data. Serves as an emergency stop.		
go	• restarts the acquisition and appends the new data to the current data set. This is helpful to improve the S/N of the spectrum by acquiring more scans		

This completes the ACQUISITION portion of the procedure

To process your data click “To Processing” button

Command	Description	Guide Icon	GUI Icon
prguide	• Opens a flowchart for processing similar to acquisition		
wm lb em	• **wm** opens window function dialog box: removes the wiggles from the base of the peak that result from incomplete decay or truncation of the fid • Without the dialog box, the line broadening parameter can be set with the **lb** command and execution of the window function is done with **em**		
ft	• Fourier transform: converts the time domain data to frequency domain data		
apk	• Automatic phase correction, adjusts the phase of the signal to give an absorptive signal		
cal	• **cal** opens a dialogue box to choose between automatic and manual calibration • Automatic calibration requires a TMS signal • Manual calibration is an interactive tool to reference or set the x- axis to the appropriate chemical shift based on residual solvent peak		
bas abs n	• **bas** pens baseline correction dialog box: auto-correct baseline using polynomial gives reasonable results for most baseline situations • Using the command **abs n** will perform polynomial baseline correction automatically without the dialog box		
pp mi, pps	• **pp** opens the peak picking dialog box: two commonly used options are the auto-pick peaks and define regions/peaks manually • Auto-pick peaks requires a minimum intensity to be set in the lower portion of the dialog box. Usually between 0.1 and 1 but dependent on the concentration of your sample • Manually defining peaks is interactive and based on defined regions or individual peak picked. Must save peaks to retain for plots and exit the mode • Can set the minimum threshold for peak picking with **mi** then automatically pick peaks using the command **pps** without using the dialog box		

.int     	• **.int** opens dialogue box for integration options - most common is to define integral regions manually. The icons are as follows: • Indicates active integration mode when highlighted green, left mouse button click and drag to define integral area • Indicates 'cut mode' is active when highlighted green, cuts the integral line into smaller segments • Undo previous action • Right click mouse to calibrate integral values, delete integral currently under cursor, or select/deselect regions • Deletes selected integral areas • Saves the integral regions and exits integration routine		
prnt plot	• Prints active window • Enters plot editor mode based on predefined layouts		
wrpa	• Dialogue box for saving data to different locations or in different formats. Unfortunately email options are not set up at this time.		

Some of the commands above are specifically for only 1D data. For 2D processing using the following commands. If a procedure is not listed below, try the command listed for 1D processing.

2D Processing Command	Description
xfb	• Fourier transfroms the 2D data in the F1 and F2 dimensions
ph  	• Opens phasing dialog box and manual processing is required. • Move cursor to a row of cross peaks that require manual phasing, right click and select “add” in the menu. Do this for two or three rows avert he 2D spectrum. • Press the **R** button at the top and it will bring you to the manual phasing window with each row that was added stack over each other. • Manually phase the 1D spectra so that all rows are phased as best as possible. • Similarly, column of cross-peaks can be phased in a similar manner, but pressing the **C** button to enter the manual phase window
bas	• Baseline correction is done through the dialog box • Select the auto-correct using polynomial and check which dimension (F2 or F1) is to be corrected • Perform again for the other dimension
pp 	• Peak picking is best done in manual mode • Define regions using the icon and draw boxes around peaks • Click on the D button to define peaks then save and exit the peak picking mode • For list of peaks, look in the peak tab