

How to create 2D plots with 1D spectra on the side

Updated to EZ NMR: 2010-05-05

There are two ways to achieve this: with the **2D with 1D** button in the Plotting section of EZ NMR P+P or by using one of two macros called **pl2d1dhh** or **pl2d1dhx** (hh for homonuclear experiments such as GCOSY, GTOCSY, TROESY etc. and hx for all heteronuclear experiments). If the button is used the software decides automatically which macro to call. The fundamental difference is that the macros give you a variety of options while the button does not.

To use the macros or the button it is a prerequisite and assumed that

- the 1D proton spectrum has been processed, phased and referenced correctly in a separate experiment
- the APT spectrum (where applicable) has been processed, phased and referenced correctly in a separate experiment
- the 2D experiment has been processed, referenced correctly and is the current experiment in VNMRJ

Experiment numbers can be freely selected but the use of the macro or button has to be from within the experiment that contains the 2D spectrum. In general, **everything is done in the experiment that contains the 2D data!**

Homonuclear experiments such as GCOSY, GTOCSY, TROESY etc. Here is what happens when using the macro **pl2d1dhh** or clicking on the button **2D with 1D** in the Plotting section of EZ P+P:

user input	system response
click on 2D with 1D or type: pl2d1dhh	This macro needs to know where the processed 1D proton spectrum is located. If you are not sure and want to start over enter 0, find out where your experiment is located, then start over by clicking on Restart 2D with 1D . Enter experiment number of the processed 1D spectrum (or 0 to quit):
2 (assuming 1D is in exp 2)	plots 2D from current experiment and 1D from exp 2 at the top and on the side of 2D
After change of expansion limits in 2D spectrum	
click on 2D with 1D or type: pl2d1dhh	plots 2D from current experiment and 1D from exp 2 at the top and on the side of 2D with spectral limits adjusted automatically, no need to re-enter location of 1D (the macro/button remembers it!)

This is the easy and most often used way for that task. More can be done but only by using the macro **pl2d1dhh** with arguments (a maximum of 5 arguments can be specified).

- To increase the vertical scaling of the 1D spectrum: type for example pl2d1dhh('x5'). Values from 2 to 99 are allowed.
- To use a different 1D than initially specified: you have to tell the macro where to look, e.g. pl2d1dhh(6) takes the 1D spectrum from experiment 6.
- You can specify to only plot positive or negative contours and a multiplier for the 1D is available too, e.g. pl2d1dhh ('pos','x3') will plot only positive contours and triple the vertical scaling of the 1D plot. Strings like 'pos' have to entered first.
- **Example with 5 arguments:** pl2d1dhh('neg','x5',3,15,1.2). The 1D is taken from experiment 3 and its vertical scale multiplied by 5, 15 negative contours spaced by 1.2 are plotted. If you want to specify contour level numbers and spacing you must specify the location of the 1D because the first numerical is interpreted as the location of the 1D spectrum. There is no way around this, however, there should be virtually no need to specify contour numbers and spacing; the default of 20, 1.5 covers a huge range of peak heights.

Heteronuclear experiments such as GHSQC, GHMQC, GHMBC etc. Here is what happens when using the macro **pl2d1dhh** or clicking on the button **2D with 1D** in the Plotting section of EZ P+P:

user input	system response
click on 2D with 1D or type: pl2d1dhh	This macro needs to know where the processed 1D proton spectrum is located. If you are not sure and want to start over enter 0, find out where your experiment is located, then start over by clicking on Restart 2D with 1D or by typing newpl2d1d. Enter experiment number of the processed 1D spectrum (or 0 to quit):
2 (assuming 1D is in exp 2)	
	This macro also needs to know where the processed C13 spectrum is located. If you are not sure and want to start over enter q, find out where your experiment is located, then start over by clicking on Restart 2D with 1D or by typing newpl2d1d. Enter experiment number of the processed C13 spectrum (or q to quit):
3 (assuming C13 is in exp 3)	plots 2D from current experiment and 1D H1 from exp 2 at the top and C13 from exp 3 on the left side of the 2D
After change of expansion limits in 2D spectrum	
click on 2D with 1D or type: pl2d1dhh	plots 2D from current experiment and 1D H1 from exp 2 at the top and C13 from exp 3 on the side of the 2D with spectral limits adjusted automatically, no need to re-enter locations of 1D (the macro/button remembers them!)

The macro **pl2d1dhh** provides the following options (a maximum of 7 arguments can be specified):

- To increase the vertical scaling of the 1D spectra: type for example **pl2d1dhh('hx5','cx3')**. In this case the H1-1D is vertically "stretched" 5-fold and the C13-1D three times. Values from 2 to 99 are allowed.
- To use different 1Ds than initially specified: you have to tell the macro where to look, e.g. **pl2d1dhh(6,7)** takes the 1D spectra from experiments 6 (H1) and 7 (C13).
- You can specify to only plot positive or negative contours and multipliers for the 1D spectra are available too, e.g. **pl2d1dhh('pos','cx3')** will plot only positive contours and triple the vertical scaling of the C13-1D plot. Strings like 'pos' have to entered first.
- **Example with 7 arguments:** **pl2d1dhh('neg','hx2','cx5',3,4,15,1.2)**. The H1-1D is taken from experiment 3 (vertical scale multiplied by 2), the C13-1D from experiment 4 and its vertical scale multiplied by 5, 15 negative contours spaced by 1.2 are plotted. If you want to specify contour level numbers and spacing you must always specify the locations of the 1Ds because the first two numericals are interpreted as the locations of the 1D spectra in the order h x. There is no way around this, however, there should be virtually no need to specify contour numbers and spacing; the default of 20, 1.5 covers a huge range of peak heights.
- The C13-1D can be at the top or on the left side, it does not matter except that a software bug limits the display of negative peaks to about 5 mm on the left side. This is only relevant if the C13-1D is an APT.
- The macro plots what is seen on the monitor. If you want to switch from the default display in a GH[(Q/B)C (H1 horizontal, C13 vertical), type **f1** then use **pl2d1dhh**. To return to the standard display format type **f2**.