

¹³C 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 ¹³ C observe.	H1>nu c13<Enter>	Required only if the prompt is not C13> .
3b	Optional: Shim sample.	C13>shim<Enter>	Follow on-screen directions. Shims are optimized. Dilute sample RD=5; Conc. sample RD=2
4	Acquire ¹ H spectrum.	C13>zgh<Enter>	Obtain ¹ H spectrum using default conditions
5	Enter NUTS and process data.	<Alt+Tab> >a2	Trim phase as required. Use cursor to determine TMS peak position in ppm, including sign.
6	Return to PNMR and enter TMS peak position.	<Alt+Tab> C13>fo<Enter> value<Enter> 0<Enter>	Enter the current position (in ppm) of the TMS peak to the first dialog box and 0 (zero) to the second dialog box. Repeat to confirm.
6b	Optional: Confirm field offset and save ¹ H spectrum for border of HETCOR plot.	C13>zgh<Enter> <Alt+Tab>, >a2 >sa filename	Acquire proton spectrum. Switch to NUTS and process with a2 link. Enter filename for ¹ H spectrum, for example <i>border_h1</i> . <Alt+Tab> to return to PNMR
7	Verify parameters.		Verify that parameters make sense; for neat samples NS=12, for 1M samples NS=60, for concentrations <1M use the BAPR program.
8	Acquire data.	C13>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.
9	Enter NUTS .	<Alt+Tab>	
10	Process data.	<Ctrl+F3> then [filename] [Open] to select a file or [Open] for default	Process using aii_C13.mac that references TMS and sets display range from 220 to -10 ppm. Does an automatic peak pick.
11	Enter line broadening.	value <Enter>	LB=0.5 Hz is a typical value.
	Optional: Pick peaks manually.	>dp <Enter>	The cursor becomes a crosshair with a DP label. <c> clears all peak picks; <k> removes a single peak pick at the cursor location. Add peaks by aligning cursor on a peak and clicking the left MB. <t> to write peak list to the table.
12	Plot Data.	>pl	
	Optional: Save ¹³ C spectrum for border of HETCOR plot.	<Ctrl+B> <Ctrl+P> >sa filename <Enter>	Remove peak labels and table displays. Enter filename for ¹³ C spectrum, for example <i>borderc13</i> .
	Optional: Add scans	C13>Go <Enter>	In case the signal to noise is too low, the acquisition can be extended.
	<u>Number of added scans</u>	scans<Enter>	For neat samples ns=12, for 1M samples ns=60, for concentration <1M use the BAPR program.
		filename <Enter>	The program will ask for a filename when finished. Use the same name as step 8.

NOTE: For weak samples use Block Averaging with Peak Registration (BAPR)