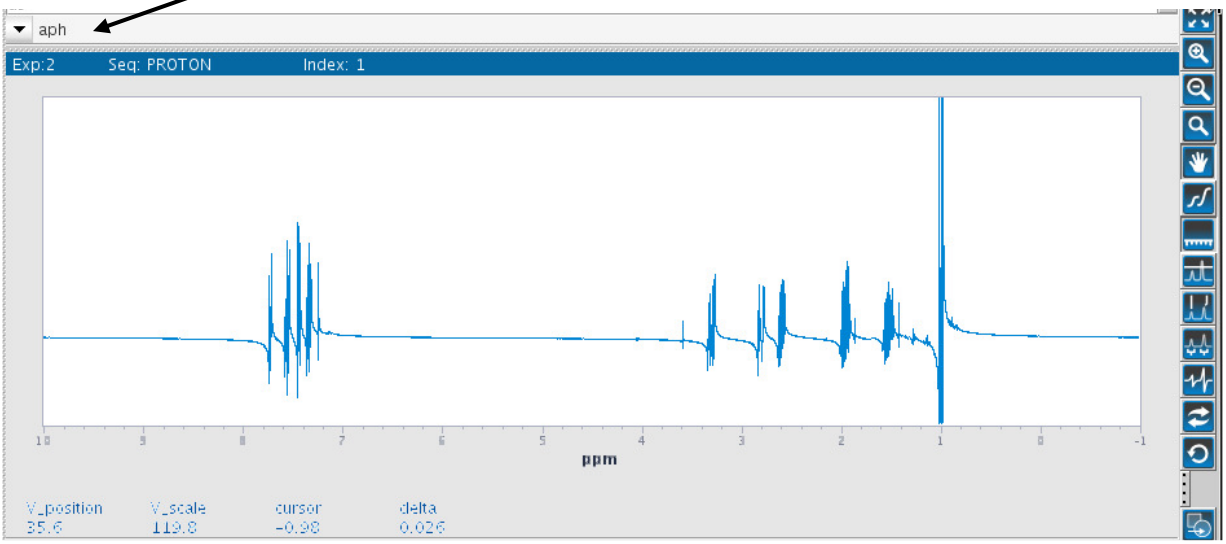
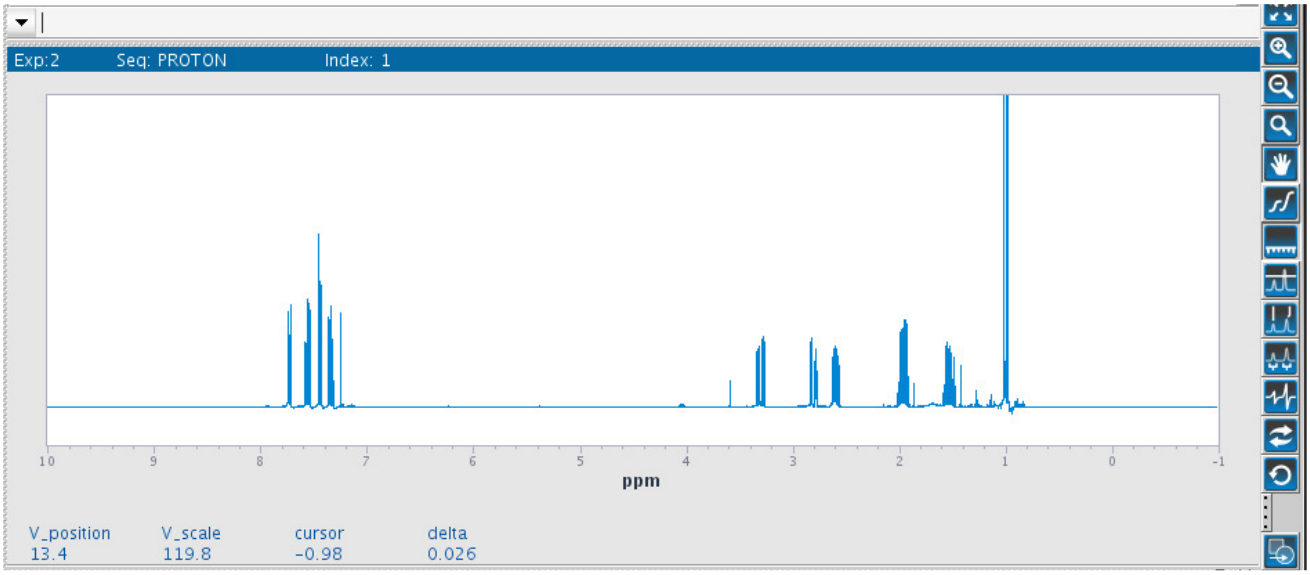
Phasing

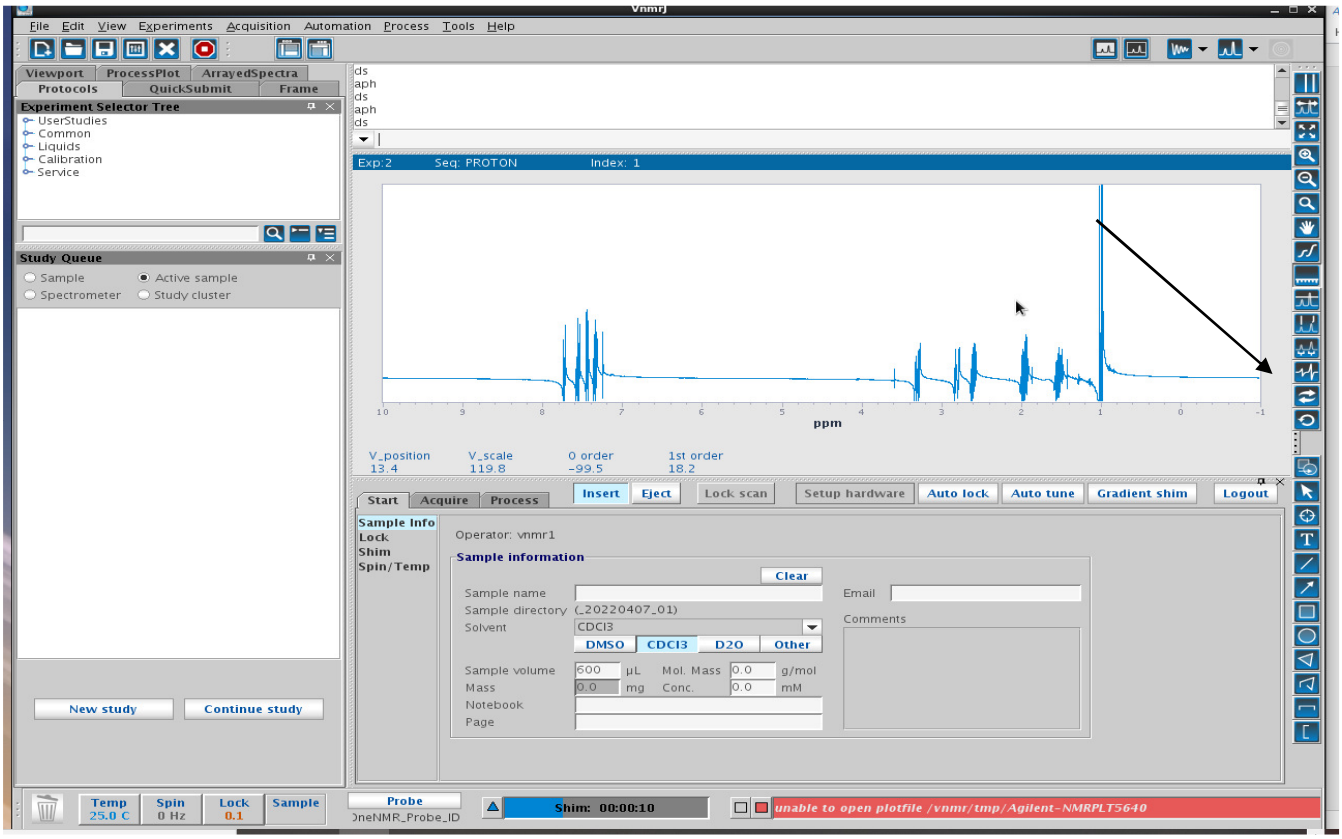
In the input window of VNMRJ type **aph** and hit Enter button to auto-phase the spectrum.



After (auto phasing):



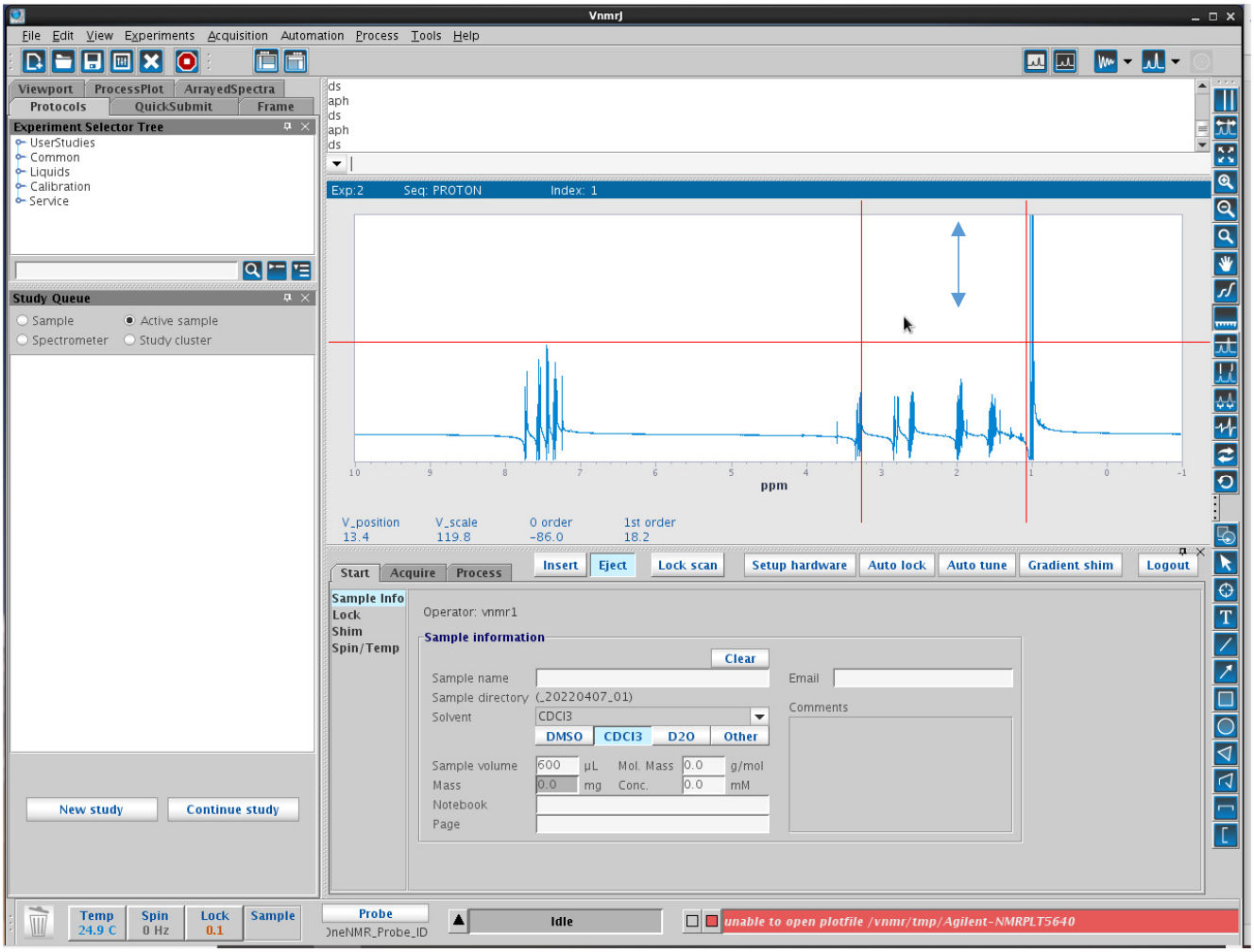
If auto-phasing does not work properly, then manual phasing must be performed. Click the **Phase** icon (location: right side of icons panel)



Adjust the phase of the peaks between the cursors by clicking and dragging up or down with the left (coarse) or right (fine) mouse button until the peaks look properly phased and the baseline is flat (see below shown Picture). If the cursor goes off the graphics window without the peak being properly phased, click on the **Phase** icon again and start over. This part of the phasing process where you phase peaks on the right side of the spectrum changes the value of the VNMRJ parameter **rp**. This is a constant (zero-order) phase correction that is applied across the entire spectrum.

Once the peaks on the right side of the spectrum are properly phased, click with the left or right mouse button on apeak near the left edge of the spectrum, and drag up or down to phase these peaks properly. This part of the phasing process where you phase peaks on the left side of the spectrum changes the value of the VNMRJ parameter **lp**. This is linear (first-order) phase correction that is zero at the place where you did the zero-order phase correction and is linearly increasing across the spectrum. Usually the magnitude of **lp** should be less than 360. If it is larger, the baseline of the spectrum may not be flat, and/or it may be impossible to phase all peaks in the spectrum at the same time. If this occurs, it may be useful to type **lp=0**, and start over with the phasing process.

If the values of **lp** and **rp** get very large (> 500), you may want to set **lp=0** and **rp=0** and start over.

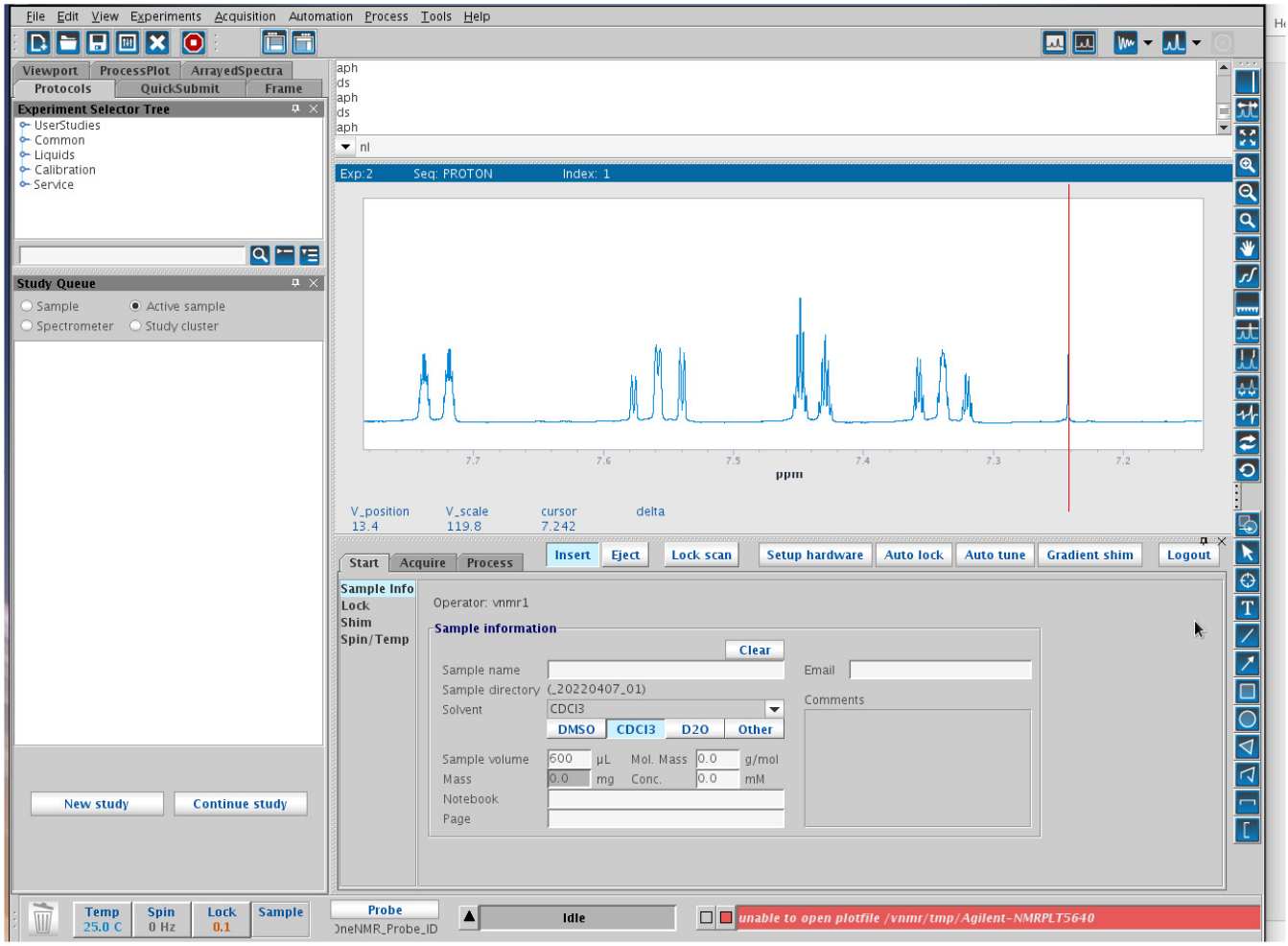

VnmrJ
File Edit View Experiments Acquisition Automation Process Tools Help
Viewport ProcessPlot ArrayedSpectra
Protocols QuickSubmit Frame
Experiment Selector Tree
UserStudies
Common
Liquids
Calibration
Service
Study Queue
Sample Active sample
Spectrometer Study cluster
New study
Continue study
ds
aph
ds
aph
ds
Exp:2 Seq: PROTON Index: 1
ppm
V_position V_scale 0 order 1st order
13.4 119.8 -86.0 18.2
Start Acquire Process
Insert Eject Lock scan Setup hardware Auto lock Auto tune Gradient shim Logout
Sample Info
Lock
Shim
Spin/Temp
Operator: vnmr1
Sample information
Clear
Sample name
Email
Sample directory (_20220407_01)
Solvent CDCl3
DMSO CDCl3 D2O Other
Comments
Sample volume 600 µL Mol. Mass 0.0 g/mol
Mass 0.0 mg Conc. 0.0 mM
Notebook
Page
Temp 24.9 C
Spin 0 Hz
Lock 0.1
Sample
Probe
Idle
unable to open plotfile /vnmr/tmp/Agilent-NMRPLT5640

Referencing and scaling in ppm or Hz

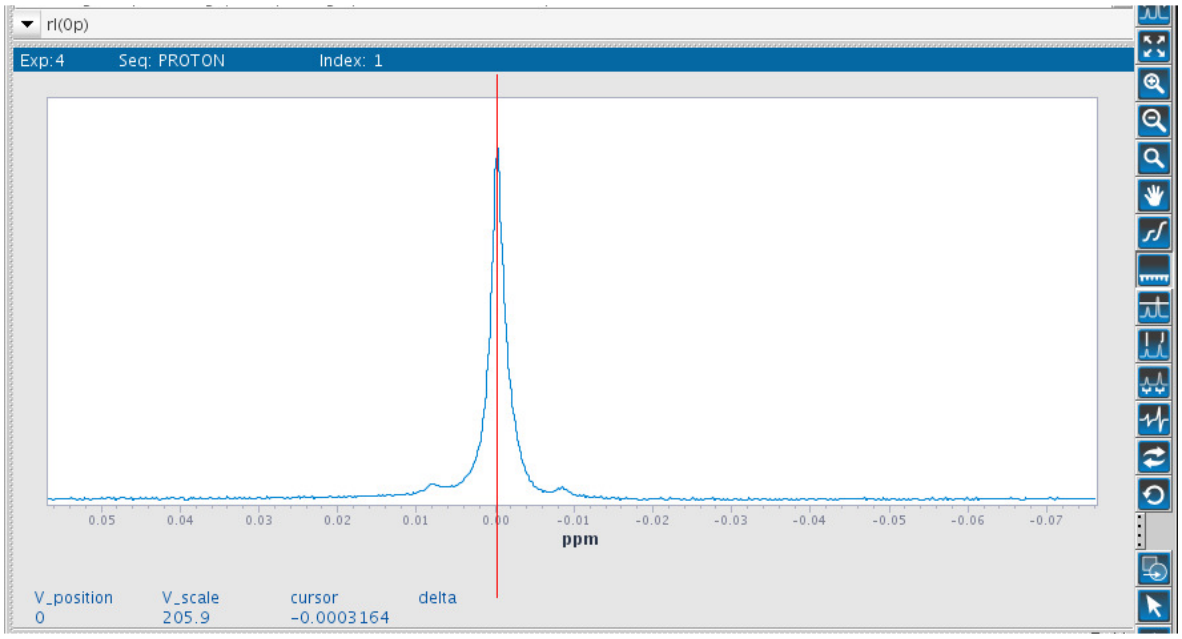
The axis for the spectrum can be displayed by typing **dscale** or by clicking on the **Icons panel**. To display the scale in hertz, type **axis='h'** before the **dscale** command. To set the scale back to ppm, type **axis='p'**. If you selected the proper solvent when setting up a proton or carbon experiment, the axis should be very close to correct, however, if you want to make sure it is exactly correct, you should re-reference the spectrum using a reference line likeTMS (0 ppm) or the solvent line (since a small portion of solvent molecules are protonated, you will usually see a solvent line in proton or carbon spectra).

To reference the spectrum, expand the appropriate spectral region to display the reference line you want to use.

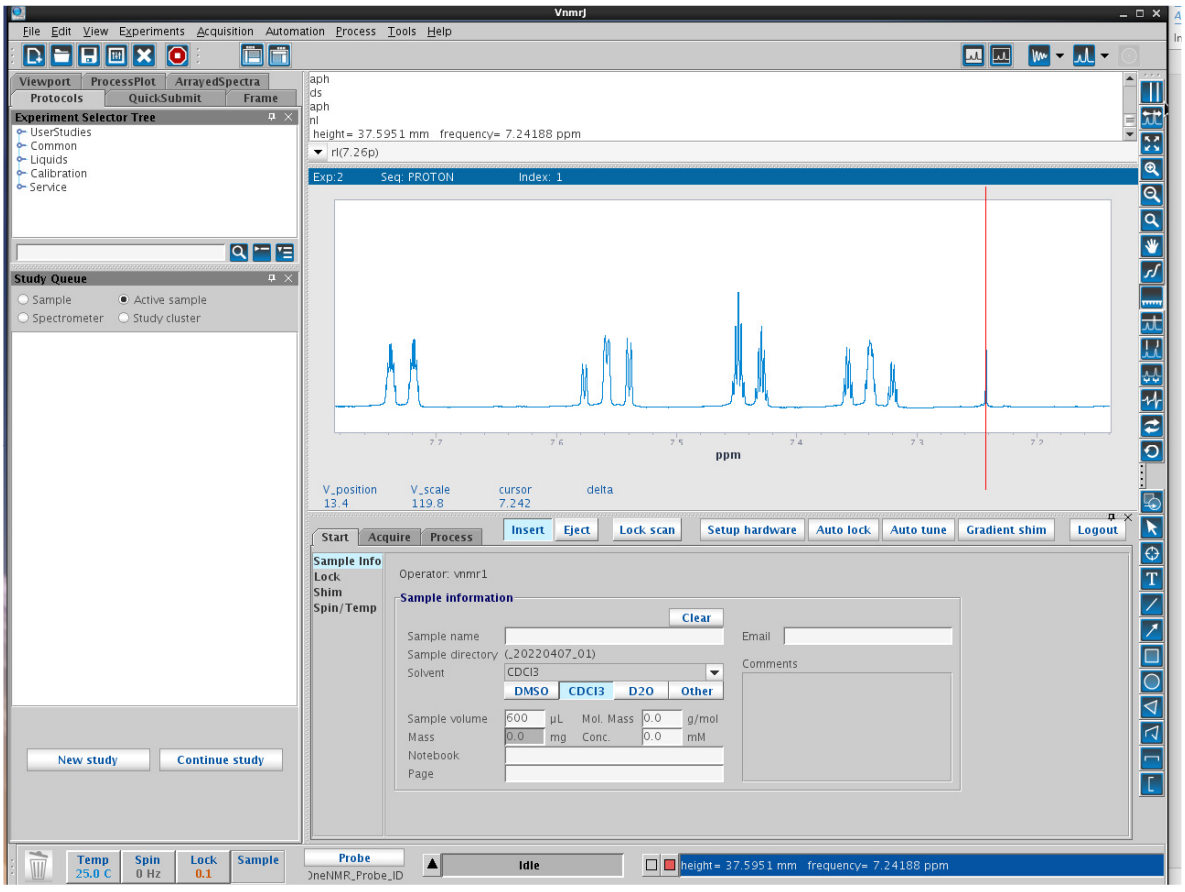
Click on the reference line with the left mouse button to move the cursor to that line and type **nl** which brings the cursor to the nearest line.



Type **rl(0p)** (for TMS) and hit Enter button



or type **rl(7.26p)** (for chloroform) and hit Enter button



Peak Picking

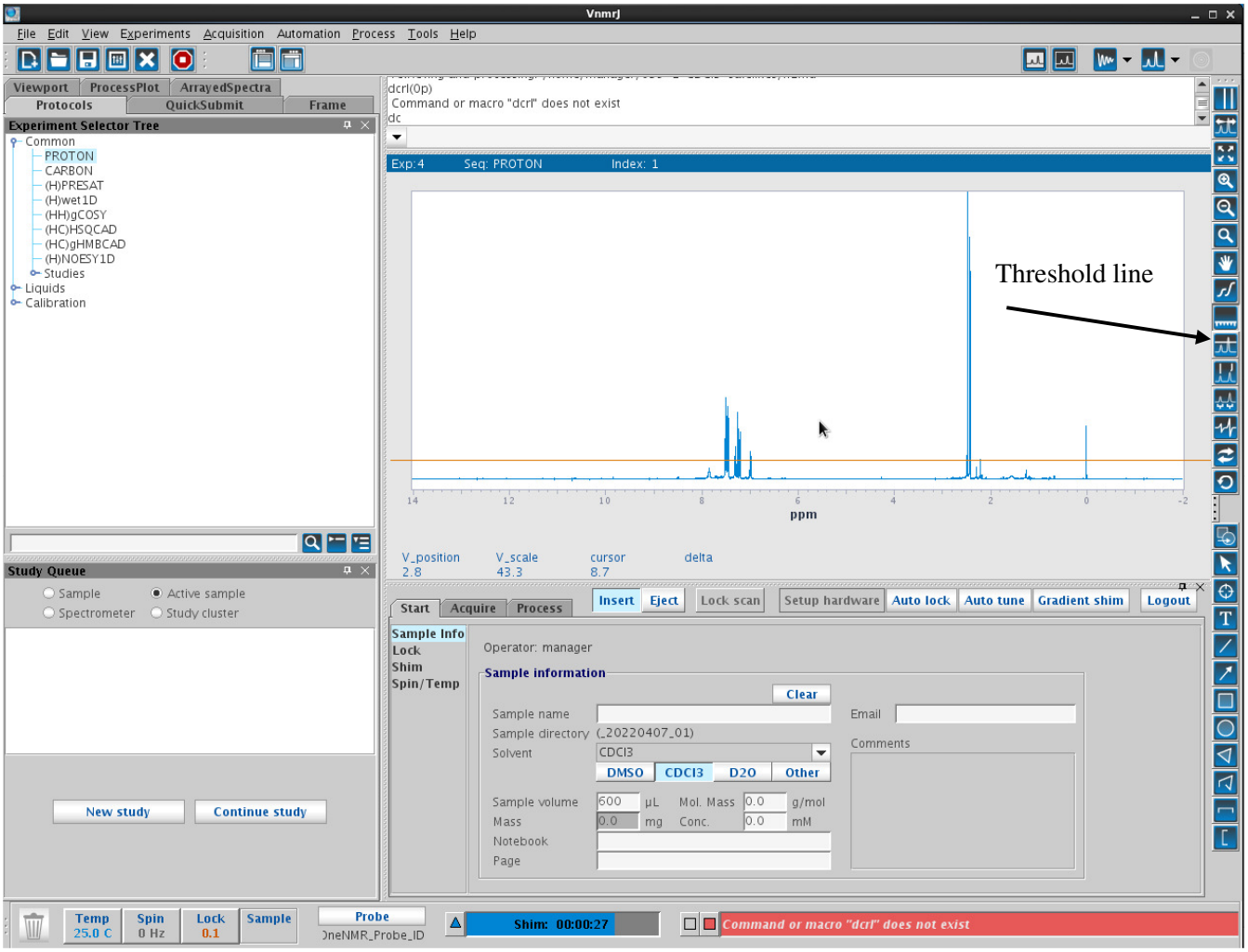
The frequencies of the peaks in the spectrum are typically the most useful information obtained from the spectrum.

To adjust the threshold (horizontal line) for peak picking, click the **threshold icon (Icon panel-**right side of VNMRJ window) in the interactive display mode.

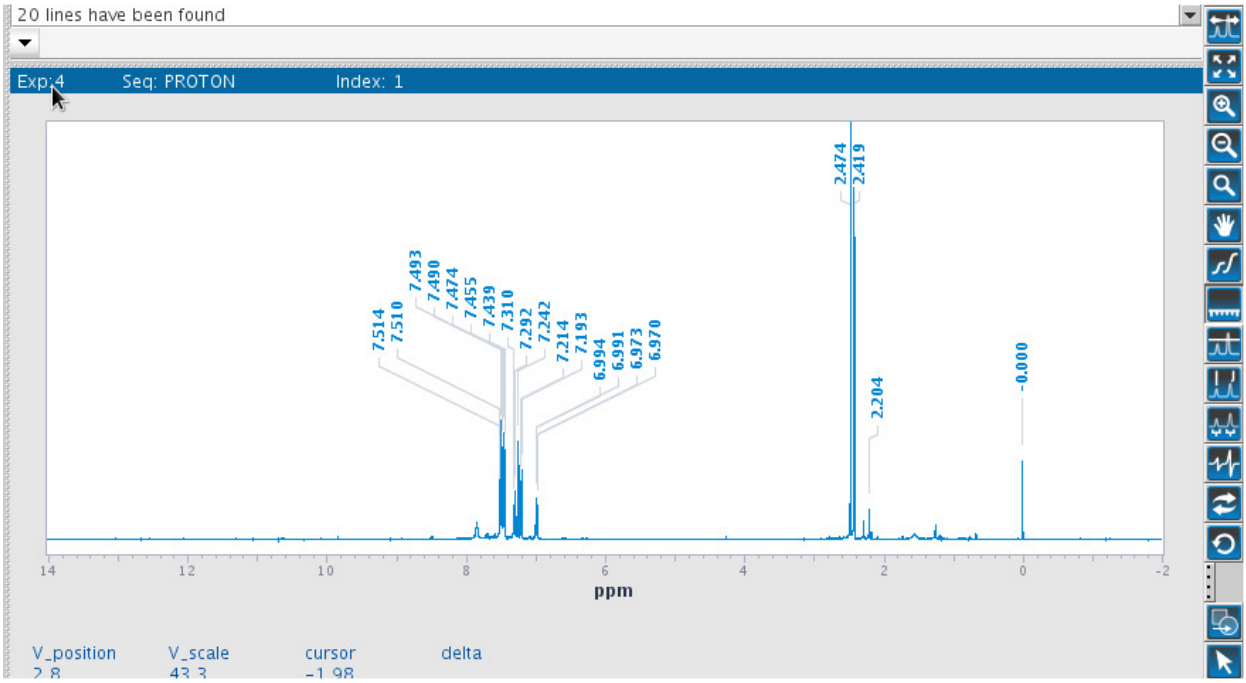
This will display a yellow horizontal line that can be dragged up and down using the left mouse button to set the appropriate level for peak picking.

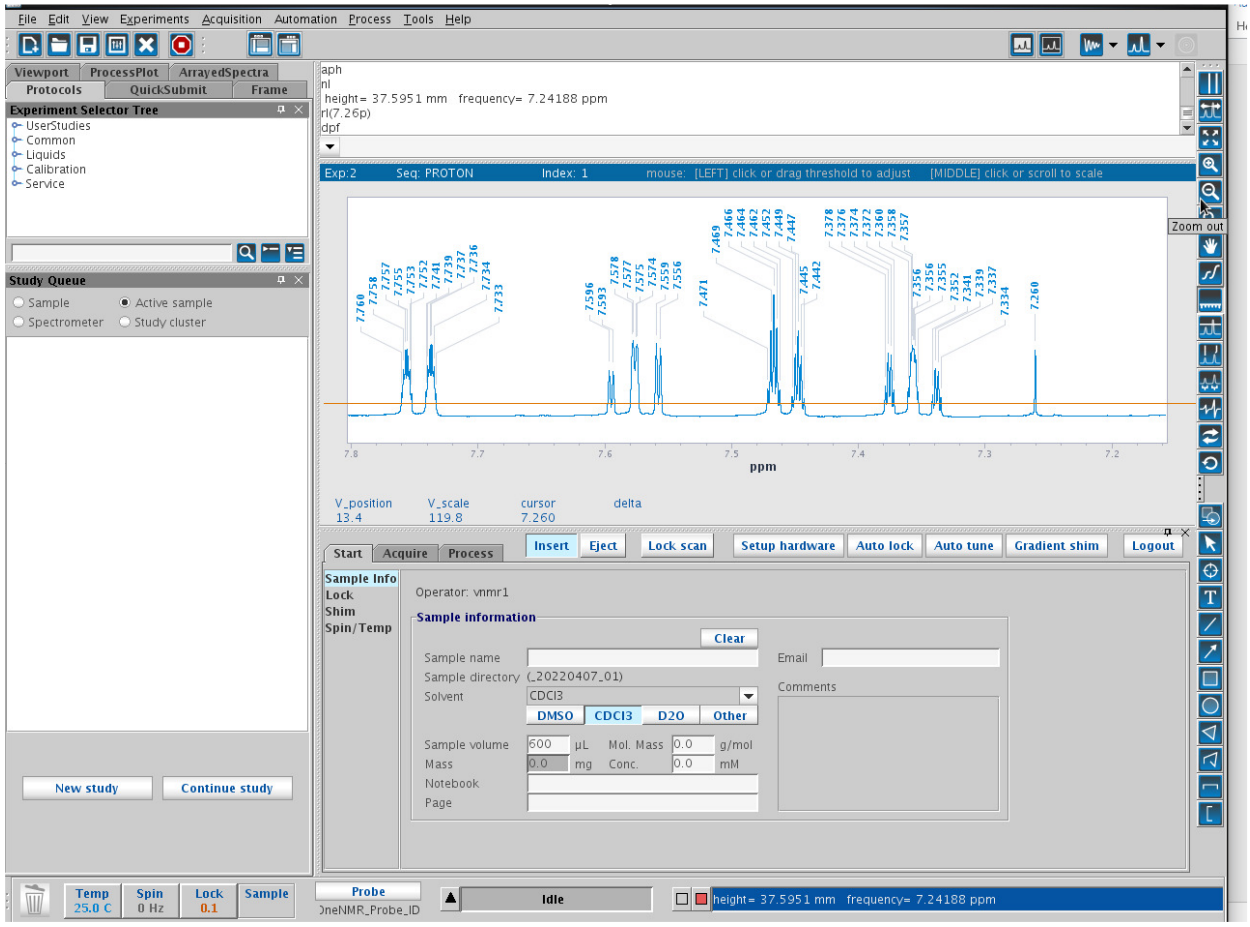
Once you've set the threshold, click on the **threshold icon** again to exit the threshold adjustment mode.

To get a listing of peaks displayed on the spectrum, the command **dpf** or **dpf('top')** can be used:



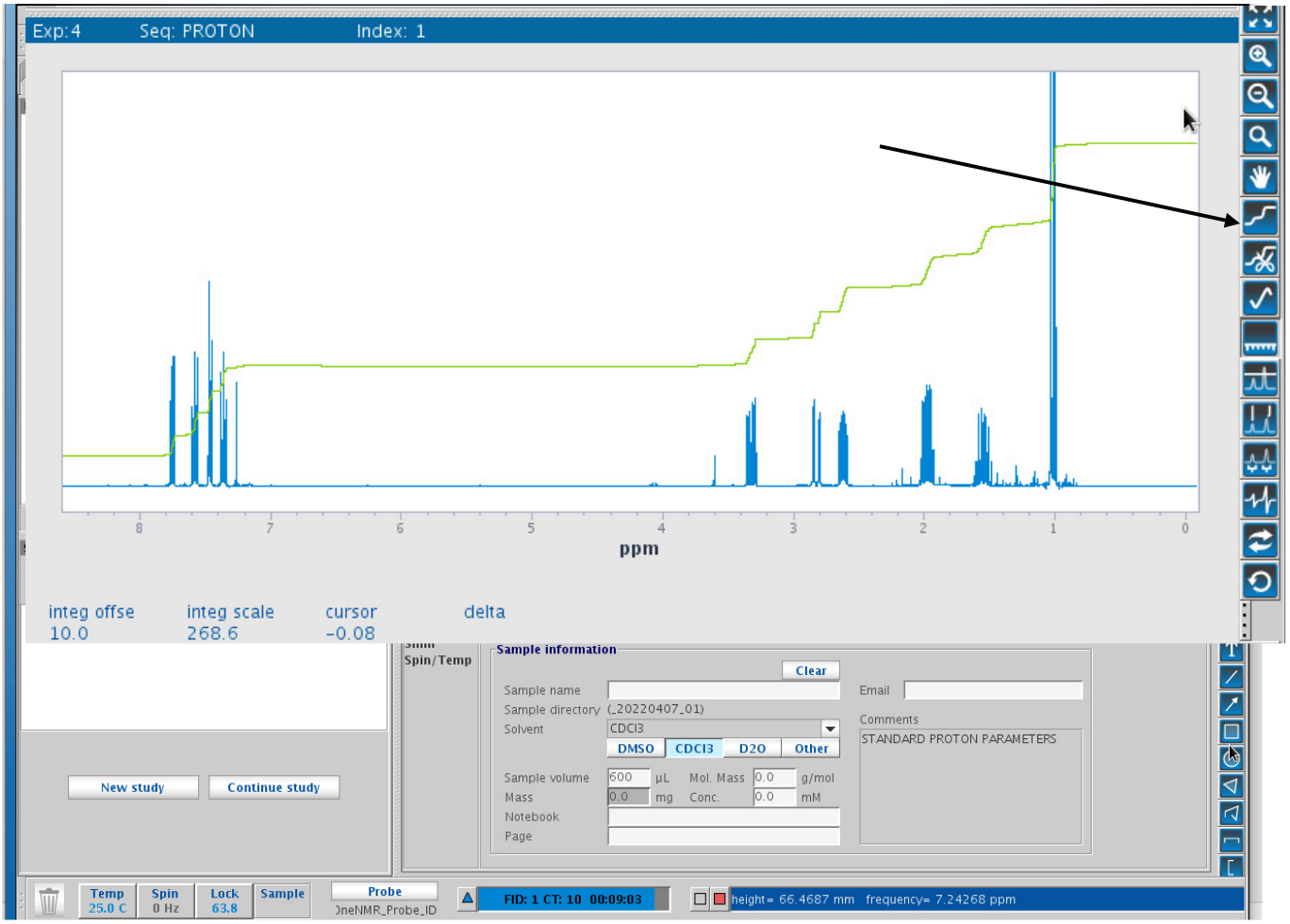
To get a listing of peaks displayed on the spectrum, the command **dpf** or **dpf('top')** can be used:
This command will pick all peaks above the threshold line and display those frequencies. Note that the **dpf** commandt fails you out of the interactive display mode. Type **ds** to return to it. A list of peaks can also be printed out to the VNMRJ text window using the **dll** command or directly to the plotter by the **pll** command.


20 lines have been found
Exp:4
Seq: PROTON
Index: 1
2.474
2.419
7.514
7.510
7.493
7.490
7.474
7.455
7.439
7.310
7.292
7.242
7.214
7.193
6.994
6.991
6.973
6.970
2.204
-0.000
14
12
10
8
6
4
2
0
-2
ppm
V_position
V_scale
cursor
delta
2.8
43.3
-1.98


File Edit View Experiments Acquisition Automation Process Tools Help
Viewport
ProcessPlot
ArrayedSpectra
Protocols
QuickSubmit
Frame
Experiment Selector Tree
UserStudies
Common
Liquids
Calibration
Service
Study Queue
Sample
Active sample
Spectrometer
Study cluster
New study
Continue study
aph
nl
height= 37.5951 mm frequency= 7.24188 ppm
rl(7.26p)
dpf
Exp:2
Seq: PROTON
Index: 1
mouse: [LEFT] click or drag threshold to adjust [MIDDLE] click or scroll to scale
Zoom out
7.760
7.758
7.757
7.755
7.753
7.752
7.741
7.739
7.737
7.736
7.734
7.733
7.596
7.593
7.578
7.577
7.575
7.574
7.559
7.556
7.471
7.469
7.466
7.464
7.462
7.452
7.449
7.447
7.445
7.442
7.378
7.376
7.374
7.372
7.360
7.358
7.357
7.356
7.356
7.355
7.352
7.341
7.339
7.337
7.334
7.260
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
V_position
V_scale
cursor
delta
13.4
119.8
7.260
Start
Acquire
Process
Insert
Eject
Lock scan
Setup hardware
Auto lock
Auto tune
Gradient shim
Logout
Sample Info
Lock
Shim
Spin/Temp
Operator: vnmr1
Sample information
Clear
Sample name
Email
Sample directory (_20220407_01)
Solvent
CDCl3
DMSO
CDCl3
D2O
Other
Comments
Sample volume
600
µL
Mol. Mass
0.0
g/mol
Mass
0.0
mg
Conc.
0.0
mM
Notebook
Page
Temp
25.0 C
Spin
0 Hz
Lock
0.1
Sample
Probe
OneNMR_Probe_ID
Idle
height= 37.5951 mm frequency= 7.24188 ppm

Integration

Click the integral icon (see arrow below) on The VNMRJ window to display the green integral line.



With the integral displayed, the middle mouse button will adjust the vertical scale of the integral instead of thespectrum. (The vertical scale of the integral can also be adjusted automatically using the command **isadj**.)

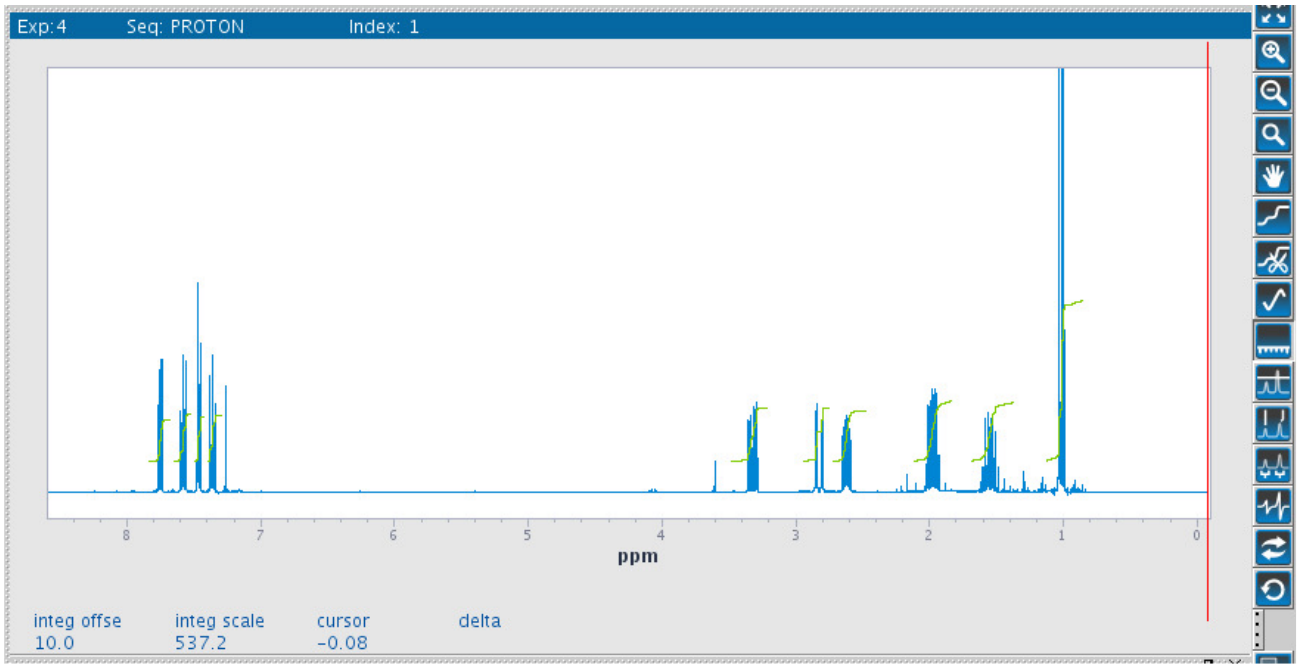
If the integral line is not flat and horizontal, you can adjust the slope and bias of the integrals. Clcik the phase integral ison. This works much like phasing. First click on an integral region towards the right side of the spectrum and drag up or down with the left (coarse) or right (fine) mouse buttons until the integral looks like it is flat in the baseline regions to the left and right of the peak. Then click on an integral region towards the left side of the spectrumand drag up or down with the left or right mouse button until that integral region looks correct. The first time you click and adjust the integral you are adjusting the slope of the integral across the entire spectrum The second time, you are adjusting the bias of the integral - a linearly increasing correction to the slope across the spectrum.

The left mouse button can now be used to select where to break the integral (set a zero) -- typically you will want to click with the left mouse button to the left and to the right of each peak in the spectrum thatyou want

to integrate. If you make a mistake when setting the integral resets, you can click with the right mouse button to remove the nearest reset. Or click many times with the right mouse button to remove all resets or type **cz** (clear zeroes). *The integrated region is the solid green line; non-integrated regions are shown as a dotted line.*

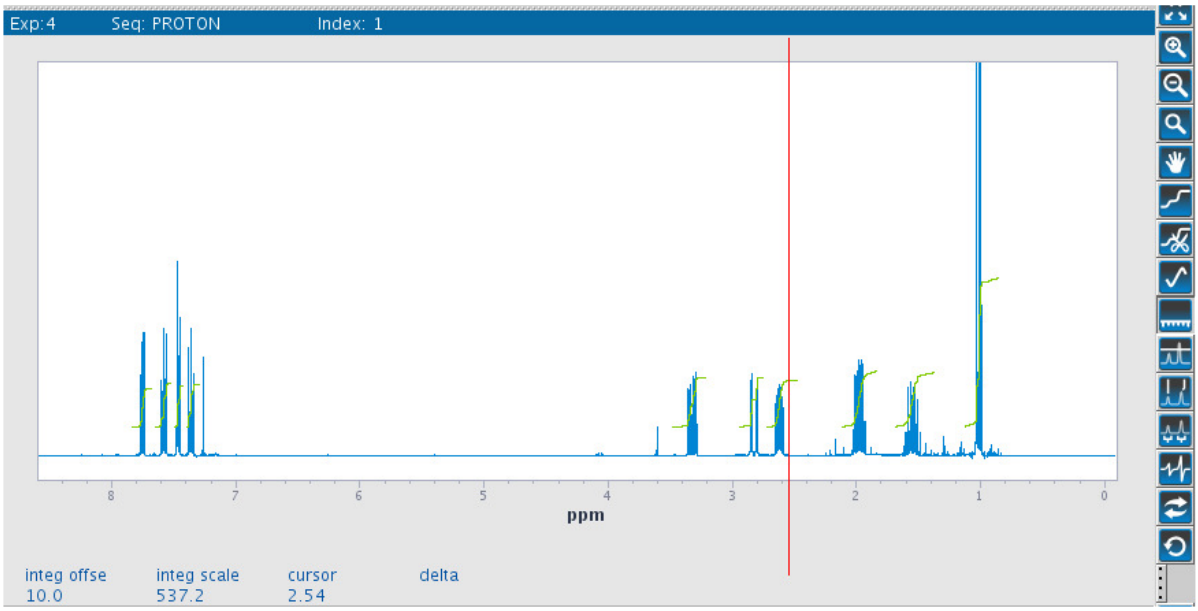
To display the integrals on the screen, make sure that **vp** is at least 12 (**vp=12**) and type **dpir** or **dpirn** (normalized).

To rescale the values displayed by either command, change the value of the parameter **ins**. For **dpirn**, set the values out of a possible 100 with **ins=100**. If you want a particular integral region to be equal to 3 (if it is a methyl group, for instance), place the cursor on that region and select the **[Set Int]** button, then type 3 at the prompt. In this case, use **dpir** to display the values.

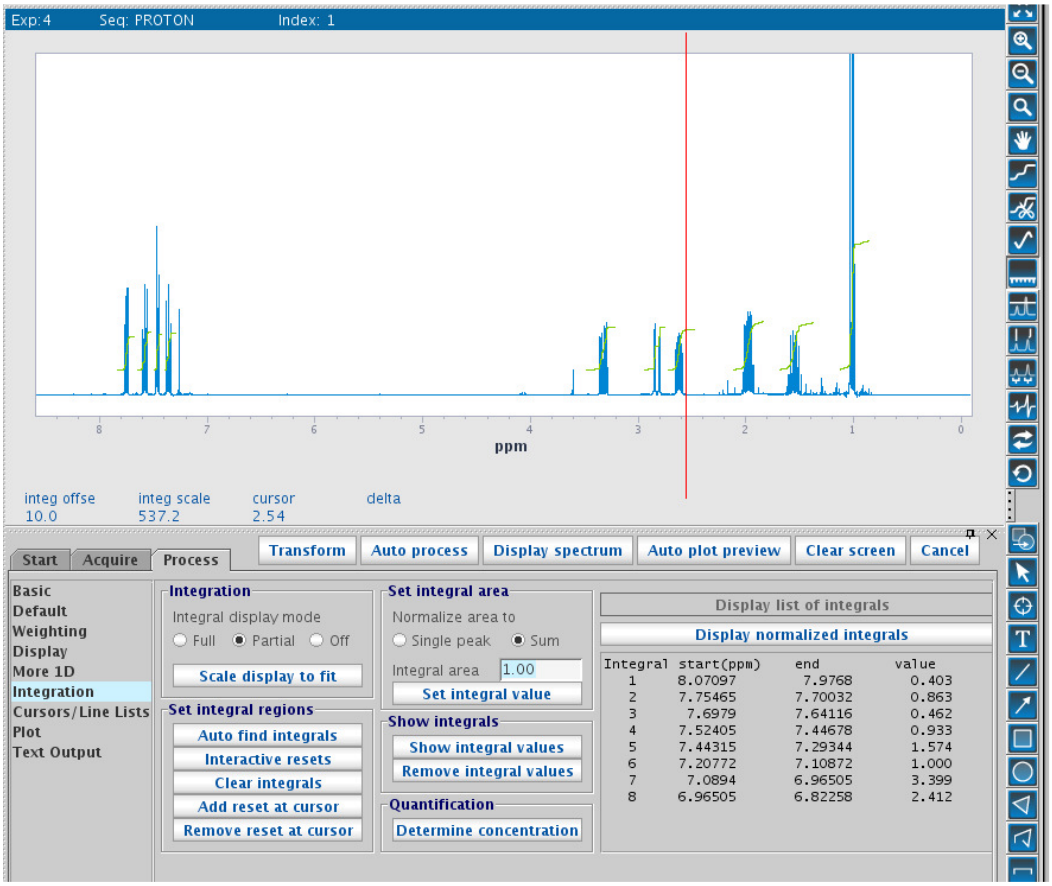


Setting integral value

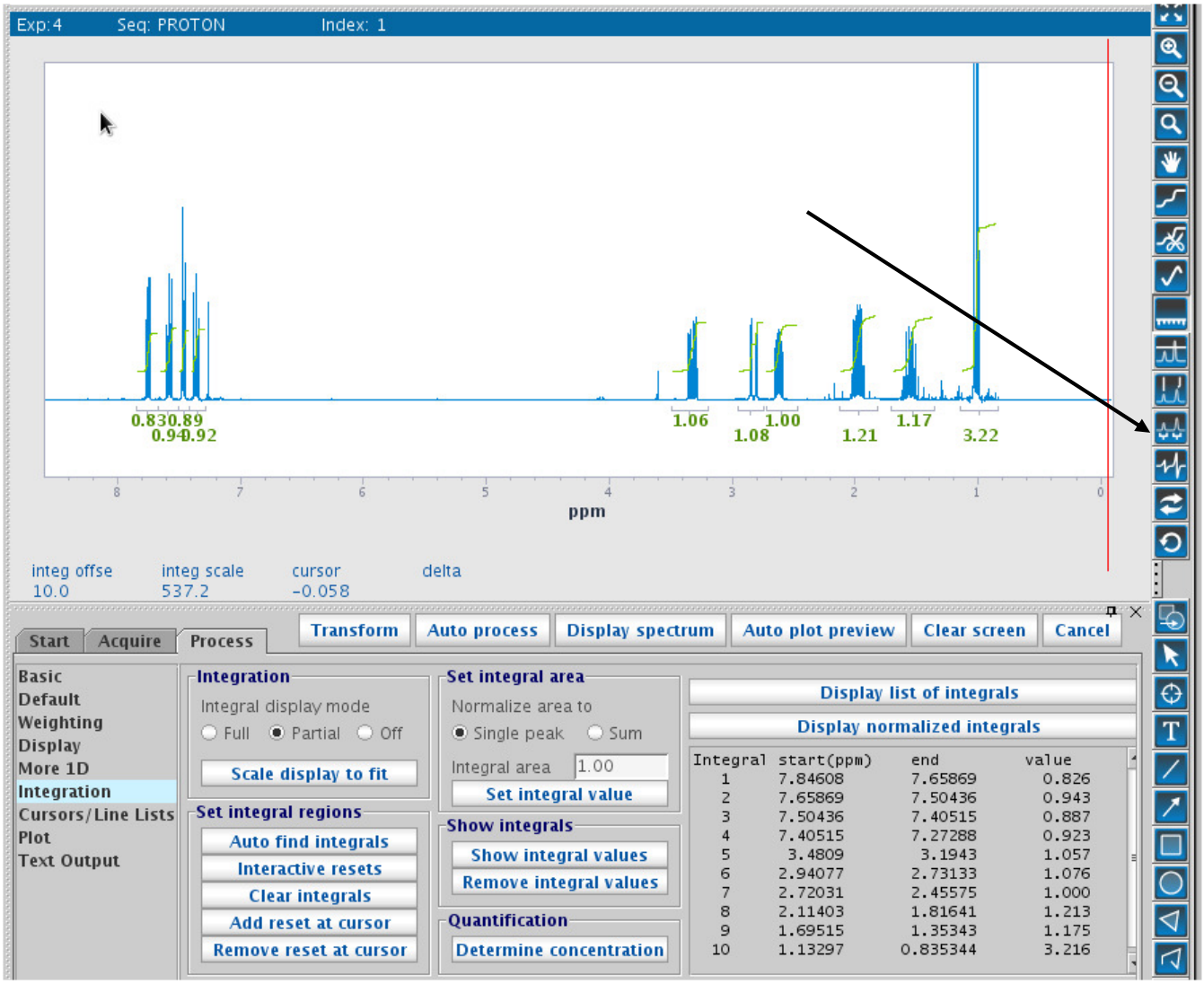
Place vertical line on the integral area



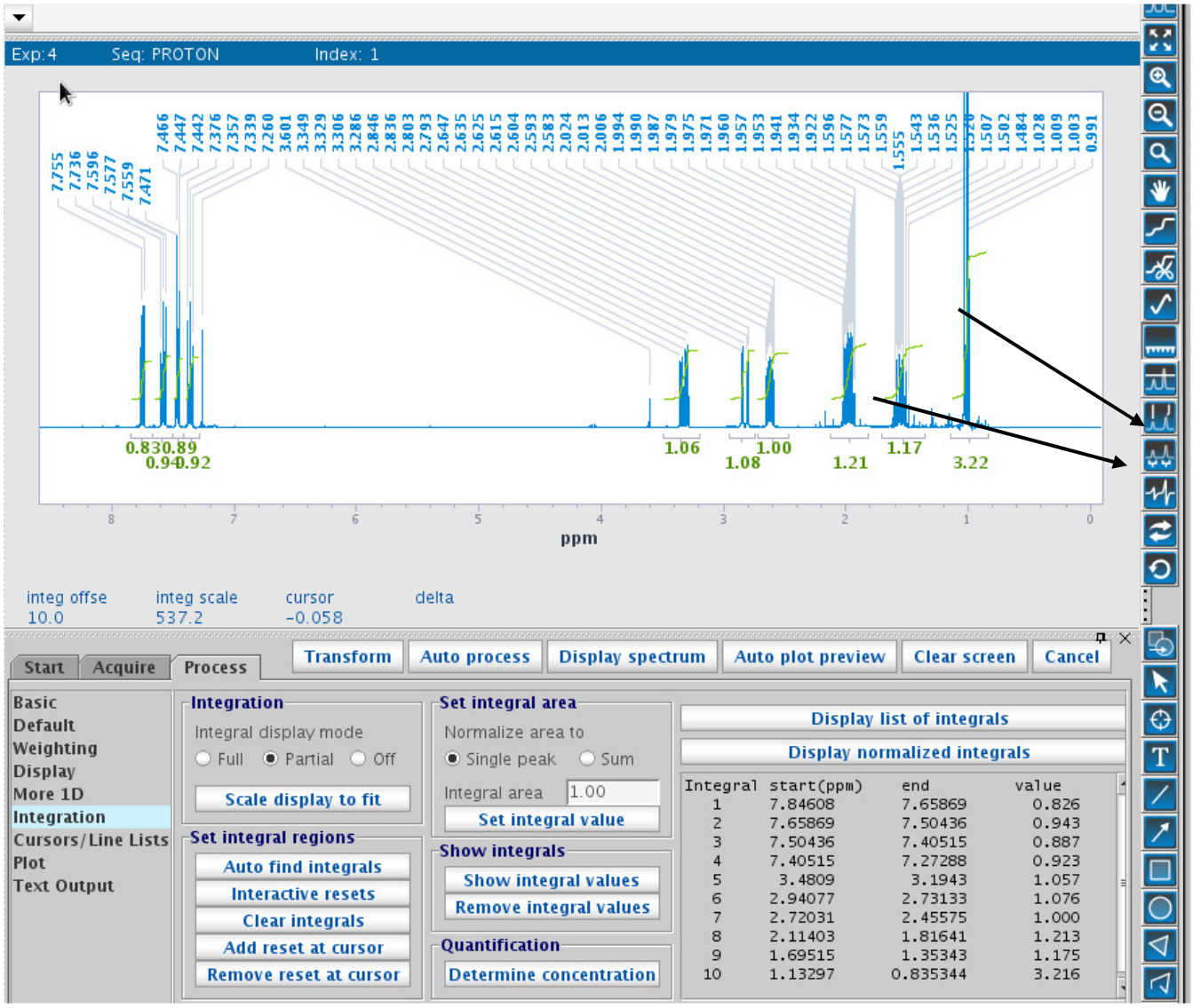
Then click **Process**, **integration** and under set integral window enter 1 and then click **Set integral value** (see below Picture)



To display the integral values under peaks type **dpir** and hit Enter button or click the **integral value icon** on the Icon panel (see arrow below).

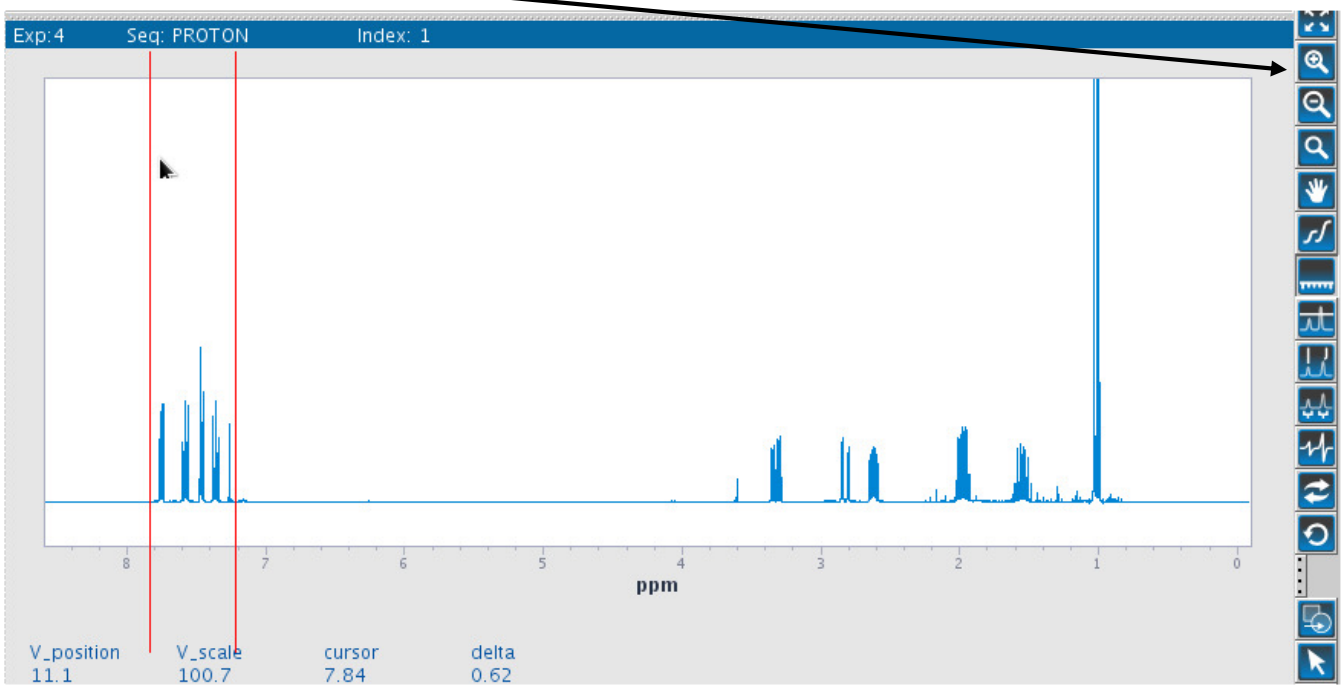


To see both (chemical shifts on the top peaks) and integral values under peaks click the appropriate icons on the Icon panel (see below shown arrows)

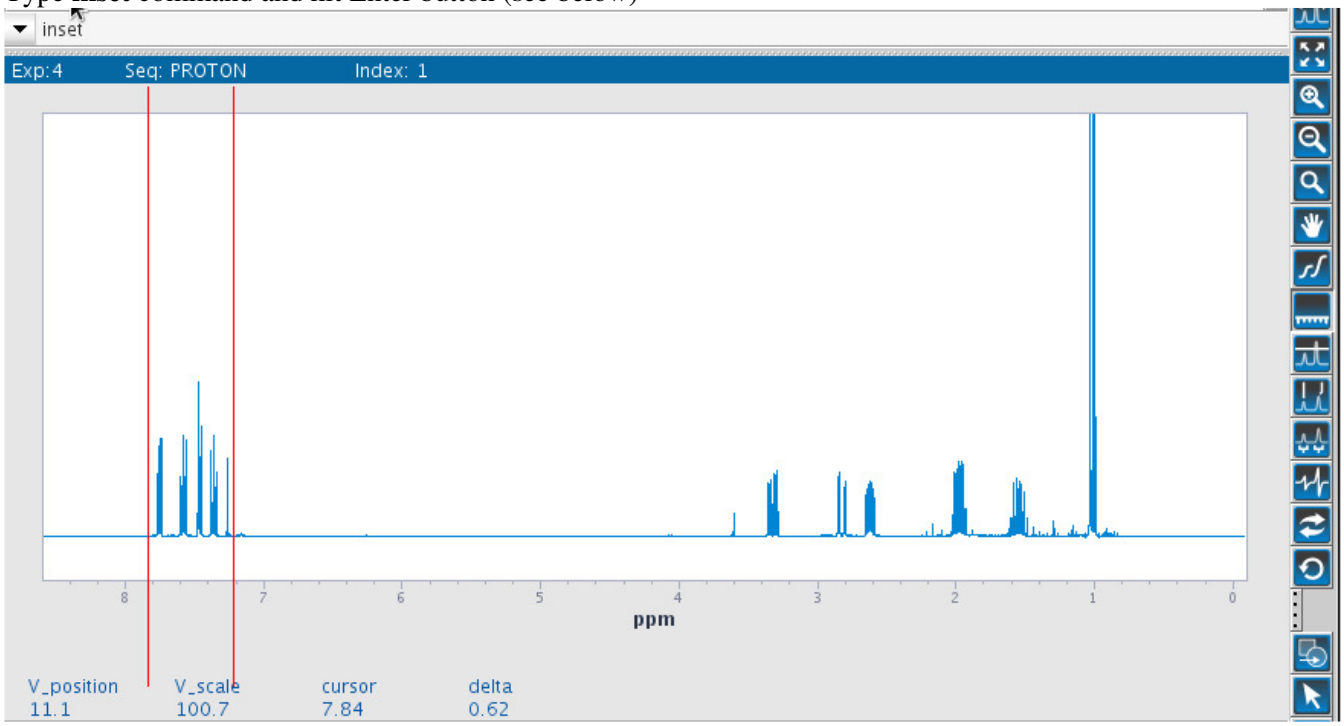


Inset command

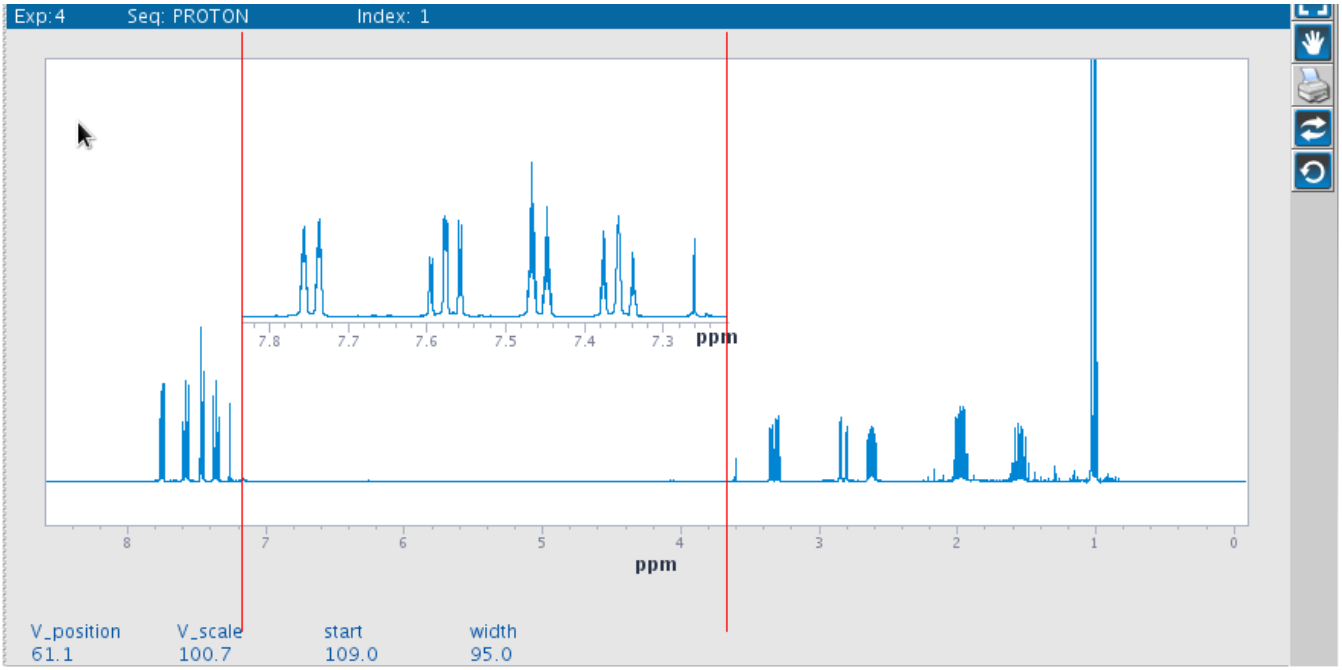
Inset command allows putting a desired region above the spectrum. To do this first select desired region with two vertical lines then click zoom in icon



Type **inset** command and hit Enter button (see below)



The selected region immediately after inset command appears above the spectrum. You can move it to the ring side or to the left side spectrum and using right side vertical cursor to do expansion of the selected region (optional)



Printing

Once the data has been processed, you will probably want to print your spectrum.

To put a title on your spectrum, type **text('title')**. The title will be printedin the upper left of the page by the command **pltext**

For printing the scale in ppm or Hz units:
pscale - plot axis under spectrum. To change the units on the axis type **axis='h'** for Hertz or
axis='p' for ppm before typing **pscale**.

For listing parameters on your spectrum, choose one of the following:
pap - plot all parameters in the upper left of the page.
ppa - plot a short list of parameters in the upper left corner of the page.
pltext - plot only the text; this is not necessary if you execute the **pap** or **ppa** commands.

For peak frequencies, choose one of the following:
ppf - plot peak frequencies above spectrum with a line going down to the peak.
ppf('top') - same, but peak frequencies are all plotted along the top of the plot.
ppf('pos', 'top') - same, but print only positive peaks.
vp=vp+80 ppf('pos', 'top') vp=vp-80 - same, but print with short lines that don't go all the way down to the top of the peak.

For integrations, choose one of the following:
pir - plot integrals under the spectrum. **vp** (vertical position of the spectrum) must be at least 12 for this to work.

To send your spectrum to the printer type **page** and hit Enter button.
page('clear') - delete everything that has been plotted so far instead of sending it to the printer.

For separate peak listings, choose one of the following:
pll - plot a list of peak frequencies in ppm and in Hz.
pli - plot a list of integrals.