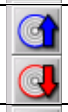
2D Processing and Printing

2D Tool Bar

Icon	Description
	Box/Cursor
	Show Full spectra
	Zoom In Zoom Out Zoom Mode
	Pan/Stretch Mode
	Trace
	Scale
	Projections
	Redraw
	Rotate
	Raise vertical scale by 20% Lower vertical scale by 20%
	Phase Mode
	Peak Picking
	Return

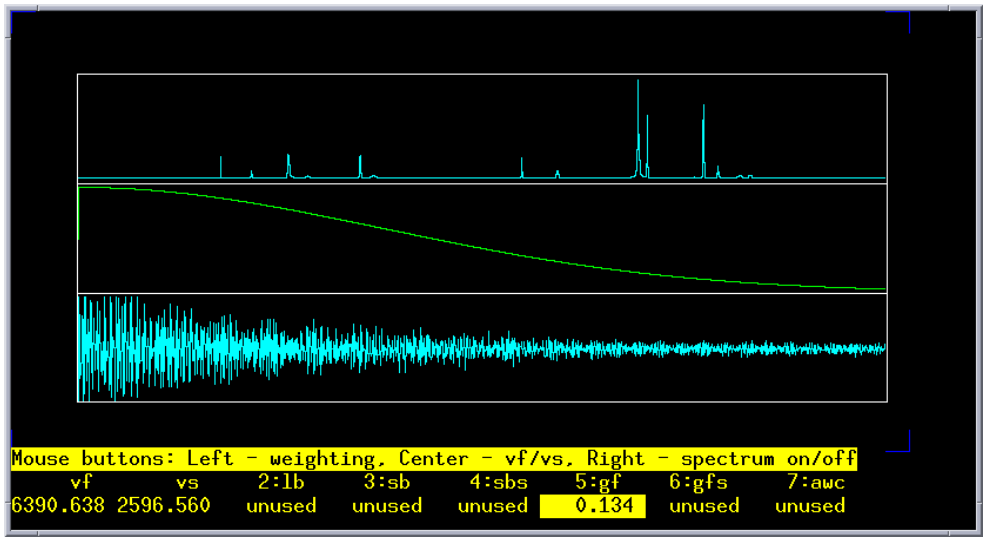
Manipulating the 2D data

Click on the appropriate icon on the tool bar to expand, zoom, and change the vertical scale of the spectra. Type dconi on the command line to display the peaks using the color map in the interactive mode. Type dpcon to display the peaks in contours. To show more contours than is automatically displayed, use a command that specifies the number of contours and spacing. To display this, **dpcon(20,1.3)** will display 20 contours at a spacing of 1.3. Other variations of this include **dpcon('pos',20,1.2)**. The modifiers 'pos' and 'neg' will display only the positive or only the negative peaks in a 2-D spectrum. To make the contour display interactive, use a variation of **dconi** such as **dconi('dpcon','pos',20,1.3).** To plot more contours, **pcon(20,1.3) pltext page**. Adjust the number of contours and spacing for the data. The 'pos' and 'neg' modifiers can also be used in the plotting.

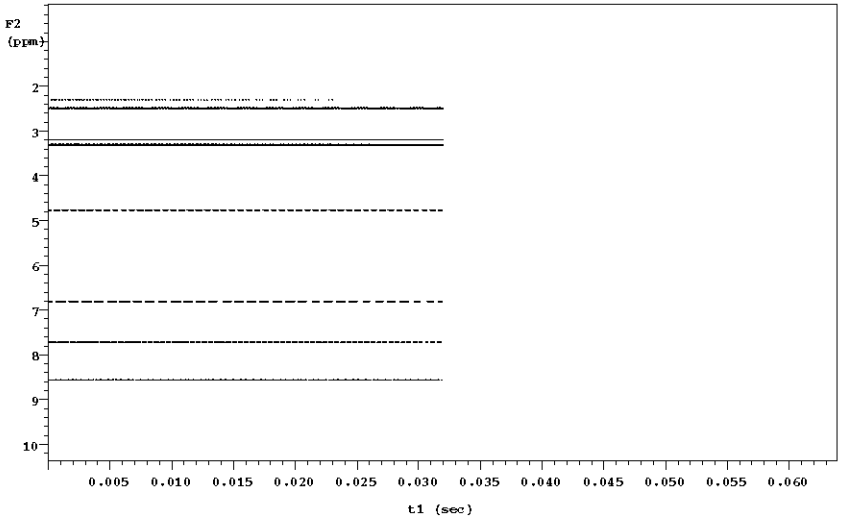
Processing 2D Data Sets Manually

This routine applies to most phase-sensitive 2-D data sets. COSY requires a slightly different approach and often uses a pure sinebell function.

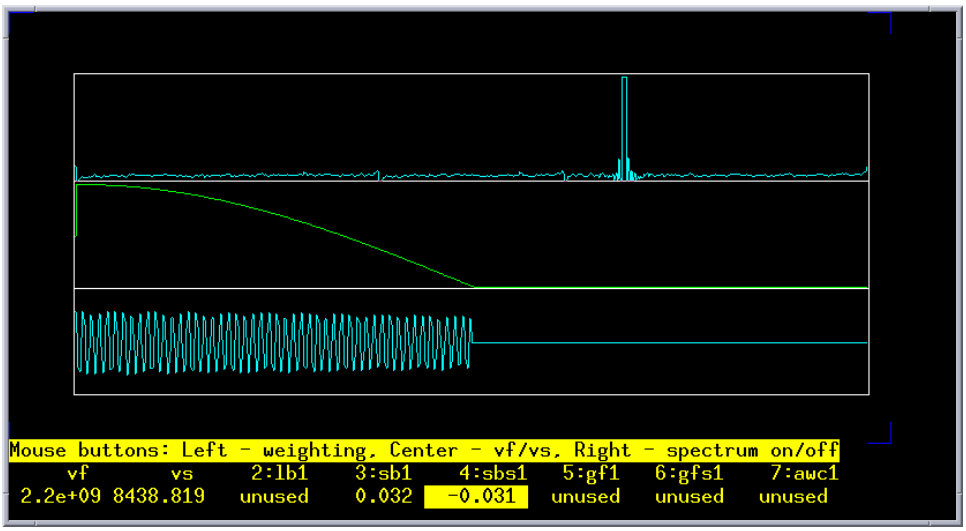
Start by processing the first increment with by typing **wft(1)** Phase this spectrum as any 1-D.Then add a weighting function to this data by typing **wti** on the command line enabling the use of the interactive weighting screen to add a weighting function. The most commonly used function at this step is a gaussian function **[gf]**.



Then process the data with by typing **wft1da.** After the data is processed, the f1 traces will be on the screen. Select a trace with the cursor. Try to use something other than solvent. Then weight this trace with **wti.**

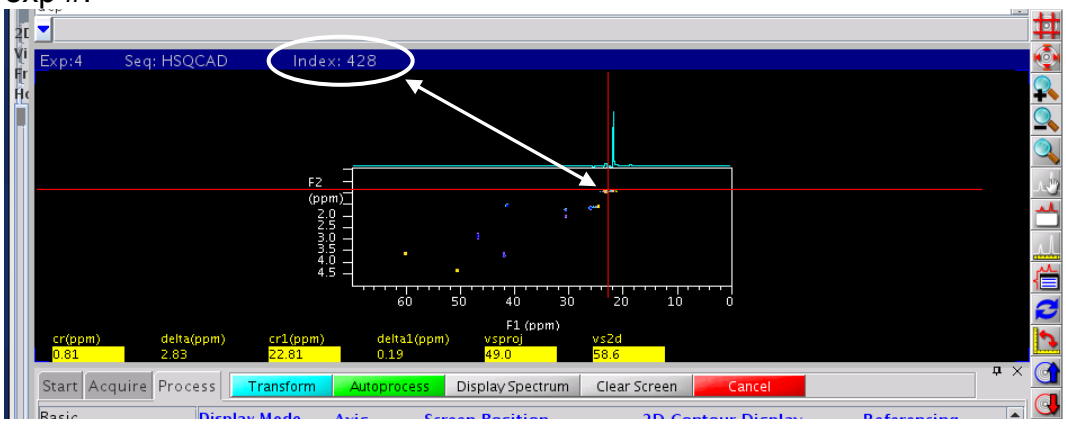


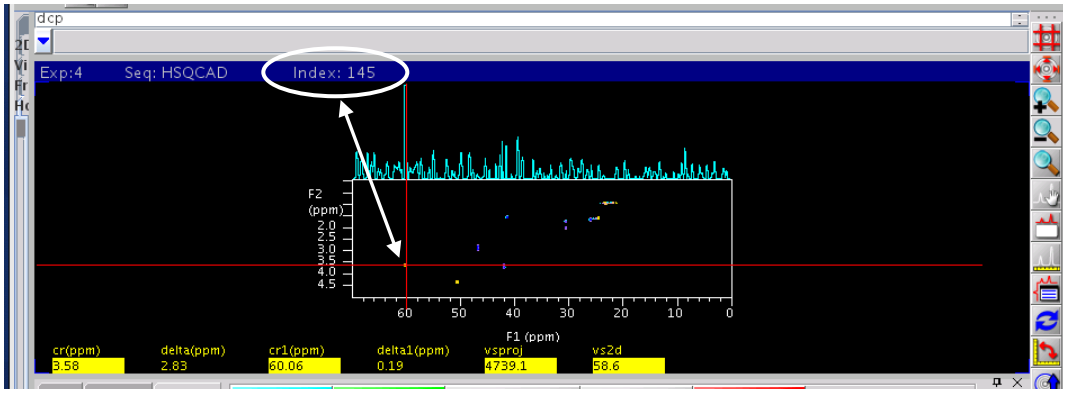
This weighting function can also be a gaussian function **[gf]**, but often a shifted sinebell is used. To put in a shifted sinebell, start with **[sb]** and move the cursor to produce a sinebell curve that is about twice the width of the interferogram. Then select **[sbs]** . Using the cursor, shift the sinebell back so the maximum starts at the left side of the interferogram. Process the 2-D data with >**wft2da**



Manual Phase Correction

Phase errors in phase-sensitive 2-D data sets can often be seen near the diagonal where the peaks may be streaked positive and negative. Display the entire 2-D spectrum. Choose 3 traces containing cross peaks near the top, middle and bottom of the spectrum and note the index #'s of each trace. The index # of the trace can be seen in the top window of VNMR next to the seq. and exp #.

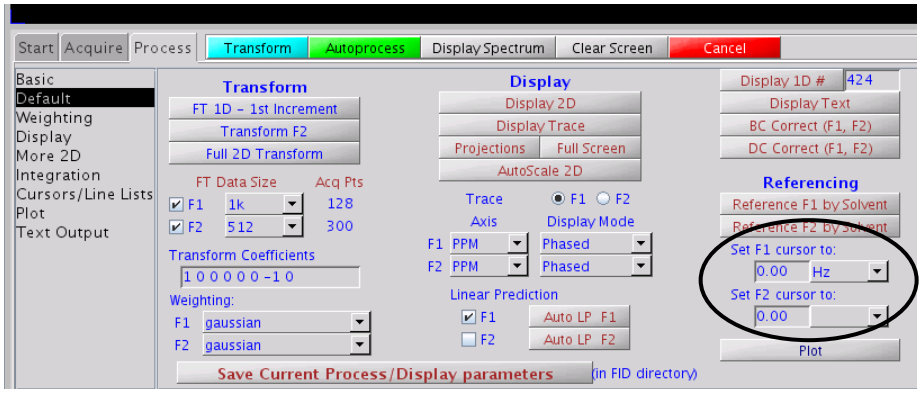




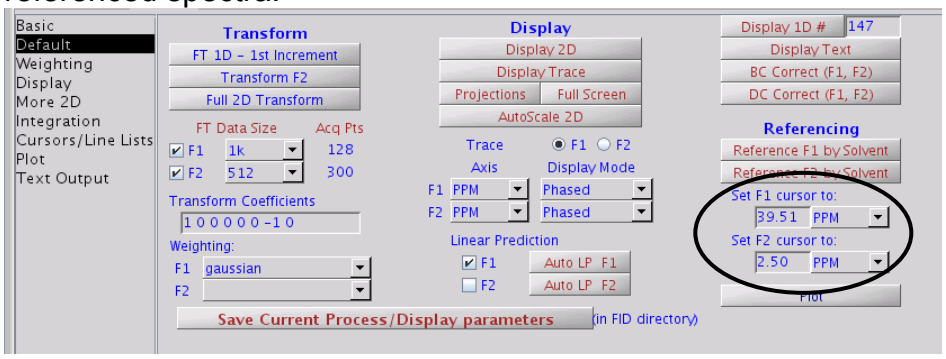
Type **r1=*index#* r2=*index#* r3=*index#*** on the command line. The values r1-r3 are place holders in VNMR. Then display the first trace: Type **ds(r1) and** Phase the 1-D trace. Display the 3rd trace. **ds(r3)** Click  . Click the left mouse button on both sides of the spectrum to accept the previous phase changes. Then phase this trace. Go back to the first trace by typing **ds(r1)** Continue phasing r1 and r3, clicking to accept phase changes in-between until they are both phased. Look at the middle trace to check by typing **ds(r2)** Then go back to the 2-D spectrum by typing **dconi.** If necessary, rotate the axis by clicking the  icon and repeat the phase correction procedure.

Referencing the 2D Data

Place the cursor on the contour which you wish to use as your reference. If the spectra is homonuclear, then type rl(#p) rl1(#p) dconi. If the spectra is heteronuclear then type rl(#p) rl1(#d) dconi. Alternatively, the spectra can be referenced by filling in the reference boxes on the Default page of the Process Tab.



Place the cursor of the desired peak, set the units to ppm, enter the correct value into the boxes, enter on the keyboard, then redraw the spectra to observe the referenced spectra.



Plotting the 2D Data

The data can be easily plotted using the buttons on the Process >Basic page or the Process>Plot page. Choosing Plot Preview will allow the option of saving the file as a pdf, while choosing Plot Page will send the printout to the printer.