Data Processing using DELTA software is optional to learn. All data processing, referencing, integration, pick picking, and base line corrections should be done on your own computer using MNOVA software

DATA PROCESSING OF 1D NMR

This section explains data processing after measurement was completed and the data were sent from the spectrometer. After the measurement and data transfer, the following is automatically executed.

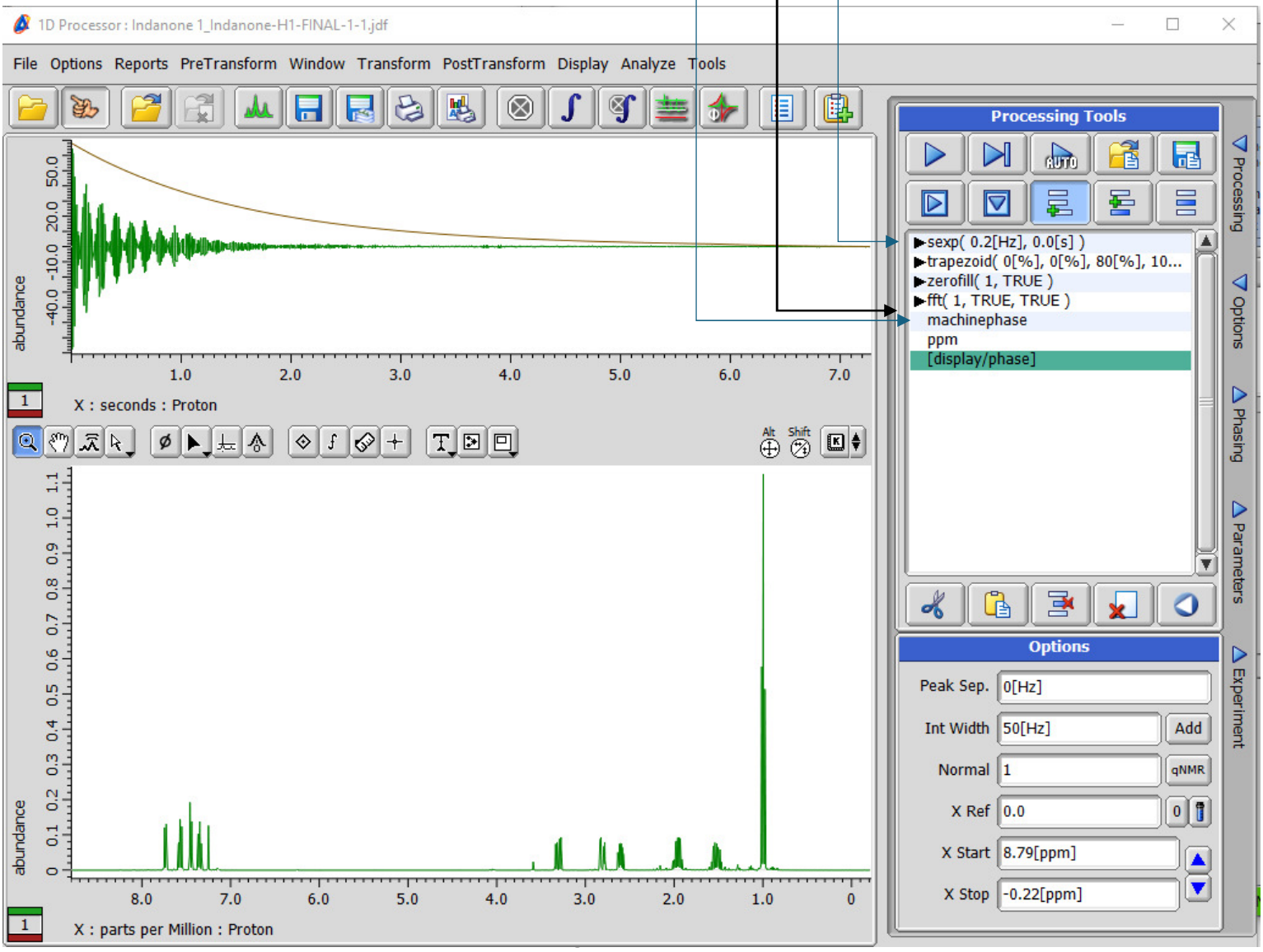
Multiplication by window functions (such as **single exponential and trapezoid**)

FFT (Fast Fourier Transformations)

Automatic phase correction

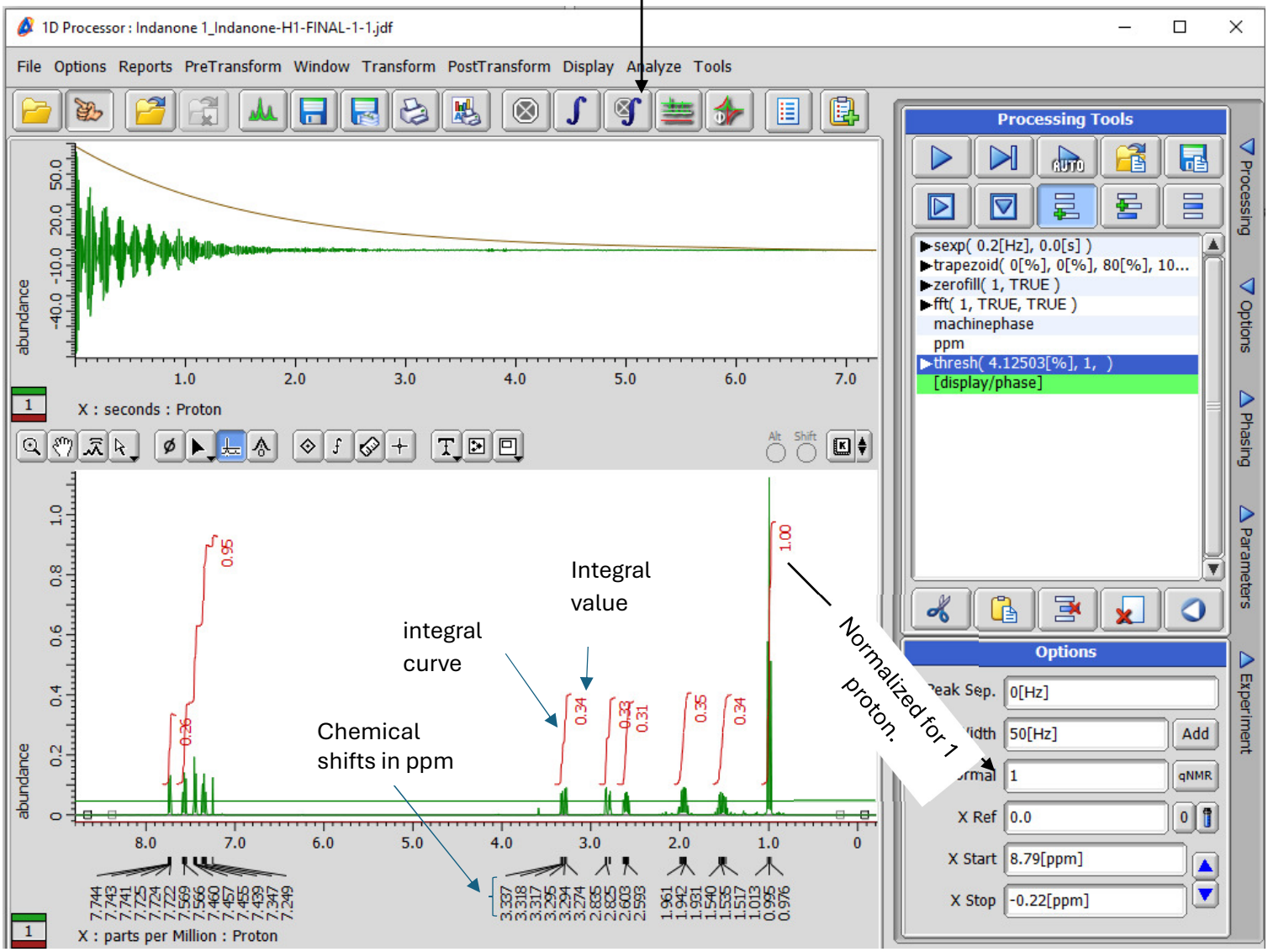
When measurement is completed, the 1D Processor window opens.

1D Processor window



Click the  button in the 1D Processor window.

Automatic peak detection and automatic integration are carried out, and the results are displayed in the lower spectral display area in the 1D Processor window.



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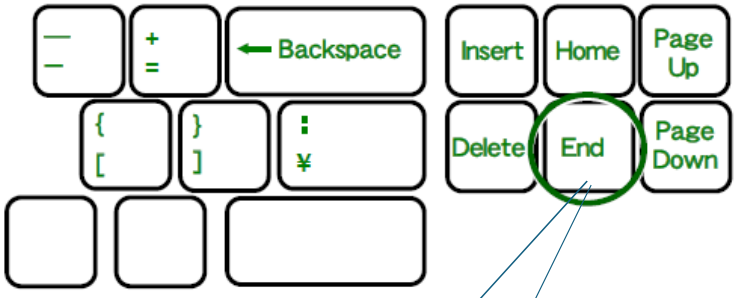
Changing the display range.

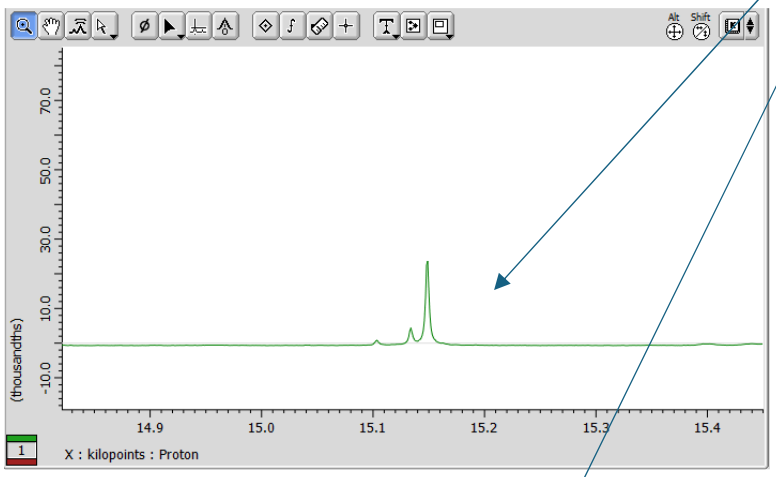
The **pointer bar** is used to expand or reduce spectra. This section explains basic usage of the pointer bar.

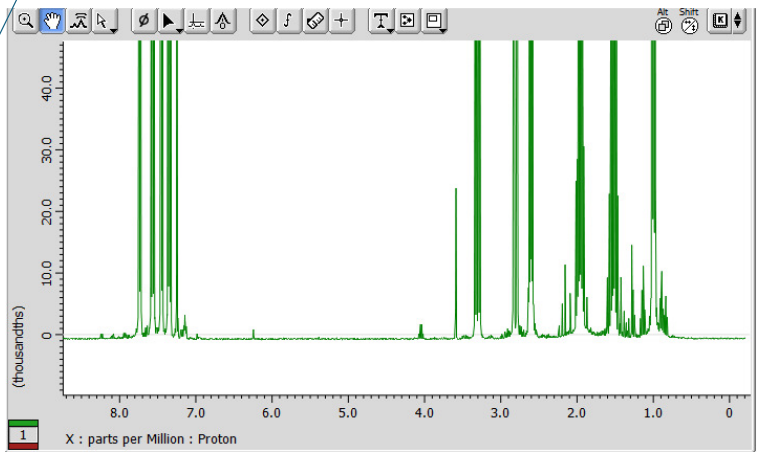
 ZOOM	To expand, reduce, or move spectra
 Pan View	To move the area after expanding spectra
 Amplitude gain	To adjust the amplitude of spectra
 Select	To select data or geometry
 Phase correction	To correct the phase of spectra
 Copy position	To copy the chemical shift of the peak
 Peak threshold	To set the position of the baseline of spectra
 Reference	To set a chemical shift reference axis marker
 Peak	To execute a peak pick
 Integral	To perform manual integration
 Measure	To measure distance between peaks
 Cursor	To display the horizontal and vertical lines
 Annotaion	To display an annotation in the geometry
 Molecule	To display a structural formula and molecular formula in the geometry
 PiP	To display a selected part of the geometry within the current geometry

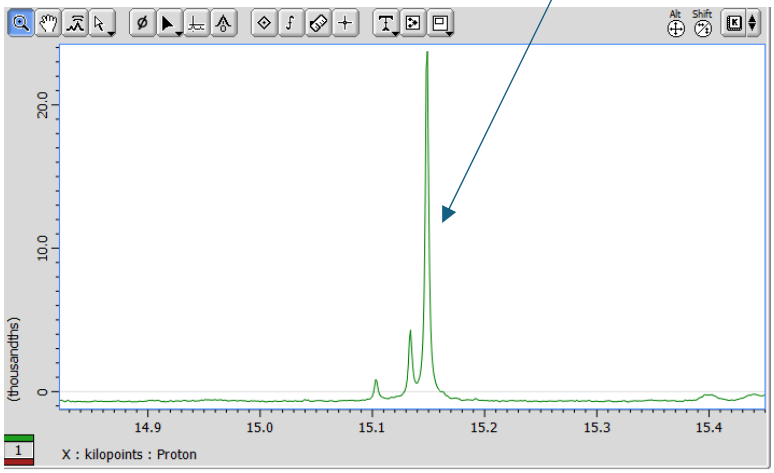
To adjust the intensity of the highest peak which is displayed. The highest peak in the spectral region displayed currently is expanded or reduced vertically to fit with screen.

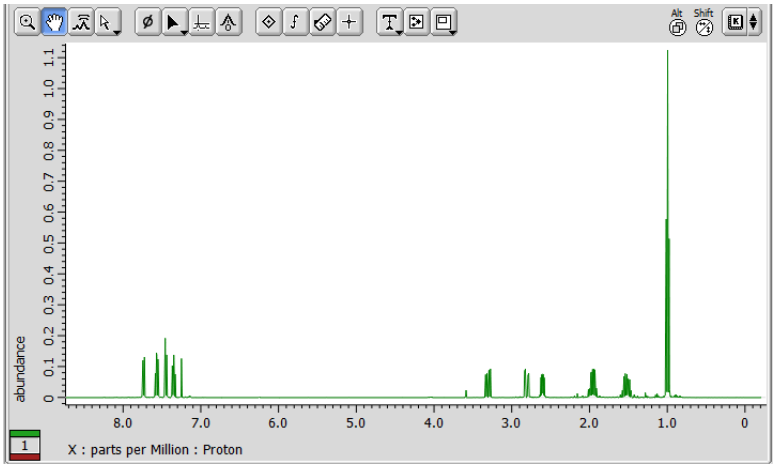
- Press the End key on the keyboard.







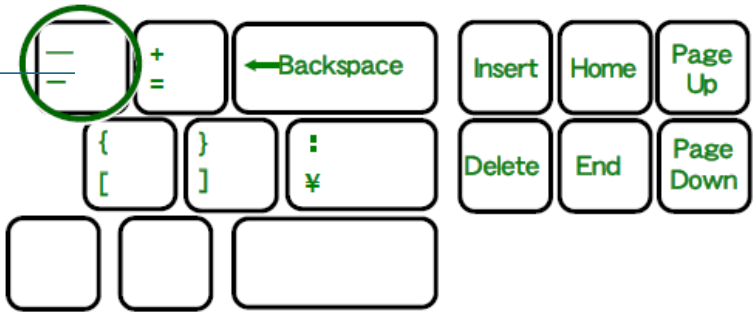


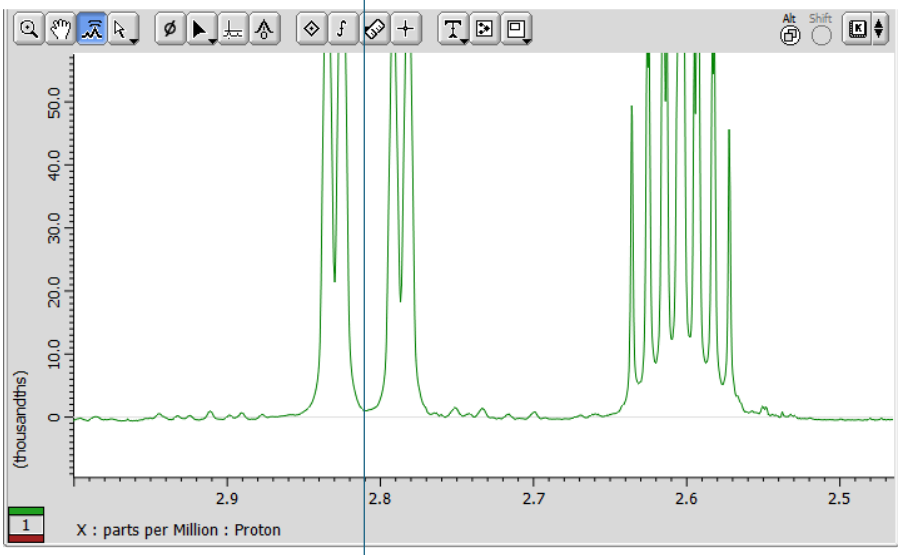


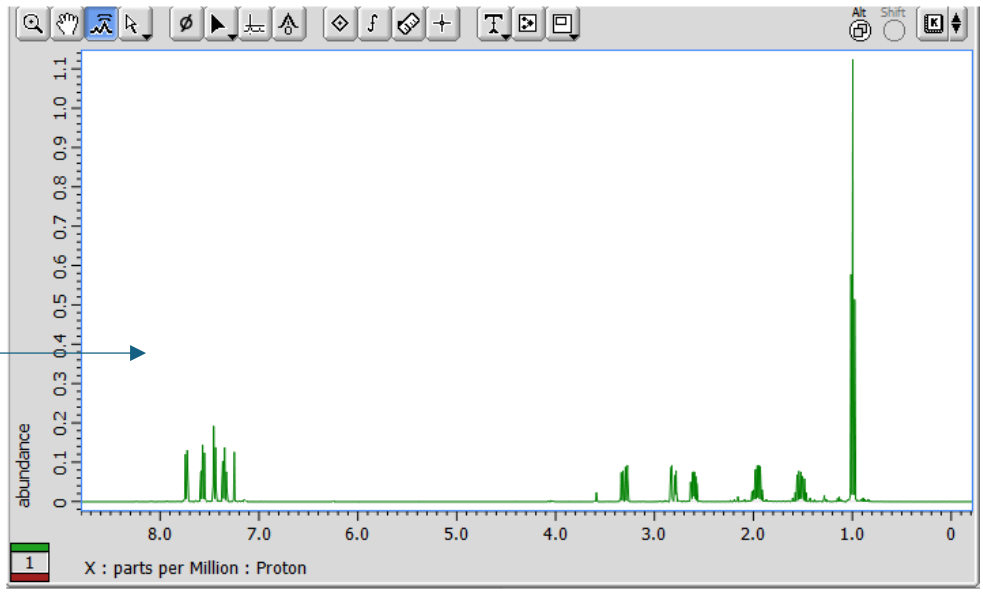
To return the spectrum display to its previous conditions

When you press the - key on the keyboard, both vertical and horizonal expansions return to their previous values . You cannot selectively return only the vertical and horizontal size to its previous value

- Press the – key on the keyboard.





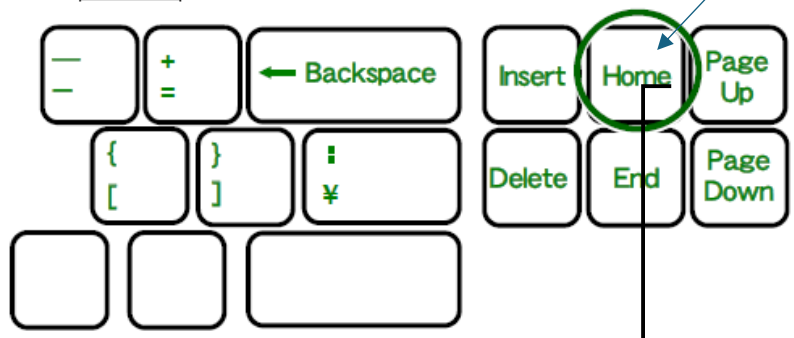


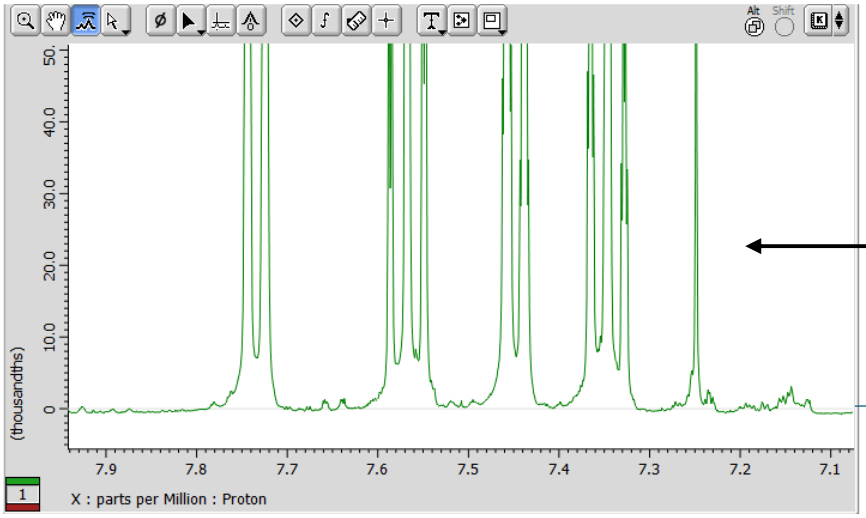
To return the spectrum display to its initial conditions.

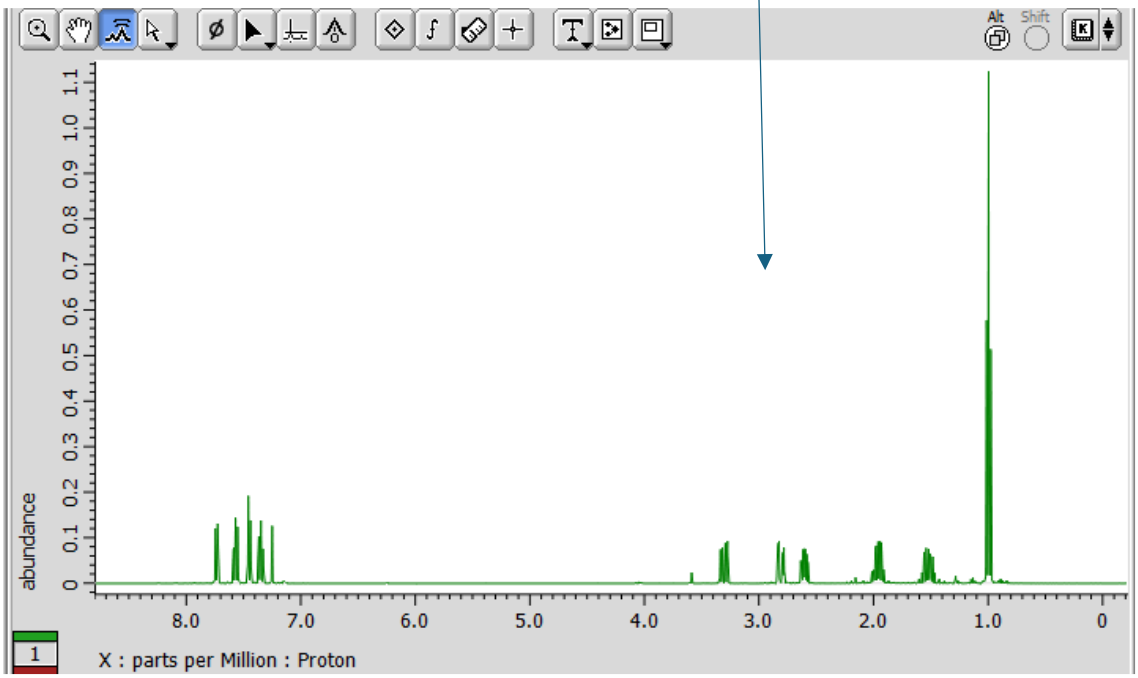
All horizontal and vertical expansion return to their initial values

Click

- Press the Home key on the keyboard.



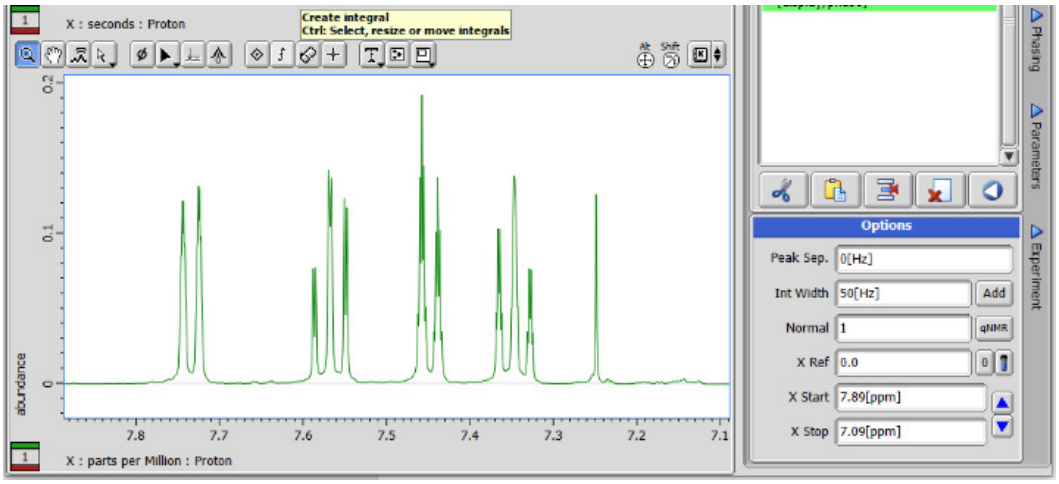


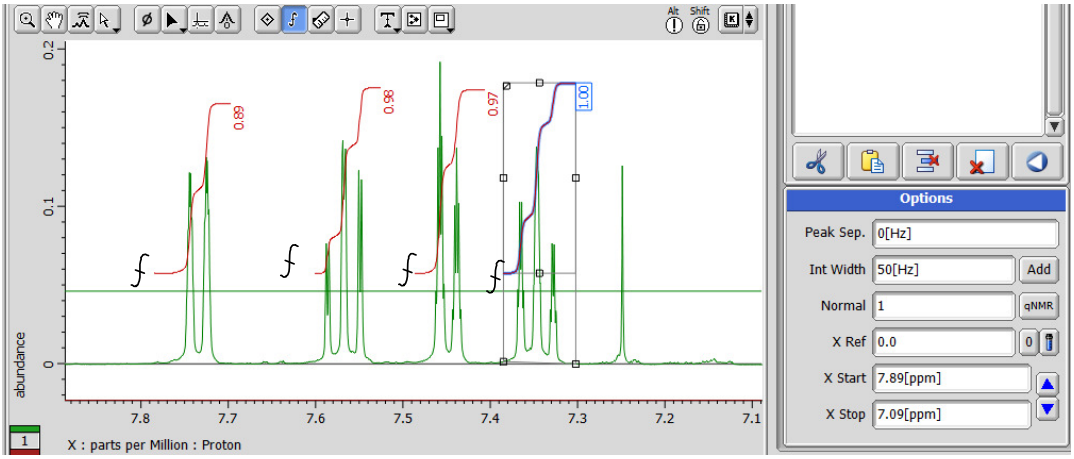


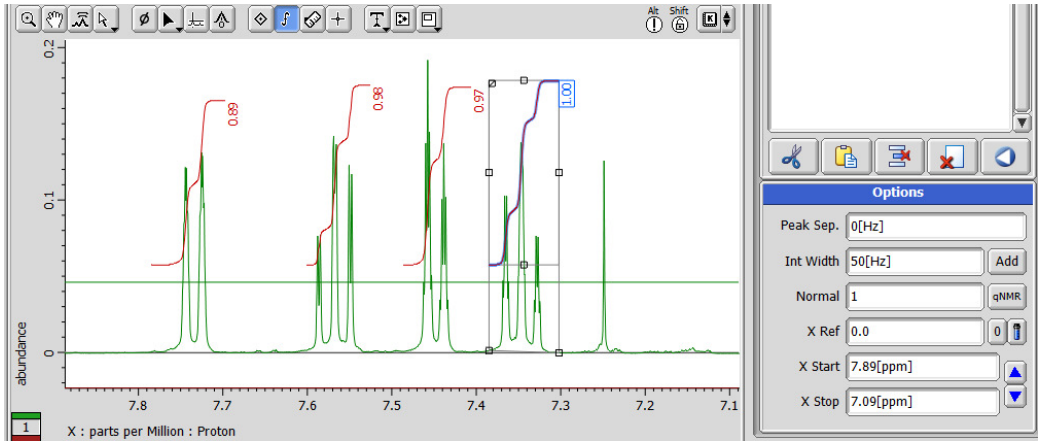
Manual integration of the peaks (singlet, doublet, triplet or multiplet etc)

Expand desired spectral region, then click integral icon  and move the left mouse button with Integral icon to the left side of desired peak (singlet, doublet, triplet or multiplet etc).

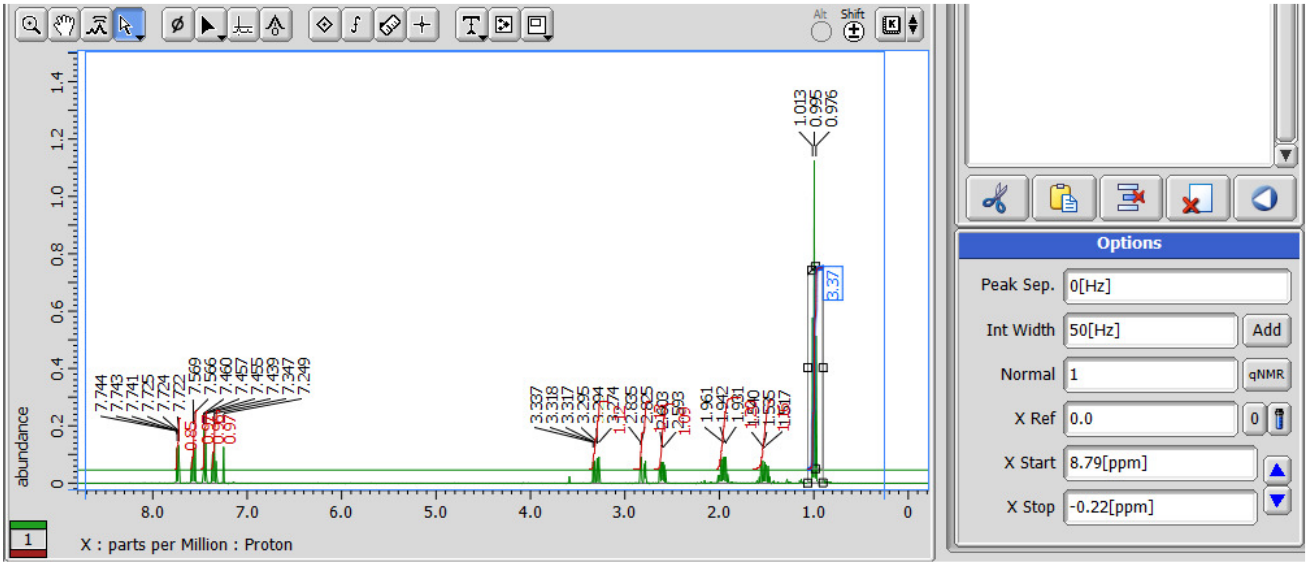
Remember the distance between the left and right end of the integral curve should be about 20 Hz equal from both sides of the peak. Hold down the left mouse button and drag the pointer in the X-axis direction (from left side to the right side of the peak and release the left mouse button while the end part of the integral curve is out of right side of peak and parallel to the base line); with the same way integrate all desired peaks. Normalizing integral: set intensity of peak to 1, 2, 3 if applicable.

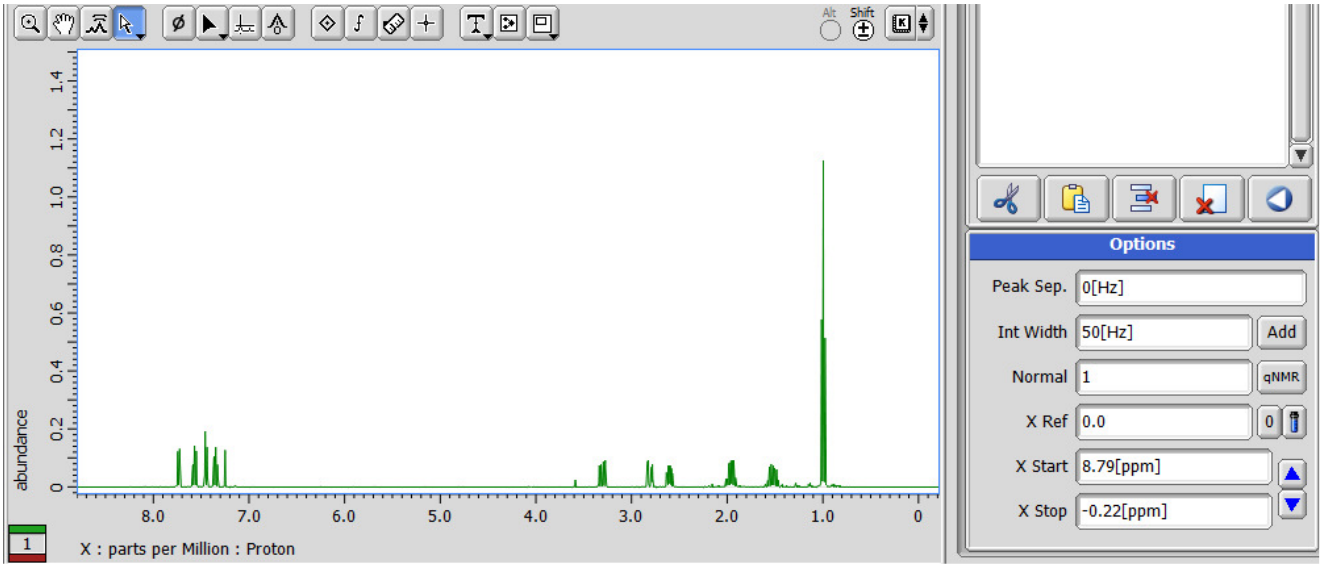




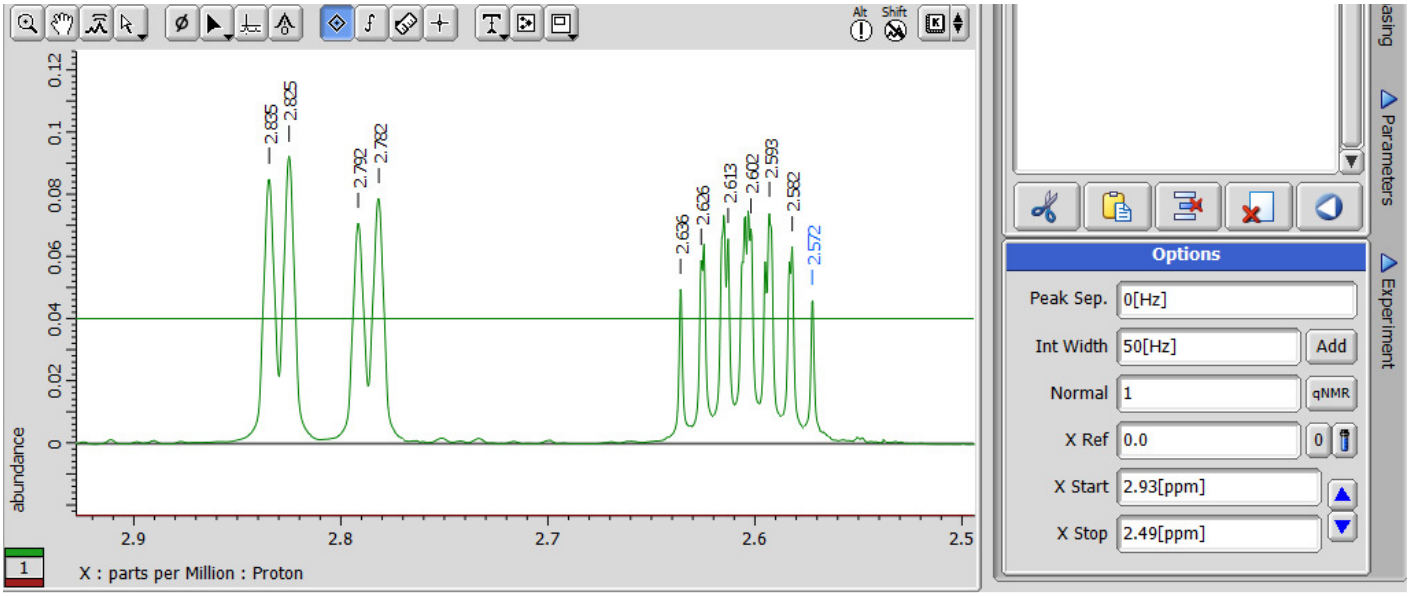


Select all integral regions and chemical shift values using the  and then hit the Delete button on the keyboard. The integral curves will be deleted.





Selecting peaks manually; click the  button to define peaks for the selected spectral region

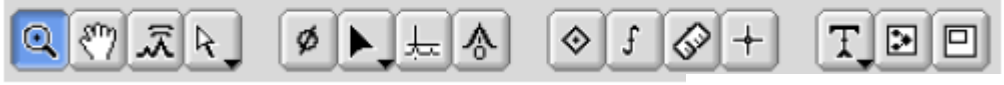


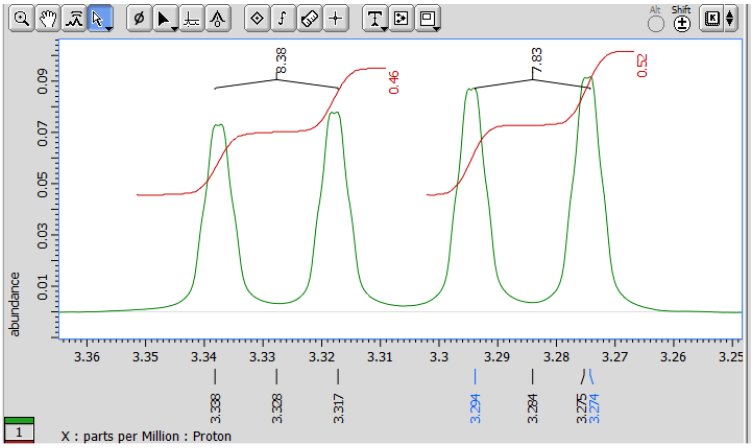
Extracting J coupling values

Process and peak pick the data set

Zoom into an area of peaks for which the "j" values need to be determined

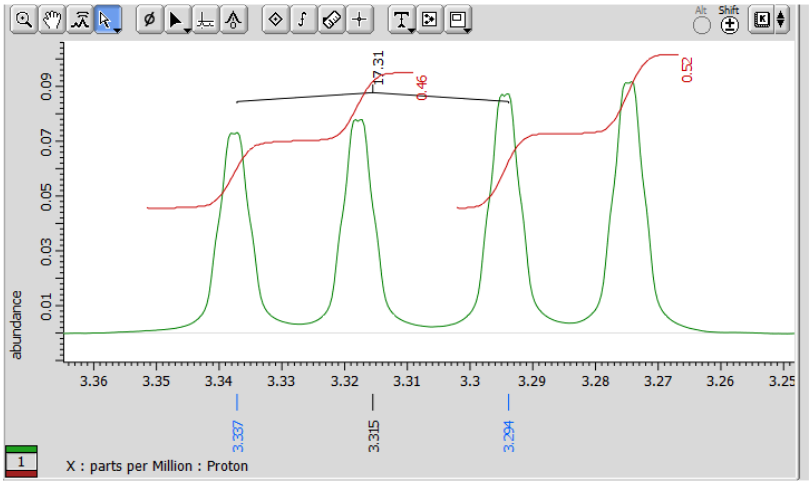
Switch to  mode from the toolbar above the 1D geometry.





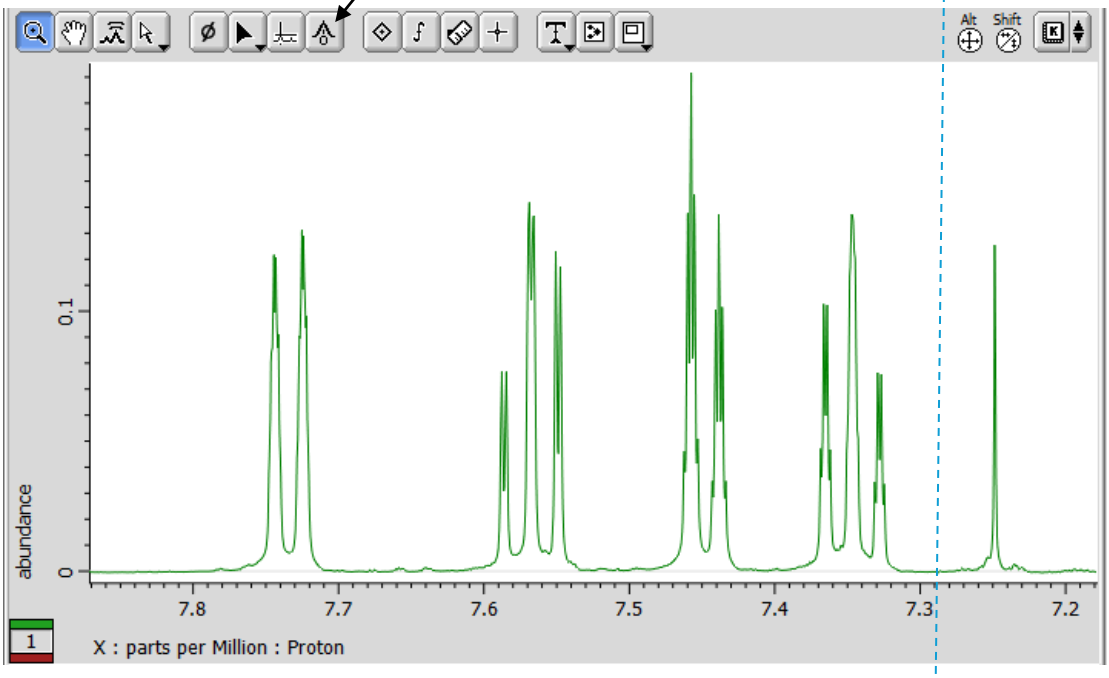
Click on the first peak to select it (it will turn **BLUE** to indicate it is selected). Hold the "Shift" key to "Add
peaks). Click on the adjacent peak to add the peak. Now 2 peaks will show up in **BLUE**.

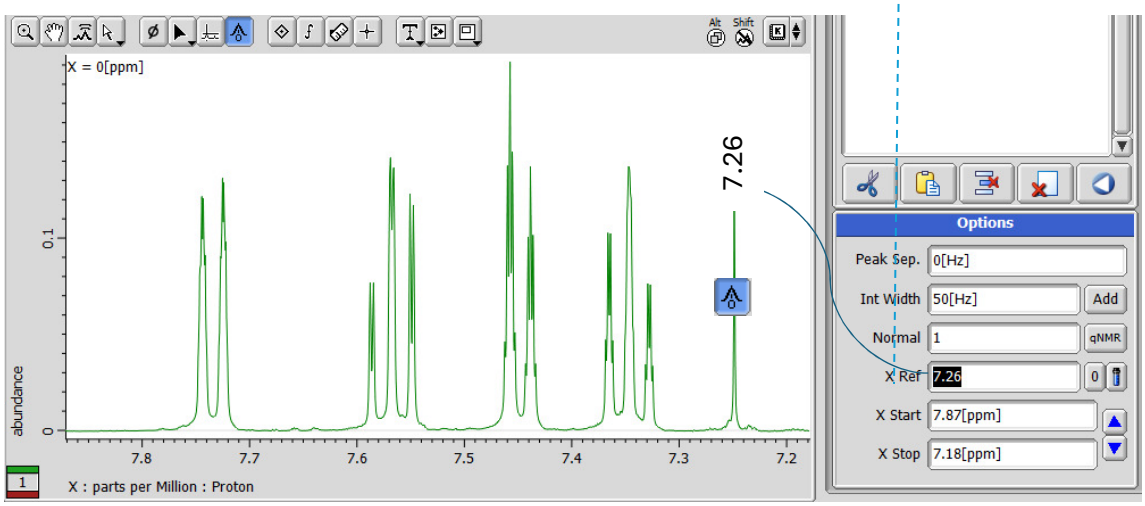
Hit "j" on the keyboard. The "j" value in Hertz will appear above the selected peaks. Repeat the process to display j's for other peaks.
Hit the "u" to un-select the peaks to start the process again.



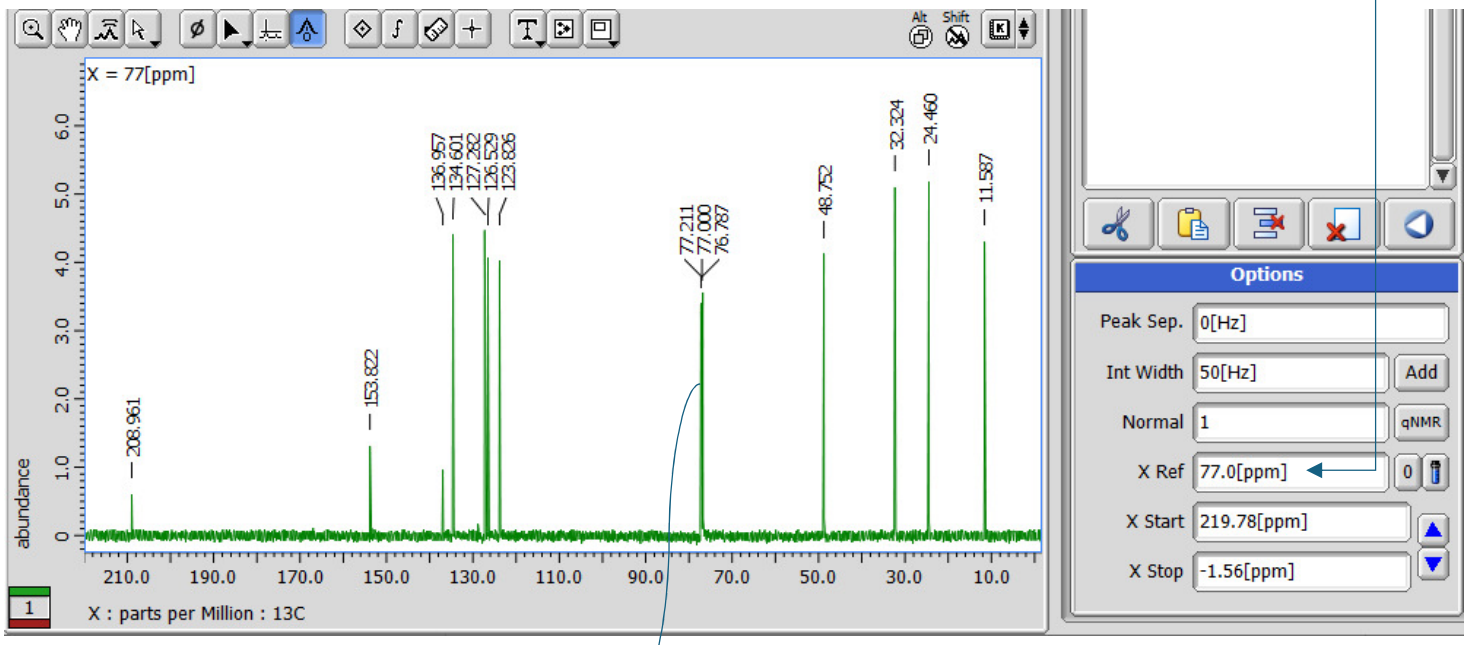
Referencing of the ^{1}H and ^{13}C NMR spectra, integration, peak peaking, and print spectrum;

Expand aromatic spectral region and find a single residual proton peak for $CHCl_3$ at ~ 7.24 ppm and change the reference value to 7.26 ppm. To do this set 1st: set X Ref to 7.26 ppm; then click the reference icon move cursor with this icon and release left mouse button when the reference icon on the peak.

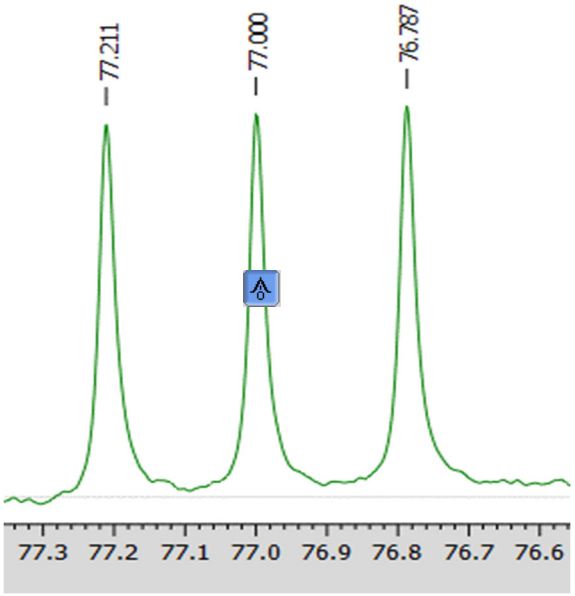




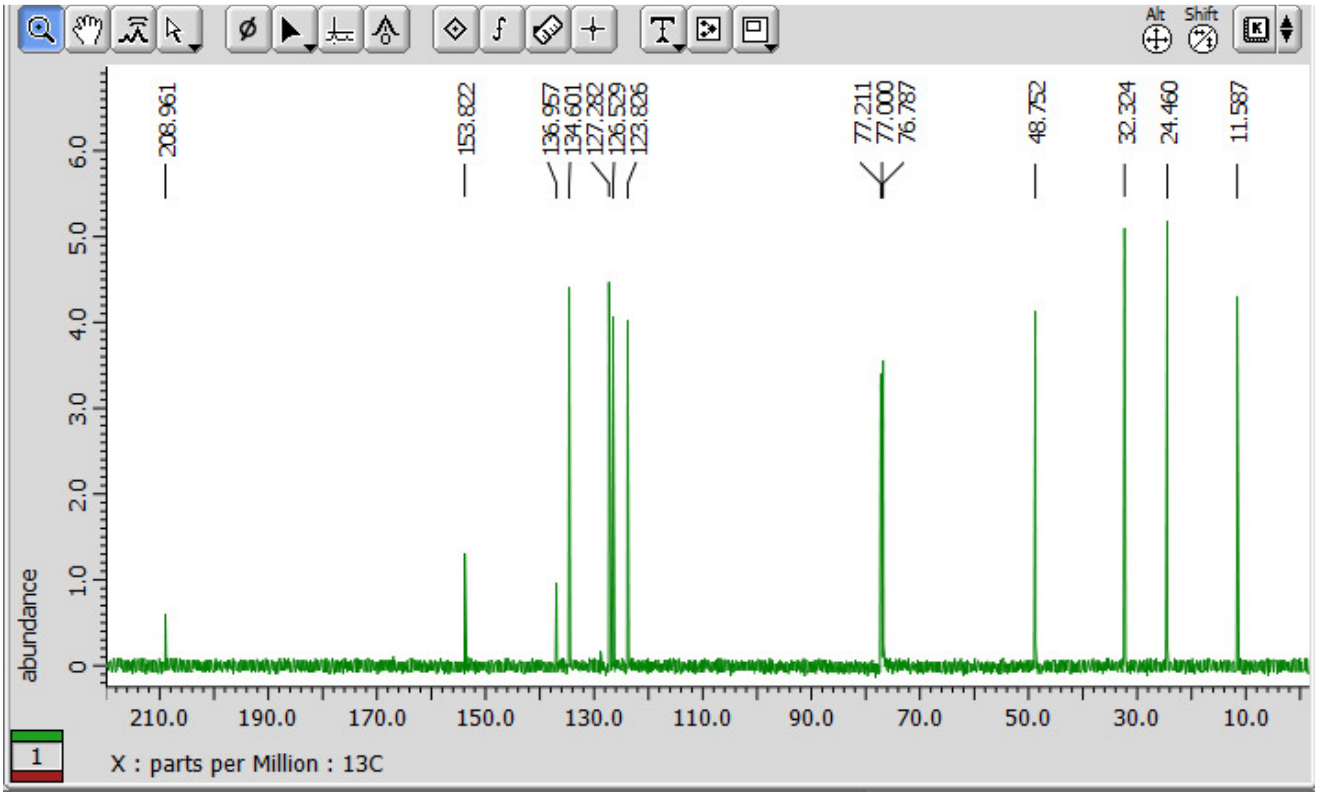
The ^{13}C NMR spectrum is referenced from the center line of the $CDCl_3$ peak at **77.00** ppm.



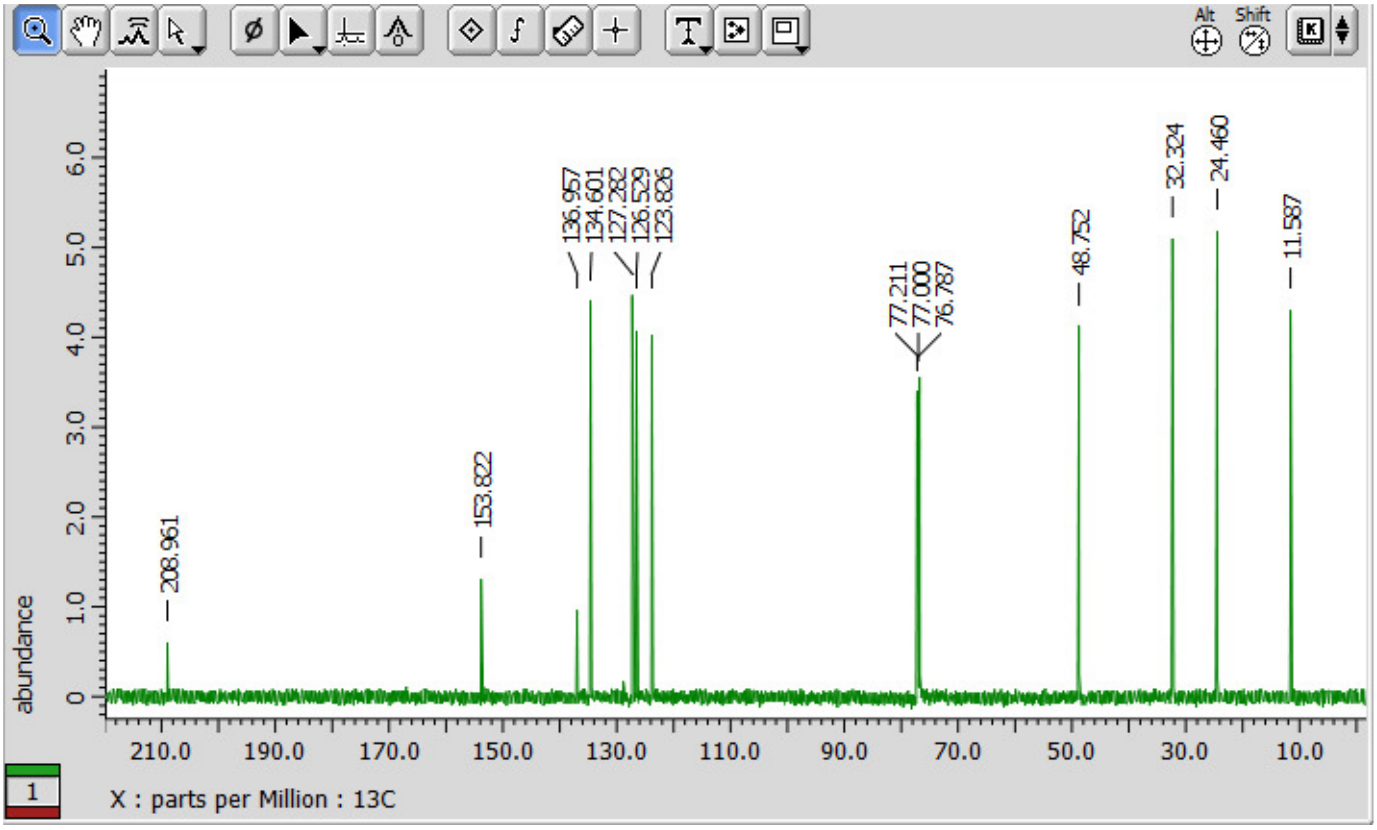
Expansion



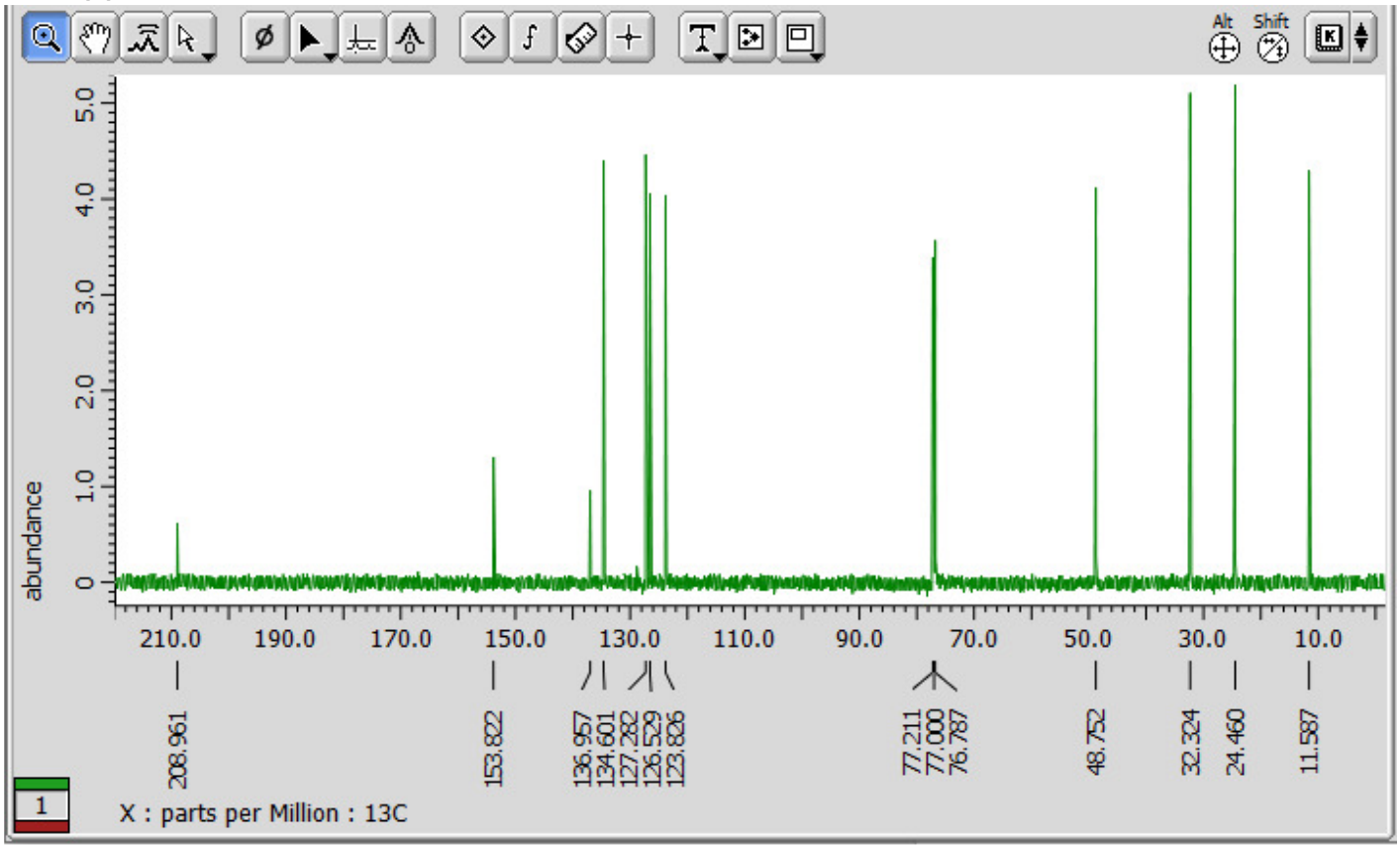
Chemical shift values can be displayed at the top peaks, near the peaks, and at the bottom of the peaks (below the baseline). While holding down the **Alt key** on the keyboard, press the **U key** on the keyboard to display all three positions (a-c) of the chemical shifts. Pressing the **U key button** should be repeated three times.



(b)



(c)


Alt
Shift
abundance
0
1.0
2.0
3.0
4.0
5.0
210.0
190.0
170.0
150.0
130.0
110.0
90.0
70.0
50.0
30.0
10.0
208.961
153.822
136.957
134.601
127.282
126.529
123.826
77.211
77.000
76.787
48.752
32.324
24.460
11.587
1
X : parts per Million : 13C