Advanced display options: viewports

We get complementary information from the different spectra we collect. When putting this together it is extremely helpful to be able to work with the different spectra at once, simultaneously. Varian's "Viewports" allow this.

Preliminaries.

Load each of the spectra to be compared into workspaces and make sure that the chemical shift axes of each are properly referenced.

You can mix 1Ds and 2Ds but in order to have them overlaid or stacked, you will need them to have at least on scale in common. (Eg. all have one 1H chemical shift axis.)

Setting up Viewports.

Join one of the workspaces that contain one of the experiments to be compared. In my case I have TOCSY in workspace 4, NOESY in workspace 1, ROESY in workspace 2 and DQCOSY in workspace 5.

Pull down the 'Edit' menu and select 'Viewports' (fourth form the bottom) (**Page 2** [1]). In the panel that opens, choose the eye-ball button next to '4' to simultaneously view four experiments. Close.

In the left-hand panel, enter the numbers of the workspaces that correspond to each of the experiments you want to view [2]. At this time you can also elect to colour-code [3}. If yes, then you can choose a colour for each experiment [4]. (All contours will have the same colour, except that two colours will be allocated for experiments where both positive and negative contours have significance.) Note that you may have to 'activate' a viewport in order to be able to alter the choice of workspace it will display etc. In order to do this you will have to draw the slider to the right [5], and this will reveal a column of eye-balls, which allow you to choose which ONE viewport you are modifying. The other way to decide which viewport is the active one, is to click on the bar on the top of the window displaying that workspace [6]. When an workspace is active, you can manipulate the spectrum in it just as you are used to doing in single-display mode, using the tools in the vertical panel [7], or the horizontal bar [8].

Choose whether you want the viewports side-by-side or one above the other [9]

Use the checkboxes to flexibly alter which of the possible viewports are actually displayed [10].

Select the viewports you want to have on the same scale, using the checkboxes. Click on 'Overlay viewports' [11].

Page 3 shows that you now have the option to 'Stack Spectra' [1]. What this means is that the software will line them up according to their chemical shift axes. When you select X and Y offsets of 0 [2], then the same chemical shift will appear in exactly

the same place in the two spectra: the axes will be superimposed and made to match one another. This will be accomplished even if you collected the data using different sw or tof, so long as both have ^{1}H chemical shift axes. If both are correctly referenced, you should see the peaks overlap perfectly where this is expected (mine is close to perfect) [3]. (If you have a collection of spectra of different types, such as a ^{1}H1D and a COSY, you will see an 'Align Spectra' button instead of 'Stack Spectra'. This allows you to line up your beautiful 1D along the edge of your 2D.)

Activate the 'Synchronize Axes' option [4] so you can zoom in on one spectrum and have the other one zoom as well. Anything done to one spectrum's axes will be done for all the other spectra too. Similarly, you will probably want to 'Synchronize Cursor' (above [4]).

At this point, I like to revert to a side-by-side display [1]. In Page 4 you see that I have loaded all four workspaces and selected them all. Each has a name (which you can change [2]), and the name appears in its title bar [3]. My synchronized cursor [4] moves the same way in all four windows, regardless of which one is the active one [5] (blue title bar instead of grey). Thus, I can move to a peak in thy TOCSY and determine whether it is present in the COSY. In this example I am looking at a spin system revealed by the TOCSY and learning from the COSY that only one of the peaks is a strong candidate for a single step. In order to make more space available for data, I often go to 'Fields' and turn them off (looses display of cr and delta [6]).

You can alter the number and spacing of contours, for whichever viewport is active [7]. Do this for each spectrum in turn to get them all displaying the desired strengths (or significance) of signals.

You can use the print screen to obtain digital figures of your display, as for single spectra. Selected the '2D' tab [8] to switch left-hand panels.

Page 5 then shows that I used Edit>Display to convert to a white background and black axes. Then and near the bottom choose to save as a file [1] (instead of printing) and then activate the 'Print Screen' [2] to enter a file directory and name, specify output type etc and SAVE.

The figure produced is shown on **Page 6**. To get the figure on **Page 7**, I exploited the synchronized zoom. With one workspace active I used the cursors as usual to delineate a spectral region of interest and then used the magnifying glass icon to zoom in. All four spectra were zoomed identically. A zoomed overlay figure is on **Page 8**. Making figures this way is extremely convenient.

The other huge convenience is the possibility of selecting one row in one spectrum and having a companion cursor move to the identical position in other spectra. This enormously facilitates the interpretation of HSQC and CIGAR (for example). You can place the crosshairs on a peak in an HSQC and this will reveal in the companion CIGAR which other ^{13}C chemical shifts are coupled remotely to the chosen ^{1}H, and

similarly which other ^{1}H chemical shifts are coupled remotely to the chosen ^{13}C. (See the notes on HMBC-CIGAR.)

Setting up inset

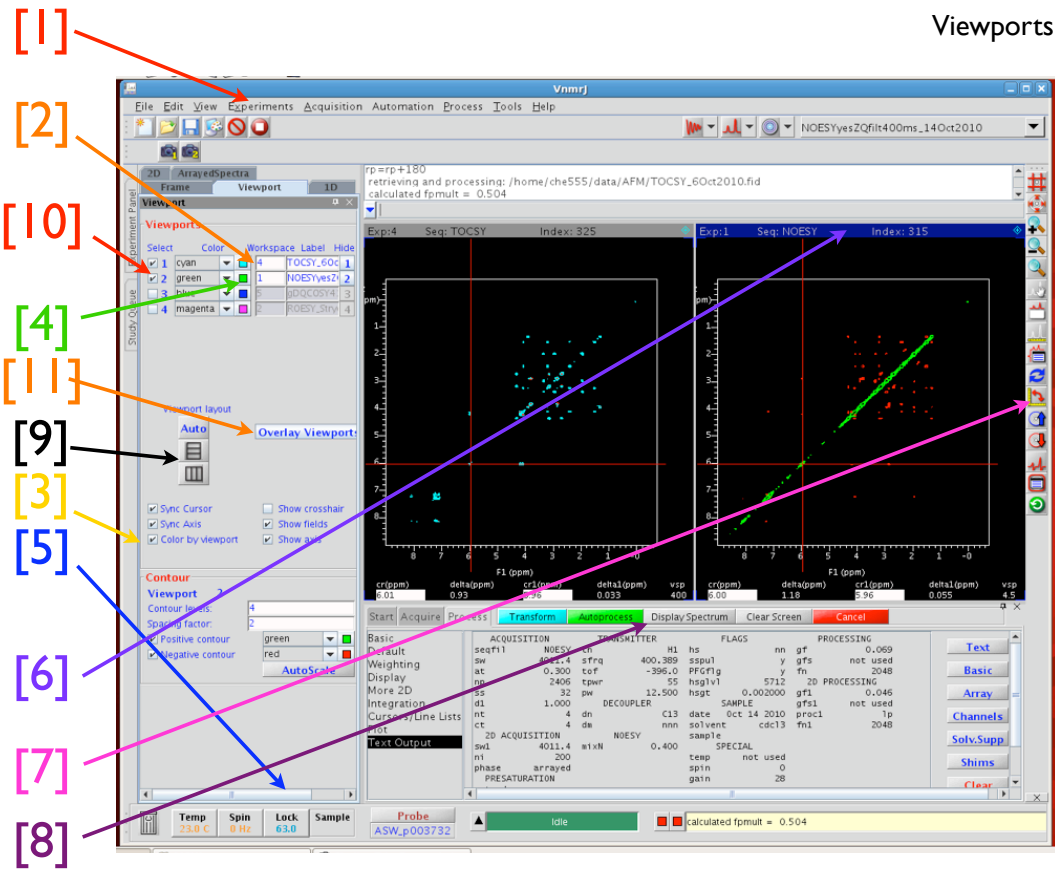
First, display the entire spectrum to suit your purpose (**Page 9**).

On the left-hand side, choose the Frame tab [1]. Click on the add inset button [2] to create a second frame inside your (full) default frame. Using the left mouse button, place the cursor at the left edge of the spectral window you want to display in the new frame. Hold the left mouse button down while dragging *to the right* until you have selected the spectral region to be displayed in the new frame [3]. Without releasing the mouse button, now drag it vertically down, to indicate the vertical height your new frame should have [4]. (This motion is like writing a capital 'L' but with the order in which the vertical and the horizontal legs are executed reversed.) Now release the mouse button. Your new frame can be moved to the desired position by dragging it by one of its edges, and it can be resized by dragging on its corners. If you have several frames, you can activate one by clicking in it (the frame now displays a border).

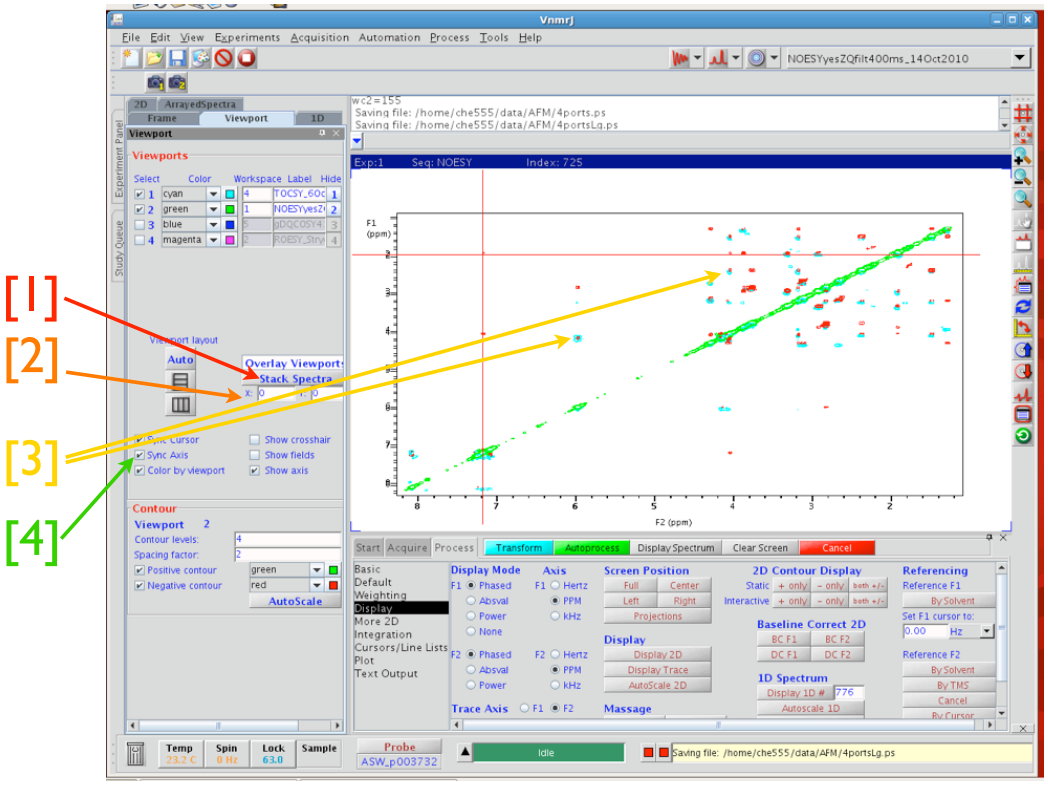
Inside an active frame, you can zoom and pan using the appropriate tools from the viewport panel (left-hand side).

The resulting spectra can be printed via the 1D panel (left-hand side) which gives you access to the Print screen (**Page 10**).

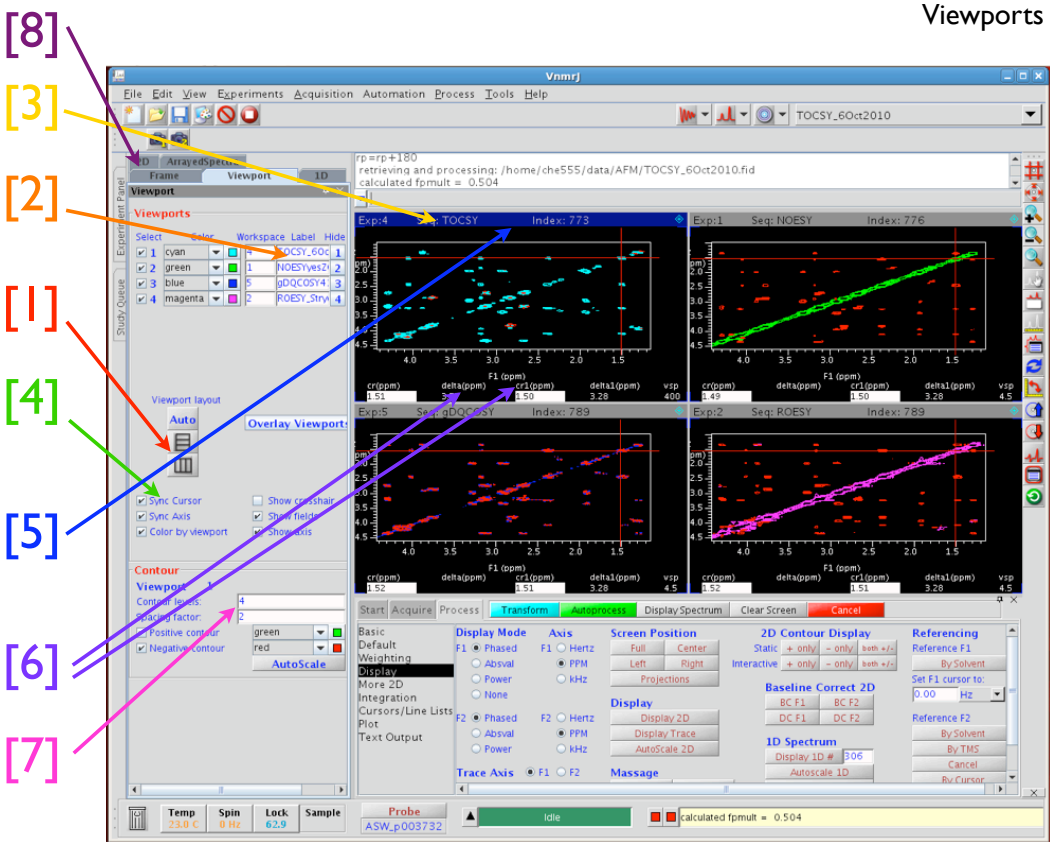
Viewports: co-analysis of multiple spectra



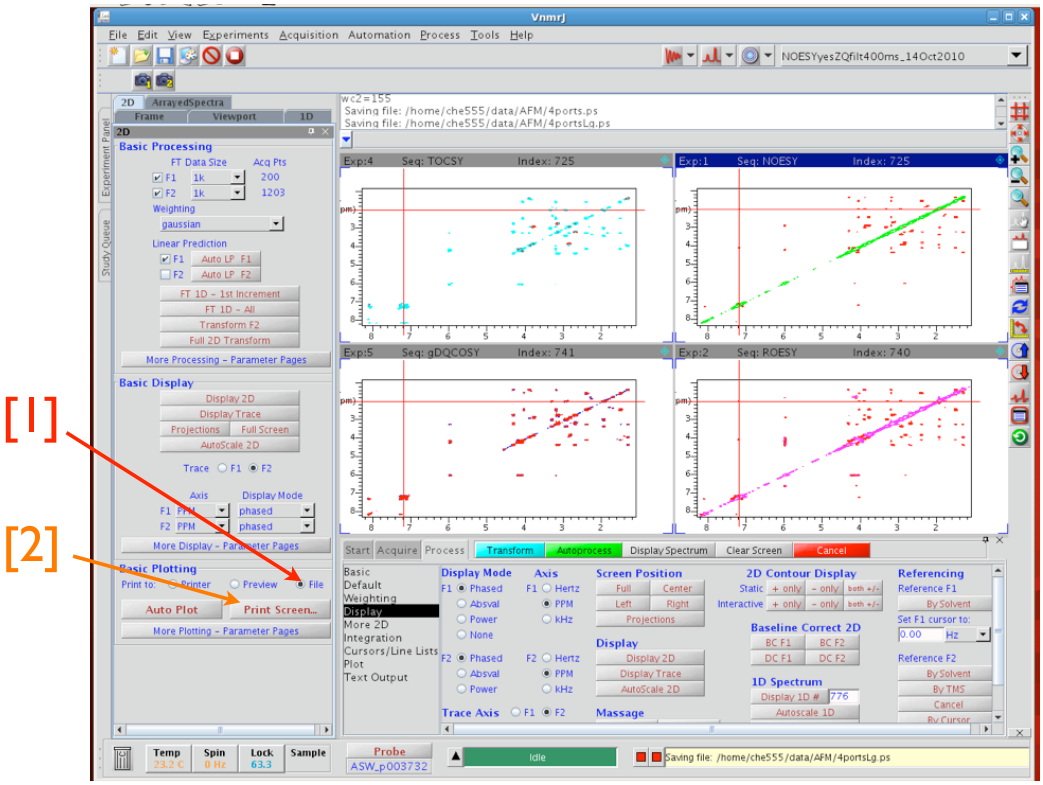
Viewports figure 3



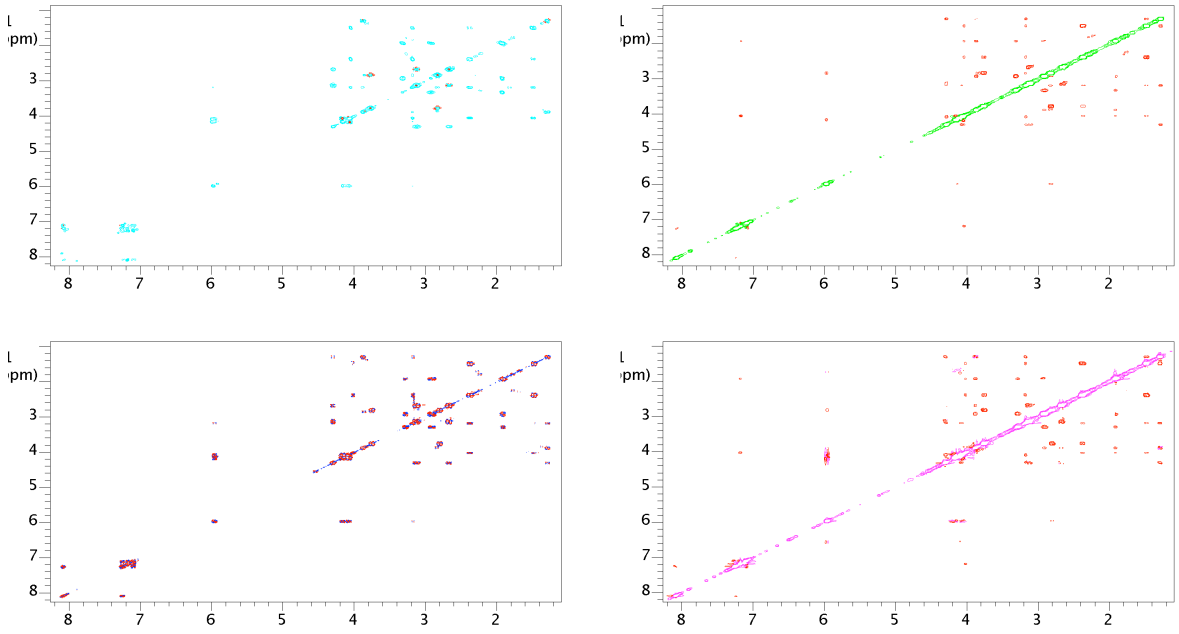
Viewports figure 4



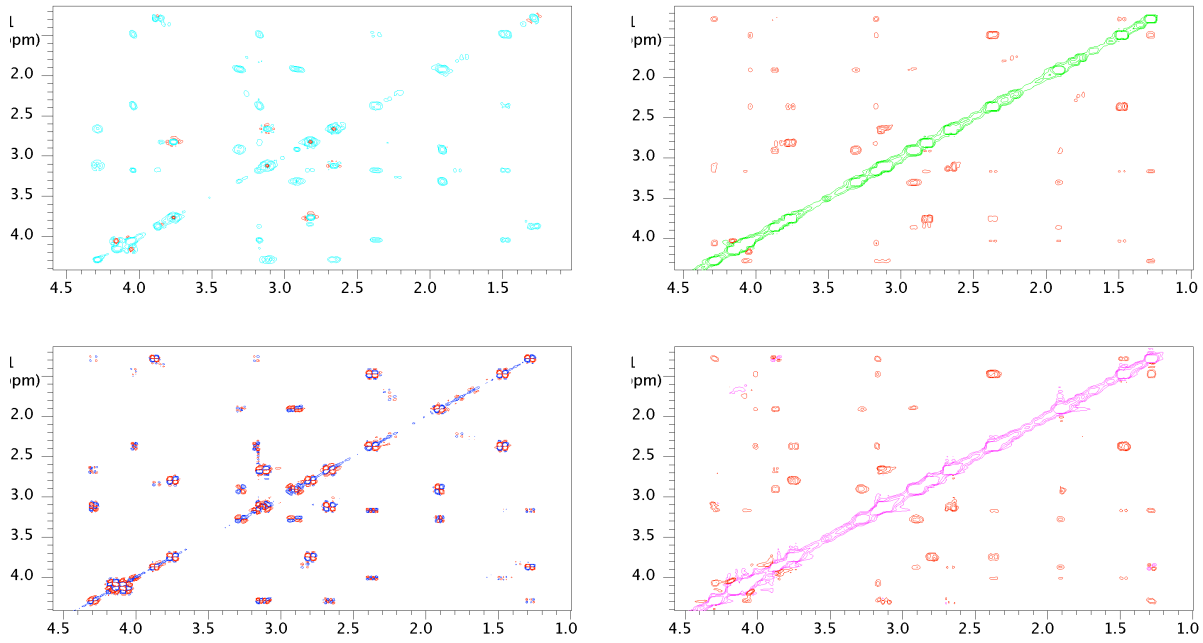
Viewports figure 5



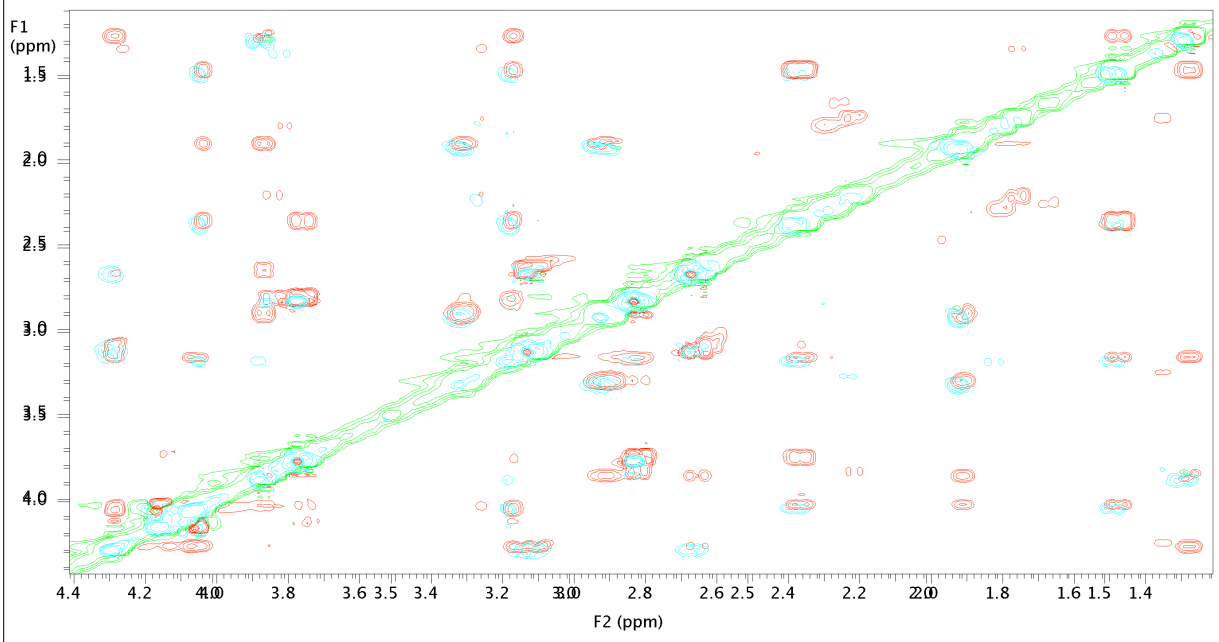
Viewports figure 6



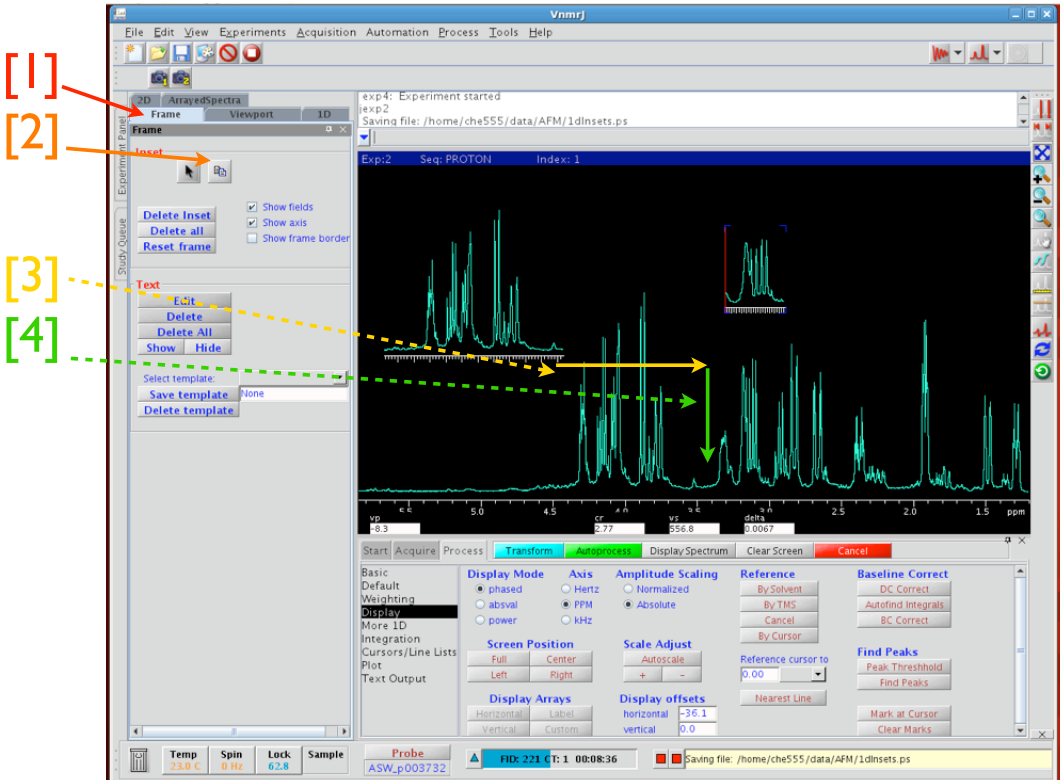
Viewports figure 7



Viewports figure 8



Viewports figure 9



Viewports figure 10