

¹H 1D Spectrum Guide

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)
3	Select ¹ H observe.	C13>nu H1<Enter>	Required only if the prompt is not "H1".
4	Verify parameters.		Verify that parameters make sense .
5	Acquire data.	H1>zg<Enter> then <i>filename</i> <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. OR, preferably:	<Ctrl+F1>	Process <u>and</u> plot using aii_proc.mac, which references TMS, peak picks, integrates, and accepts spectral information and plots.
7b	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. Expansion zo, integration id, peak picking pp or dp, and plotting pl may be done manually.
8	Enter zoom routine.	>zo	Set up for phasing.
9	Select two regions of interest. (see comment)	<1> then <2> <Enter> to exit "zo"	Drag cursor over a strong peak on left. Press <1> to assign as region 1. Drag cursor over a strong peak on the right and press <2> to assign as region 2.
10	Trim phase.	>pe <Enter> to exit "pe"	Phase left side peak by pressing and holding left MB while dragging mouse side to side. Repeat using the right MB to adjust the right peak.
11	Fit baseline.	>fb <L> <Enter>	Enter fb subroutine, remove stripes on or too close to peaks, press the letter "I" for Least Squares fit, save result and exit fb with <Enter>.
12	Enter integral display.	>id	
13	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.
14	Pick Peaks a. Automatic or b. Manual	>pp or >dp <c> <Enter> to exit "dp"	a. Automatic peak pick - Vertical red lines indicate selected peaks. Use MH and RM to change peaks selected. b. Manual peak pick -The cursor becomes a crosshair with a DP label. <a> automatically picks peak; <c> clears all peak picks; <k> removes a single peak pick nearest the cursor. Add peak by clicking the left MB near any peak. <t> writes peak list to the table. <Ctrl+B> toggles peak pick table on/off. <Ctrl+P> toggles the peak labels on/off.
15	Expand selected region.	>zo <Enter> to exit "zo"	Select expansion region with mouse or <f> to enter fixed offsets with information dialog box. <Ctrl+E> gives the expanded region <Ctrl+F> gives the full spectrum.
16	Plot Data.	>pl	