Quick Start

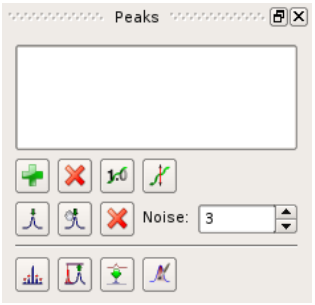
24 May 2011

Introduction

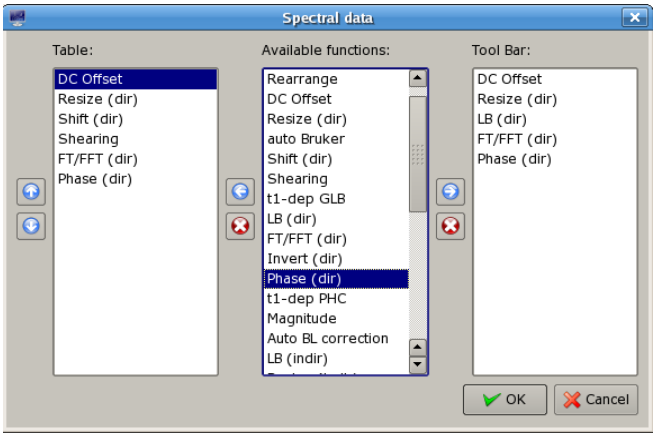
In these short notes a simple one-dimensional (1D) processing of an example data, taken from the Varian Inova spectrometer will be explained. GSim is possibly not the simplest NMR processing software for novices, and this script is aimed to assist this kind of users.

Customisation

GSim is a very customisable program. It is likely that following this document you would be not able to get access to some of the described functionality. The most likely cause, of course, that your version is customised in a slightly different way that required in this tutorial. Below is a description how to get an access to the functions required by this short notes.
First of all, let ensure that you have an access to the panel called “Peaks”.
It should look like this:



If, by any reason, it is not available in your system, you can call it using main menu command ‘View->Tools’ and select ‘Peaks’ entry there.
Secondly, we have to customise our toolbar, responsible for the processing operations. Start main menu command ‘View->Options’. On the tab called ‘Processing’ press ‘Edit’ button. A new screen should appear.



At the moment we are interested in two right panels here. The central panel contains a list of all available functions whereas the right panel contains the functions which would have a button on the processing toolbar. Delete all functions from the right panel clicking on the right button with a red cross. Then copy functions needed for this tutorial by selecting them in the central panel and pressing button with blue right arrow. The functions we needed for the simple proccessing are:

```
DC Offset
Resize (dir)
LB (dir)
FT/FFT (dir)
Phase (dir).
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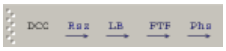
The right panel should looks like on the screenshot above. Close the dialog and ‘Options’ dialog

pressing ‘OK’ buttons. Now you should find a toolbar like this:



If, by some reason, it is not there, ensure that you have selected a menu entry in ‘View->Tools->Processing toolbar’.
Also check that ‘Plot toolbar’ and ‘Main toolbar’ are selected there as well.
Ensure that the ‘Move/Scale’ mode is selected (green 4-side arrow symbol) on the plot toolbar:

Now we are ready to proceed.

Opening datafile

The datafile, used in this tutorial can be found in ‘gsim-extras’ package in ‘tutorial’ folder. Download this package from the GSim website if you haven’t done this yet. The data is taken from Varian Inova spectrometer. Activate command ‘File->Open’ and choose file ‘fid’ in the original directory. Press ‘OK’. You should see 1D FID on the screen.

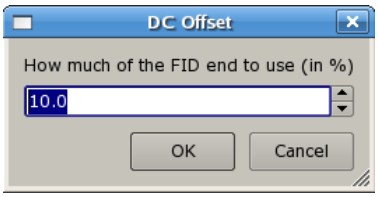
Processing

NMR processing normally includes several processing operations. Below you can find a description for a simplest 1D NMR case.

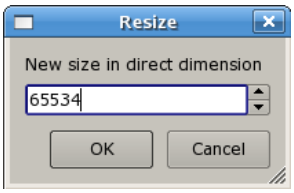
Processing can be done by pressing consequently buttons, created on the processing toolbar.

Below is a short description what should be done for this particular ^{13}C NMR spectrum.

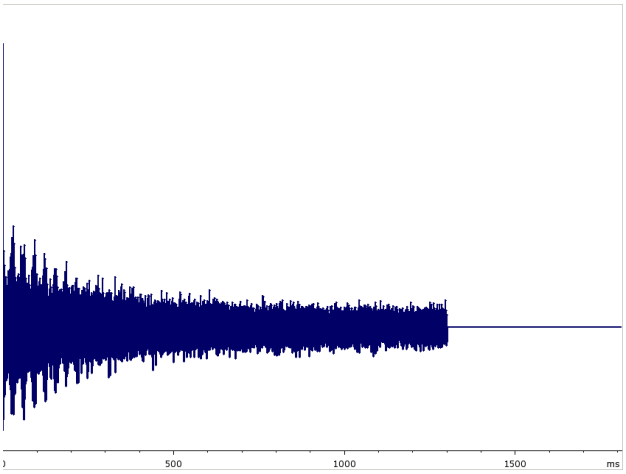
Pressing button with ‘DCO’ icon should perform a so-called DC offset correction. This function ensures that the experimental FID decaying to zero value at the end. Leave a default value of 10% in the dialog box. That means the average value of the 10% of FID points will be taken at the end of the FID to find an overall offset of the data. Press ‘OK’:



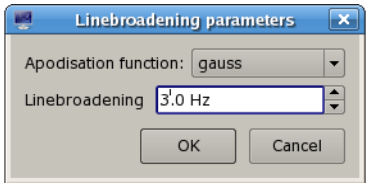
Pressing button with ‘Rsz’ icon you will apply resizing (zero-filling) of the current dataset. Zero-filling changes the number of datapoints in the final FID. See specialised literature for details. It is advisable to use a number of points equal to power of 2, *i.e.* ..., 256, 512, 1024, 4096, 8192, 16384, ... In our case type ‘65534’ in the prompt dialog and press OK:



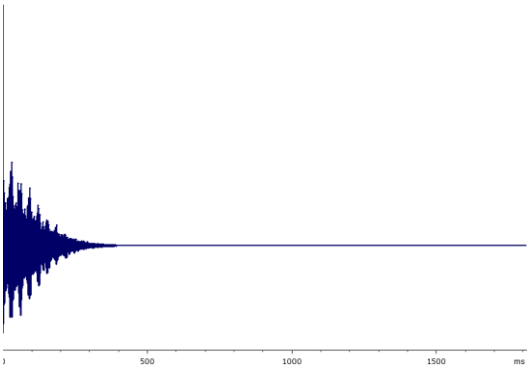
The main screen should looks like:



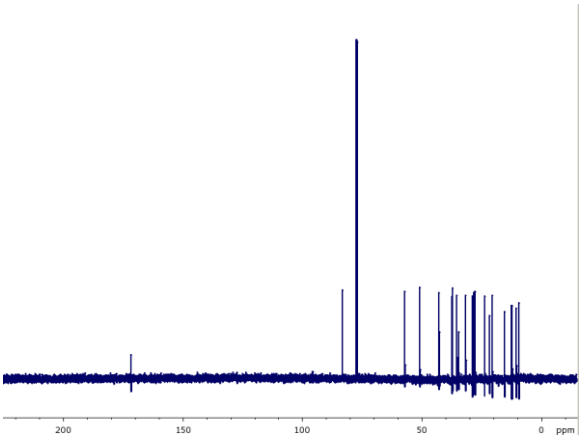
Pressing button with ‘LB’ label you will apply line-broadening (apodization) for the current FID. See specialised literature for details. Choose ‘gaussian’ type of broadening of 3 Hz linewidth in the prompt dialog:



The main screen should looks like this now:



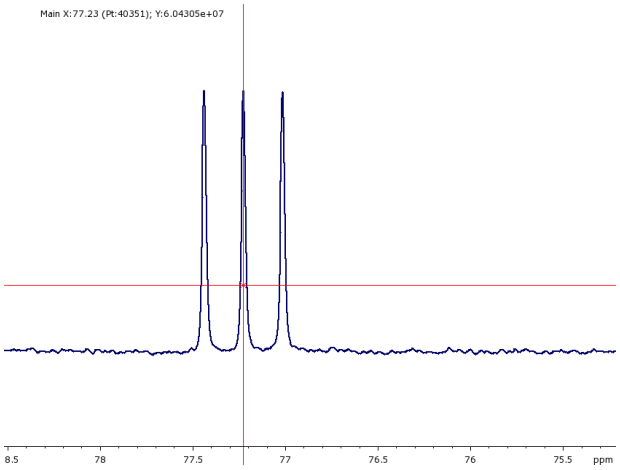
Pressing ‘FTF’ button the Fourier transformation of the time-domain FID into frequency domain spectrum is applied. The main screen should looks like:



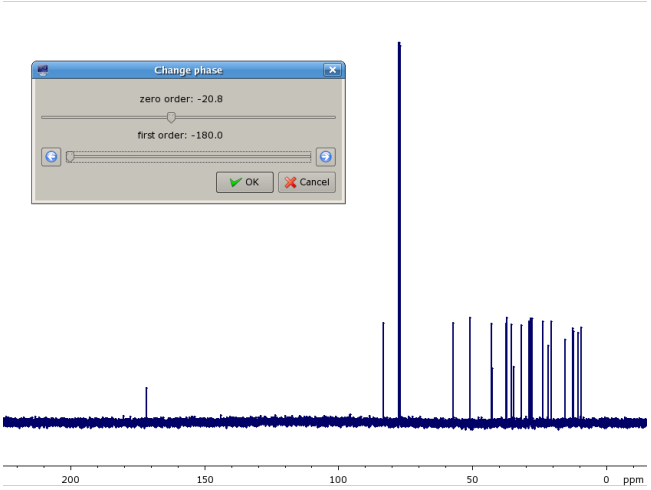
If the units are not ‘ppm’ then keep clicking on the unit label (bottom right corner of the main screen) while ‘ppm’ units have appeared.

Now we need to apply phase correction pressing ‘Phs’ button on the processing toolbar. The zero-

order phase correction looks all right (at least for peaks around 77 ppm) and we are not going to change it. Dragging mouse extend the region around peaks at 77 ppm and set the main marker at the centre of the group:



Using mouse again, shrink a spectrum a bit to see all peaks and use ‘First order’ phase correction sliced till all peaks have a pure absorption (positive) lineshapes.



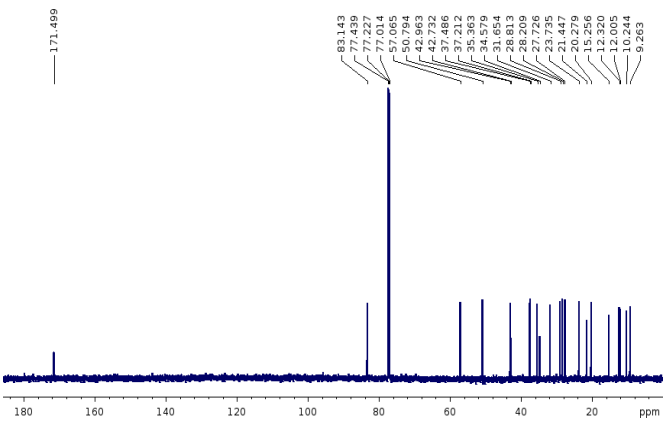
Now the basic 1D processing is finished.

Analysing spectrum

We will perform automatic peak picking and integration of some lines in this section.

Let start from the peak picking. Set the main marker above noise level pressing the left mouse button. Then press  button on ‘Peaks’ panel:

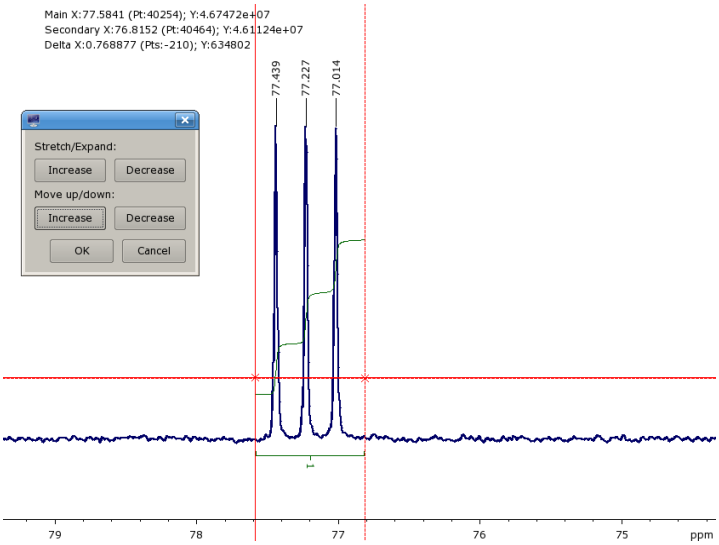
All peaks, found above the main marker position should be labelled. For spectra with high level of



noise you can adjust peak picking sensitivity changing ‘Noise’ parameter in ‘Peaks’ panel. Higher

value corresponds to less sensitivity.

In order to perform integration set the main marker (clicking left mouse button) and secondary marker (clicking right mouse botton) at the edges of the integration region. Then press button in ‘Peaks’ panel. You may require to zoom the region of interest first. Pressing button you can adjust the position and size of the integral curve.



Repeat this procedure for all needed spectral lines. You can remove markers from the screen either by pressing button or pressing ‘M’ on your keyboard.

The current view can be exported by several ways. You can print it (File->Print’), export to PDF (File->Export to PDF), export to vector graphic format, ready for the editing in external graphic applications (File->Export to vector graphics) or simply copy bitmap to the system clipboard (Edit->Copy Screen).

What’s next

Just read the manual for the full description of the GSim functionality. It is worth noting that a processing method described here (which uses processing toolbar) is, probably, the simplest, but not the most effective. Read a section of the manual where the usage of the ‘Processing’ panel is described. You also can use a command line to type your processing command (*ala* VNMR or Xwin-NMR).

Bruker users can have problems processing data, acquired from recent Bruker spectrometers equiped with digital filtering. It is likely you have to use a processing command called ‘autoBruker’ to fix the problem. For the most recent Bruker hardware this command can fail too. Then a manual shift using ‘Shift (dir)’ command can be used. See the command descriptions in the manual. GSim also has special linebroadening functions (bruker_gauss and bruker_lorentz) to deal with this situation.

And finally, have a fun and don’t forget to send your feedback to me!