UNIVERSITE CATHOLIQUE DE LOUVAIN

GROUPE DE RMN

Processing Manual

VERSION 1.1

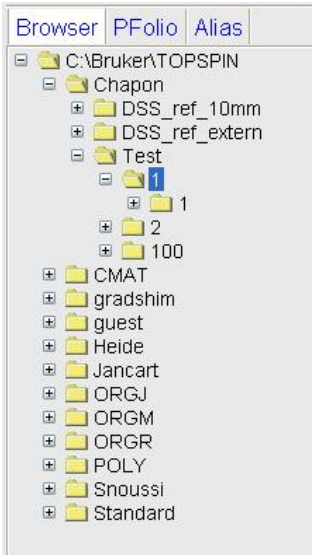
by Dr David Chapon -21/06/06

1. Display Description

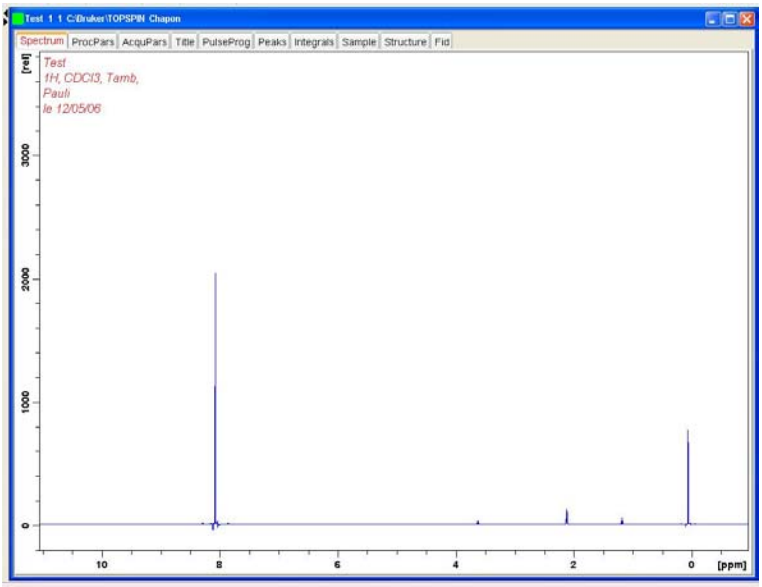
- The menu line

- Two icon lines

- The browser



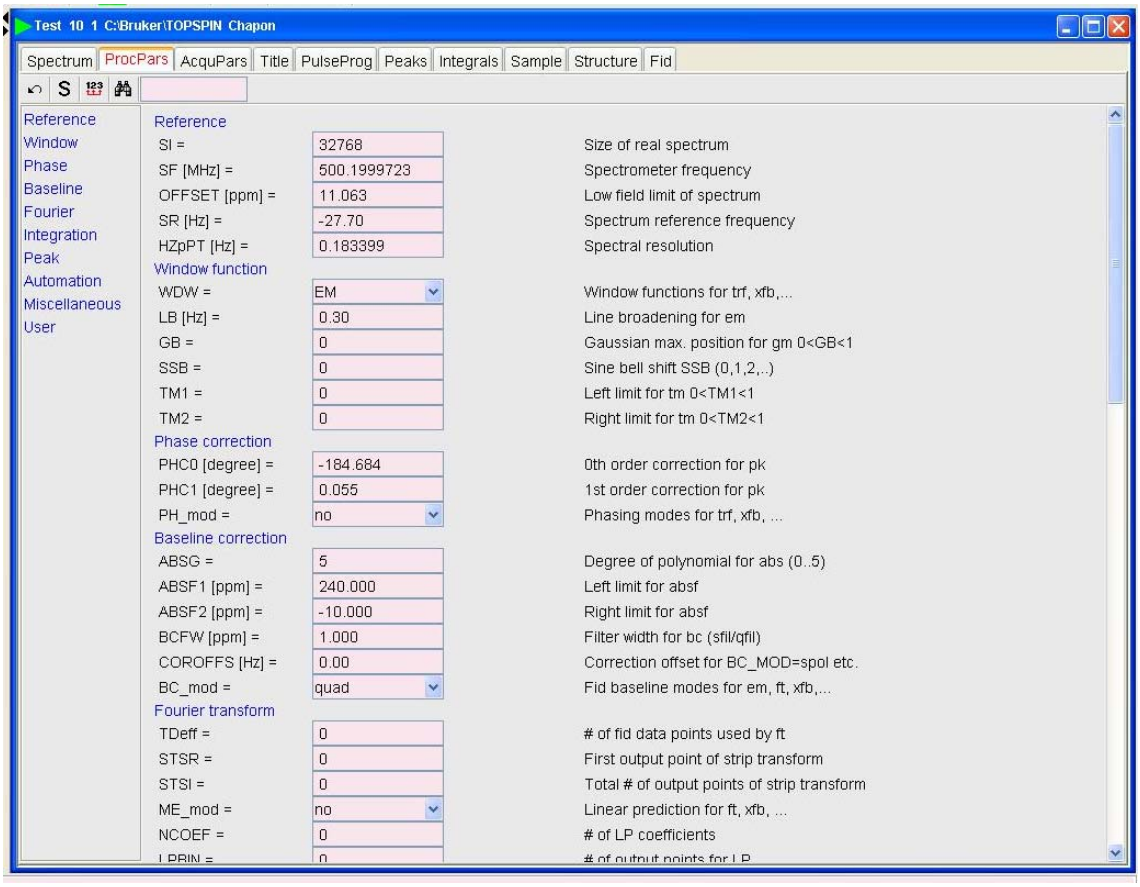
- The spectral window



- The command line

2. 1D Experiment Processing

- Open your spectrum by double clicking on its name in the browser window or dragging it from the browser to the spectral window.
- Check the processing parameters in the process parameter window (ProcPars menu) before doing the Fourier transform of the signal.



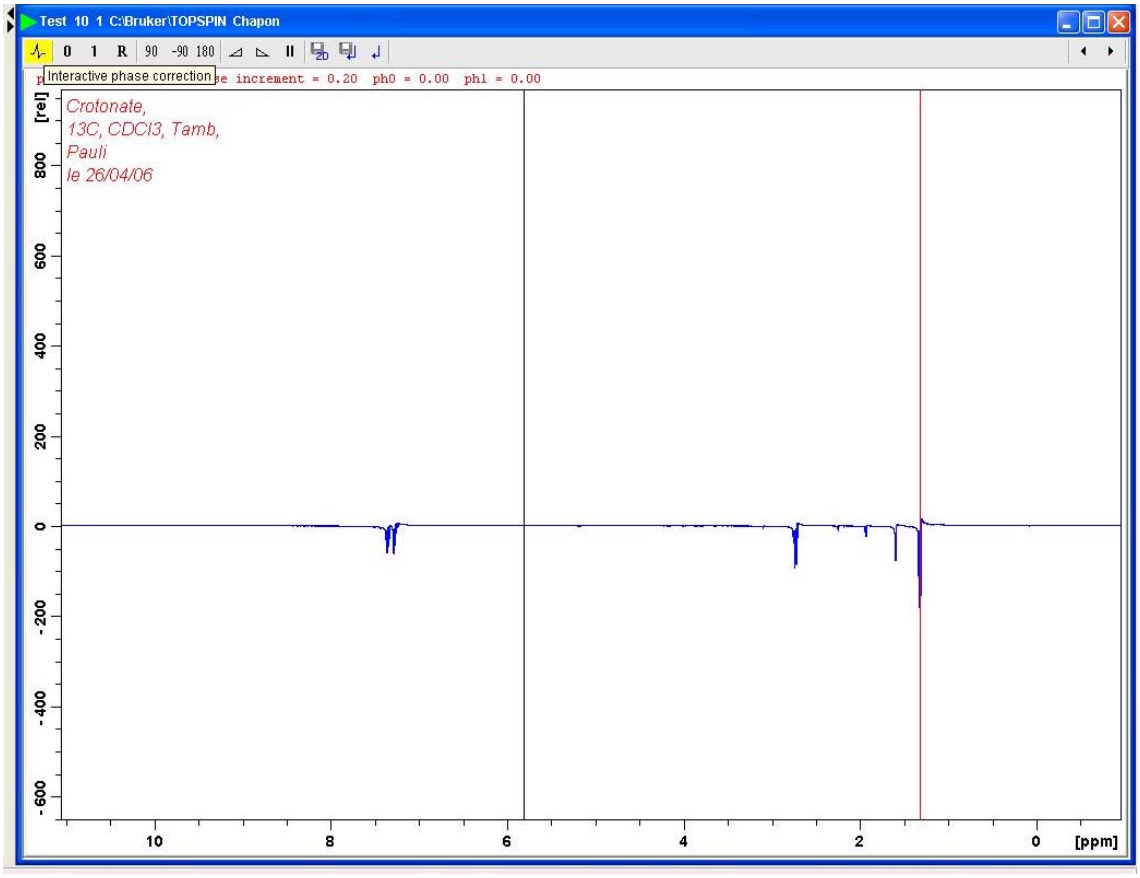
Essential processing parameters for 1D treatment
• SI: Number of points in the frequency domain. If SI > TD/2, the FID is zero filled (TD: Number of points in the acquisition time domain: AcquPars menu). • SR: Spectrum reference. Parameter to report in each 1D spectrum to calibrate them in the same way (the spectrum calibration is correlated to this parameter).

- WDW: Choose EM to apply an exponential multiplication to your FID.
- LB: Factor of line broadening for EM. Enter 0.3 as standard for ^{1}H and 2.0 for ^{13}C.

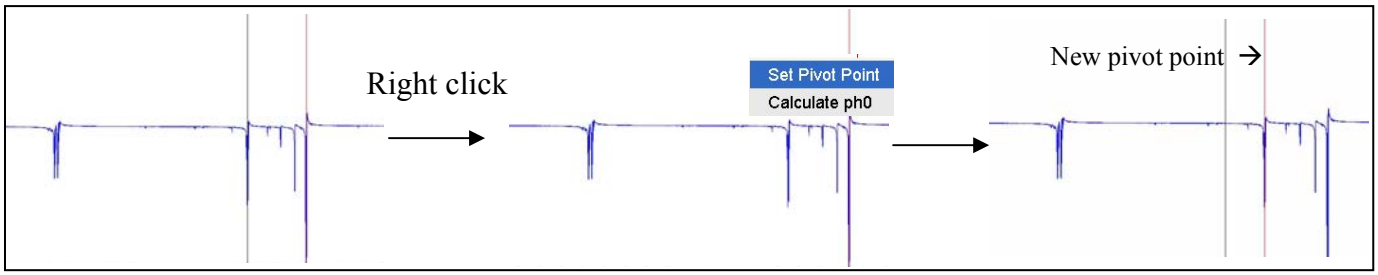
➢ Click on Process 1D in the icon line to do a Fourier transformation, an automatic phasing and a baseline correction.

1. *Phase Correction*

➢ If the phase is not correct, phase the spectrum manually by clicking on  icon. You will move in the following window.



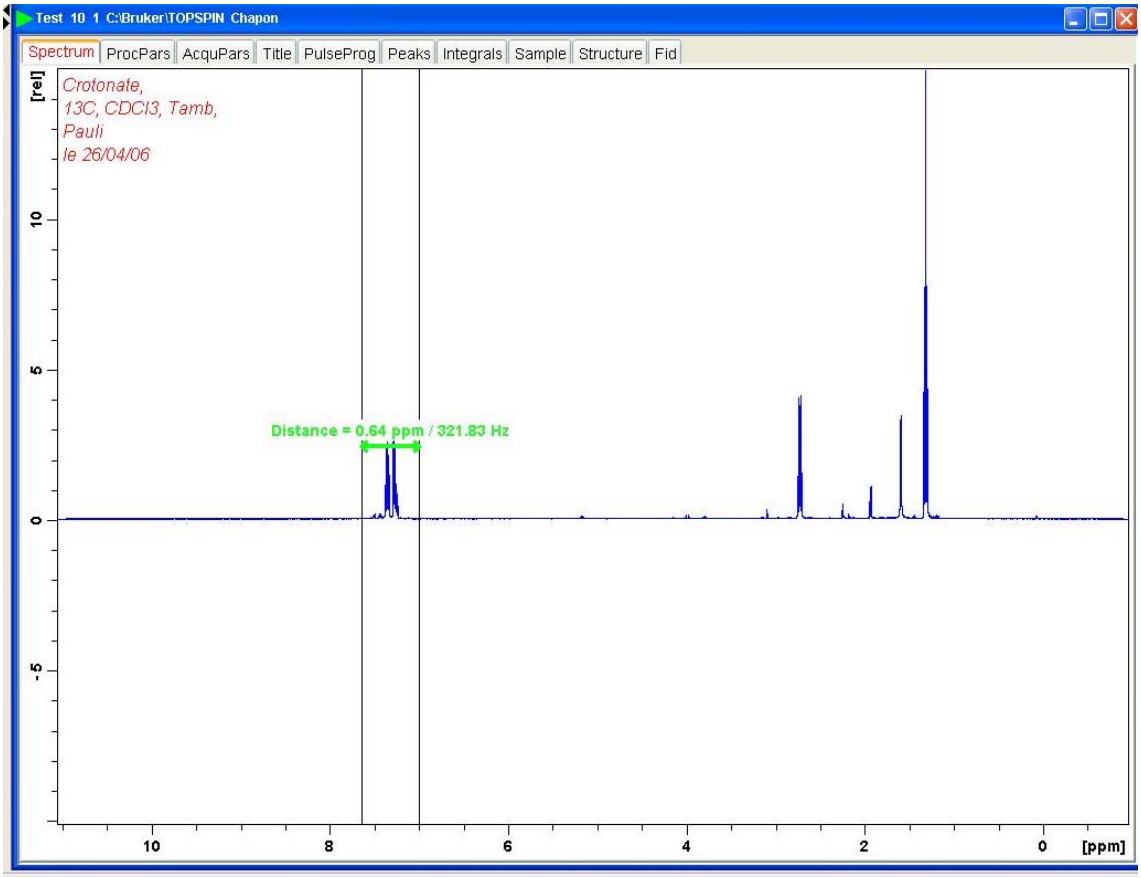
- The red cursor on the spectrum is the pivot point for the first order phase (by default the biggest signal). If you want to change this pivot point put the black cursor on another signal. Click right with the mouse, and select Set Pivot Point.



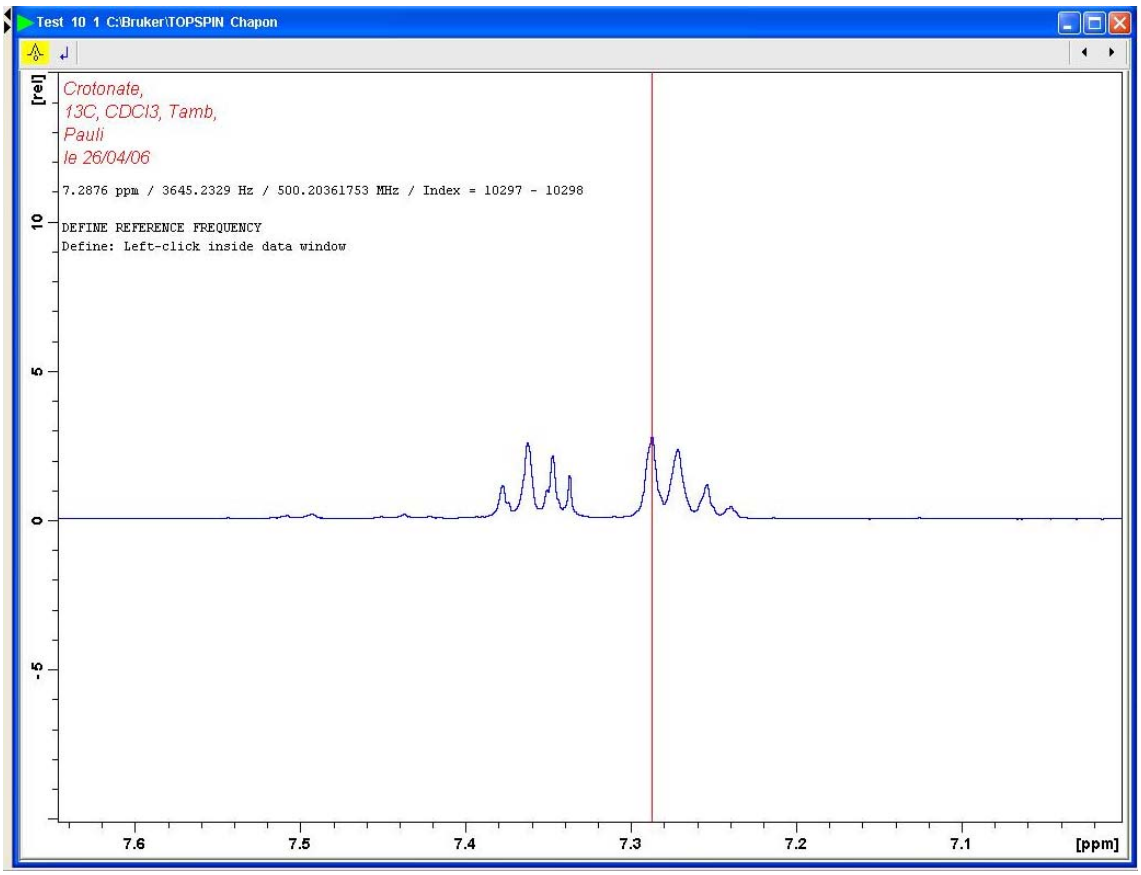
- Phase to zero and first orders by keeping clicking the mouse left button respectively on the two icons 0 (zero order) and 1 (first order) and moving the mouse vertically.
- When the spectrum is correctly phased click on to save the phase and return to the classical spectral window.

2. *Calibration*

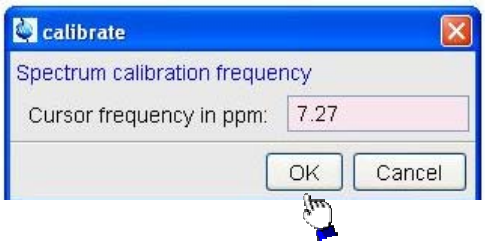
- Do an expansion of the signal you want to calibrate by keeping clicking the mouse left button and moving the mouse from one side to the other side of the selected signal (with  icon activated).



- Calibrate the spectrum by clicking on  icon. You will move in the following window.



- Put the red cursor on the top of the signal you want to calibrate and click left.
- The following window appears.



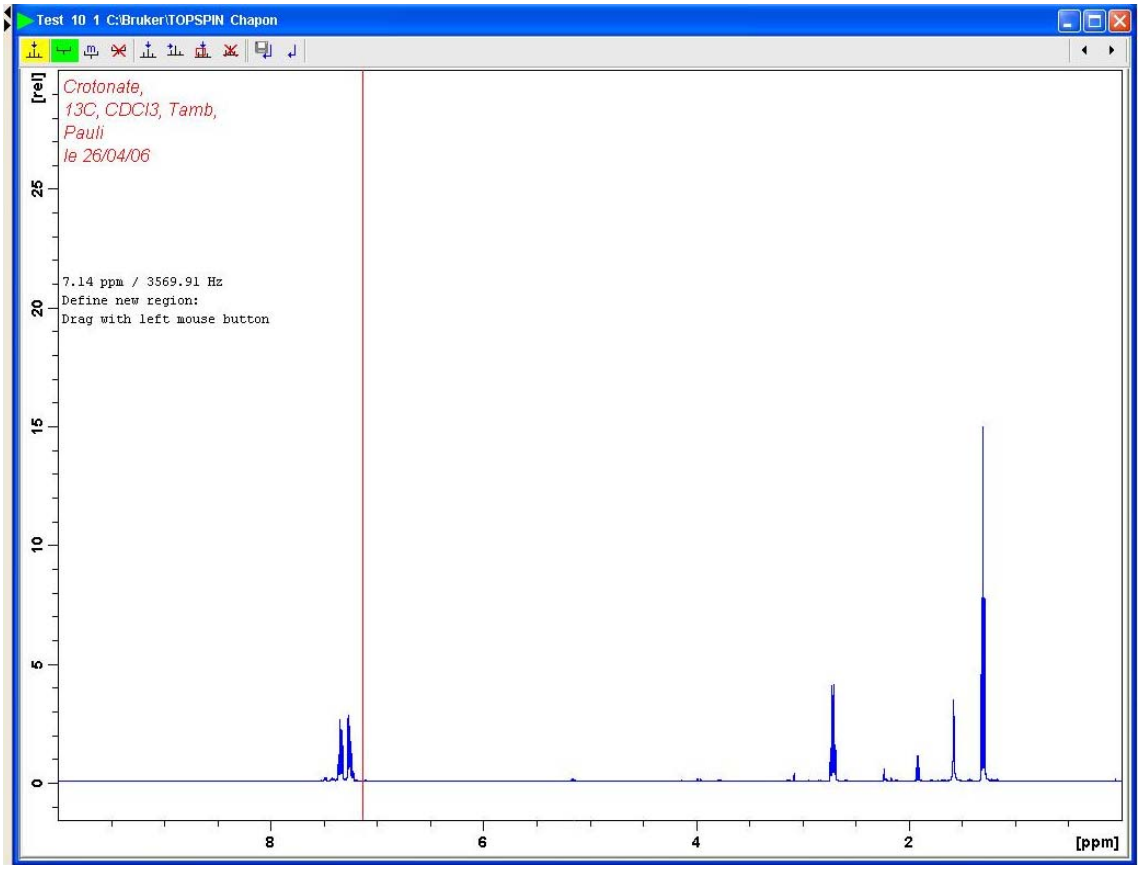
- Enter the new value of chemical shift (in ppm) and click on OK. You will automatically quit this calibration window.

3. *Baseline Correction*

- You can click on  icon to do a specific baseline correction. The easiest way is to enter ‘abs’ in the command line, it will do a classical baseline correction + automatic integration of the main patterns. You could change the integration of these patterns in the integration mode. Enter ‘abs n’ in the command line to do only a baseline correction without integration.

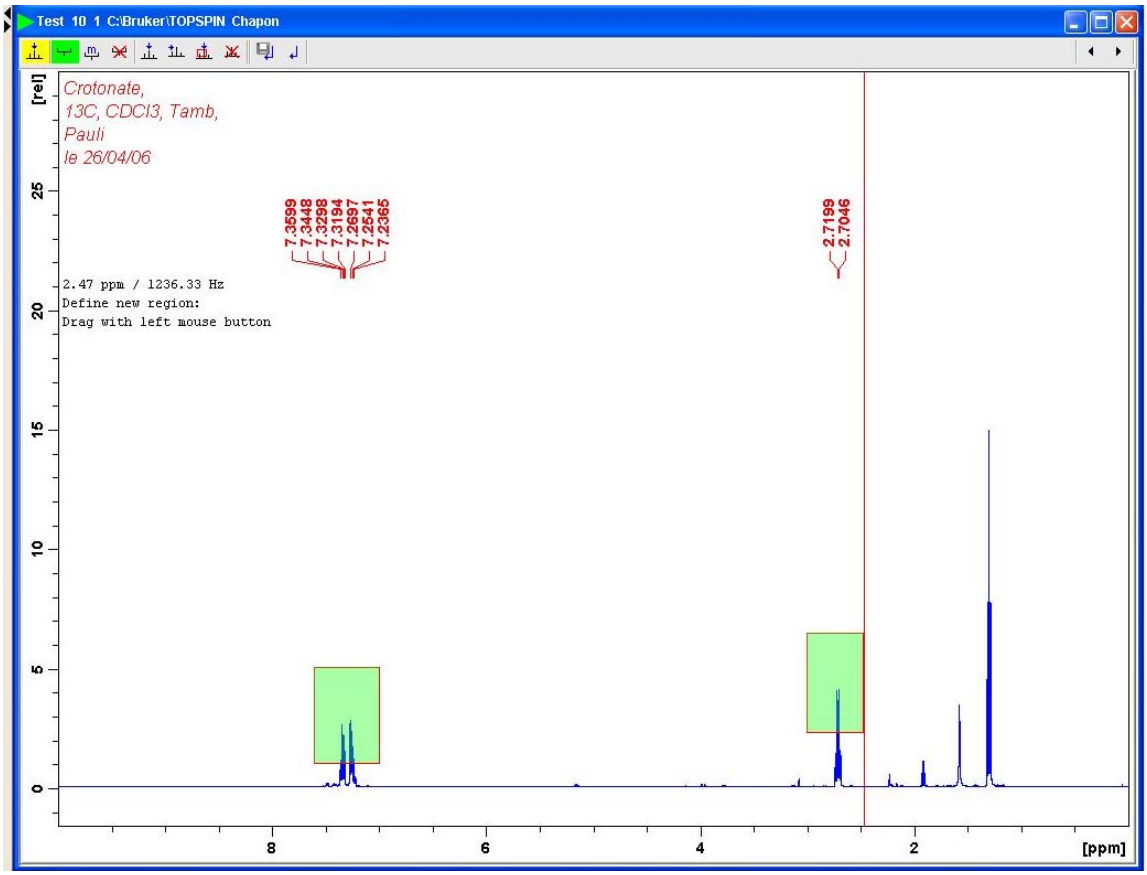
4. *Peak Picking*

- Click on  icon to enter the peak picking routine. It will open the following window.



- The icon  is activated by default.

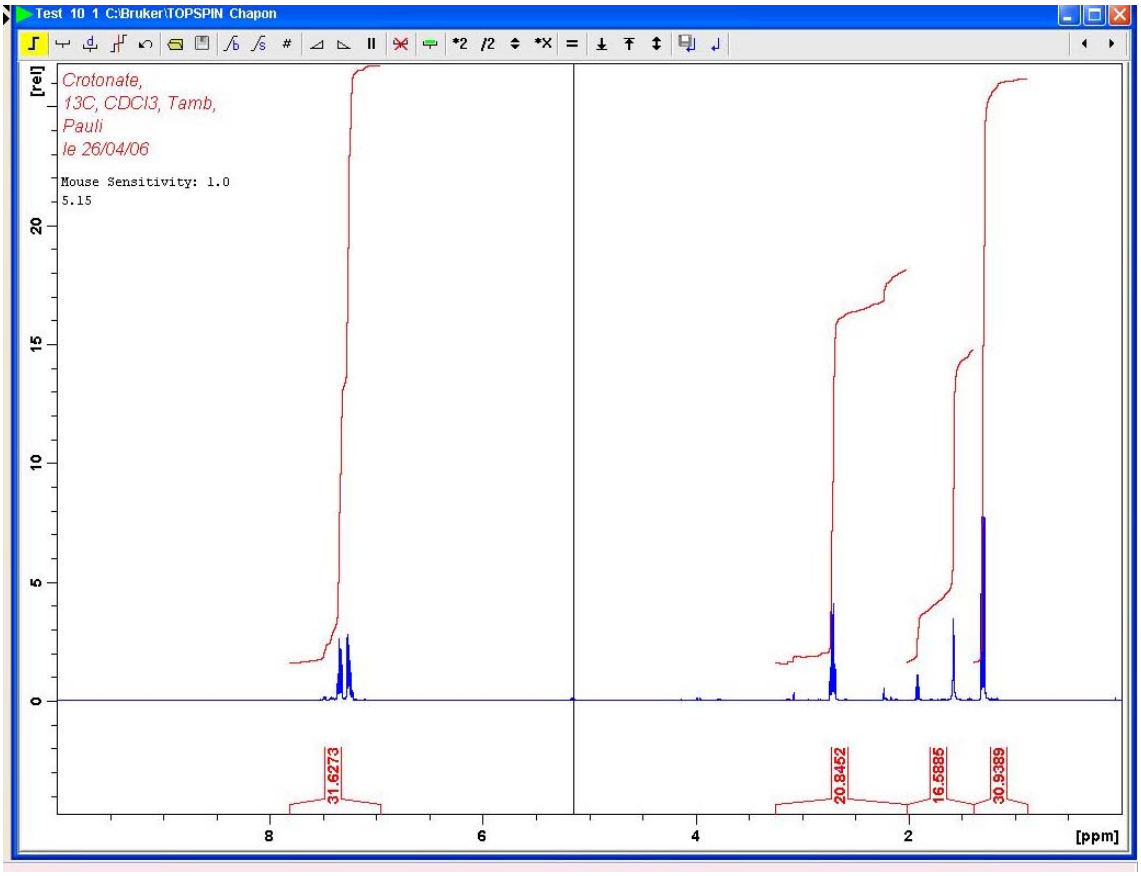
- On the signals you want to peak pick, draw a green region with the mouse (by keeping clicking the left button of the mouse) as in the following window. For each selected region the peak picking appears in red at the top of the window.



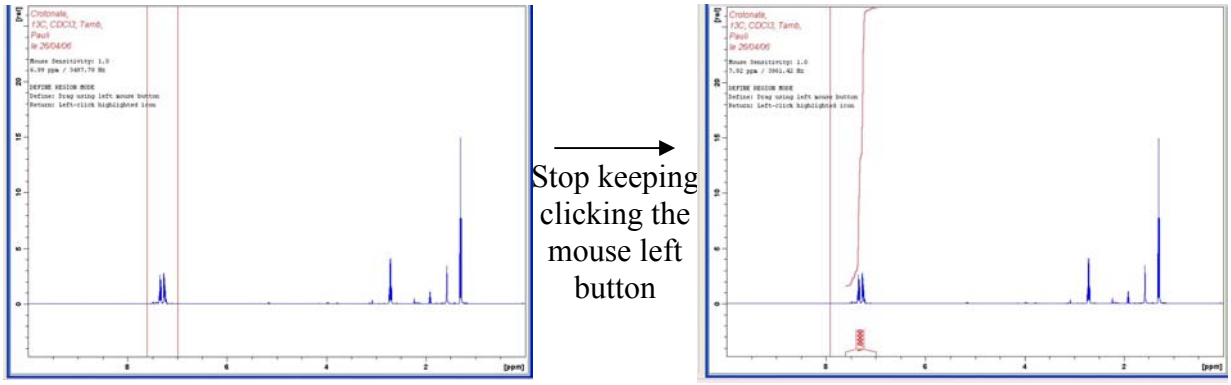
- You can expand the selected regions by activating the icon, and move the limits of each green region with the mouse.
- You can delete the peak picking or the selected regions by clicking respectively on or icon.
- When you have finished with the peak picking click on icon to save it and return to the spectral window.

5. *Integration*

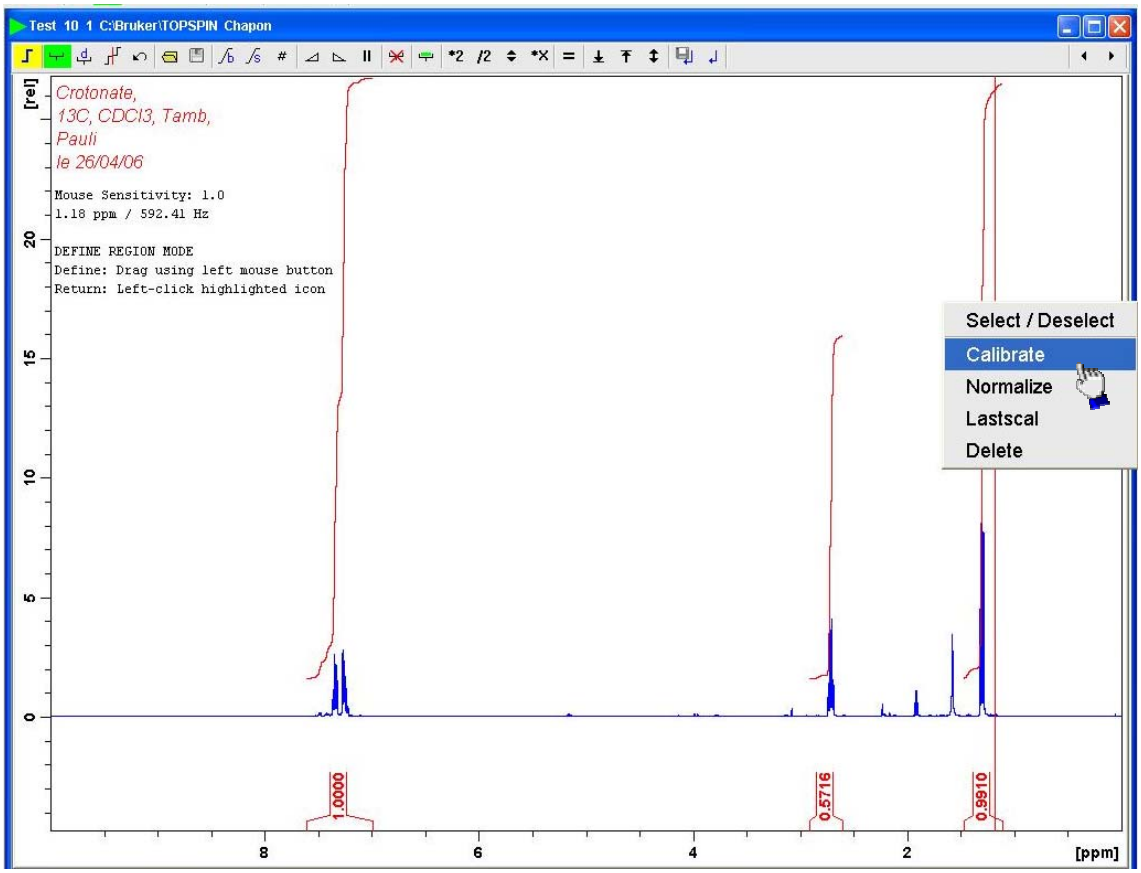
- Click on  icon to enter the integration routine. It will display the following window.



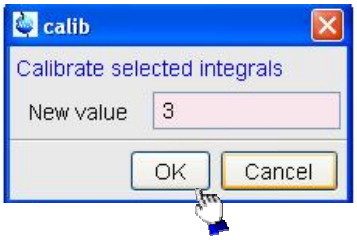
- If you have some integrals displayed, there are those obtained before with the 'abs' command. If you want to delete them: First click on  icon to select all the integrals (all the integrals labels are then coloured in green) and click on  icon to delete them. It will ask you whether you are sure to delete all the integrals: Click on OK.
- Click on  icon to do a manual integration (it is activated when it is green).
- Create your integral by keeping clicking the left button of the mouse and move the mouse from one side to the other side of the signal you want to integrate as in the following window.



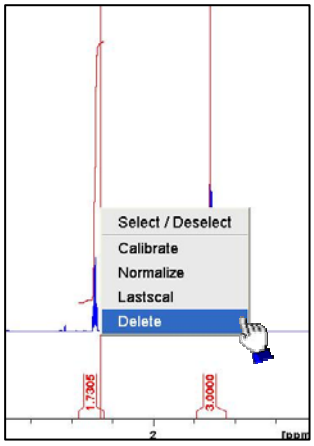
- The first integral defined takes by default the value 1.
- Proceed with all your signals in the same way.
- To calibrate one integral put the cursor under it, click right and select the line Calibrate.



- In the open window, enter the new value of your integral, and click on OK.



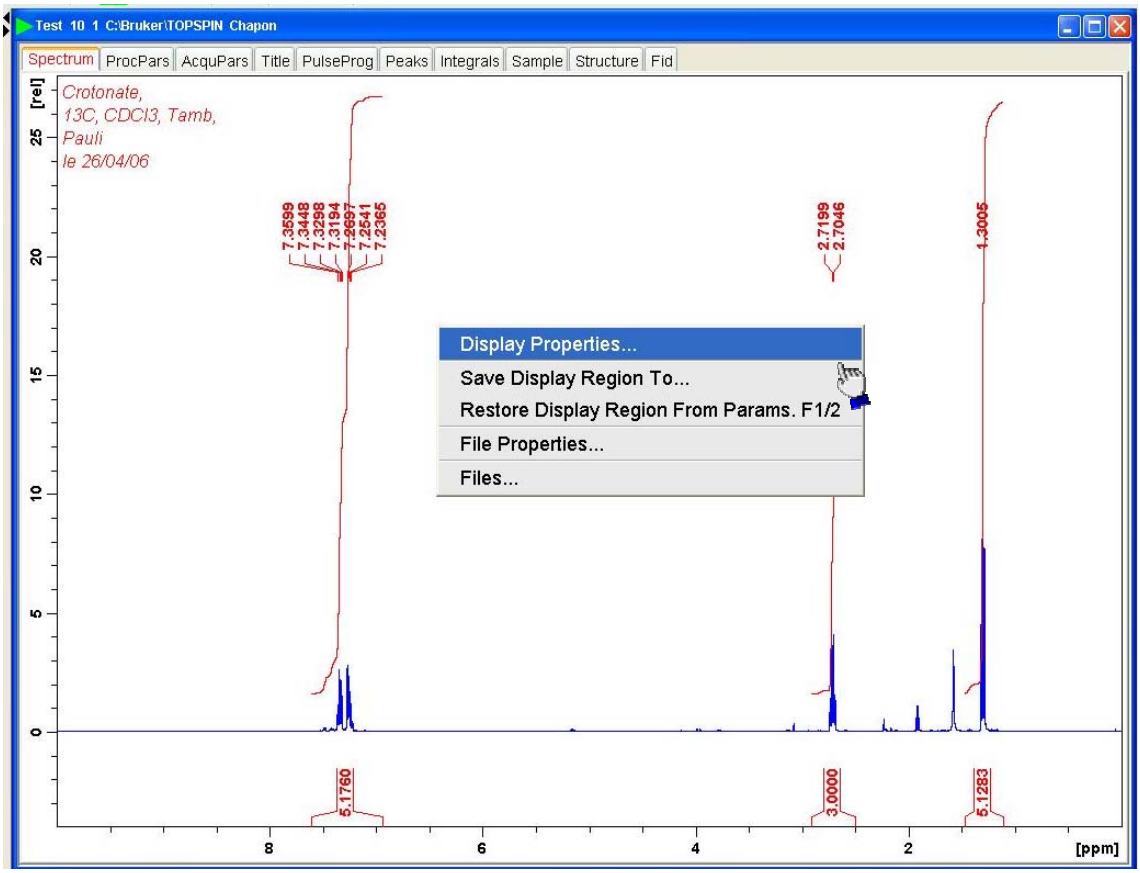
- If you want to delete one integral, put your cursor under it, click right and select Delete.



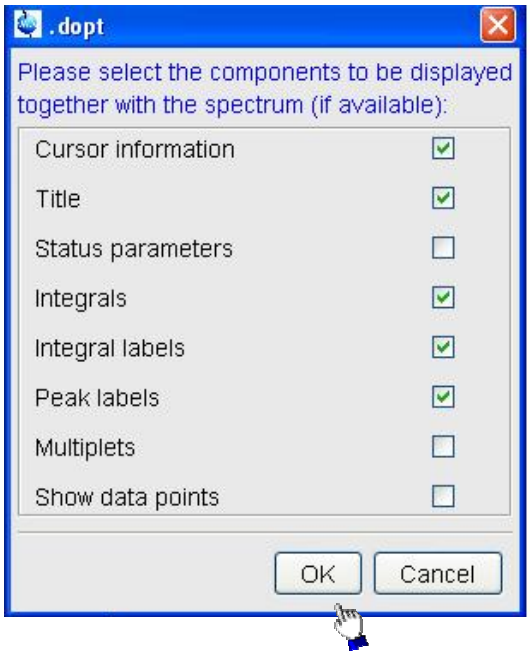
- If you want to adjust the slope or the bias of one integral, select it by a right click with the cursor under the integral. When it is selected the integral value is coloured in green. Change the slope and the bias by keeping clicking the mouse left button respectively on the icon  and  and moving the mouse vertically.
- When you have finished with the integration click on  icon to save it and return to the spectral window.

6. *Printing*

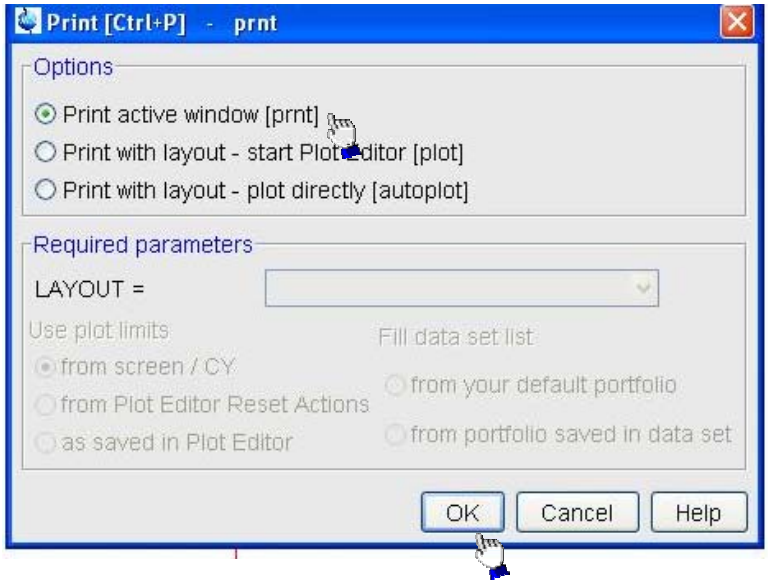
- Display in the spectral window what you want to print. Thus click right in the spectral window and select Display Properties.



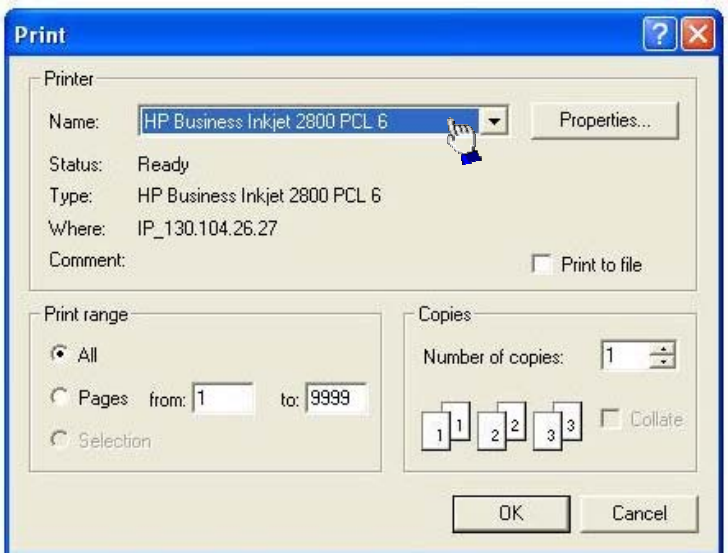
- Select the parameters you want to display on the following window.



- When you have all your desired parameters on the spectral window, click on  to print. The following window appears.

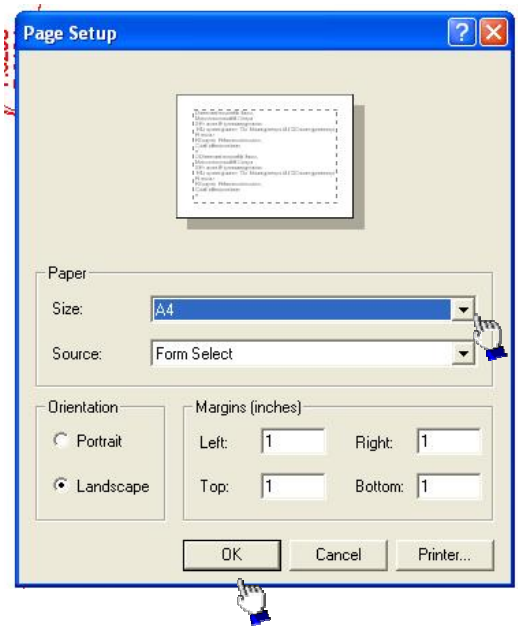


- Select Print active window, the following window appears.



- Select your printer and click on OK.

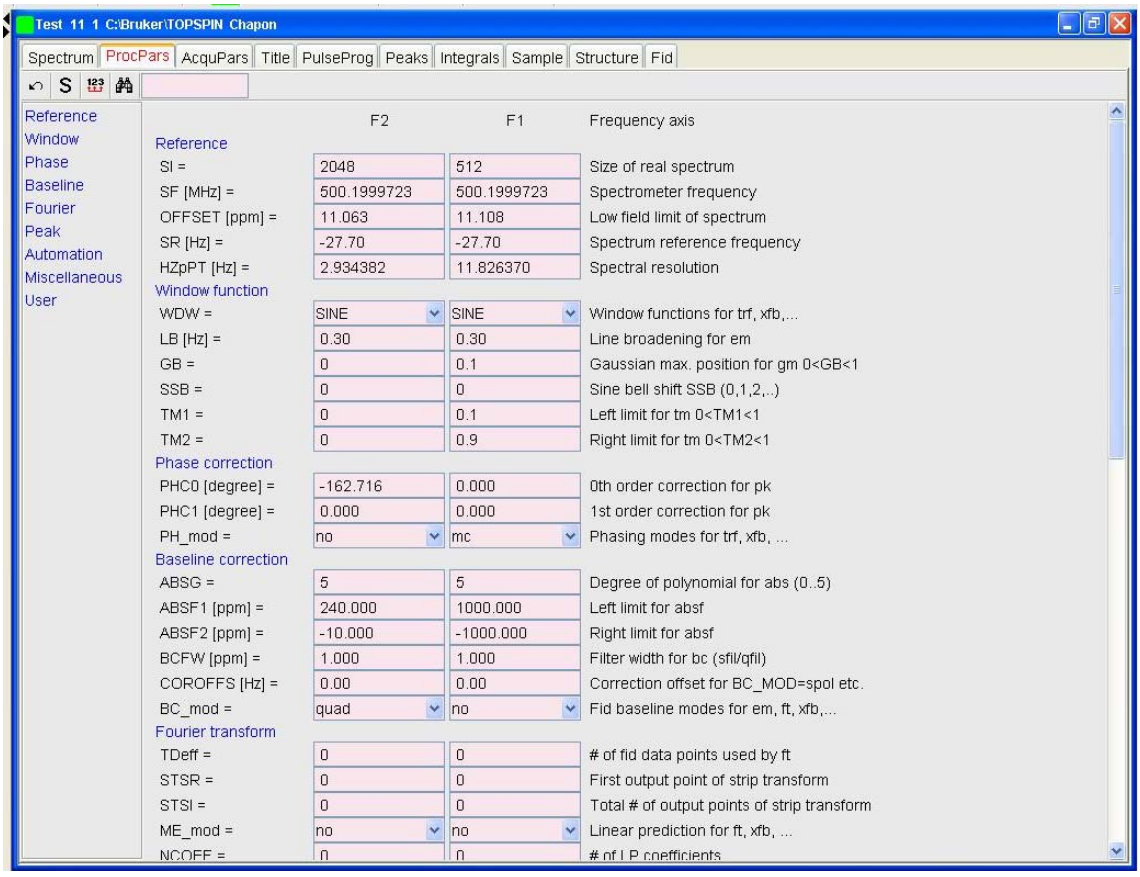
- The following window appears.



- Select the size of your desired paper (A3 or A4), and click on OK.

3. 2D Experiment Processing

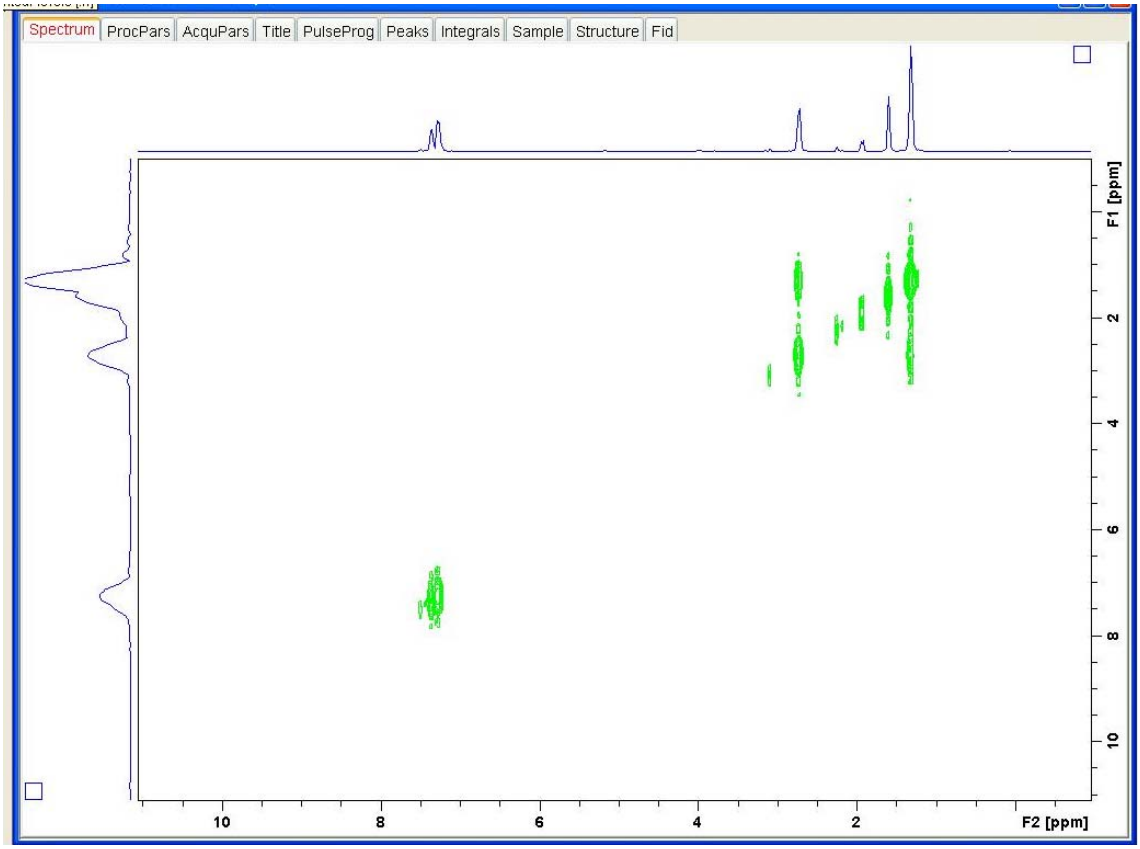
- Open your spectrum by double clicking on its name in the browser window or dragging it from the browser to the spectral window.
- Check the processing parameters in the process parameter window (ProcPars menu) before doing the Fourier transform of the signal.



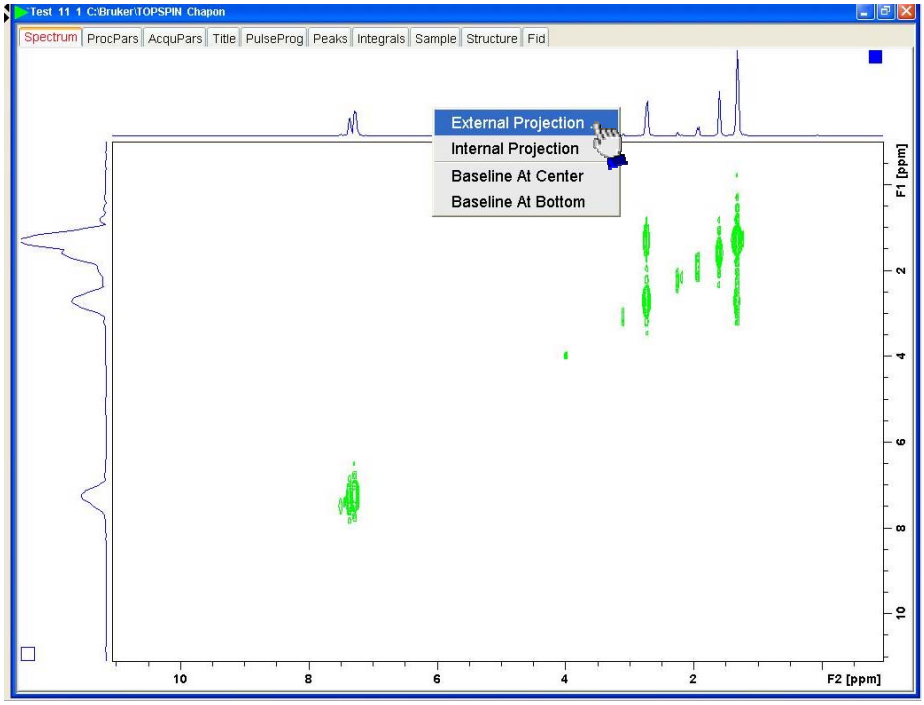
Essential processing parameters for 2D treatment
• SI (F1/F2): Number of points in the frequency domain. For each dimension, if SI > TD/2, the FID is zero filled (TD: Number of points in the F1/F2 time domain: AcquPars menu).

- SR: Spectrum reference. Put the same value of 1D spectrum to calibrate each dimension of the 2D experiment as the 1D experiments.
- WDW: Choose EM to apply an exponential multiplication to your FID.
- LB: Factor of line broadening for EM. Enter 0.3 as standard for ^{1}H and 2.0 for ^{13}C channel.

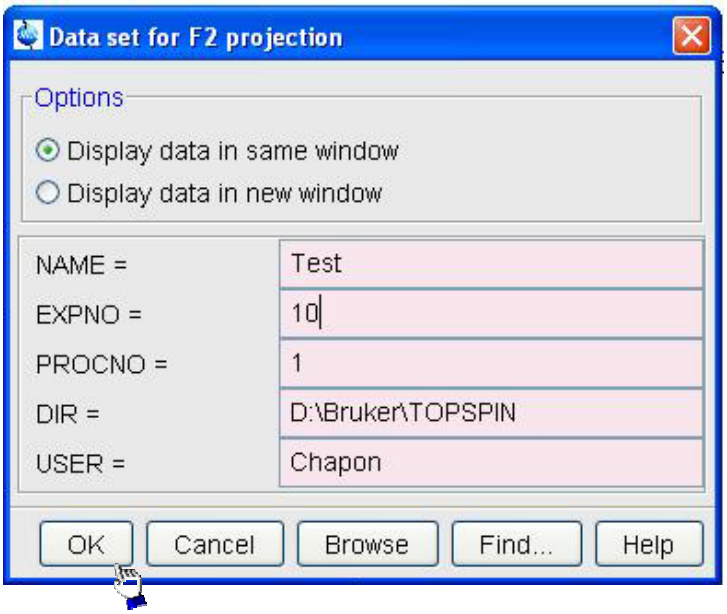
➢ Click on Process 2D in the icon line to do Fourier transforming. You will have the following display in the spectral window.



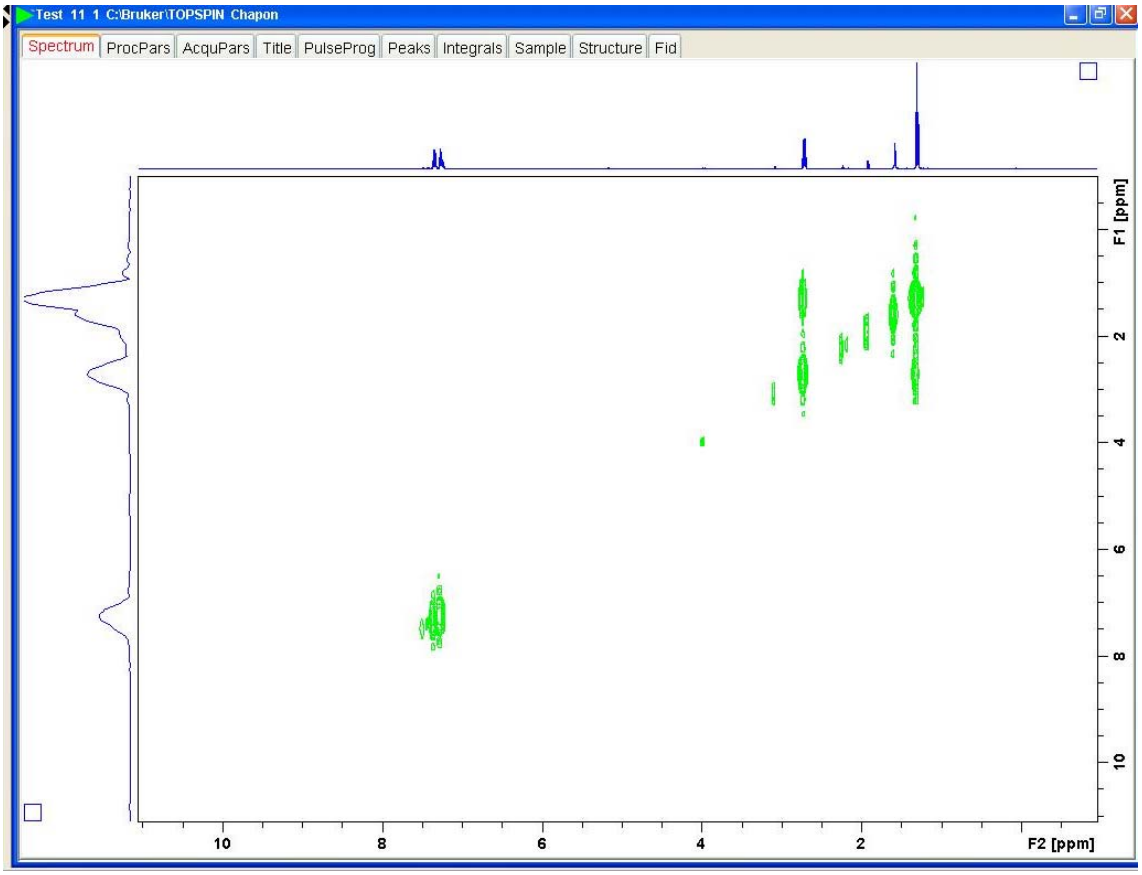
- Add the correct 1D external projections on each side of the 2D by clicking right on a 1D projection, and select External Projection.



- Fill the following window with the user, the name and the experiment number of the 1D experiment, and click on OK.

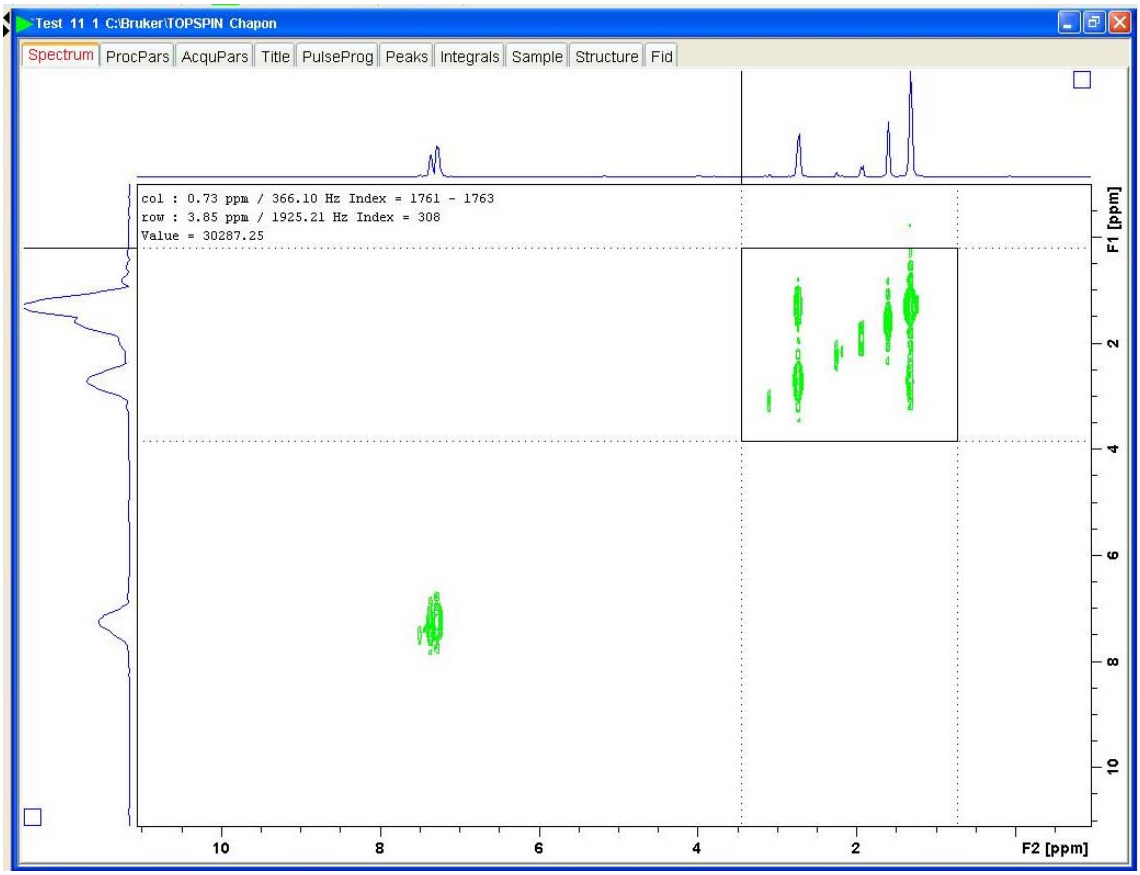


- It will display the select 1D spectrum as in the following window.

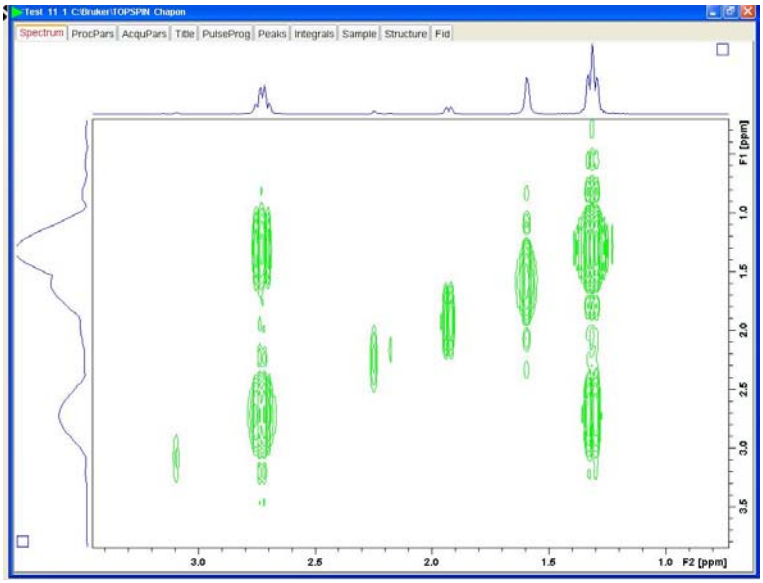


- Proceed with the second dimension in the same way.

- To do an expansion on the 2D spectrum, keep clicking the mouse left button and draw a square from one corner to its opposite as in the following example.



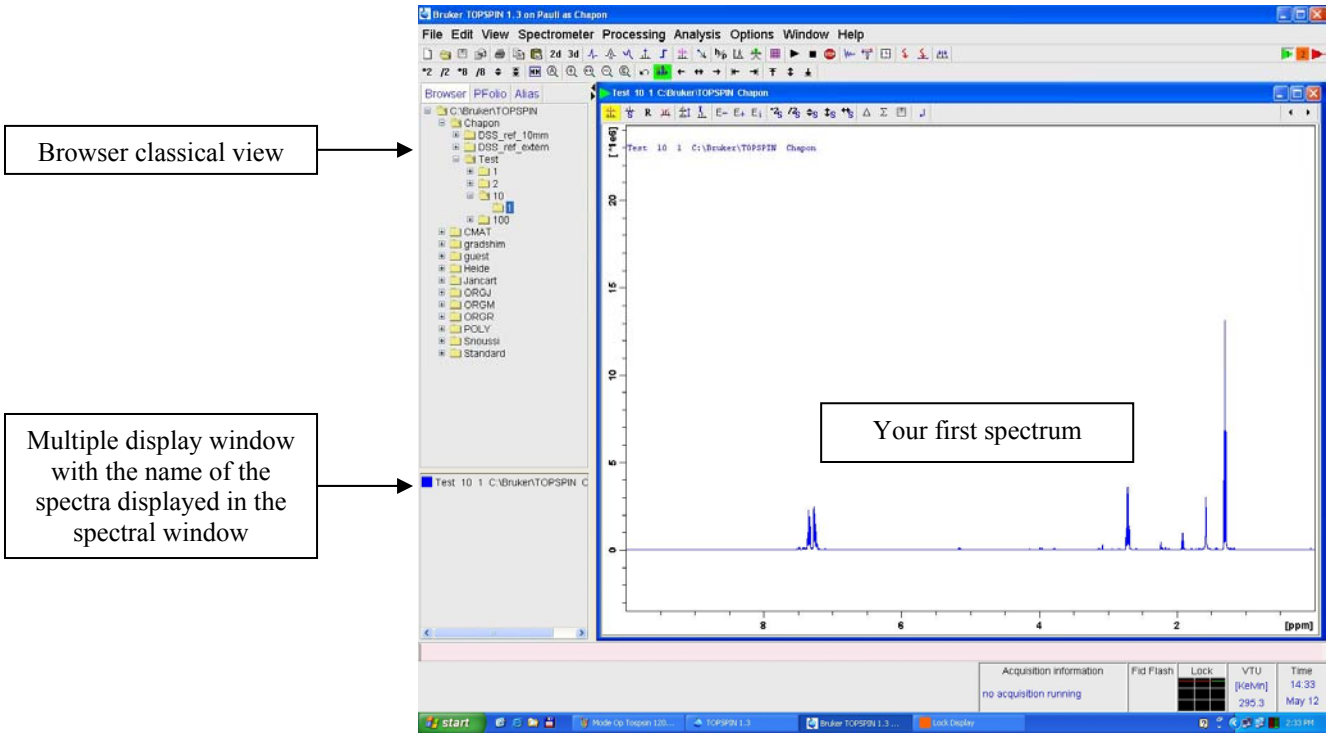
- Stop keeping clicking the mouse button, and your expansion automatically appears.



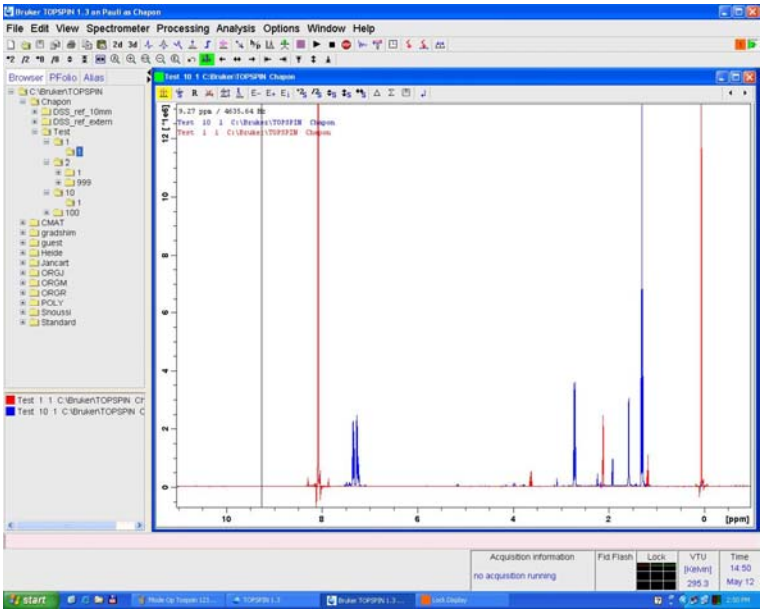
- To print, display what you want on the spectral window and proceed as with a 1D experiment (see p.12)

4. Superposition of several spectra

- With a first spectrum opened in the spectral window, click on  icon to enter the multiple display menu. You will obtain the following window on the screen.

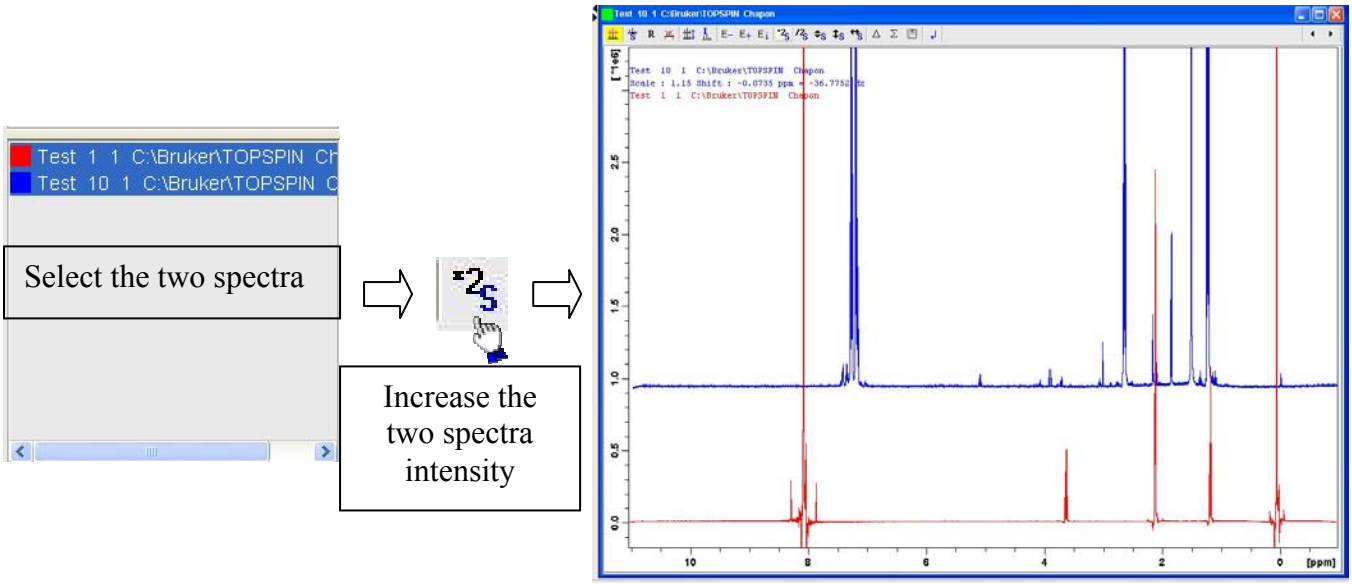


- Select the second spectrum you want to display in the browser and double click on the experiment number or drag it in the spectral window; it will automatically appear in red in the spectral window and in the multiple display window.

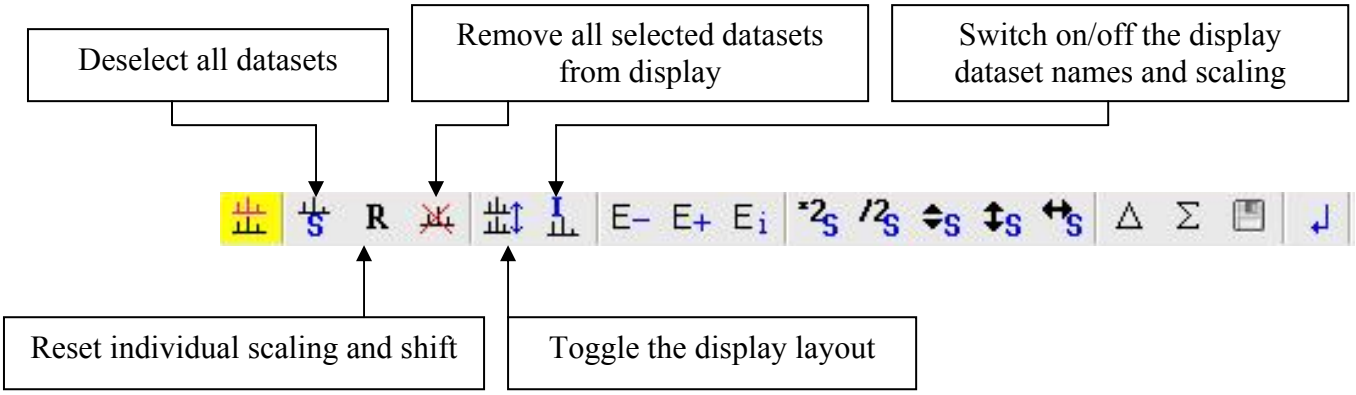


- Select one of the spectra in the multiple display window.

- On the first icons line of the spectral window, move up or down the selected spectrum by keeping clicking the  icon with the left button of the mouse and move the mouse vertically.
- You can increase/decrease the intensity of the selected spectrum or both by selecting your spectra in the multiple display window and click on  icon.



- In the same way, click on  icon to move the selected spectra horizontally.
- Click on  or  icons to respectively do the difference or the sum of the two spectra.
- You will find in the following window the details of the rest of the most interesting icons:



- You can now add a third spectrum by processing it in the same way.

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