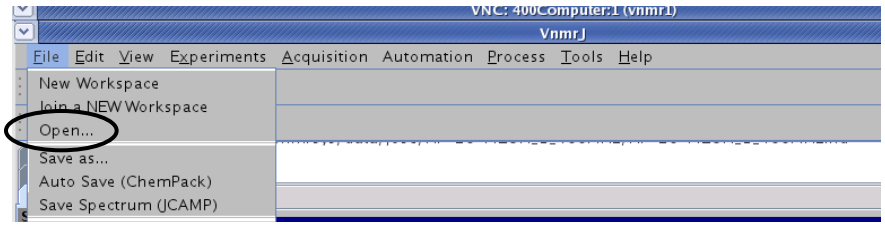
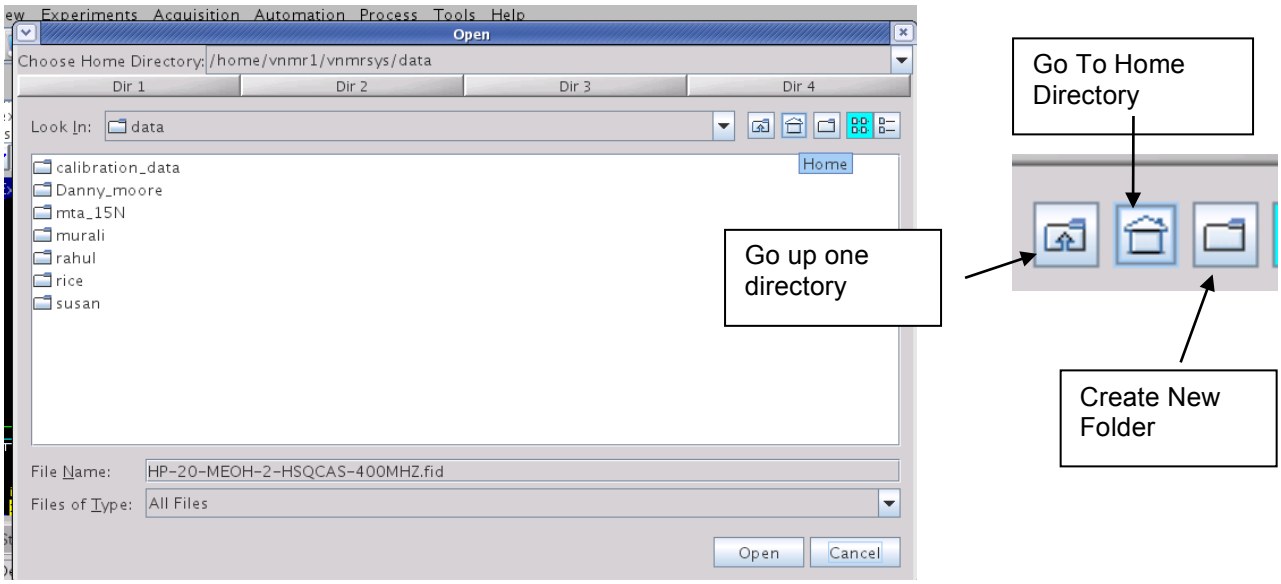
## Basic 1D Processing

### Opening Saved Data

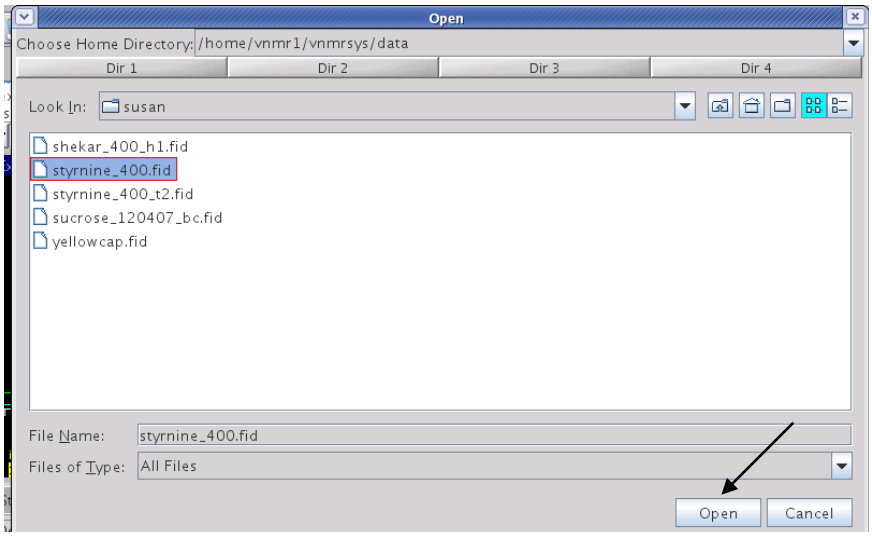
Start the VnmrJ software. "Click File > Open".




This will open a pop-up window. Clicking "Home" will take you to the data directory within your account. You can create folders here using the create folder icon.




Highlight the desired spectrum and click "Open". The spectrum will processes automatically and appear on the screen. Use the toolbar icons to access cursors. If the spectrum seems to "freeze", either click the redraw icon on the toolbar or type *ds* in the command window. The vertical scale can be changed with the mouse wheel or by typing in a numerical value for vertical scale (i.e. *vs=5000*).



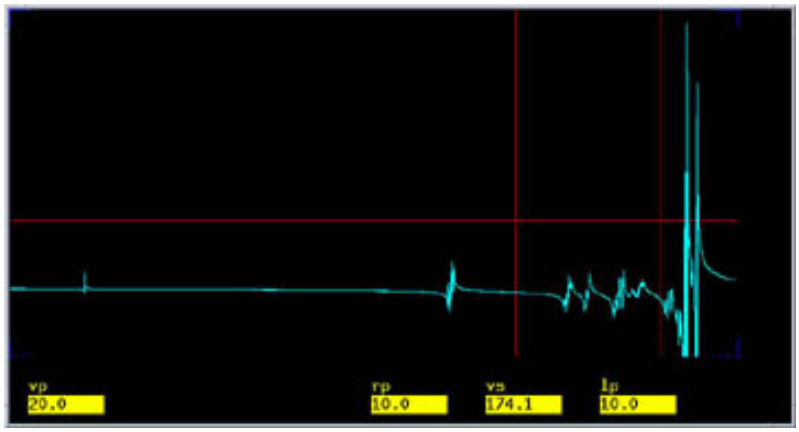

**Toolbar Icons**

| | | | |
|---|---|---|---|
|  | Access one cursor click again to access a second cursor |  | Pan and Stretch More |
|  | Show the full spectrum |  | Integration |
|  | Reset to full display |  | Show/Hide Scale |
|  | Zoom In |  | Show/Hide Threshold |
|  | Zoom Out |  | Phase Mode |
|  | Zoom More |  | Redraw Spectrum |

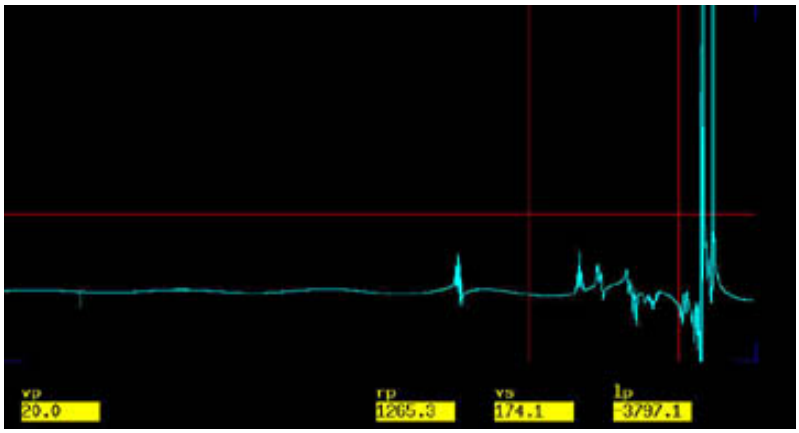
## Phasing

To display the spectrum on the screen, type *ds* Type *f full* to see the full spectrum in the full screen. The spectrum will likely need to be phased. Simple spectra can be phased crudely with by typing ***aph*** (automatic phasing).

To manually phase the spectrum, click on the phase icon on the toolbar  . Use the left mouse button to click on a portion of the spectrum. Hold down the left mouse button and move the mouse to flatten the spectrum's baseline and makes the peaks symmetrical. The right mouse button will make fine adjustments and the center mouse button will increase or decrease the vertical scale. The spectrum below is a newly acquired spectrum, which needs to be phased.



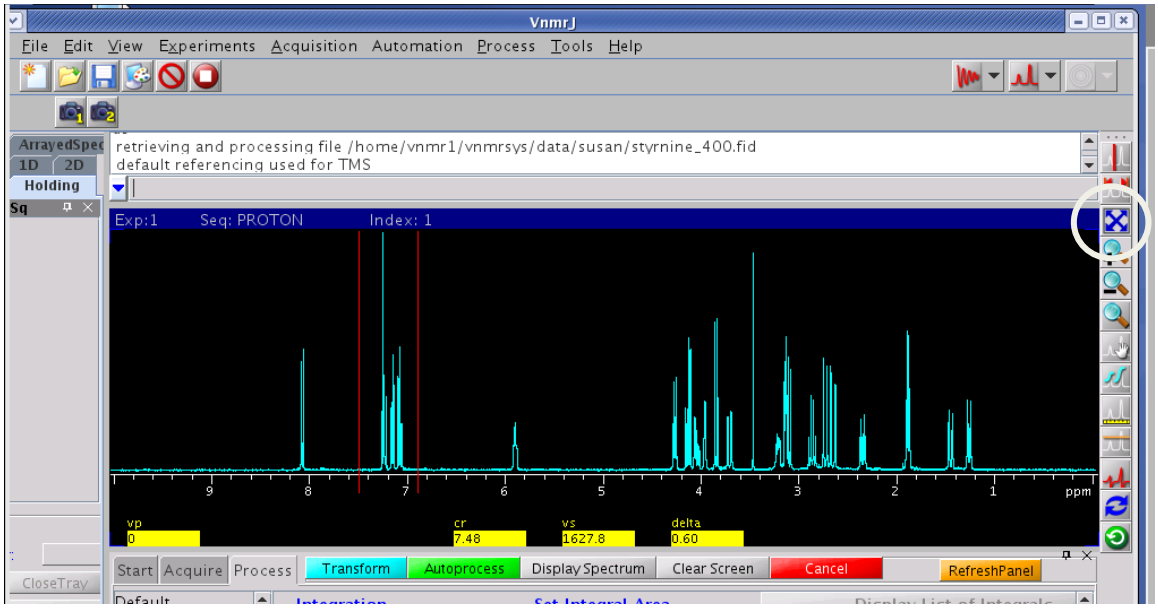

This spectrum has been “wrapped around” by bad phasing. It can be corrected by setting *lp=0* and *rp=0* and then phasing again.



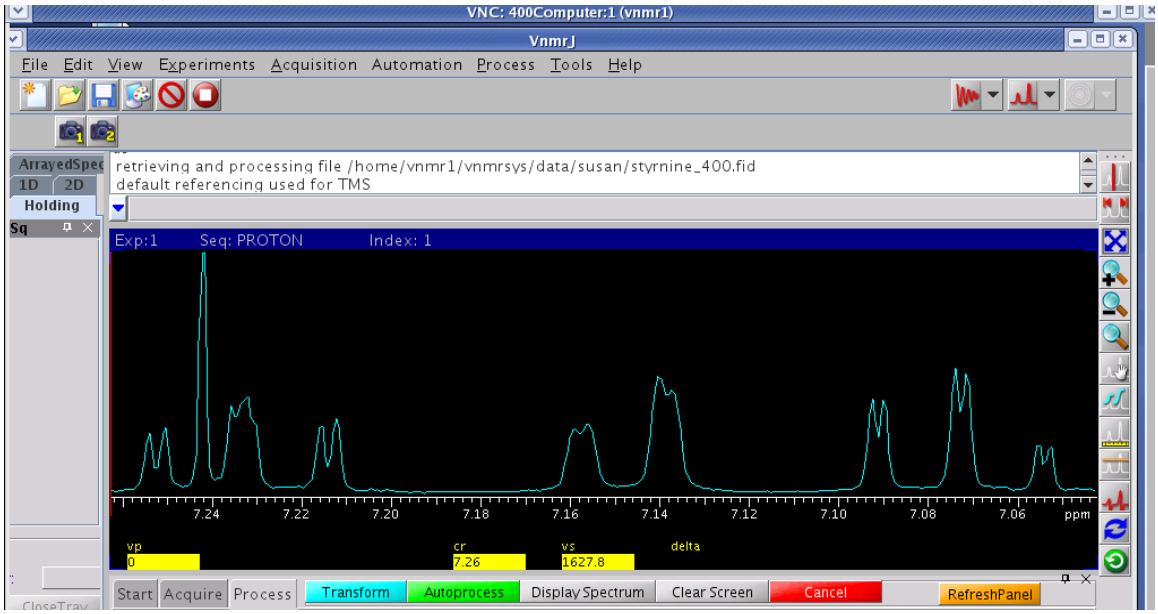

Beware of becoming dependent on *aph* since autophasing does not always work and often leaves small errors in the phase that are better corrected manually. The *lp*, or left phase, value corresponds to a first order phase correction that is frequency dependent, meaning it affects peaks differently. The *rp*, or right phase, value corresponds to the zero-order phase correction and is an error seen in all peaks.

## Referencing the Spectrum

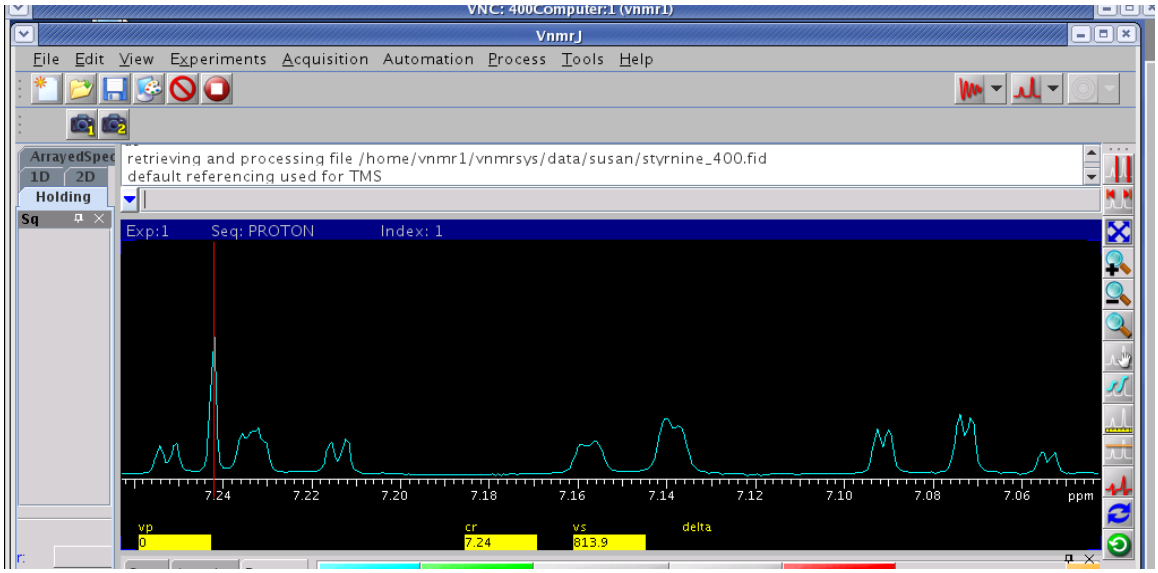
The spectrum may be manually referenced using the cursor. Expand the region around the peak you wish to reference by placing a cursor on either side of the peaks and clicking the zoom in icon.



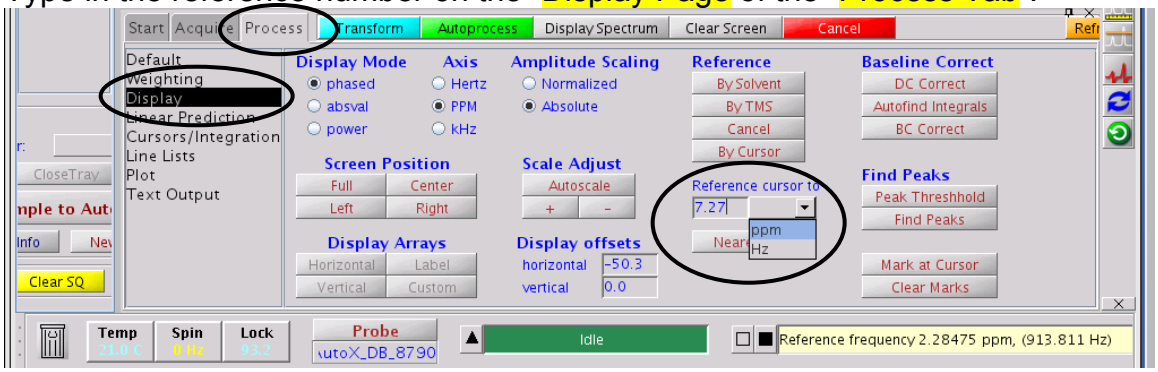

Lower the vertical scale to bring the desired peak to scale. This can be done by clicking the mouse wheel under the scale (To raise the vertical scale click the mouse wheel at the top of the black part of the screen).



Put the cursor on the peak. In this example, it is the chloroform peak.




Type in the reference number on the "Display Page of the "Process Tab".



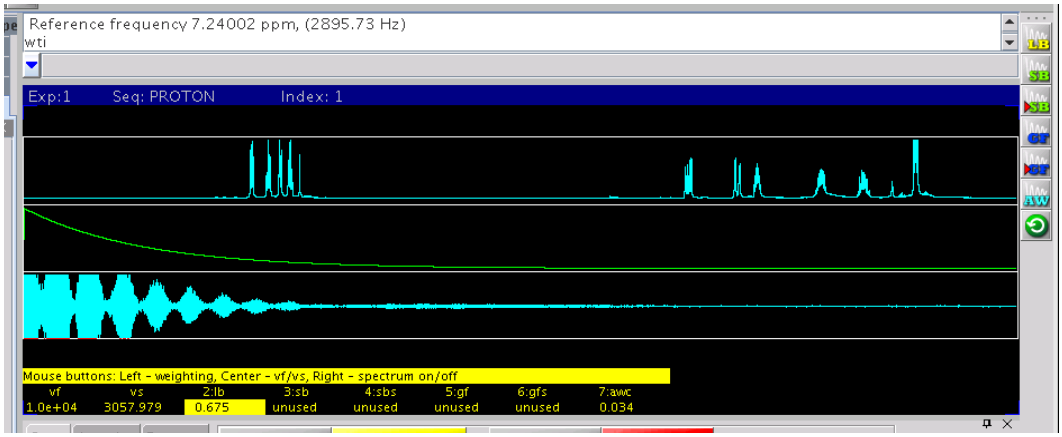

## Weighting Functions

To add a weighting function to a FID, type *wti* on the command line. This opens the weighting function screen. The mouse controls are shown on the screen. The right mouse button toggles the spectrum (top box) off and on, the center button controls the vertical scale of the FID (bottom box) and the spectrum, and the left mouse button controls the adjustment of the weighting function (green line in the center box).

Start by clicking on line broadening icon on the toolbar. 

This should bring up an exponential function in the middle window (green line). Click on the right mouse button in the top box to see the spectrum. Use the left mouse button to adjust the green line (weighting function) and observe the change in the

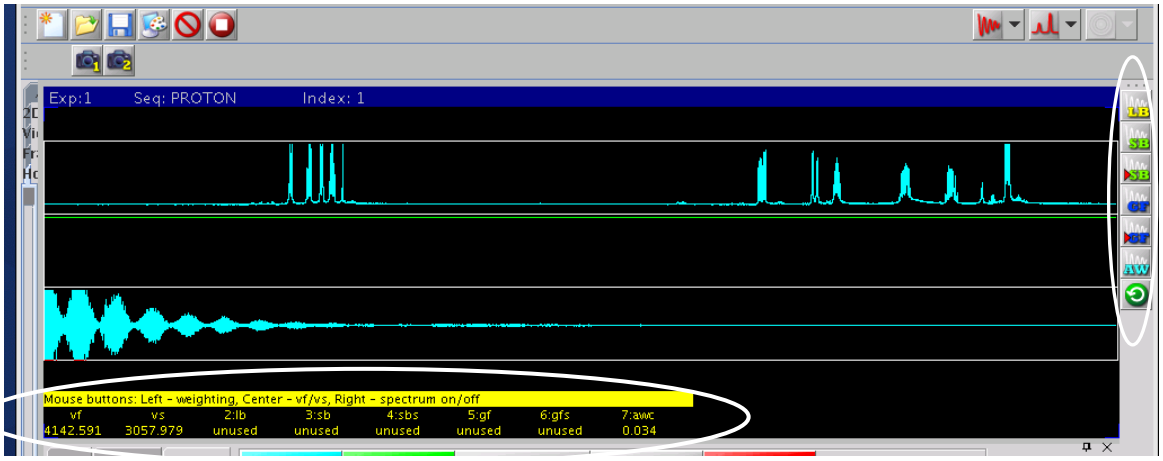
spectrum. The value of the line broadening (*lb*) is shown on the bottom of the screen.




The interactive weighting screen displays the FID, spectrum, and the weighting function applied. Above, an exponential function, line broadening (*lb*), is applied to the FID. Line broadening improves signal-to-noise at the expense of resolution. Larger values also can improve FID truncation artifacts. Negative values of *lb* can improve resolution, compared to the unweighted spectrum, at the expense of signal-to-noise.

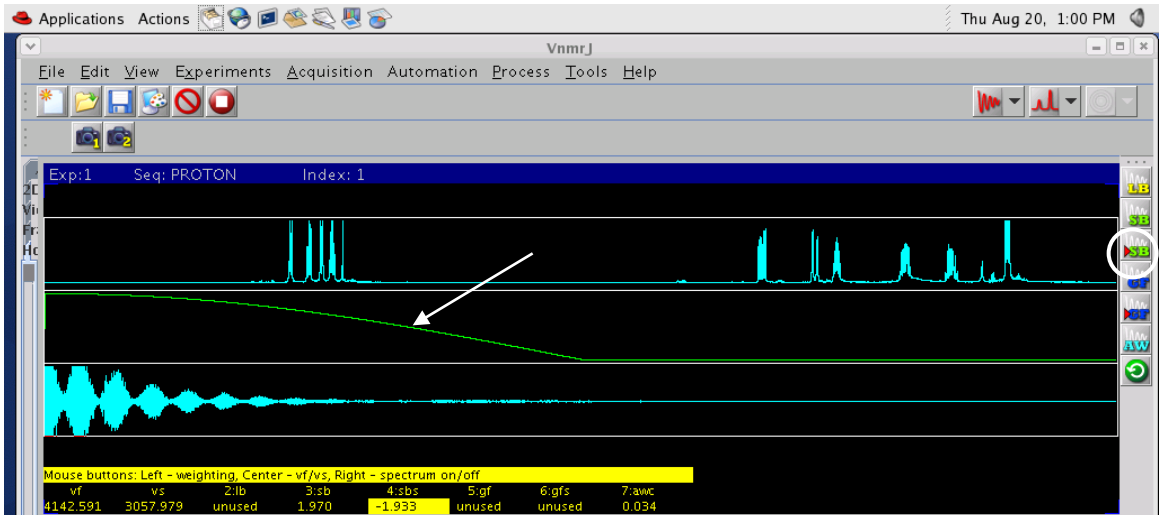
After a good adjustment is found, type *wft* in the command line. This performs a weighted Fourier transform and applies the weighting function. The spectrum may need to re-phased slightly after this.

A sinebell function can also be used for resolution enhancement. To use a weighted function like a shifted sinebell, go to the interactive weighting screen by typing *wti* on the command line. Turn off any weighting functions by clicking the *lb*, *sb*, and *gf* toolbar icons until all of the weighting functions say “unused”.



Set the sinebell function to be about double the width of the data in the FID to be kept.


Next click the sinebell shifted icon on the toolbar and shift the sinebell over so that it just covers the FID.




After a good adjustment is found, type *wft* in the command line. This performs a weighted Fourier transform and applies the weighting function. The spectrum may need to re-phased slightly after this.

**Zero-Filling**

Zero-filling is handled through the *fn* parameter. The Fourier number, *fn*, is normally set to 'n' or not used. In this case, the number of points (*np*) are the actual data points. To use zero-filling, setting the *fn* to a number larger than the *np* will zero-fill. This number is typically a power of 2. For example type *fn=16k* or *fn=32k* or *fn=np*2* on the command line and the computer will automatically adjust to the correct number. Re-transform (*wft*) the data after changing this parameter to see the result. Using a *fn* smaller than *np* will use fewer than the actual number acquired.

## Measuring Signal-to-noise

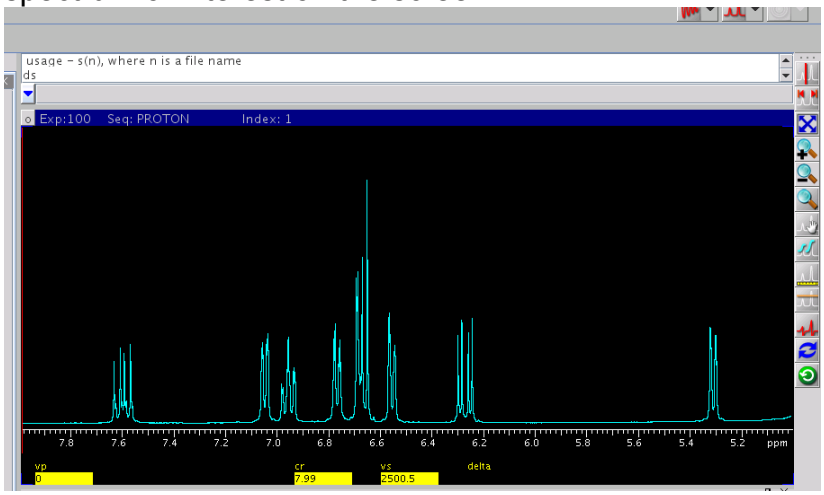
Measure the intensity of the largest peak in the spectrum. (Use the cursor to move onto the line and type *nl*.) Then move the cursor over and enclose an area of noise with two cursors. Type *dsnmax(200)* on the command line for a display of signal-to-noise. This command can be found in the Command and Parameter Guide. For this to be an accurate measure between spectra, use the same peak and the same window of noise each time.

## Finding Digital Resolution

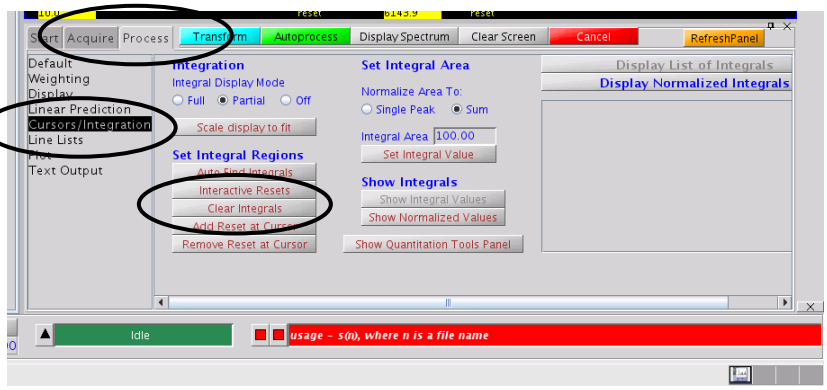
Place the cursor near the maximum of the peak to measure. Type *nl dres* on the command line for a display of the digital resolution (width at approx. half height).

## Integration

Display the spectrum of interest on the screen.

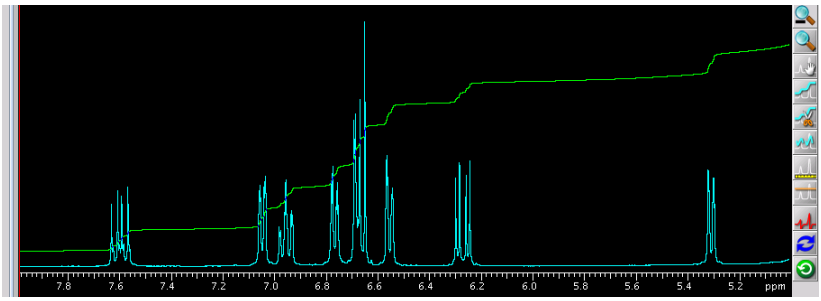



Clear any existing integrals by clicking Clear Integrals on the Cursors or "Integration Page" of the "Process Tab" or by typing *cz*.

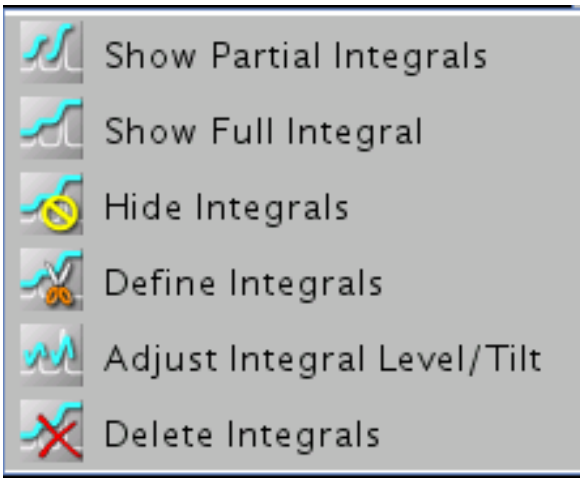



Click the integral icon on the tool bar to access the integration mode.

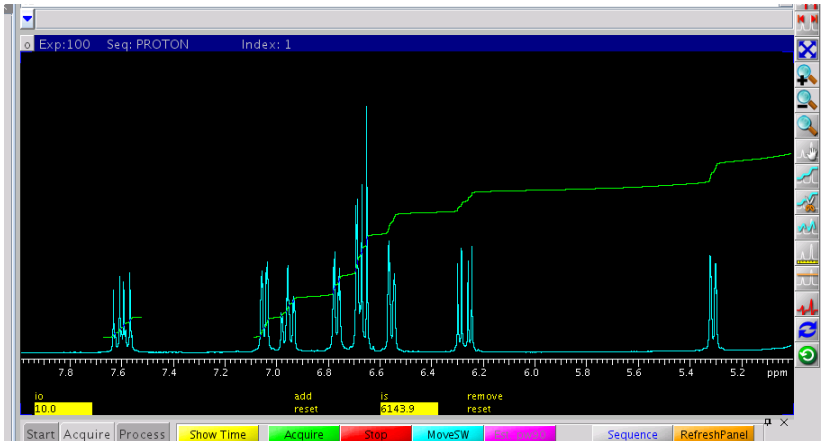
This will cause a green integration line to appear on the screen.



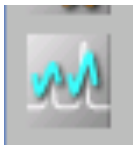

The different integration icons are shown below.



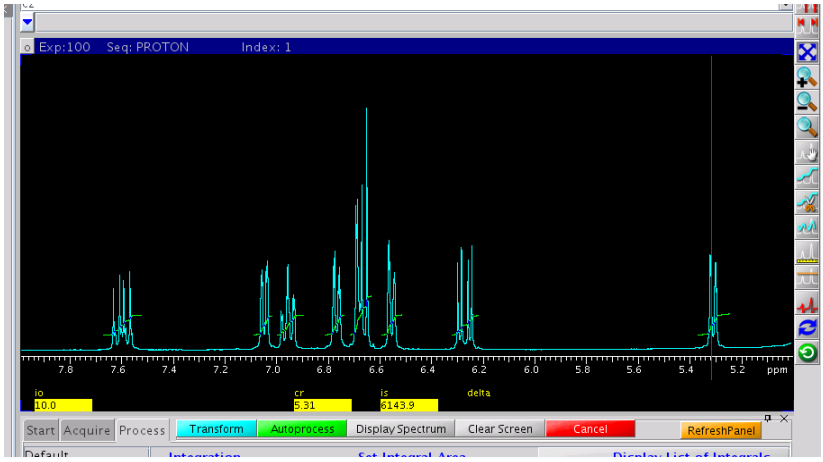

Click the define integrals icon on the toolbar, then click the left mouse button to cut the green line on either side of the peaks of interest. Clicking the right button will cause the cut to be erased.



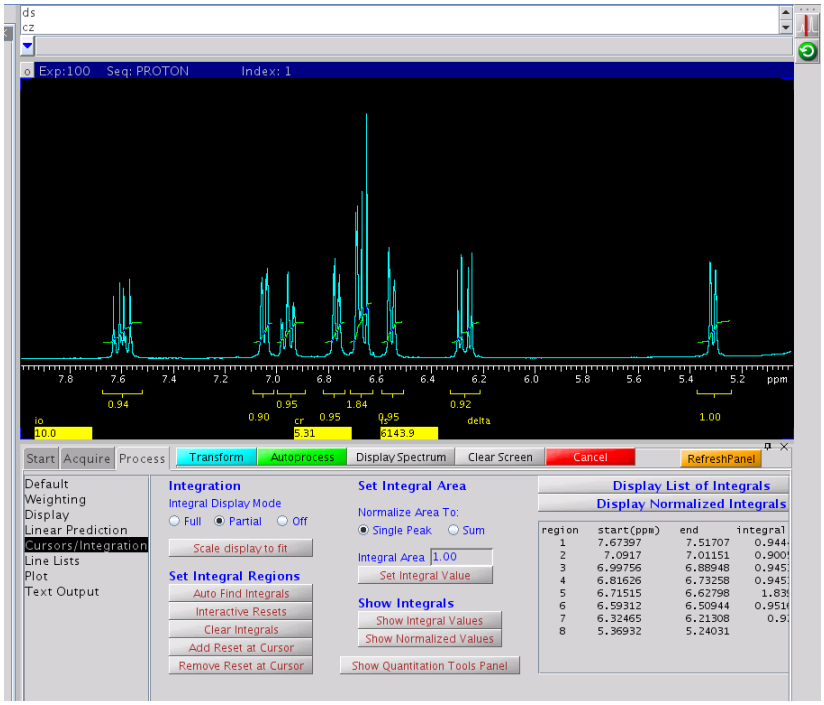

To correct leveling and tilt errors in the integral click the level/tilt integration icon



and adjust the integral similar to phasing the spectrum. To set the integral values, put the cursor on one of the peaks and type a numerical value into the Integral Area Box.

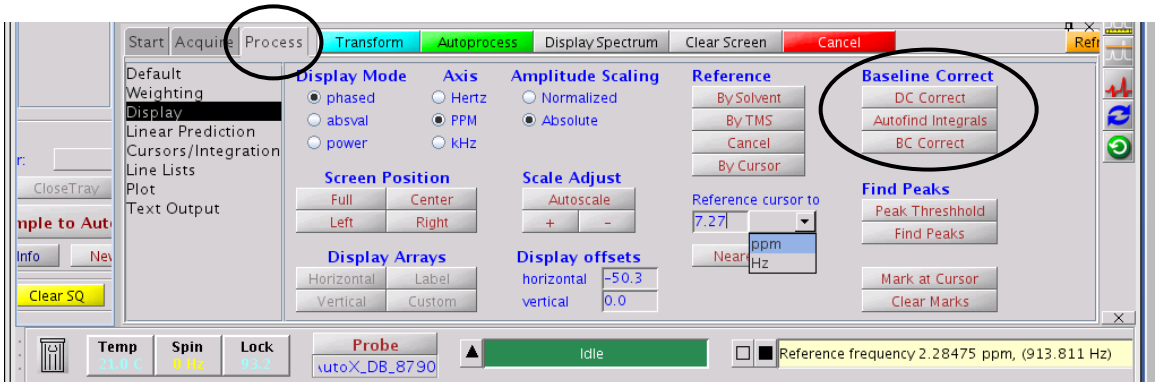



Click Set Integral Value and Show integral value to see the integral values on the screen.

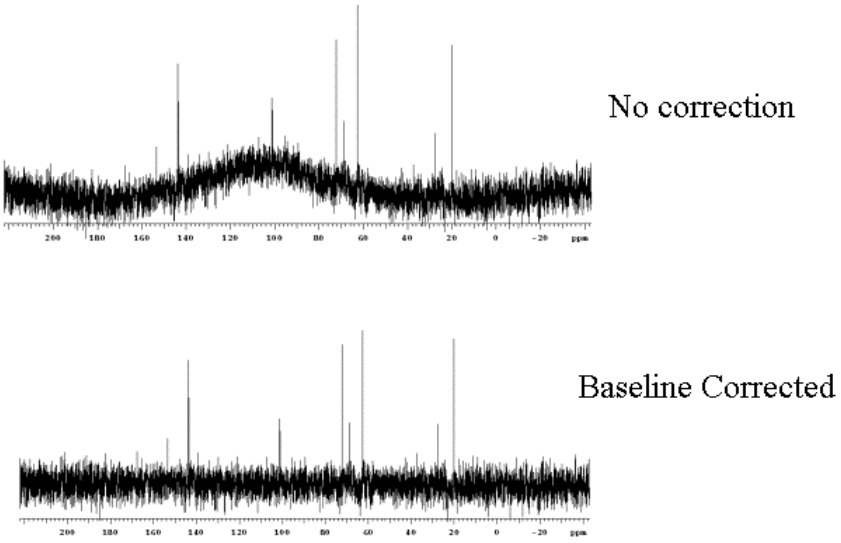


## Baseline Correction

After integral regions have been specified on a spectrum, the baseline can be corrected to reflect these regions as peaks. To baseline correct, type *bc* on the command line or click the BC Correct button found on the Display page of the Process Tab. This baseline correction assumes everything in a defined integral region is a peak and flattens the rest. To work properly, everything that is or might be a peak must be in an integral region. To massage this further, see the Varian parameter guide on *bc*. This command can have many modifiers to produce a better correction.

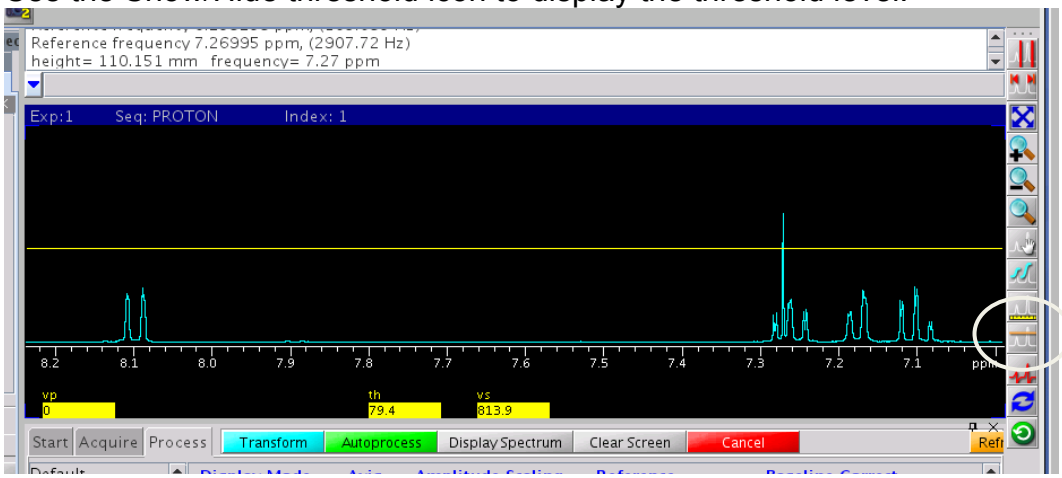



The spectrum below illustrates the use of the baseline correction in a $^{13}C$ 1D spectrum.

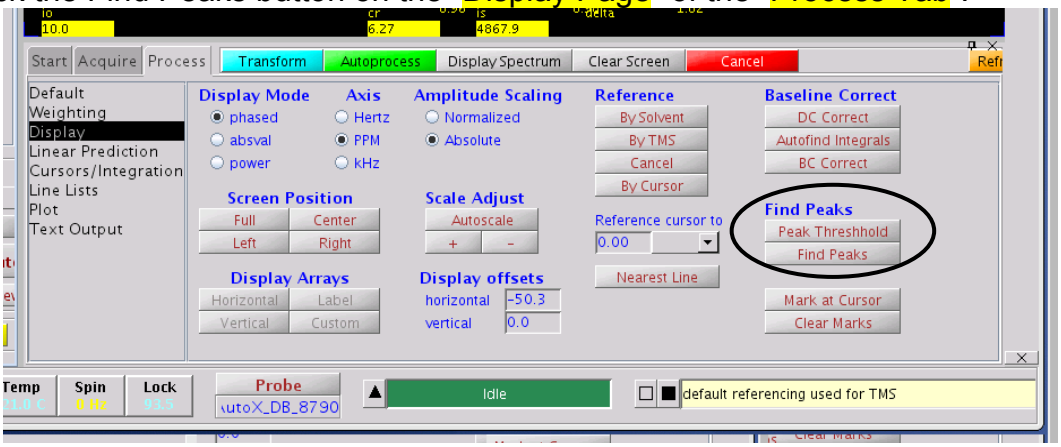


## Peak Picking

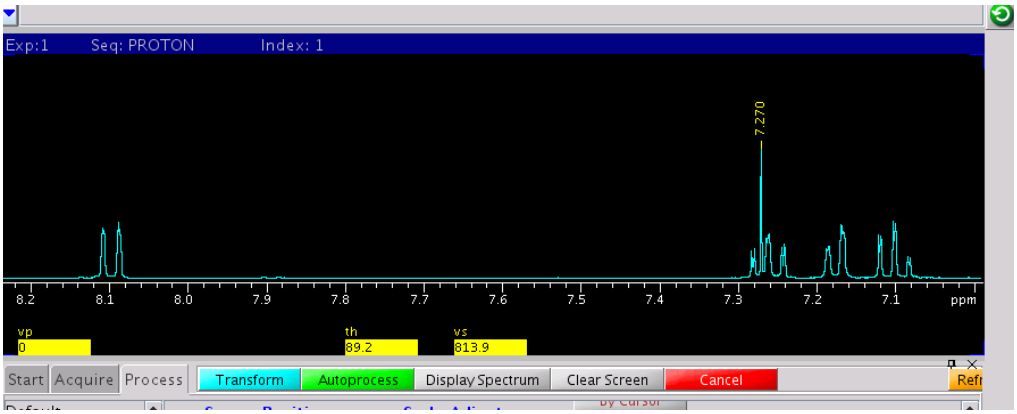
Use the Show/Hide threshold icon to display the threshold level.



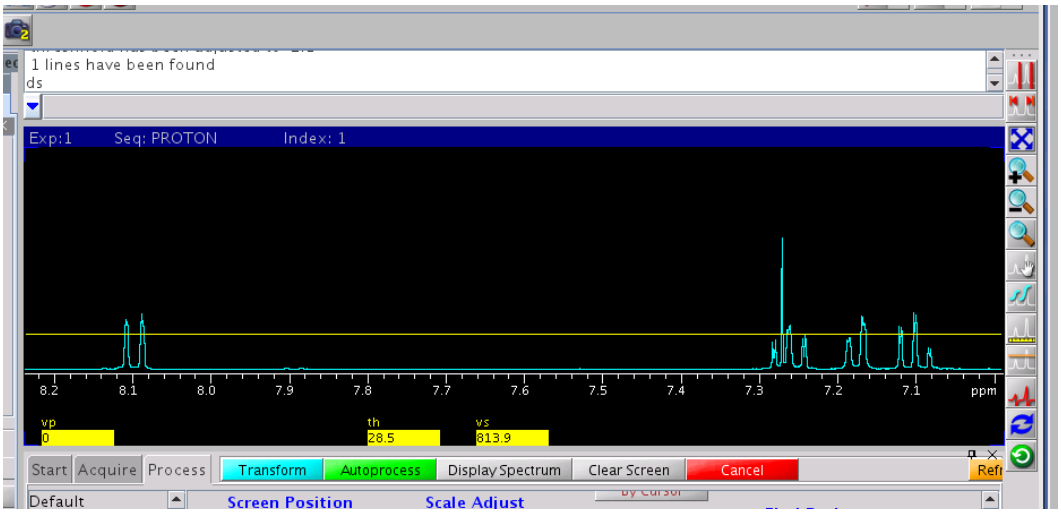

Click the Find Peaks button on the "Display Page" of the "Process Tab".




This will display the peak frequencies on all of the peaks, which cross the threshold.




Readjust the threshold by clicking the Show/Hide Threshold icon. Move the yellow line with the left mouse button.




Click the Find Peaks button to display the peak frequencies.


**Basic 1D Plotting**

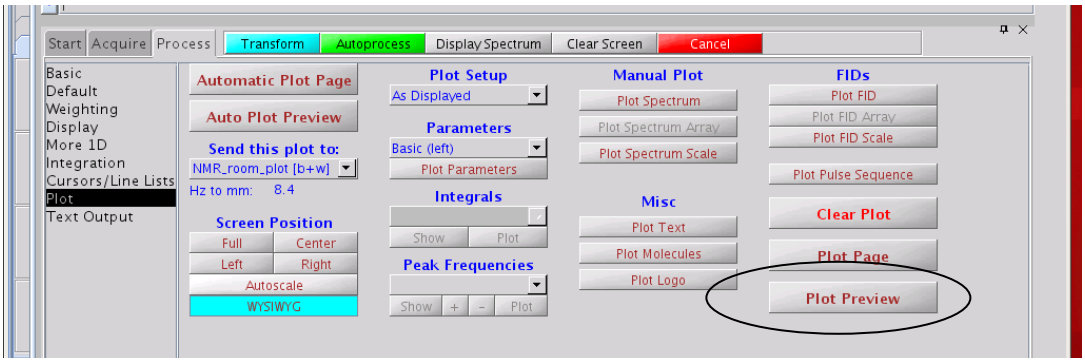
The simplest way to print is with a list of commands. These commands are listed below. The following commands should be typed in the vnmr command window to print the following options. They should be typed in a string separated by spaces ending with the command page. All commands are optional except for page. The spectrum will be plotted at a width of 250 mm, unless you specify different. You can change the width of the plot by typing wc=200. This will change it to 200 mm.

| | |
|---|---|
| pl | prints spectrum |
| pscale | prints scale |
| pap | prints all parameters (long list) |
| ppa | prints primary parameters (short list) |
| pir | prints integration ratios horizontally |
| piv | prints integration ratios vertically |
| ppf | prints peak frequencies |
| page | sends file to printer |

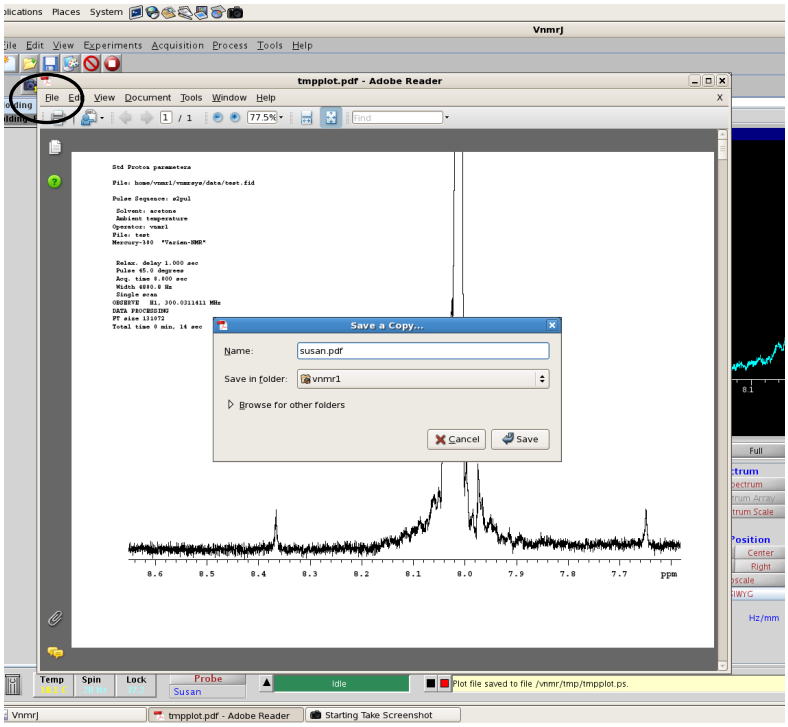
You may also use the buttons on the Process>Plot page. Simply click the options that you would like to print and then click Plot Page.

**Making a PDF Files**

To make a pdf file from your spectra, choose the features that you would like to print, then simply click Plot Preview instead of Plot Page.




Adobe Acrobat will open and show you your pdf file. Click File>Save As> to save the pdf file.




**Converting 1D Data to ascii Format**

Spectra can be plotted by excel or other programs if it is first converted to ascii format. To convert the FID, first process, phase and reference the data. Take note of the frequency at which it was collected. (Type sfrq? on the command line and write down the number). Type *writexy* on the command line. There will be no indication or message that anything was written, however, the file should have been created inside of the experiment directory. For example, if the vnmr1 group was working inside of exp1, then the output file named xytrace.1 would be found inside of /home/vnmr1/vnmrsys/exp1/ directory. The file will have two columns. The first column is frequency and the second column is intensity. After opening the file in excel, divide the first column by the sfrq value noted earlier to convert it into ppm. Plot data as desired.