

# Process 2D NMR data

After the 2D NMR experiment finishes, click just finished 2D data name or click "File -> Open ...." to load the 2D data. In here, a 2D HMQC spectrum (proton-carbon) is used as an example.

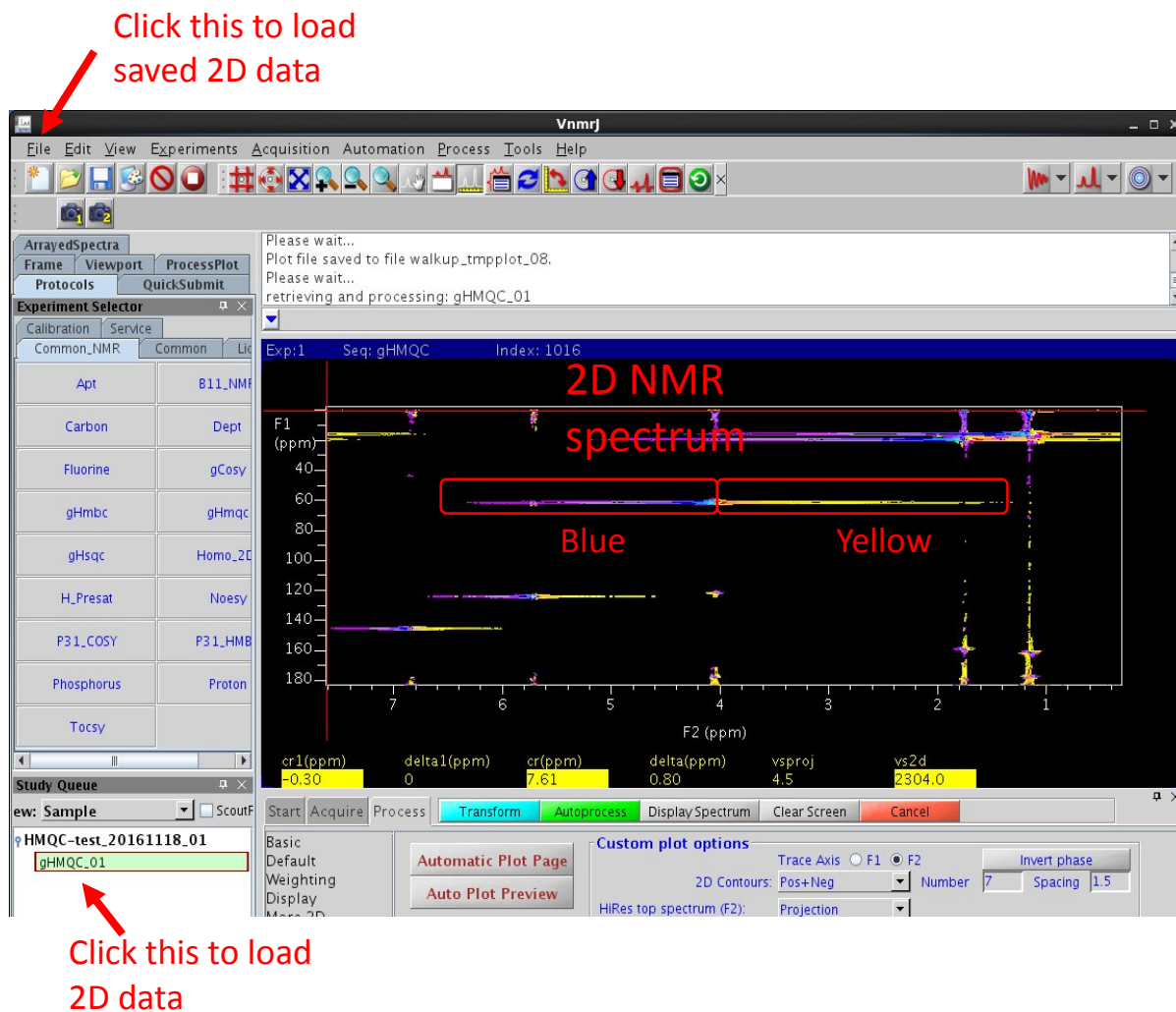


Fig. 1

The 2D NMR spectrum will be displayed in the rectangular box, horizontal is the F2 (H) scale, and vertical is F1 (C) scale. You may notice that there are horizontal lines in the spectrum in which one side is blue (or purple) and the other side is yellow (or red), this means that the phase of the 2D spectrum needs correction.

## 1. Phase correction

Put the red cross cursor on the center of a peak located right upper area, in this example at 1.4ppm (Horizontal) and 14ppm (vertical). The index of the horizontal trace (horizontal line of the cross cursor) is 931, record this

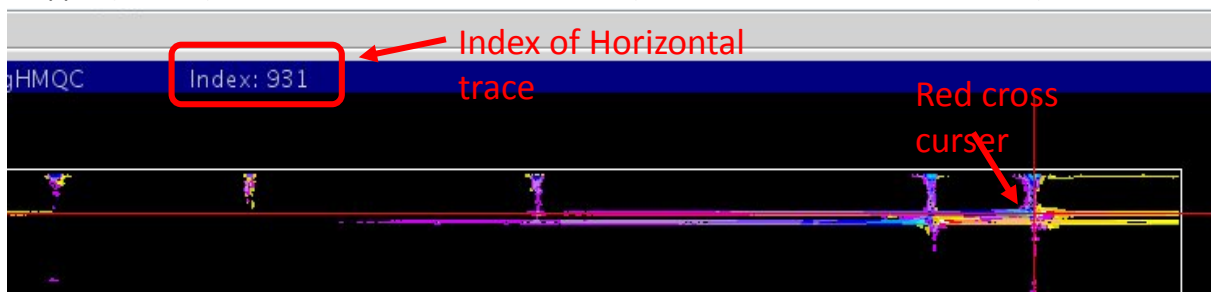


Fig. 2

number for later use. Moves the cross cursor to the center of the peak located at the left lower area, in this example, at 6.8 ppm (horizontal) and 144ppm (vertical), record the index (209) of the horizontal trace.

At the command line, type ds(931), a 1D spectrum appear, this 1D spectrum is the trace of the 2D spectrum at index 931 shown in Fig. 3 You can see that the phase is not good, so, phase this 1D spectrum with normal 1D phasing procedure.

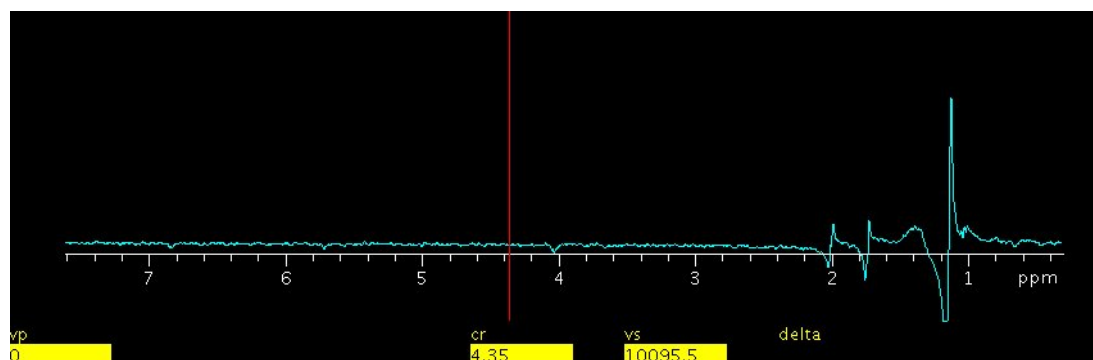


Fig. 3

After phase correction, it looks like in Fig. 4.

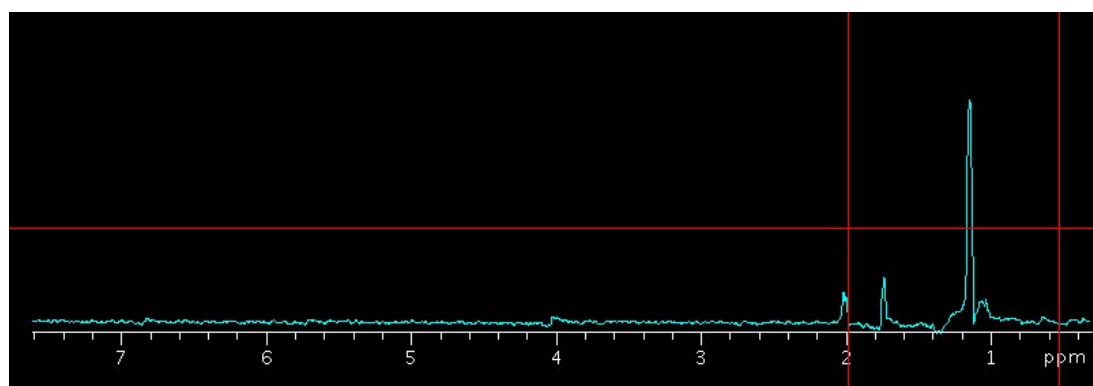


Fig. 4

At command line, type ds(209), the trace of index 209 of the 2Dspectrum is shown as in Fig. 5.

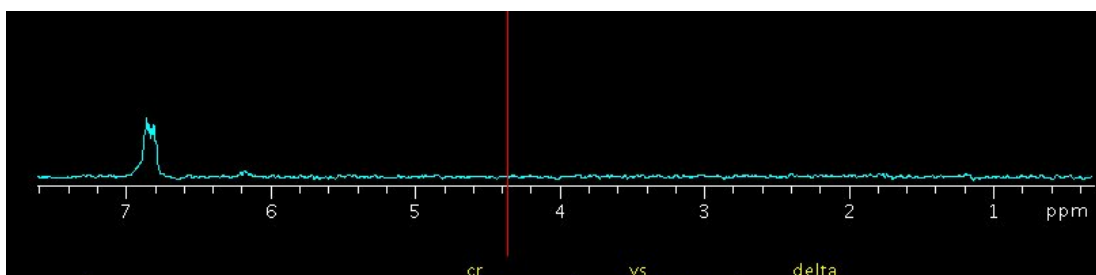



Fig. 5

The peaks of this trace may be good or may need further phase correction. After phase correction of this trace, you need go back to trace 931, to check if the phase is ok, if not ok, then you have to phase it again, then back to trace 209... until you are happy with both traces. Sometime you cannot make the two traces "perfect", you have to compromise.

After phase correction, click  button to display 2D spectrum shown as Fig. 6

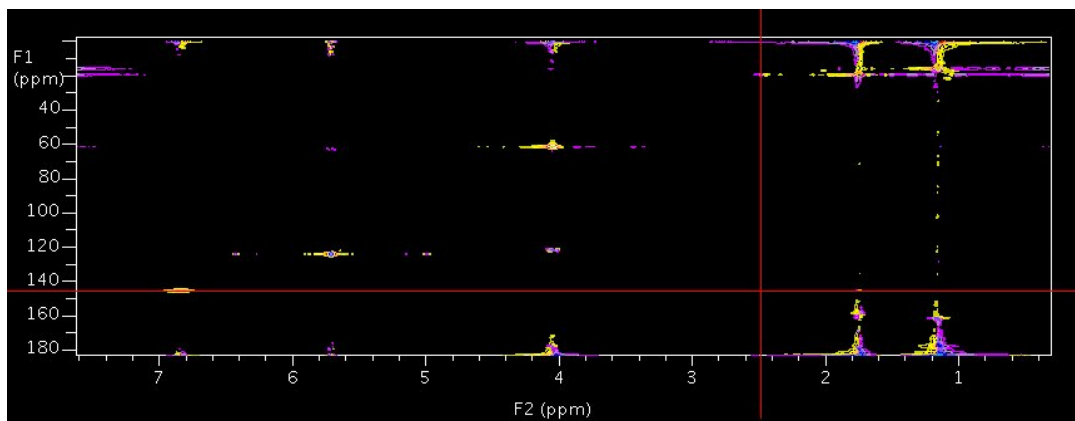


Fig. 6

This 2D spectrum may not look good with a lot of artifacts (noise), but you may adjust the intensity scale by



clicking button many times, the 2D spectrum will look very good as Fig. 7, very clean, it may still have some artifacts, but it is acceptable.

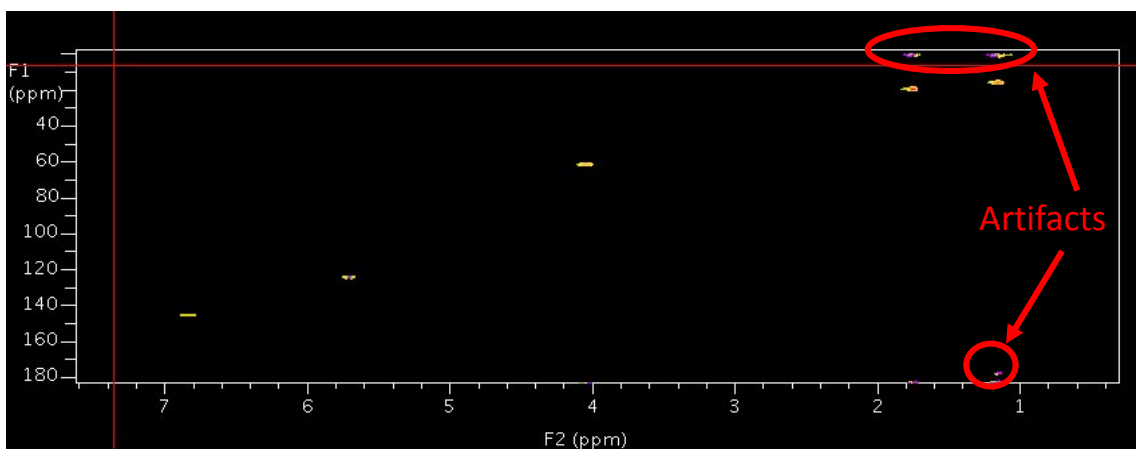


Fig. 7



In some cases, the phase in vertical direction may need correction, so you need to click button to rotate the 2D display (vertical to horizontal, horizontal to be vertical), follow the steps above to correct the phase. Then rotate the 2D spectrum back.

## 2. Reference

The ppm scale may not be accurate, so you may need to reference the 2D spectrum. Some 2D spectra (COSY, NOESY) may have solvent peaks which can be used for reference, some 2D NMR spectra may not have solvent peaks for reference, then you need to identify a 2D peak which you know its ppm values. Click "Display" in

- Basic
- Default
- Weighting
- Display
- More 2D
- Integration
- Cursors/Line Lists
- Plot
- Text Output

, for more accurate reference, you may need to expand one peak by putting the two cross cursors on that peak (shown in Fig. 8)



Fig. 8

Then click  to expand it as Fig.9,

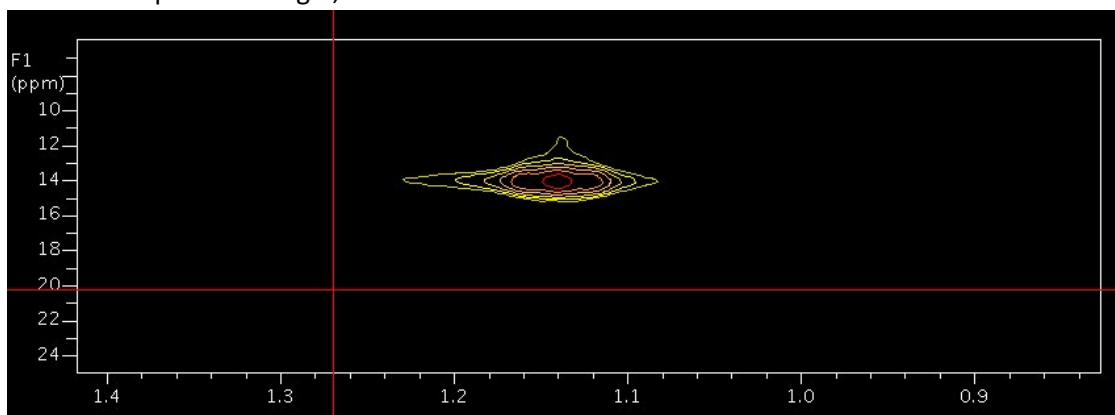


Fig. 9

then put one cursor on the center of the peak shown in Fig. 10.

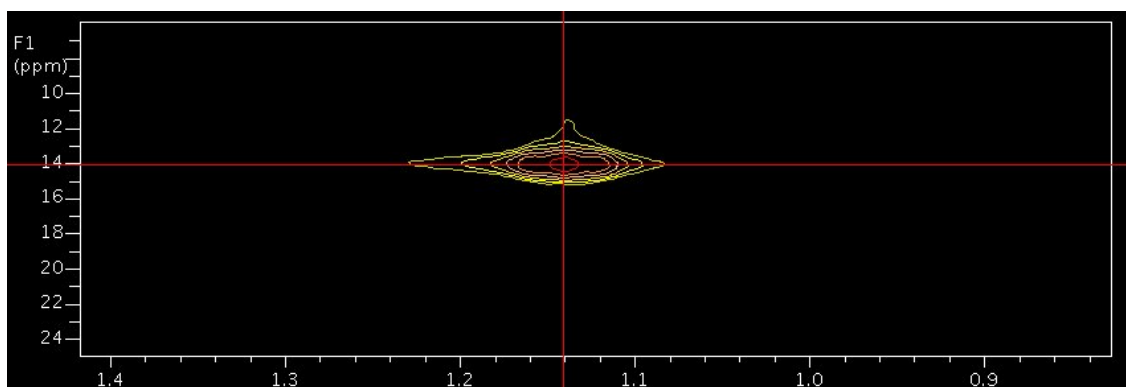


Fig. 10

Type in the ppm values in "Reference" section shown as Fig. 11. In this example, Carbon peak (F1) is 14 ppm, and Proton peak is 1.14 ppm (F2)

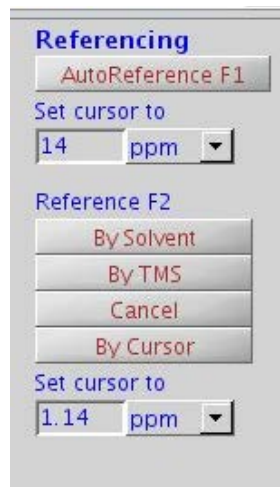

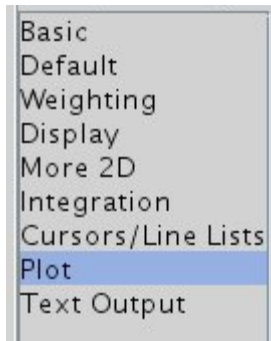


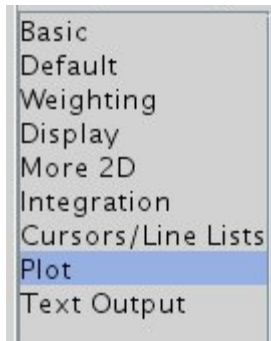
Fig. 11




Click  to refresh the display, it should have the correct ppm scales now.

### 3. Prepare for the plot



Click "Plot" in . To make the plot as pretty as possible, select the area with less

noise/artifacts, shown as in Fig. 12. Click ,

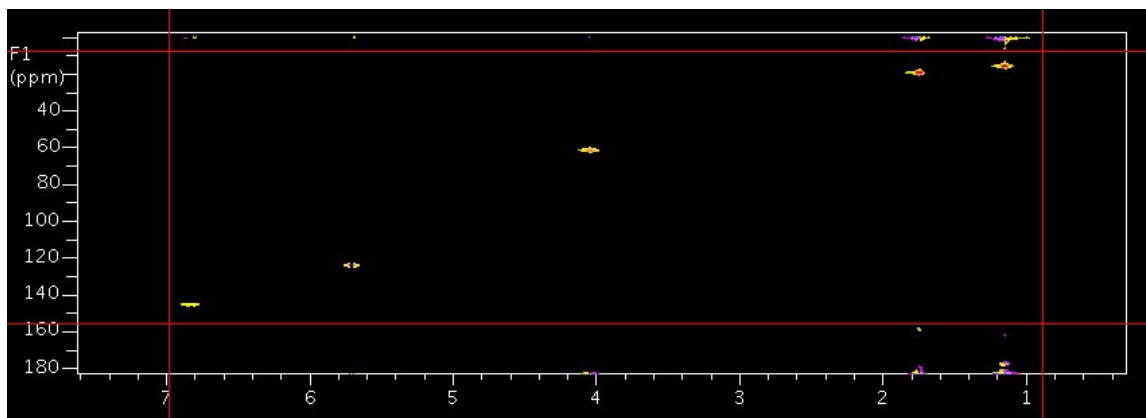


Fig. 12

The plotting area is shown as Fig. 13. This plotting area only has the 2D NMR peaks, very pretty.

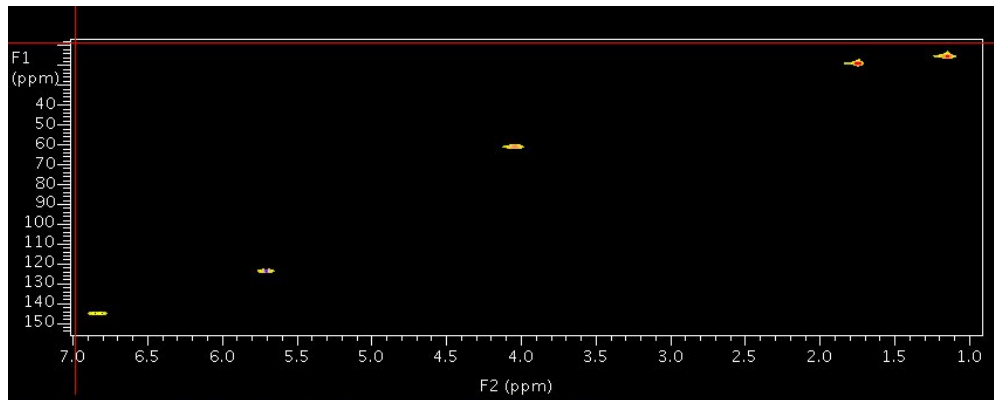


Fig. 13

If you want to put the projections on the top and side of the 2D spectrum, you may click

, the size of the 2D spectrum will be smaller shown as Fig. 14 to give some room for projections.

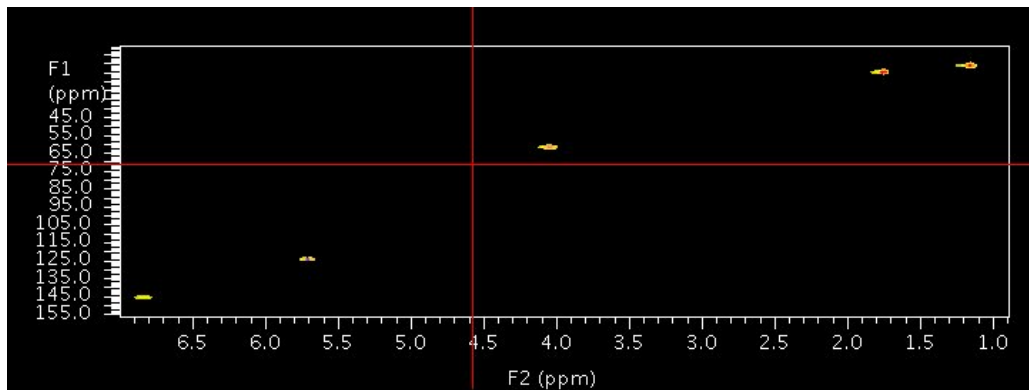


Fig. 14

click  to display the horizontal project on the top of 2D spectrum shown as Fig. 15.

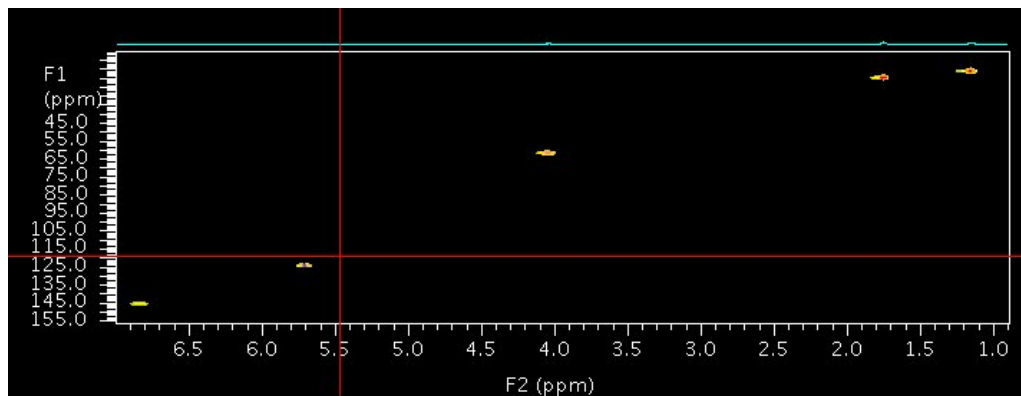


Fig. 15

The intensity of the project may look small, you can adjust it by putting the mouse on the projection line, press and move the middle mouse to adjust the intensity, when you are happy with it, release the mouse, click

, the vertical projection is on the right side of the 2D spectrum as shown in Fig. 16

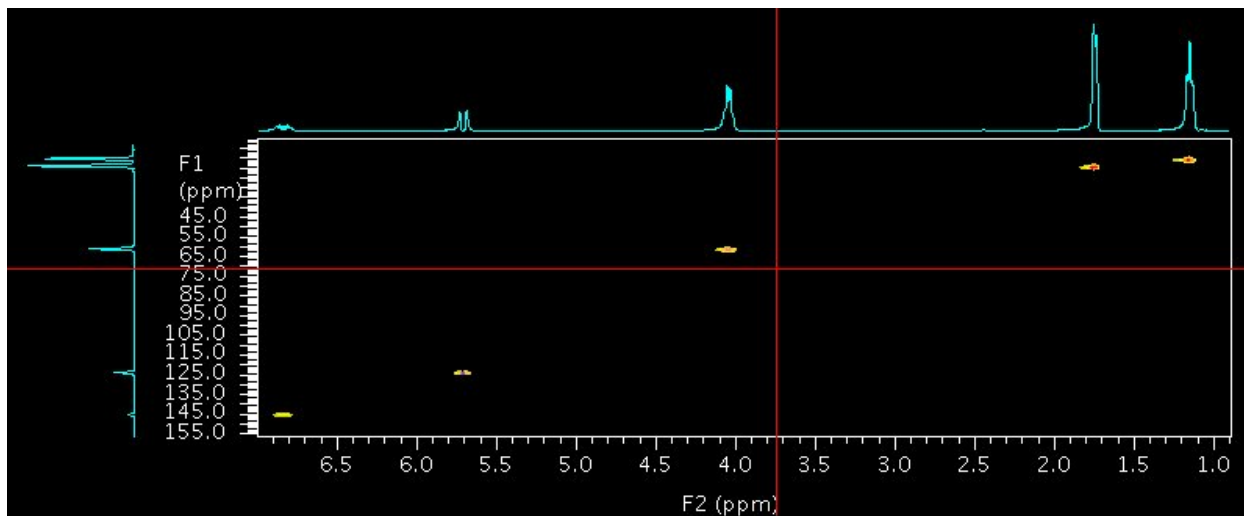


Fig. 16

Now it is ready to plot.

#### 4. Plot and save the plot as PDF file



Click each **plot** in

to plot what you want, then, click



to get paper print of the spectrum. You may want to save the plot as PDF file, so, do

not click **Plot Page**,



, a pop-up window appears with default

file name and directory shown in Fig. 17,

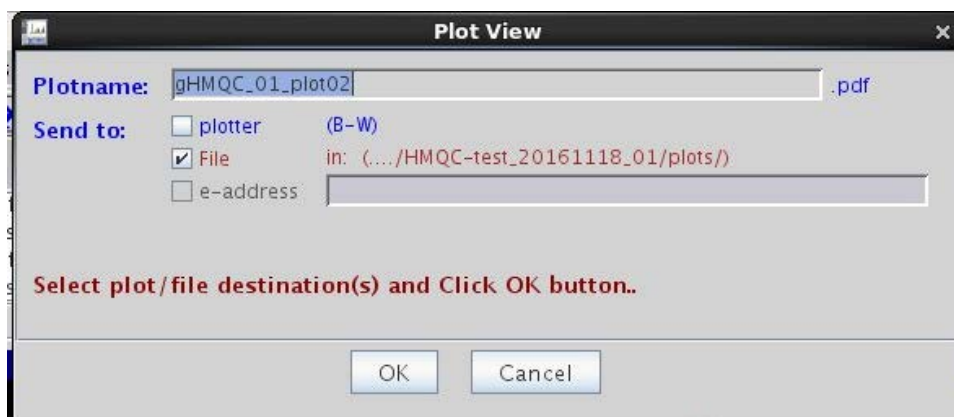


Fig. 17

you may type in the filename, check the “File” box  File , click “ok” , the PDF file is saved in directory of the sample file data directory like in: (.../HMQC-test\_20161118\_01/plots/).