

# <sup>1</sup>H 1D Spectrum Guide (modified)

Step	Function or Dialog Box	<Keystroke>/[Select]/<Data Entry>	Comment
1	Sample		See Sample Preparation Guide. Position sample spinner using the depth gauge, place in probe
2	Enter PNMR program.	<Alt+Tab>	(If necessary - this is a standard "Windows" command)
3	Select <sup>1</sup> H observe.	<b>C13</b> >nu H1<Enter>	Required only if the prompt is not "H1".
4	Shim the magnet	<b>H1</b> >shim <Enter> then 2 <Enter>	A value of 2 is usually used; 5 is for viscous degassed samples (rare).
5	Acquire data.	<b>H1</b> >zg<Enter> then filename<Enter> or <Enter> for default	Enter file name if desired but it is usually better to use the default (pnmrfid) unless intending to save the data long term. Use acq <Enter> to shim and automatically set RG
6	Enter NUTS.	<Alt+Tab>	
7	Process data.	<Ctrl+F2> then [filename][Open] to select a file or [Open] for default filename	Process using aii_H1.mac to show the entire spectrum referenced to TMS. Enter any Comments (e.g., sample name) and User (operator's name or initials) in the appropriate fields, then click OK.
8	TMS at zero (0) ppm	click left MB on peak	Place cursor on right-most peak, verify that it's at 0 ppm, otherwise adjust using FO command in PNMR. (ask instructor)
9	Enter zoom routine.	>zo	Set up for phasing.
10	Select two regions of interest. (see comment)	<1> then <2> <Enter> to exit "zo"	Drag cursor over a <b>strong</b> peak on left. Press <1> to assign as region 1. Drag cursor over a <b>strong</b> peak on the right and press <2> to assign as region 2.
11	Trim phase.	>pe <Enter> to exit "pe"	Phase left side peak by pressing and holding <b>left</b> mouse button while dragging mouse side to side. Repeat using the <b>right</b> mouse button to adjust the right peak. Don't forget to press <Enter> when done.
12	Fit baseline.	>fb <L> <Enter>	Enter fb subroutine, remove stripes on or too close to peaks, press the letter "l" for Least Squares fit, save result and exit fb with <Enter>.
13	Enter integral display.	>id	
14	Integrate data.	two clicks of left MB, then one left click <Enter> to exit "id"	For each broken integral, click left MB twice on left side of peak(s) then once on right side. To assign a relative integral value place cursor on integral, click left MB, press <v> and enter number. <Ctrl+I> toggles integrals on/off.
15	Expand selected region. Standard range is: 10 to -0.5 ppm	>zo <f> <Enter> to exit "zo"	To select standard expansion region type <f> to enter fixed offsets with information dialog box. <Ctrl+E> gives the expanded region <Ctrl+F> returns to the full spectrum. (If peaks are present 10 ppm, then standard range is either 12, 14, etc., to -0.5 ppm until peak is displayed on the screen)
16	Prepare for Plot	Check Printer Setup  then Adjust spectrum height  >id	At the Base Level, under File menu, choose Printer Setup and select Landscape under Orientation (if necessary). Using the scrollbar at right adjust the height of the tallest peak in the spectrum (not the TMS peak) to the top of the page. Finally, display the integral with integral values.
17	Plot Data.	<p> <b>or</b> >p1	If still in the ID mode (or ID and ZO mode), just type <p>, otherwise in the Base Level type >p1.

