PSU NMR Facility
Acquiring ^{1}H NMR spectrum
(Quick instructions for Topspin)

If you need assistance, please contact:
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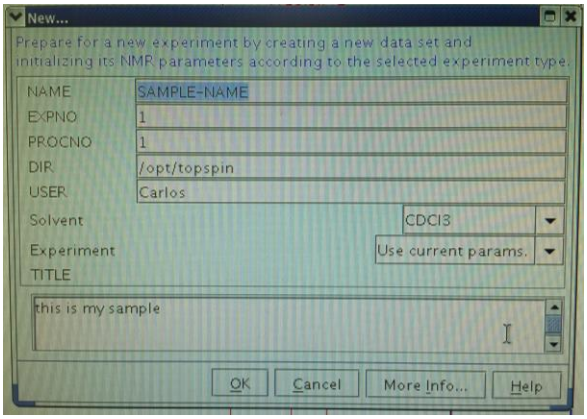
- Dr. Debashish Sahu -- Room#10 - desahu@psu.edu

Place your sample in the spinner and carefully adjust the NMR tube depth in the gauge.

1) Turn on the lift air using BSMS (or type ***ej*** *<enter>* at the command line*)*.
   a. If BSMS window is missing, type ***bsmsdisp*** *<enter>* at the command line.
   b. ***Always wait for the sound of the lift air at full power before placing your sample on top of the magnet!!!***

2) Turn off lift air from BSMS (or type ***ij*** *<enter>* at the command line).

3) Create a new data set by typing ***new*** *<enter>* at the command line or click  on the toolbar (or type ***edc*** at the command line)



NAME -- (filename for your compound)
EXPNO -- suggestion: Set 1 for a ^{1}H, 2 for a ^{13}C
PROCNO -- set to 1
DIR -- set to /opt/topspin/
USER -- should be <your_Professor-name>
SOLVENT -- your deuterated solvent from the pull-down menu.
EXPERIMENT -- "Use current params"
TITLE – the title of your sample (can be as descriptive as possible)

4) Read a good shimfile with ***rsh***<*enter*>: choose the **stdshims** file from the list, which is the standard shimfile name for all NMRs.

5) Type ***lock*** <*enter*> at the command line and choose the appropriate solvent from the lock table.
   a. If the lock window is missing, type ***lockdisp*** <*enter*> at the command line.

6) After the lock process is finished, shim **z1** and **z2**.

7) Type ***rpar PROTON all*** <*enter*> at the command line.

8) Type ***getprosol*** <*enter*> at the command line.

   a. For instruments running **Xwinnmr,** type ***eda*** <*enter*> and set prosol to ***TRUE***.

9) (**OPTIONAL**) Adjust **SW** and **o1p** values.

10) Type ***rga*** <*enter*> at the command line

   a. Adjust the number of scans - **NS** - as appropriate if necessary; default for ^{1}H is 16, for ^{13}C is 1024).

11) Type ***zg*** <*enter*> at the command line to start the experiment.

12) Type ***acqu*** <*enter*> at the command line if you do not see your FID (raw NMR data).

13) Your NMR data is automatically saved **at the end** of the experiment.

DATA PROCESSING

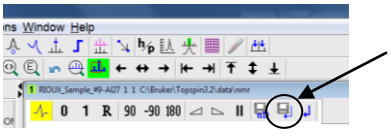
((It is highly recommended to carry out the NMR processing on the *off-line* PC at the NMR Facility – room #10, where you can also back your NMR data up))

14) Type **ef; apk** <*enter*> at the command line to perform Apodization (**e**), Fourier (**f**) Transformation, and automatic phase adjustment (**apk**).

15) If needed, further optimize the phase of the spectrum manually, **using the phase correction icon**.

Click on the phase icon: 

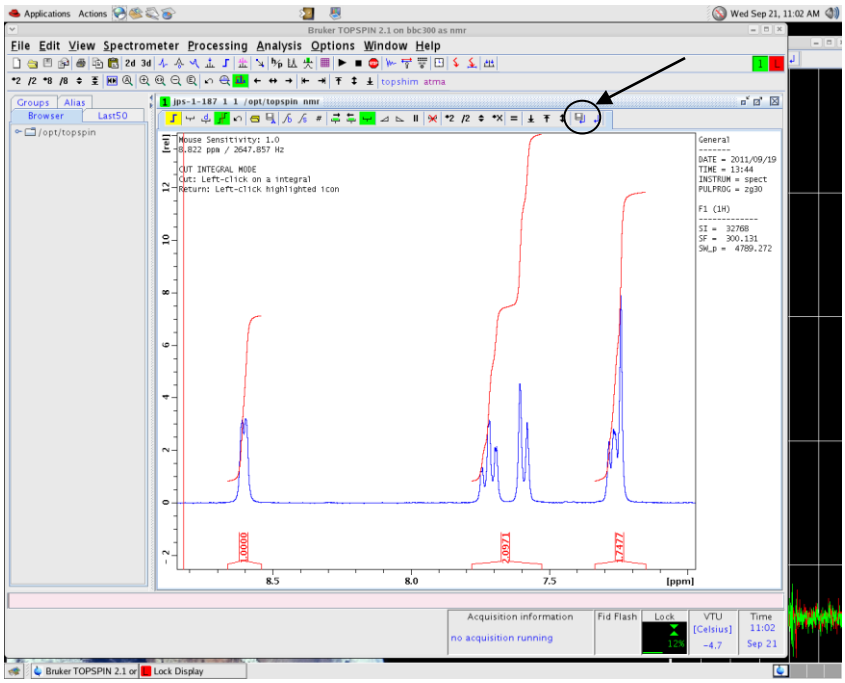
Left-click **0**, hold the mouse button to correct phase **at** the vertical cursor.
Left-click **1**, hold the mouse button to correct phase **away** from the cursor.
Click on the SAVE icon to exit the phasing window.



16) Calibrate your spectrum using a known chemical shift (residual solvent peak or TMS). Click on the icon  at the toolbar. Set the reference and return.

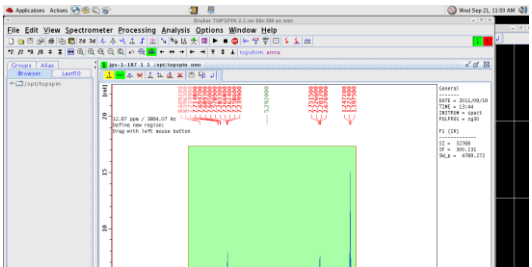
17) Type **abs** to flatten the baseline. There is a manual baseline flattening: 

18) Integrate the spectrum manually with  -- This takes you into a subroutine:



Integrate the spectrum, save the integrals before exit the window.

19) Peak picking can be done with the icon  and drawing a green box around the peaks:



Save the peaks before exiting the window (using the same icon as the phasing and integration).

20) Type ***plot*** <enter> to open the plot editor (for instruments running TopSpin) and then print.

a. For instruments running Xwinnmr type ***view*** *<enter>* to print preview and type ***plot*** *<enter>*.

21) Print.

22) Save your data on the PC at Room #10

a. Save your NMR data **ALSO** on a thumb drive.
   i. Email the NMR data is also possible at the off-line PC.