# HOW TO: OBTAIN A 1H NMR SPECTRUM ON THE 300 MHz BRUKER NMR

Open the TopSpin program if not already open.

## I. ACQUIRING A SPECTRUM

*1) Create your data file*

Type “new” and enter the name of your sample. If you are running multiple experiments on this sample, you may change the experiment number as well.

*2) Remove current sample/insert your sample*

Remove the black cover of the bore. Eject (“ej”) will pop up the current standard sample. Remove the sample, and exchange the spinner to your sample using the depth gauge (failure to do so may damage the probe). With the air flow still on, place your sample onto the bore so that it is floating on the air. Return to the computer and type “ij” to inject your sample. You should hear a slight clicking noise after it is lowered.

*3) Choose your experiment*

Type “rpar” to bring up a menu of common experiments. Select “PROTONSTD” for a routine 1H NMR, click the READ button, and hit OK on the next window. This loads all the parameters necessary for this experiment.

*4) Lock your solvent*

Type “lock CDCl3” to lock your sample to the deuterium signal of your solvent. If you are using DMSO-d6, type ”lock DMSO”, etc. Wait for the process to complete.

*5) Tune*

Type “atma” to tune the probe to your desired nucleus.

*6) Spin your sample*

Type “ro on” to turn on the spinning for your sample. You should hear a continuous, slight whirring noise from the air flow. [THE “7. spin” TAB DOES NOT CURRENTLY WORK]

*7) Shim your sample*

Type “topshim” to begin an automated shimming program. Lucky you! – manual shimming is mostly a thing of the past. Wait for the process to complete.

*8) Load pulse sequence*

Type “getprosol”. This process completes almost automatically.

*9) Set gain level and number of scans*

Type “rga”. Wait for the process to complete. Type “ns” to enter the number of scans you want.

*10) Zero and Go*

Type “zg”. This command will begin the experiment, and you can see the number of scans begin to accumulate in the mid-center window below the FID.

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## II. ACQUIRING THE SPECTRUM AND BASIC PROCESSING

1) Type “tr” to transfer the current number of scans. When transferred, type “efp” to perform the Fourier transform. Note this will not stop the experiment (scans will continue).

2) To autophase the spectrum, type “apks”.

3) To begin processing the data, click the Process tab at the top:

   a) Calibrate Axis: Left click to set your x-axis (typically to solvent or TMS).

   b) Peak pick: Left click and drag to select peaks you desire.

   c) Integrate: Left click and drag to integrate your peaks.

   For more details, consult the Avance Bruker Guide or Dr. Walvoord.

## III. PRINTING YOUR SPECTRUM

1) Type “plot”. Click on the button next to “Print” and select “Print” from the drop-down menu.

2) Click on your spectrum, then enter your desired plot limits (x axis).

3) Click on Properties to select Black/White printing, then print.

## IV. FINISHING UP YOUR EXPERIMENT

1) Type “halt” to end your experiment (you may transfer your extra scans and work them up if you’d like).

2) Turn the spin off (type “ro off”).

3) Eject your sample, and inject the standard sample. Refer to step I.2 above.

4) Lock the standard sample (type “lock DMSO”).

5) Replace the black cap and leave the standard locked and with no spinning. Leave TopSpin program on.