

## Plotting NMR Spectra with TOPSPIN-PLOT

These notes provide a brief introduction to plotting NMR spectra with the BRUKER TOPSPIN-PLOT interactive plot program using TopSpin 3. Please see the handouts *Introduction to the TOPSPIN program* and *2D Acquisition and Processing* for further details on spectrum manipulation within the TopSpin 3 NMR program.

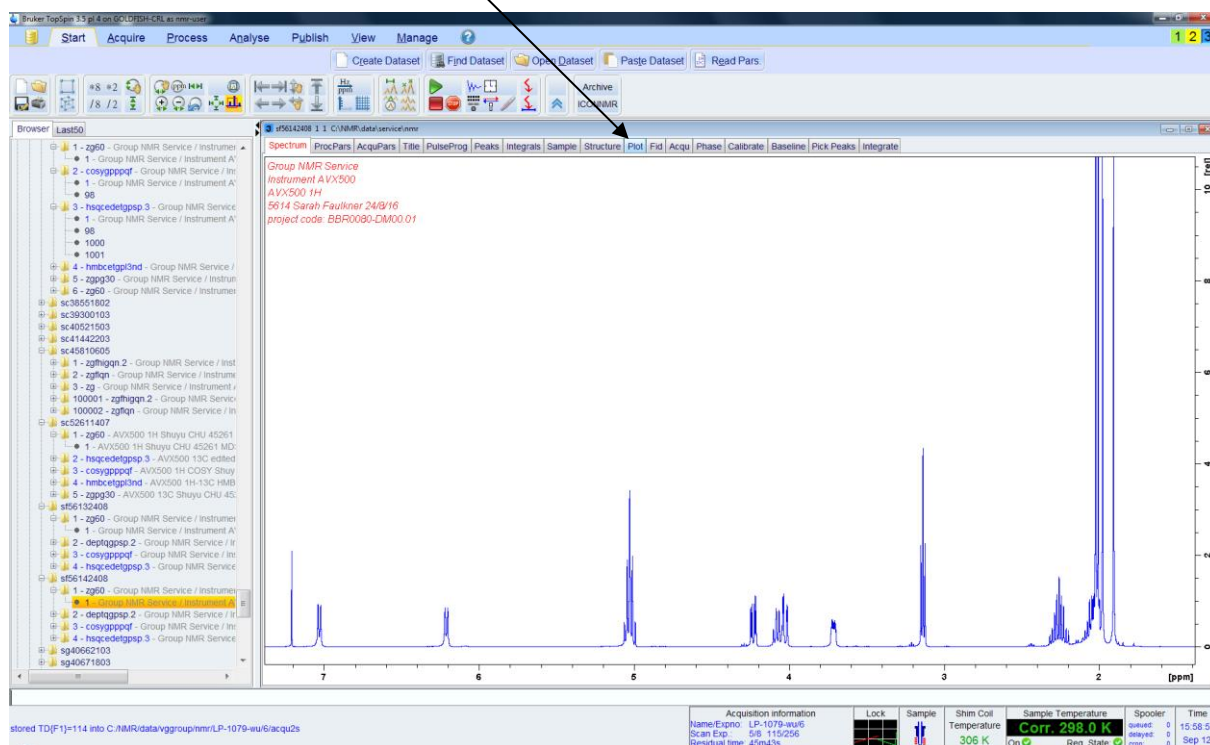
For details of how to access your data from your PC see <http://nmrweb.chem.ox.ac.uk/> and see sections *Software* and *Data access*.

Process your data within TopSpin described in the appropriate handout above. For a 1D proton spectrum the usual procedure would be:

1. Transform with *efp*
2. Phase correct with *apks*
3. Baseline correct and integration with *abs* (or generate integrals manually).

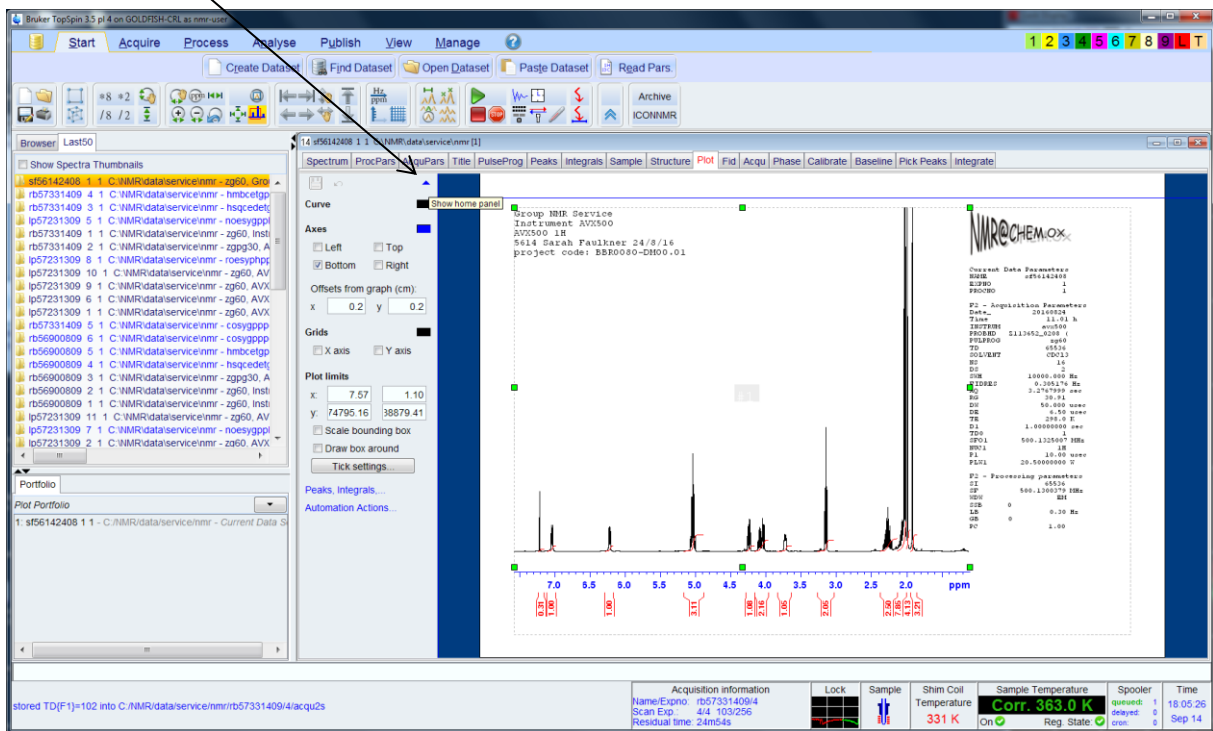
### 1) Simple Plotting of 1-D Spectra

From the spectrum window, select the *Plot* tab.



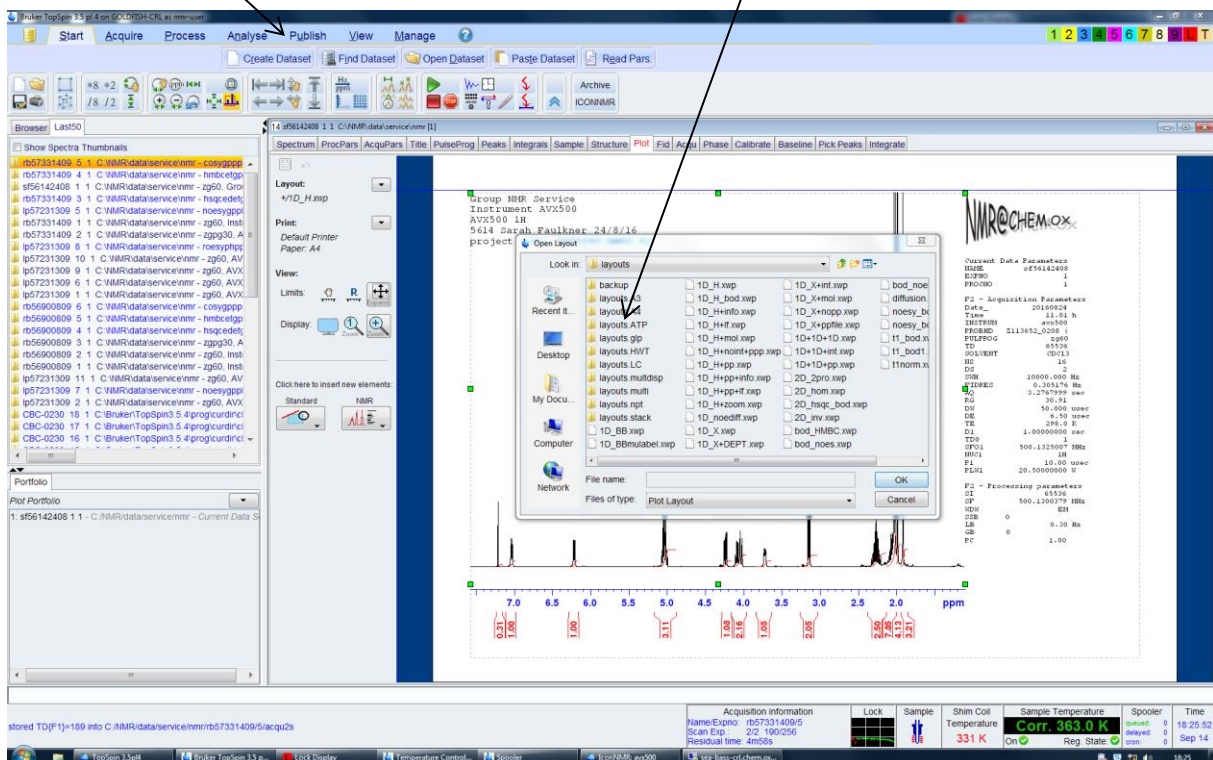
In the Topspin Plot window (see below), click *home panel* on the top left hand corner and select different *plot layouts* by clicking the down arrow in the layout section. Plot layouts define where on the page all features are placed, including the spectrum, title, parameter lists, labels, images etc. Choose one to suite your requirements; the basic proton plot is *1D\_H.xwp*. All plot layouts have *.xwp* extension. You can compile your own and save it as a *.xwp* plot file. At this point you can print or export your spectrum from the file icon (top left hand corner) in the following formats; pdf, png, ps, tiff, tif, jpg, jpeg, bmp (defined by the file extension you use). Exporting PNG files is most appropriate for use directly in Word or Powerpoint documents, but exporting as Postscript files (by using the *.ps* file extension) will allow the images to be imported into graphics editing programs such as Coreldraw where the files can then be fully edited and labelled etc.

## Show home panel (blue triangle)



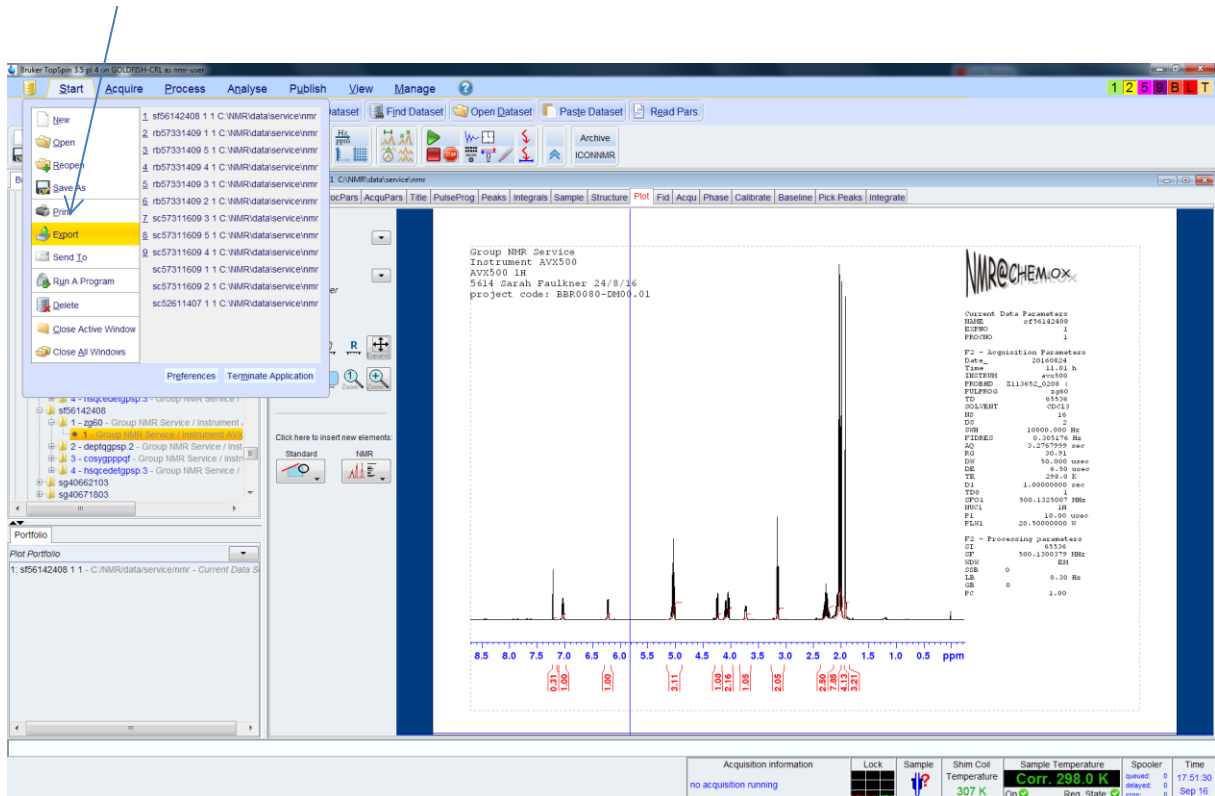
## Publish tab

## Choose a plot layout



You can plot or export the spectrum by selecting **Publish** tab and then the **Print** or **PDF** icon to access different export options. Alternatively you can print and export from the **Command** icon (gold block in top left corner of program).

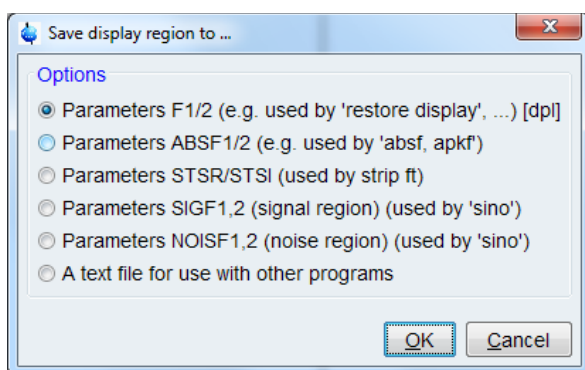
## Print and export



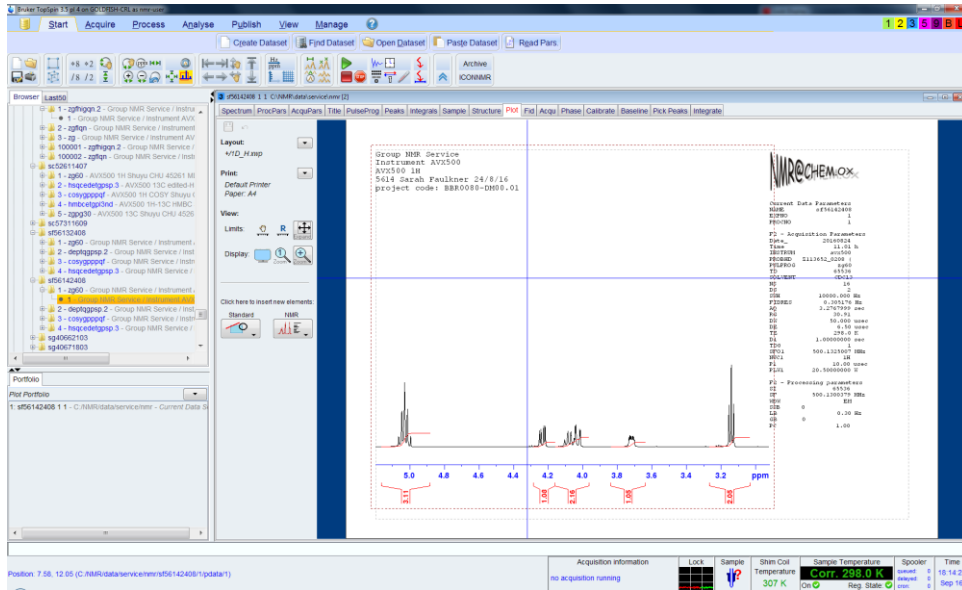
Individual parts of the display (spectrum, parameters, title, logo etc) can be moved, scaled (with middle mouse button) and edited independently as in any graphical drawing program. The currently “active” window for editing is highlighted with green boxes around its perimeter, as seen in figures above. Changes to fonts, colours, display options etc within the active window are made via the options within the left hand panel of the Plot window.

You can go backwards and forwards between the spectrum and the plot (although in older TOPSPIN versions the plot can revert back to the default one, which can be annoying because if you do not save the layout you can lose your design by moving between spectra!).

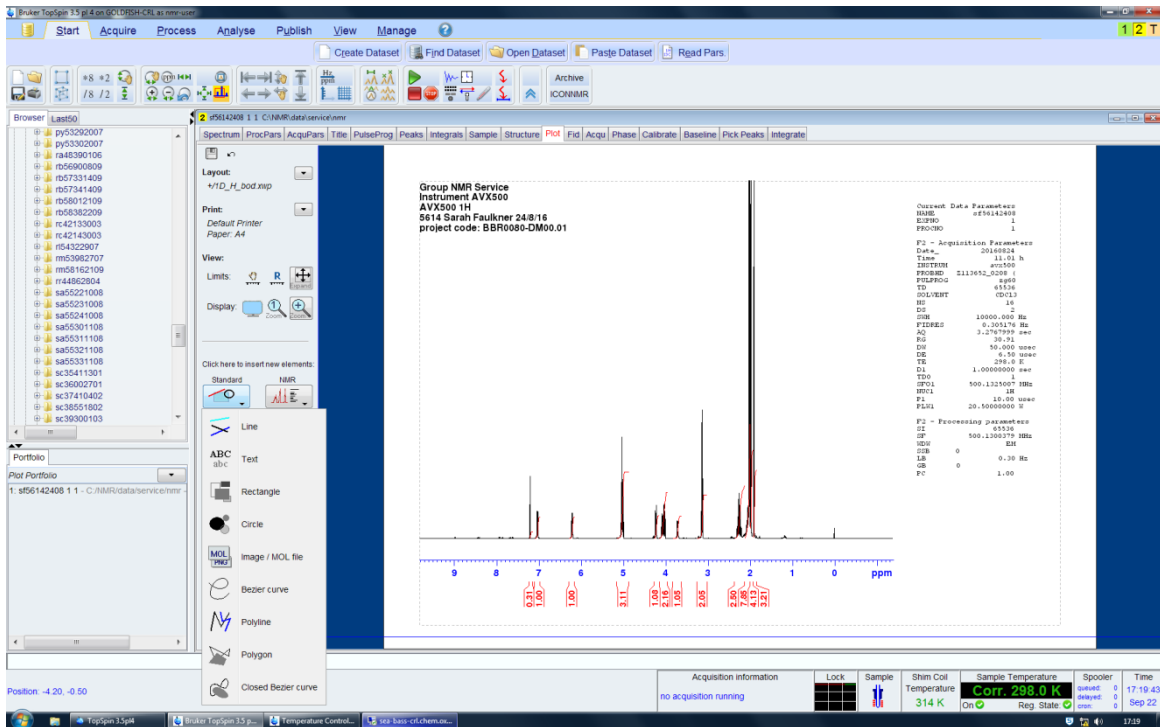
You can define a selected region of the spectrum for plotting from the main **Spectrum** display by right clicking then *Save display region to..* as shown below;



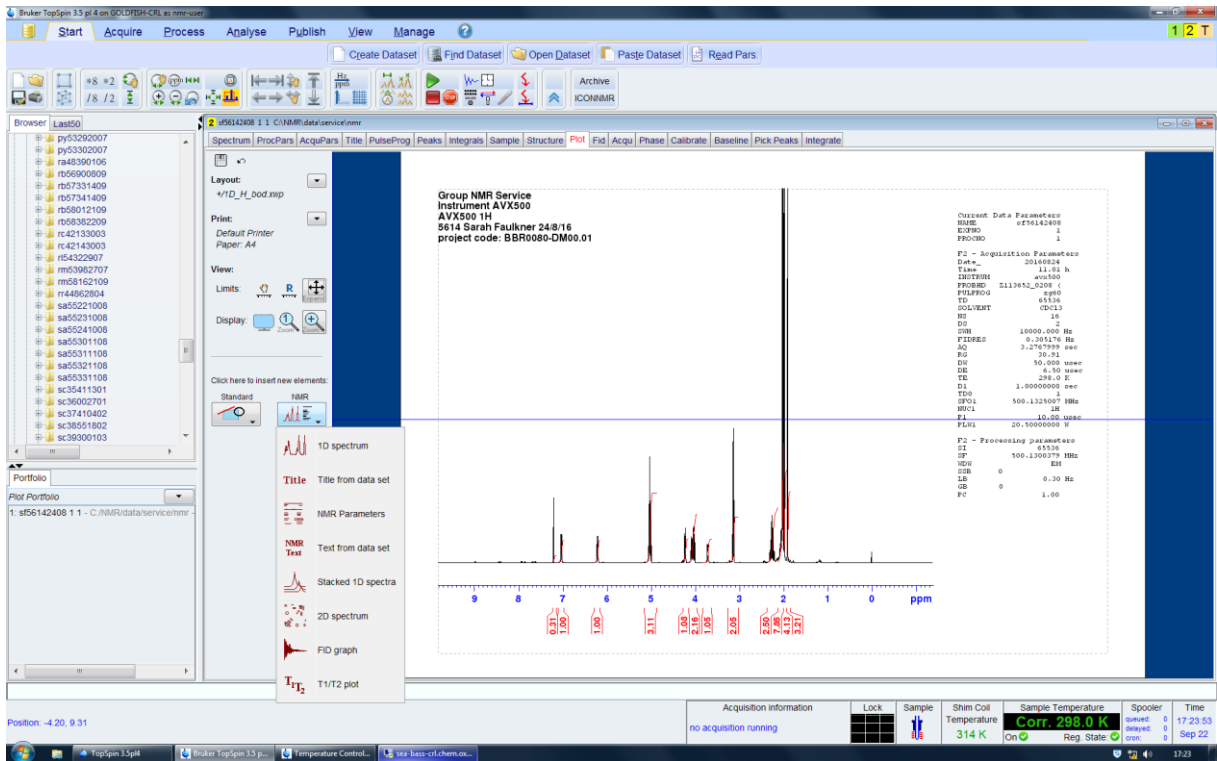
Then opening up the **Plot** tab should reveal the same expansion (if not, right click in the plot window and select *Reset Object*);



You can insert graphic objects like lines and arrows by clicking outside the spectrum window and selecting insert new elements '**Standard**' in the options area of the left.



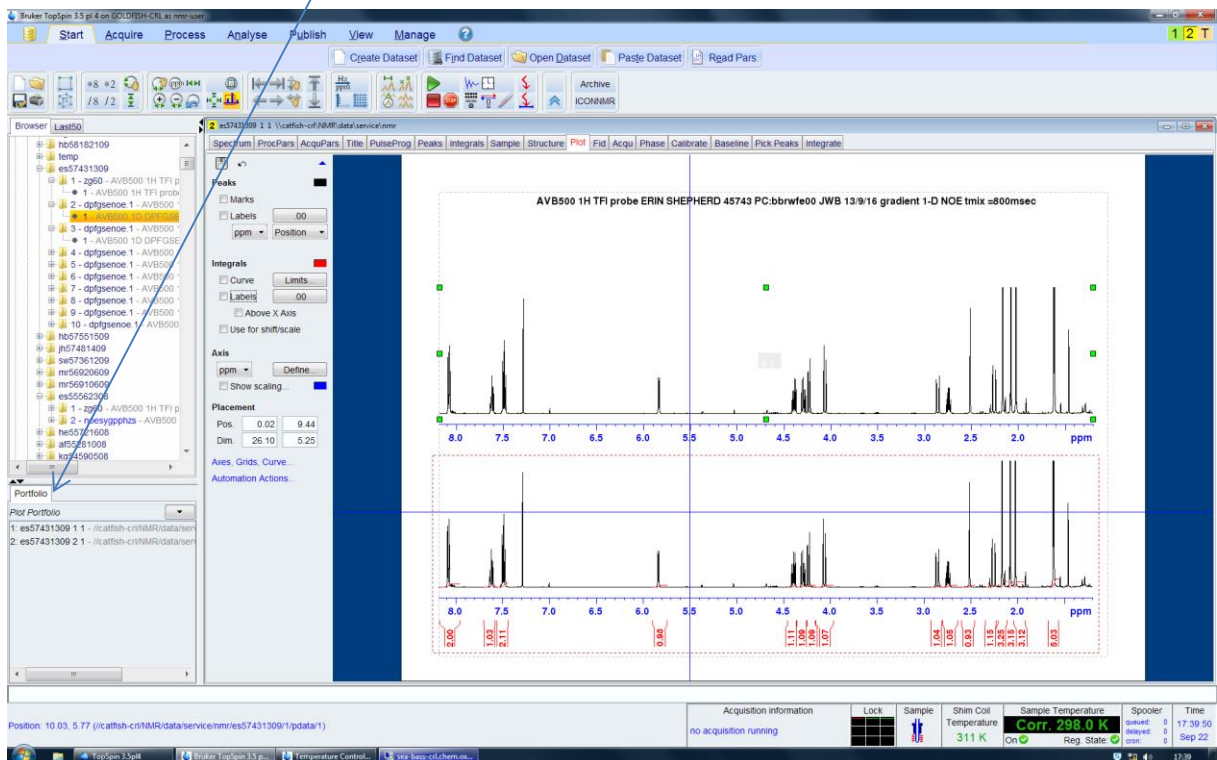
Likewise, you can select titles, spectra, parameters etc. for display from the '**NMR**' option. Once selected, drag to create a new window containing the selected object in the main plot area.



## 2) Overlaying 1-D Spectra

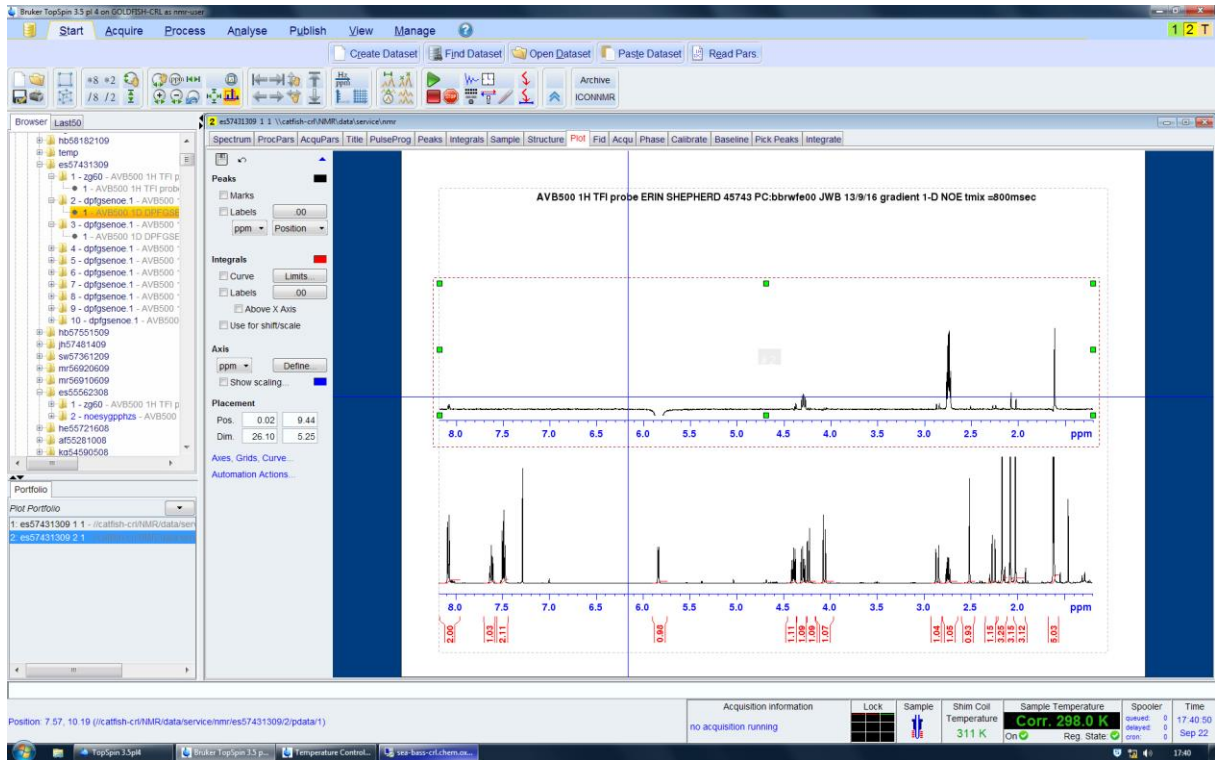
Select the starting spectrum and arrange the objects in the desired way to receive the overlay, then copy and paste the original spectrum where the subsequent spectrum of interest is intended to be. Select the subsequent spectrum of interest from the browser area and drag and drop it into the plot portfolio below so that it appears in the portfolio list.

### Plot Portfolio

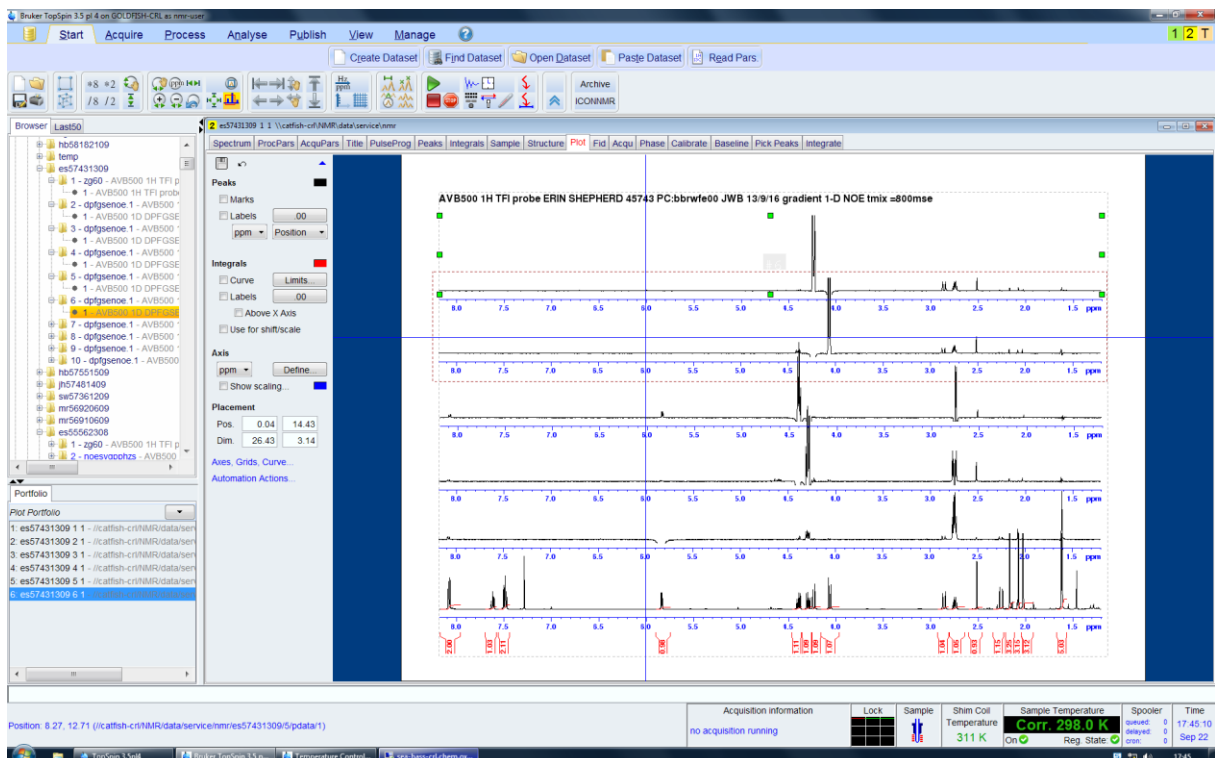


Then drag and drop the intended file from the Plot Portfolio into the plot window as shown below;





You can continue selecting other plots provided they are listed in the Plot Portfolio in the same way;

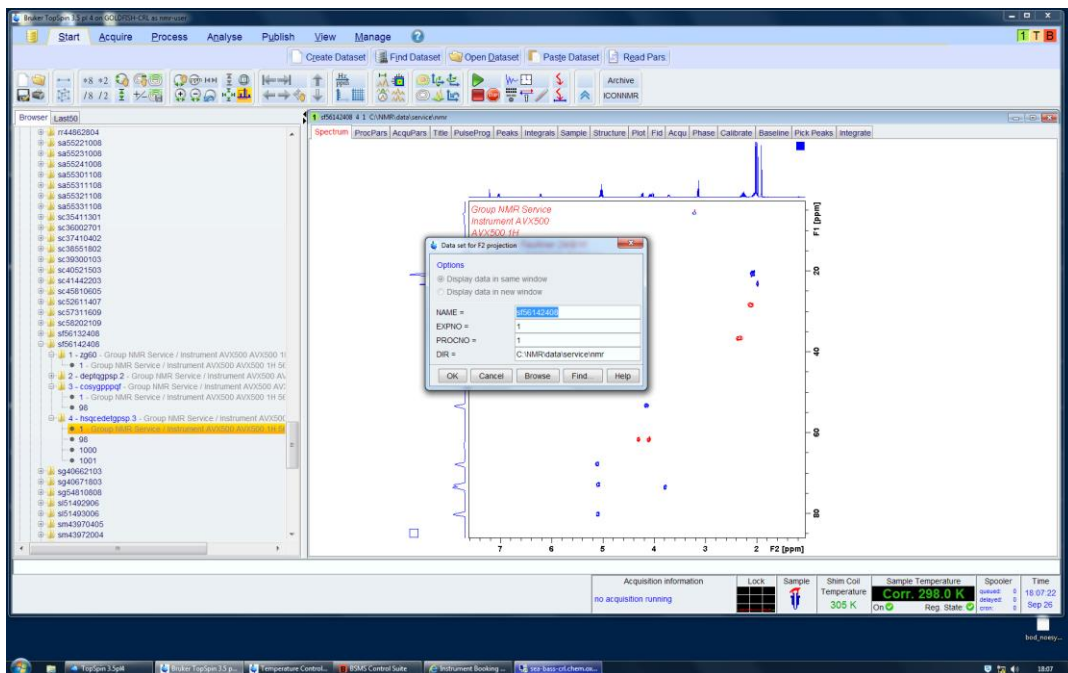


An easier option is often to display your spectra overlaid in the main **Spectrum** tab using the multiple display mode. Then in the **Plot** tab under the Portfolio window, use the down arrow and select "Load collection from multiple display mode" to populate the Plot Portfolio with the same spectra.

Remember, if you leave the plot window without exporting it to a plot format you may lose your precious plot forever and you will have no option but to start all over again ! This is easily done if you accidentally double click another spectrum in the browser.

### 3) Plotting 2-D Spectra

Have your 2-D spectrum in the spectrum window of Topspin. If you have selected the 1-D spectrum projections beforehand by right clicking the blue square in the top right hand corner for proton and selecting the correct 1-D spectrum as shown below, the correct 1-D projection spectrum will also accompany the plot. By selecting the plot button a default 2-D plot will appear before you, with the 1-D projection and 2-D files listed in the Plot Portfolio. If you also have a  $^{13}\text{C}$  -1D spectrum in the browser you can double click it and transfer it to the Plot Portfolio and drag it also to the 2-D plot for a HSQC. By moving the mouse middle button you can raise the level of the 1-D projections if you hover over them, and you can increase/decrease the contour levels of the 2-D plot in the same way.



It is now up to you to design your 2-D plot. By selecting levels you can colour code edited-HSQC spectra in the same way as they appear in the spectrum window. Likewise, you can change the axes, plot limits, title etc. If you are working hard to get the desired plot, again please remember to save the plot layout or else all may be lost!

