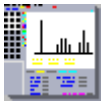
Instruction for 1D NMR data processing with VNMRJ2.2C

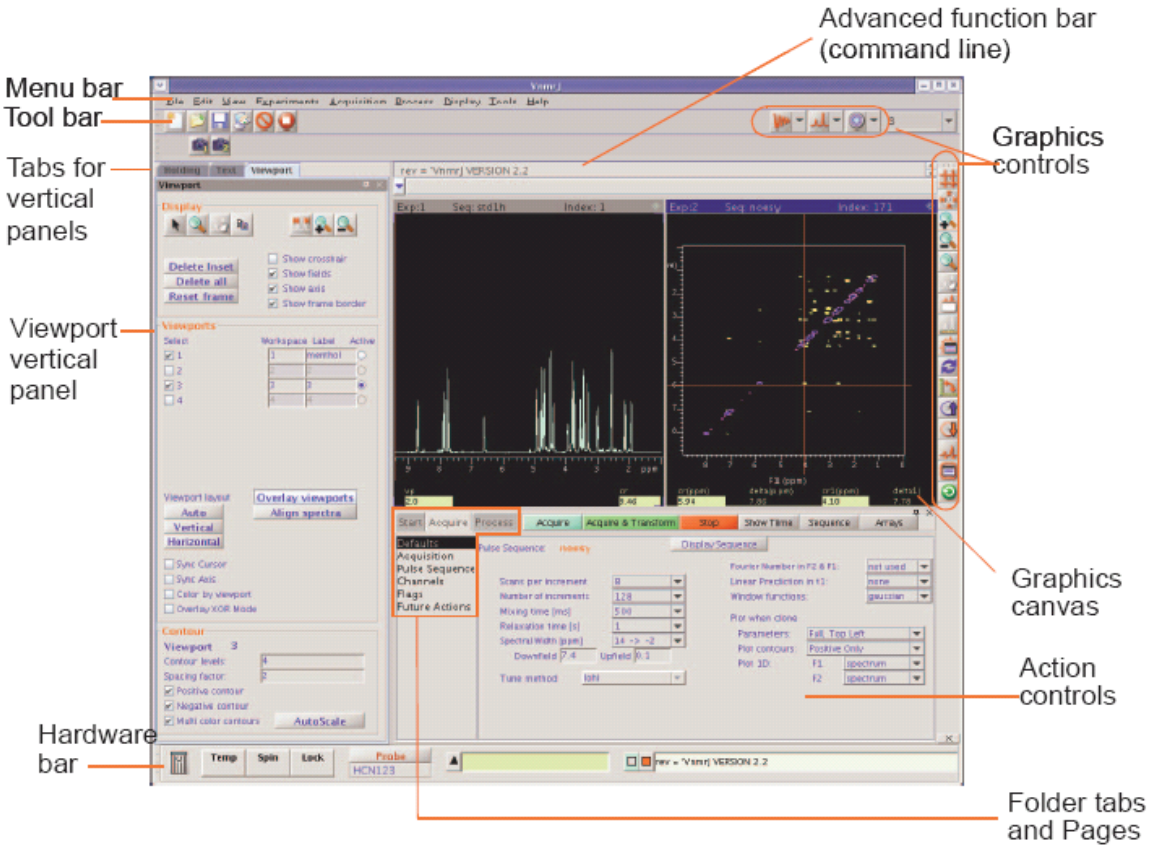
Login

Login to the Linux system by entering your username and password.

Starting vnmrj

Click vnmrj icon  to start vnmrj program.

The window below is what you will typically see. Get familiar with this window. Your files will be displayed in File Browser area.



VnmrJ Experimental Interface

Icon Description


Zoom in.


Zoom out.


Select zoom region.


Redraw display.


Return to previous tool menu.

Display Spectrum Toolbar Controls


One cursor in use, click to toggle to two cursors.


Two cursors in use, click to toggle to one cursor.


Click to expand to full spectral display.


Pan or move spectral region.


Display integral.


Display scale.


Toggle threshold on or off.


Phase spectrum.

Display FID Toolbar Control


One cursor in use, click to toggle to two cursor.


Two cursors in use, click to toggle to one cursor.


Click to expand to full fid display.


Pan and stretch.


Click to show real and imaginary.


Click to show real and zero imaginary.


Click to show real only.


Toggle scale on and off.


Phase fid.

These buttons function as follows:

Cursor or Box	
Box	Change to the box mode with two cursors.
Cursor	Change to the cursor mode with one cursor.
Expand or full display	
Expand	Expand the area between the cursors.
Full	Display the full area.
Set integrals	The first click displays the intregal function buttons. The second click displays the No Integral and Clear Resets buttons.
Full integral	Display all integral regions.
Integral resets	Open an interactive integral reset mode. The left mouse button defines an integral reset at the current mouse position. The right mouse button removes an integral reset closest to the current mouse position. The middle mouse button adjusts the scale. The integral does not have to be displayed. However, if the integral is displayed in the "partial" mode, the normally blanked regions are displayed as dotted lines. To clear the integral reset points before beginning, click the Clear Resets button.
Integral Lvl/Tlt	Open interactive zero- and first-order baseline correction mode, see See "Interactive Zero- and First-Order Baseline Correction Mode".
Scale	Display a time scale under the spectrum in units specified on the Display page.
Grab and Move	Opens the interactive spectral windowing mode. Use the left mouse button to adjust the starting time of the display and move the display left or right. Use the right mouse button to adjust the width of the display.
Threshold	Toggles the display of a horizontal cursor. The left mouse button positions this cursor at the mouse arrow position. The middle mouse button adjusts the scale.
Phase	Opens the interactive phasing mode. Use the left mouse button for course adjustments (180°) and right button for fine adjustments (20°), where full scale corresponds to 180°. See "Spectrum Phasing". Use the middle button to adjust the vertical scale of the display and to apply the latest phase correction to the entire spectrum.
Refresh	Open an interactive integral reset mode, see below.
Return	Returns to the last menu.

Create workplace (known as exp#)

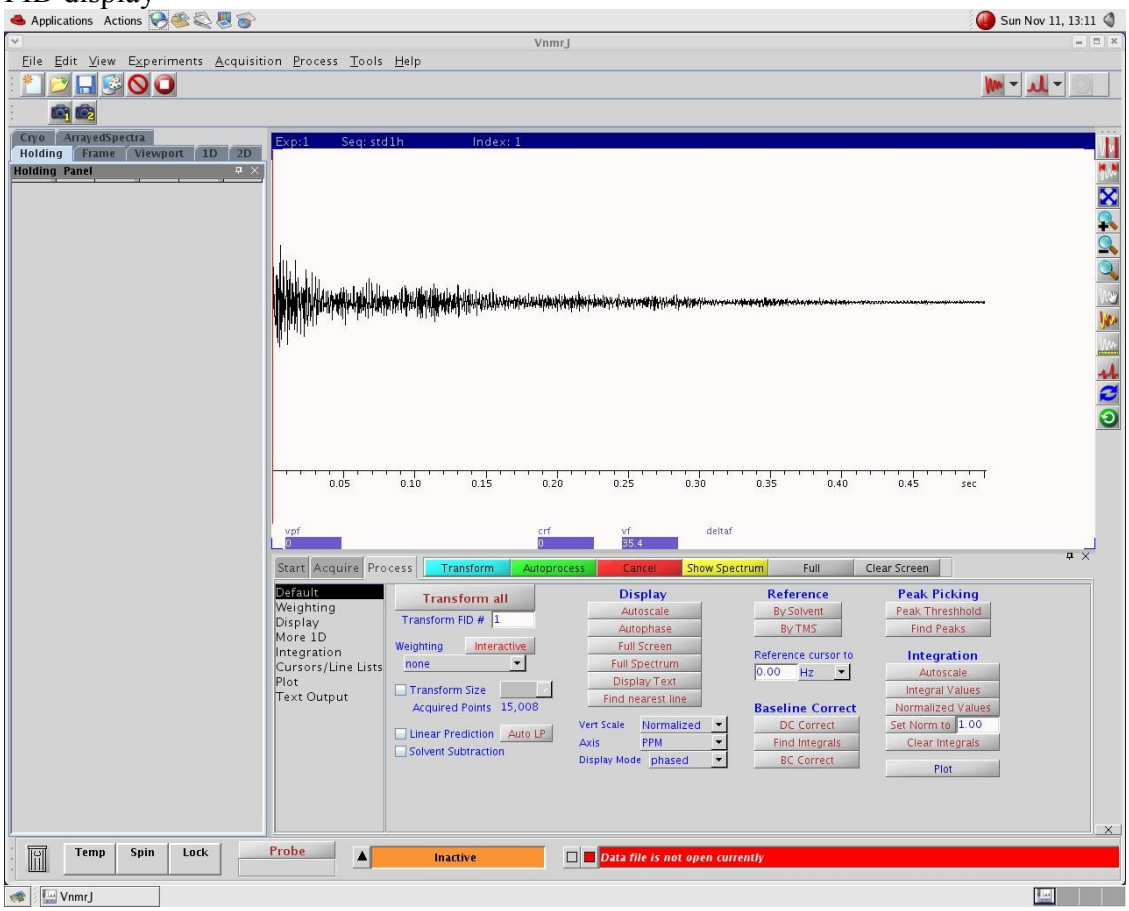
Click Files → New Workplace, each time you click New Workplace, a new exp# is created, # is a number from 0 to 99. Different jobs can be performed in different exp#. For example, You may use exp1 to acquire 1H NMR and use exp2 to setup 13C nmr experiment and use exp3 to setup a 2D NMR experiment or process the data.

Input nmr data to the graphics canvas

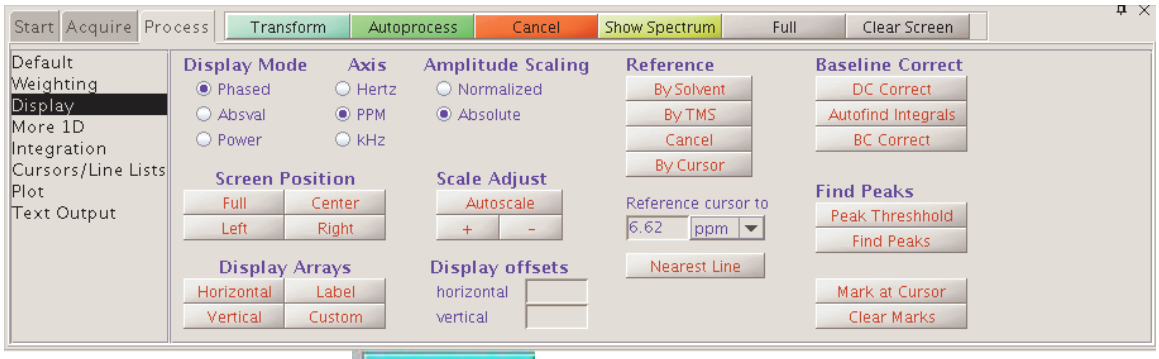
Click File → Open , your data folder is opened, double click the data file to open (you may use mouse to drag the file to the canvas). For practice, open a proton file **proton-test.**

The NMR spectrum may appear with automatic transform. You may click  to see the FID.

FID display



Process penal

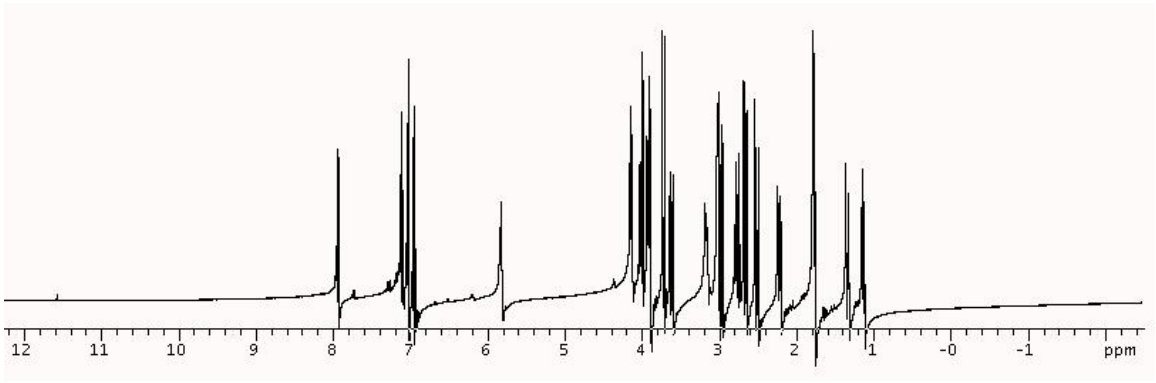


Click Fourier transfer icon 

at the bottom of the graphics canvas or click  , the NMR spectrum is displayed and graphics control bar changes. If you do not see this button, click **Process** tab to display FT button. The central button adjusts the intensity of the spectrum

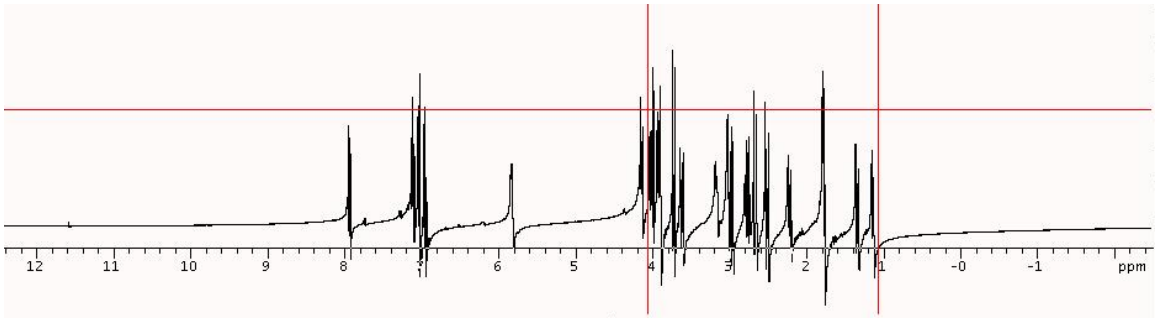
The phase of the spectrum may be good, may be not. If not (like the spectrum bellow), then phase correction is needed. If it is good, but for practice, follow the following steps to get familiar with the procedures.

NMR spectrum

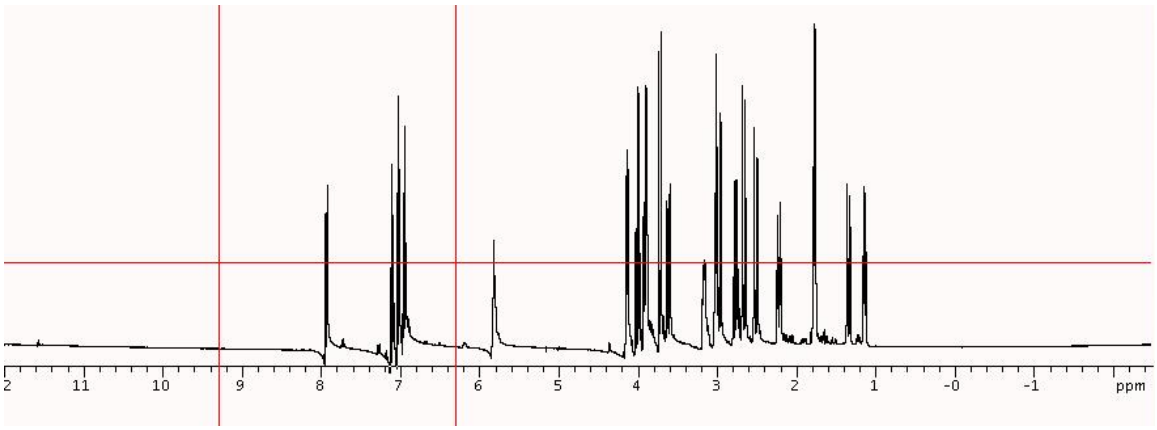


Phase correction

The spectrum above is out of phase, click phase correction button  , move mouse to the right portion of the spectrum as below

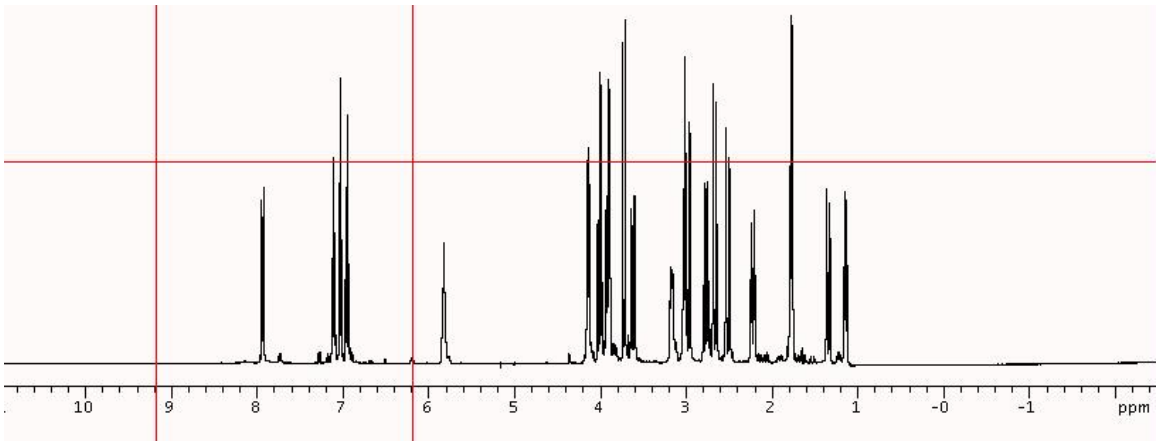


Press the left button and hold, move the mouse up/down, the spectrum changes with the mouse until the phase of this portion is right, shown below, but the phase of the right portion is still not correct.



Release the left button, move the mouse to the right portion of the spectrum shown above,

Press the right button and hold, move the mouse up/down, the spectrum changes with the mouse until the phase is correct shown as below, release the mouse.



Baseline correction

Click the **Display** in the left menu under the Process Tab. Then click **DC correction** and **BC correction** for base line correction.

Add text

In command line, type **text('your text is here')**.

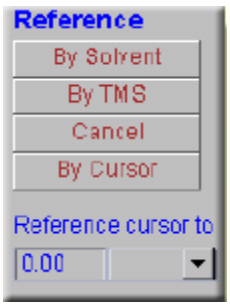
Reference

Click the cursor button  , making sure there is only one curser on the spectrum, move the cursor to the peak to be referenced, then you may do one of the followings,

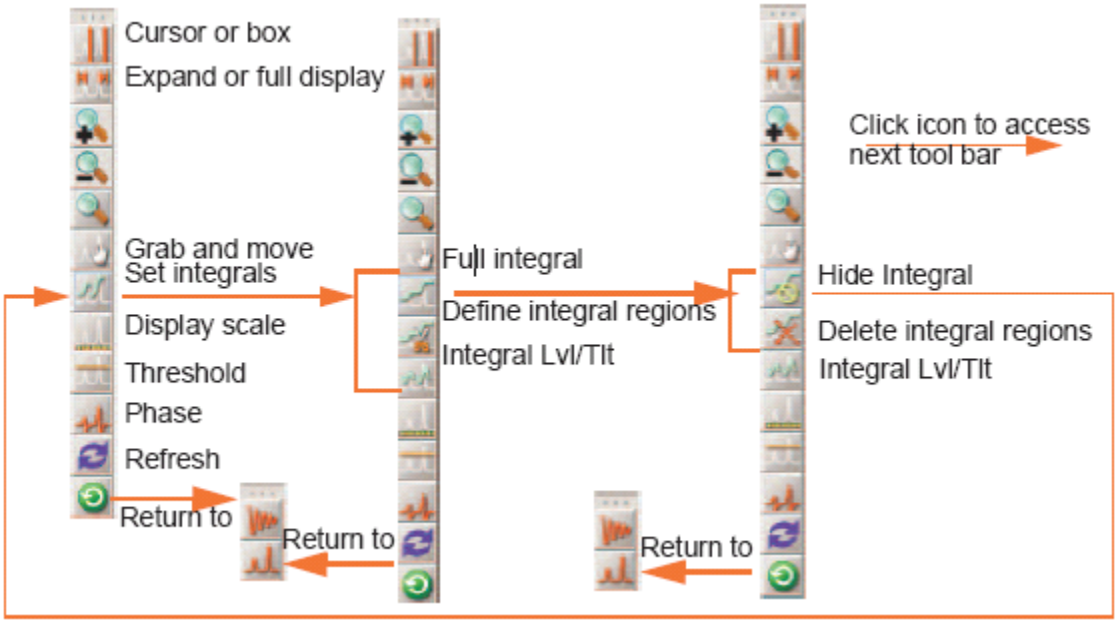
1. At the command line, type **nl rl(xxx.xxp),** here the "nl" means going to the nearest line, "rl" means the reference line, and "xxx.xxp" is the chemical shift value in unit of ppm (p means ppm).

or

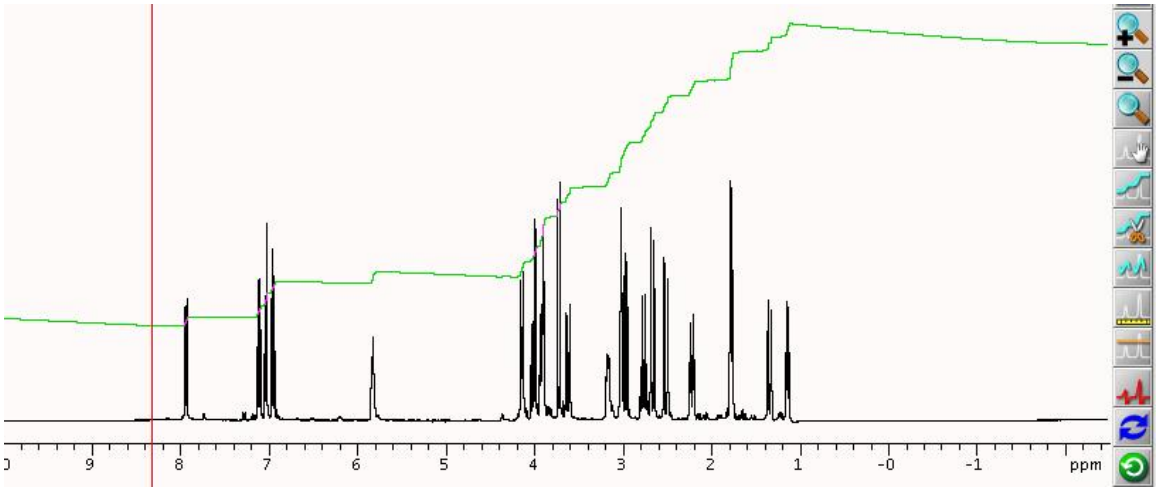
2. At the process panel, click button "Find Nearest Line", type in the chemical shift value in the box "Reference cursor to"., and click the down arrow to specify ppm or Hz, and hit enter.



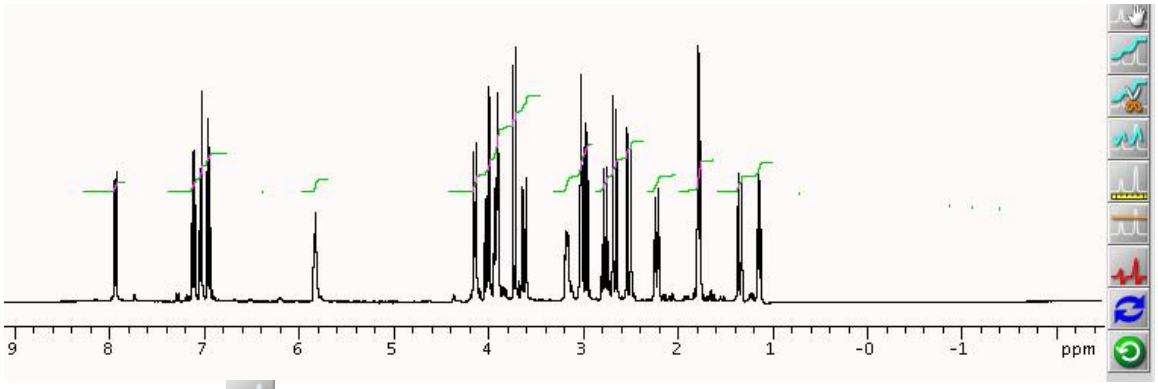
Integration (for Proton spectrum only)



Click the integration button, three integration buttons , and appear and a green integration line appears on the spectrum. You can also click Integration on the left menu under the Process tab to access more integration buttons. Under this menu, click the "clear integrals" button or type CZ. The line would be completely solid.



Click the Define Integral Regions button, and the line should be completely solid. Move the mouse to the left side of the peak, click left button, the left side of the integration line at the clicking point will turn to dash line. Move the mouse to the right side of the peak and click the left button, the section of the integration line in between the two clicks remains solid, but the other sections of the line become dash lines. Move the mouse to the left side of another peak, and click the left button, then move the mouse to the right side of the peak, click the left button, repeat this for all remaining peaks. If you make a mistake in clicking reset point, you have to start over by typing **cz** in the command line or clicking **Clear Integrals**.



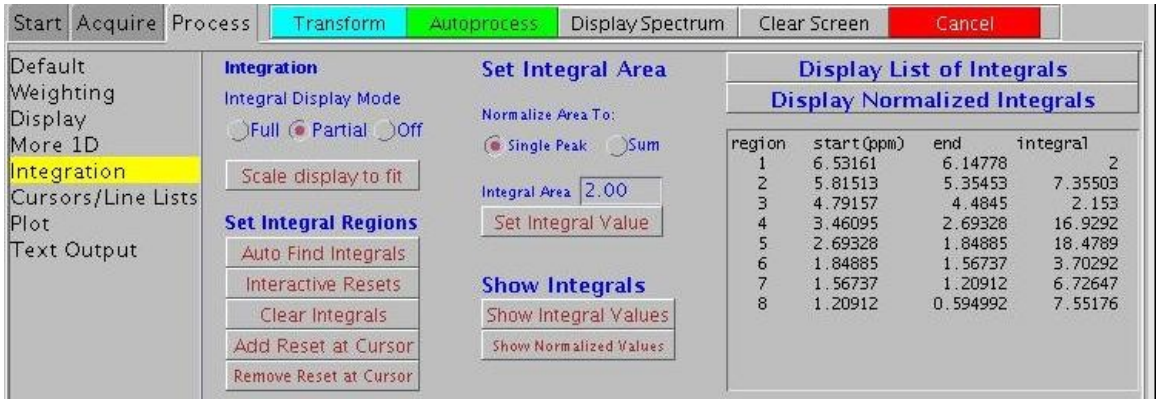
Click the button to activate integration baseline correction (Lvl/Tlt), and move mouse to the integrals and press the left button and move to do Lvl/Tlt.

Process penal

Assign integration value to an integral

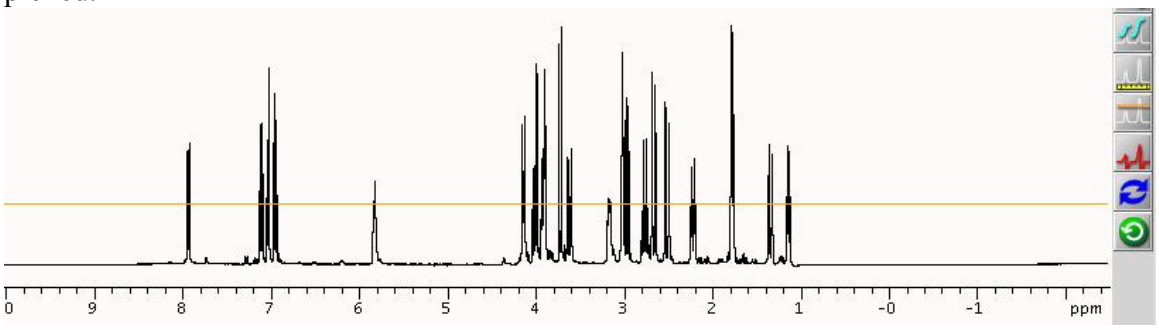
You may assign a specific value to the integral of a peak. Move the single cursor into a integral section, and click **Integration** at the left side of process tab. Under the **Set Integral Area,** click **Single Peak (** or you may click **Sum)**, type in the integral value you

want it to be, then click **Set Integral Value**. All integrals will be adjusted according to this new value and displayed at the right side of the panel. You may have to click **Display Normalized Integrals** to refresh the list.

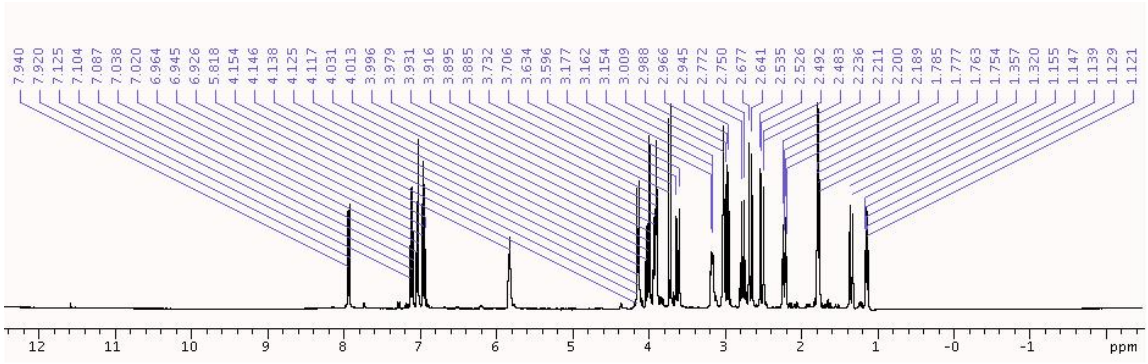


Peak picking

Click the threshold icon,  a yellow line appears on the spectrum, move the mouse to the yellow line and press the left button, hold and move the mouse, the yellow line will move with the mouse, release the mouse when the line is at the position you want. Any peaks below the line will not be picked and peaks above the line will be picked.



To show the peak picking on the top the of peaks, click **Find Peaks** under the **Process** Tab and **Display** menu. The chemical shift value will be displayed on the top of each peak which is above the threshold.



Plot

Click **Plot** at the left side of process tab, then click buttons for plotting what you want. Note: if you want to plot integral, click the **Plot Integrals**, when the red message "pir requires minimum vp of 12" at the bottom, go to command line, type "vp=12", then click **Plot Integrals** button again. The peak picking will be automatically printed on the When you are done, click **Manual Plot** to send all plot requests to the plotter. If this button is not clicked, nothing will print out. *If you want to make inset, do not click* **Manual Plot** until you finish the inset (see below). Before you do the inset, you have to type **ppf** at the command line in order to print the peak frequencies on the top of the peaks. If no spectrum is plotted and you see a message "**no plotter on system or plotter undefined**" at the right bottom, this means that the plotter is not activated. Click Files → Printers → select printer and plotter.

Or type the plotting commands at the command line:

pl	print spectrum
pir	print integrals
pscale	print scale
pltext	print text
pap	print acquisition parameters
pll	print peak locations (ppm and Hz) and peak height
ppf	print peak frequencies above each peak
page	eject page from printer (actually print on the paper).
vp=xx	(xx is the digital number to adjust the vertical position of the spectrum)

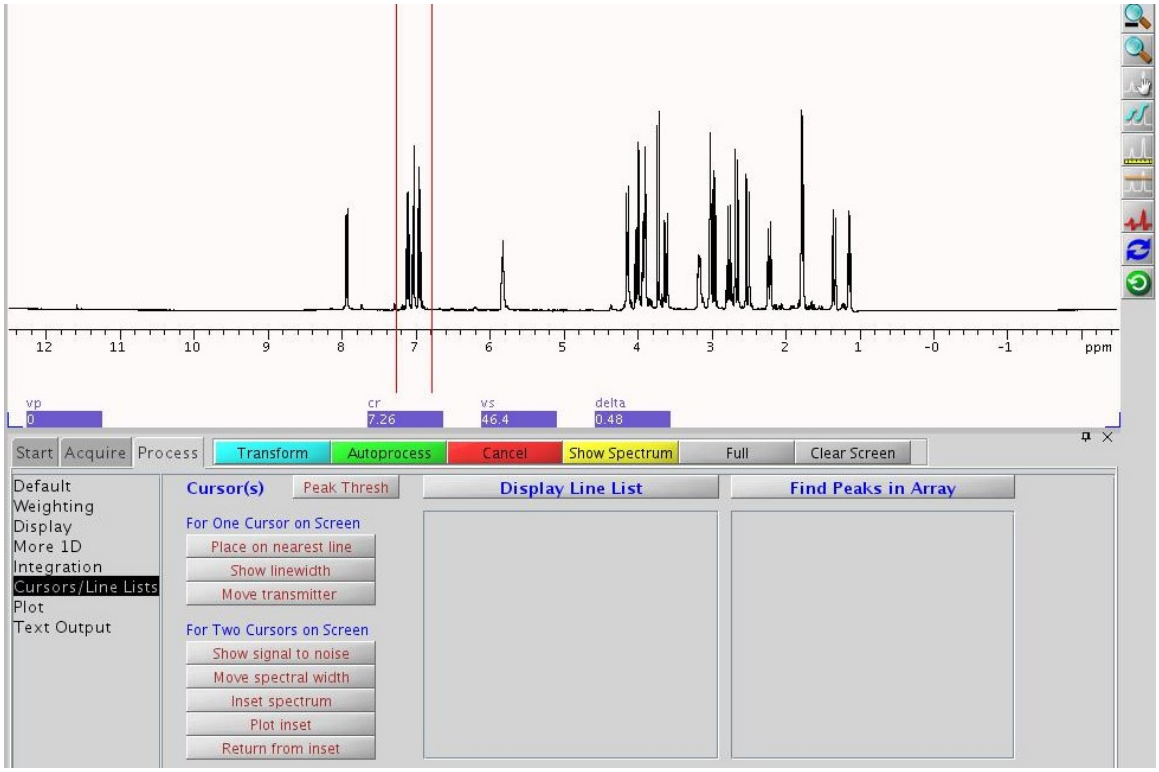
*** For plotting the peak picking, the position of the peak picking plotting can be adjusted by following at the command line:

pl pscale pir vp=vp+80 ppf('pos','top') vp=vp-80 page

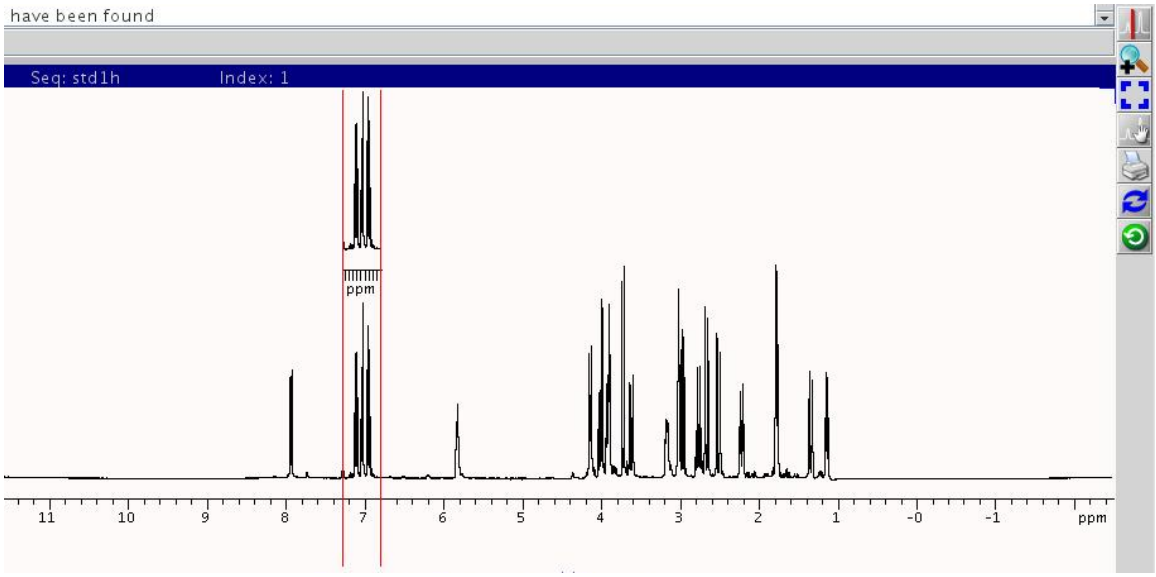
(the number 80 can be adjusted according to what you want)

Create an inset

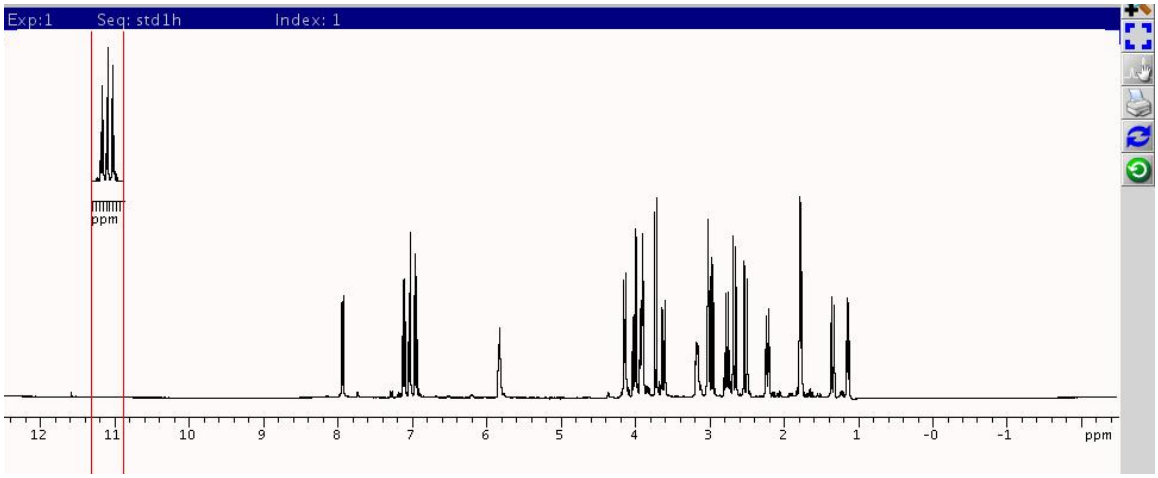
Put two cursors on the two sides of the section of the spectrum to be insetted,



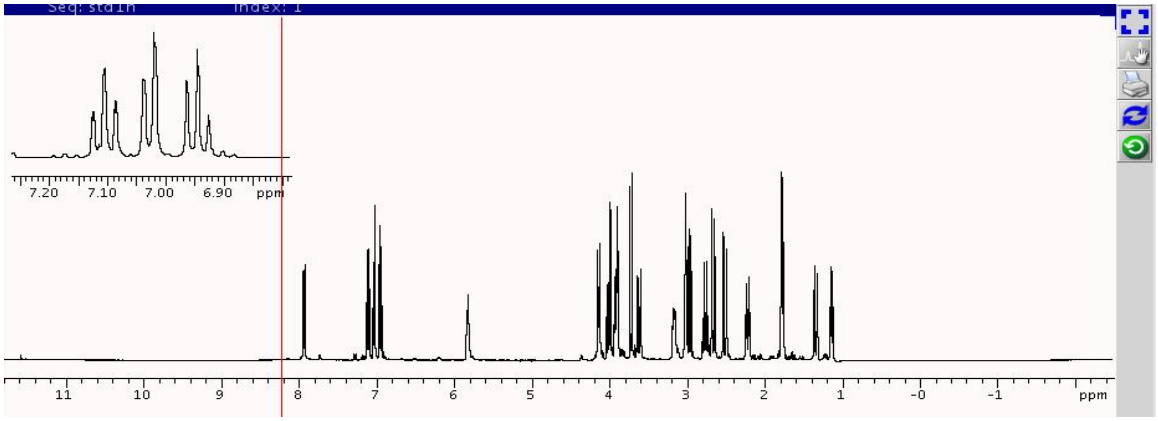
Click the **Cursors/Line Lists** at the left side of **Process** panel, click **Inset spectrum**, the inset is placed above the original spectrum and graphics control also changes.



Click the inset shift position icon  and use mouse to move the inset to the desired position. .



press the right button, then move the mouse to right side (or left side) to expand/ shrink the inset.



You may adjust its vertical position by typing vp=xxx, here xxx is a number from 0 to 100.

Plot inset

Click inset plot button  or click **Plot Inset Spectrum** to plot the inset. Click **Plot,** click **"Manual Plot"** to print the spectrum with the inset.

To save the spectrum into an image file:

Click File →Create a Plot Design, then follow the JDesign instruction.

Logout Click **Actions** at Linux bar (either at top or bottom), click **logout**.