

NUCLEAR MAGNETIC RESONANCE RESEARCH RESOURCE

Plotting 1D NMR Data with Layouts in TopSpin 4

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The TopSpin (TS) plot editor is an object-oriented, WYSIWYG program for producing high quality plots of NMR data. Once you have mastered the basics, the editor is an invaluable presentation tool; however, my experience has been that researchers often have a difficult time mastering the basics. Thus, this guide has been created to address this need. In this guide, instructions are provided on how the plot editor can be used to produce figures containing 1D NMR data (a separate document is available for 2D data). At the end of the guide, a FAQ repository is provided.

Please note that the TS plot editor is **NOT** designed to process NMR data. Rather, its role is as a graphics editor for the creation of high-quality figures displaying data you have previously processed. Consequently, I will not address processing strategies in this document; other documents are available from the facility website for this purpose.

(1) Understanding Layout Files and the Plot Portfolio

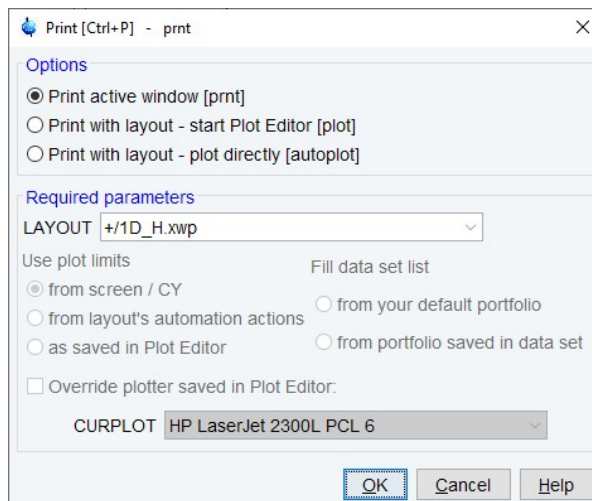
When you launch the TS plot editor from an NMR data set, the editor consults a special template file called a *layout file* to instruct it how to arrange the various objects (spectra, titles, parameters, etc.) on the display, along with default dimensions and attributes. The default TS installation contains numerous layout files which you can of course use “as-is”. However, part of the great utility of the plot editor is that users can customize and save new layout files to suit their individual needs. To determine the current file specified and /or to change it prior to launching the editor, go to the TS PROCPARS tab and search for “LAYOUT”. Alternatively, you can simply type **layout** in the command line.

Another important plot editor concept to understand is the *plot portfolio*. The portfolio is a list of one or more NMR data sets; NMR objects defined within the plot layout get filled with data specified in the portfolio. The first portfolio entry is **ALWAYS** the TopSpin dataset from which the plot editor has been launched. Consequently, if your layout only creates a single NMR object, that object will be filled automatically with the NMR data that was displayed when you launched the editor. However, the use of the portfolio becomes crucial with layouts that contain multiple NMR objects. The two most common situations where this is needed is plotting 2D NMR spectra with projections as well as the generation of stacked plots. Detailed instructions for customizing the plot portfolio will be provided later in this document.

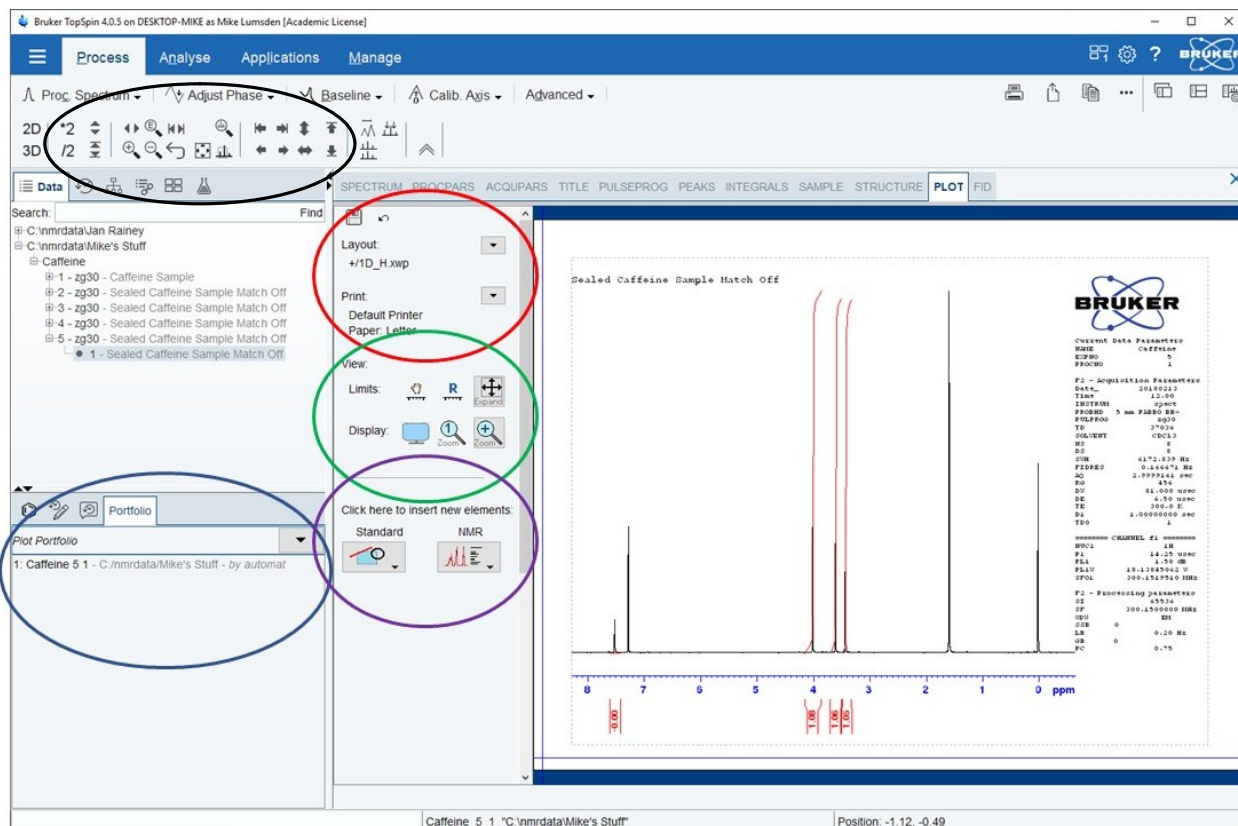
(2) Launching the Editor

Like most tasks within TS, the plot editor can be launched in multiple ways. For example:

- Simply type **plot** in the TS command line
- Click on the “Plot” tab in the dataset tab bar
- Type “CTRL P” which will open the print window shown in the adjacent figure. Selecting the “Print with layout – start Plot Editor” option and clicking OK will launch the editor. Note that this interface allows you to view the layout file specified in PROCPARS and change if necessary. Some of the other options available in this interface will be addressed in the FAQ section.



The following figure shows the result after launching the plot editor from a 1D ¹H experiment using the 1D_H.xwp layout. The spectrum was processed and analysed (integration and peak picking) prior to launching the editor.

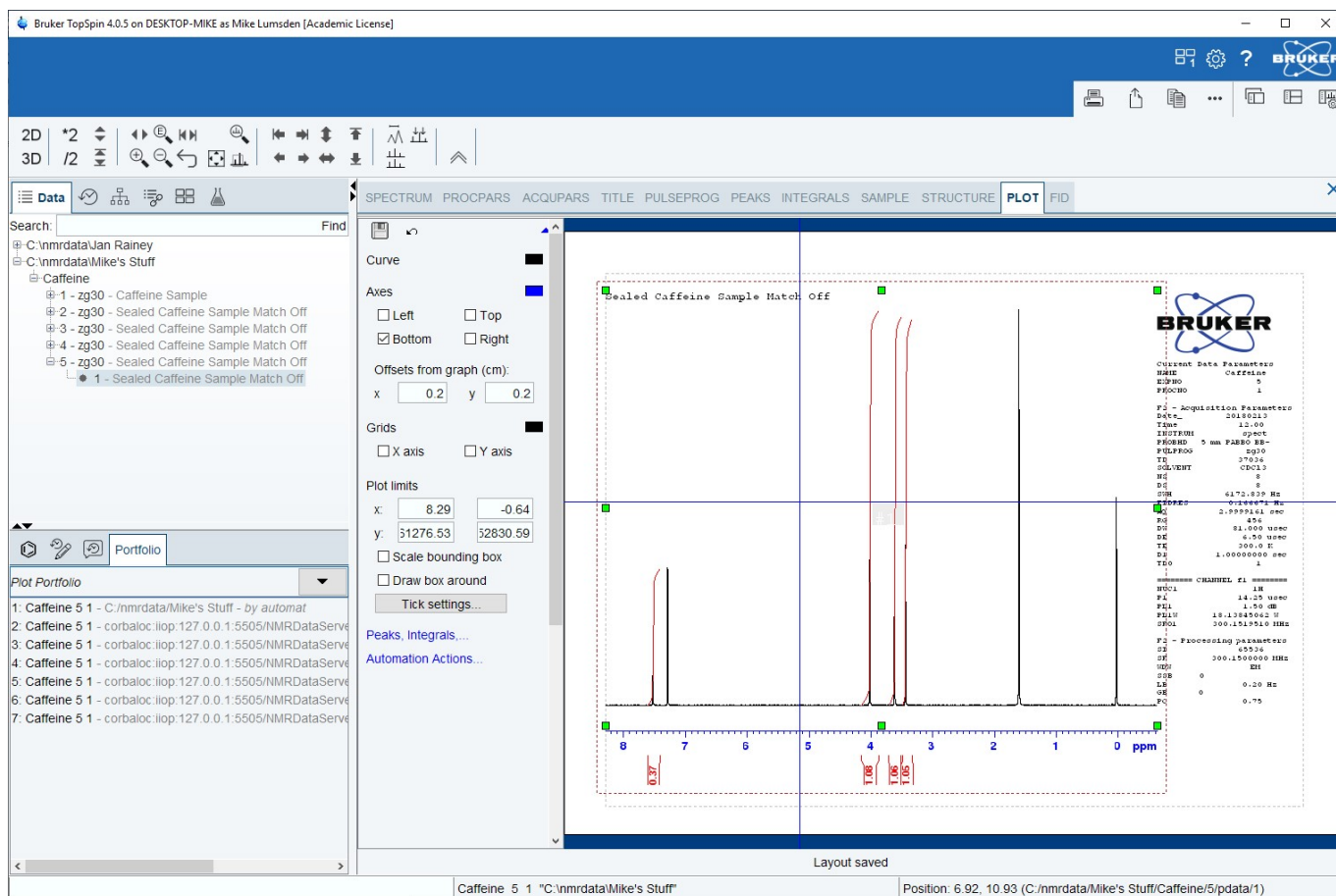


One can see from the figure that the 1D_H.xwp layout file specified the display of a single 1D spectrum along with the parameters, integrals, title and a logo above the parameters. To the left of this display is the editor main menu. A description of the regions indicated by the colored circles is as follows:

- Black → The majority of these icons can be used to move or scale spectra vertically or horizontally both within the spectrum tab as well as the plot tab.
- Blue → Plot portfolio window which in this case contains a single entry (by default the experiment from which the editor was launched).
- Red → The floppy disk icon at the top is for saving modified layouts. Beside that is an undo arrow. Below that is a display of the current layout and plotter/paper size. Changes can be made to the defaults via the adjacent drop-down arrows. In the layout dropdown, one can load a different layout (**Open...**), create a new one from scratch (**New**), or save changes to a modified layout (**Save** to update an existing layout or **Save As** to generate a new layout). In addition, one can export the current layout as a graphics file (**Export...**).
- Green → View menu which allows expansions of spectra as well as zooming. Of particular use are the following:
 - adjusts the spectral display limits to match what you had in the spectrum tab.
 - perform an interactive expansion; click and then drag a box around the area you wish to expand.
 - adjust the display to full screen (CTRL-D to return to normal view)
- Purple → Use to insert new elements into the layout. Select the element to be inserted from the desired dropdown and then click and drag to insert it into the layout. There are two categories of elements available:
 - “Standard” elements include lines, arrows, text, shapes, and curves.
 - “NMR” elements include experimental NMR data (FID/1D/2D NMR data), NMR parameters, titles, T1/T2 relaxation curves, etc.

(3) Modifying Layout Objects

The objects within the layout can be modified provided they are first “marked” by selecting them with the mouse. Once an object is marked, a border is created around it with a series of green rectangles as shown in the below figure (1D spectrum object is marked). Left clicking and dragging the green markers will resize an object whereas dragging an object with the left



mouse button will move it. In addition, right-clicking on an object will open a useful menu where you can perform several actions such as a rotation, duplication or deletion of an object.

Also evident in the figure is that the left side editor menu is context sensitive. It provides access to a variety of attributes that can be modified when an object is marked. When the marked object is a 1D NMR spectrum, there are three attribute menus available (1) Peaks, Integrals... (2) Axes, Grids, Curve... and (3) Automation Actions. The first two are more important for the average user and are described in the next figure. Note that the various colored rectangles present (adjacent to Peaks, Integrals, Axis, Curve, Axes, Grids) all permit color changes for the specified item. Some items will also allow specification of a fill style and color (Integrals, Axes and Curve) and most provide the ability to change line thickness. Lastly, font changes can also be made in this same manner for 1D spectrum items containing text (peak labels, integral labels and axes).

This figure provides a detailed view of the context-sensitive control panels in the software. It highlights specific settings and their functions:

- Peaks Panel:**
 - Turn on/off peak picking (Labels) & tick marks (Marks)
 - “.00” controls number of decimal places
 - “ppm” dropdown changes peak picking units
- Integrals Panel:**
 - Turn on/off integral trails (Curve) & integral values (Labels)
 - “.00” controls number of decimal places
 - “Limits...” button allows integral trail scaling
 - “Above X Axis” allows position of labels above or below the chemical shift axis
- Axis Panel:**
 - Control chemical shift axis units and scaling
- Placement Panel:**
 - Specify exact placement and size of the object
- Curve/Axes Panel:**
 - Controls position of the shift axis (bottom or top) as well as the y-intensity axis (left or right)
 - Control the offset of the axis/axes from the spectrum
 - Turn on/off horizontal/vertical grid lines
 - Specify plot limits and vertical scaling numerically
 - Tick settings... controls the number and the spacing of the axis ticks/labels. Number of decimal points also controlled here.

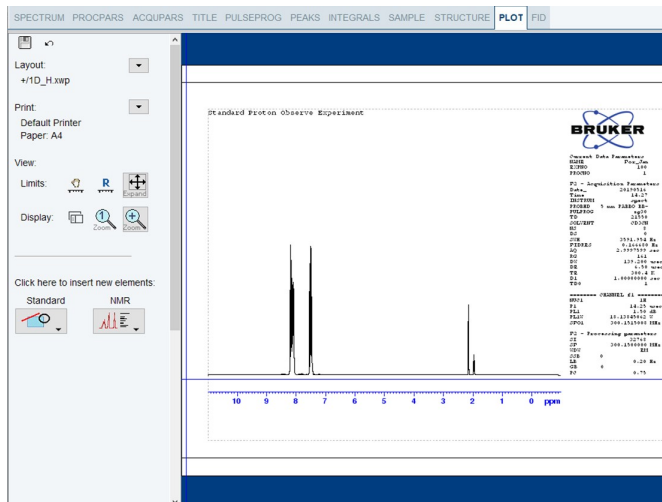
(4) Learn by Doing

At this point, it is hopefully clear that you can use pre-defined layouts to generate NMR figures in addition to modifying these layouts as you deem necessary. Modifications come in the form of changing existing objects (resizing, moving, deleting, marking and changing attributes) as well as using the insert menus to introduce new objects (either standard or nmr objects). Modified layouts can of course be saved for future usage. In this section, I will discuss using the editor to perform a couple of common tasks (expansions and stacked plots).

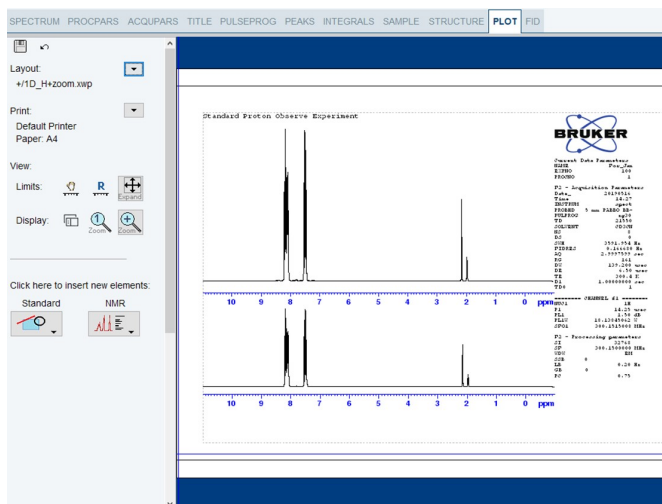
Common Task #1: Overlay an Expansion on a 1D NMR Spectrum

Method #1 – Using a Pre-Defined Layout

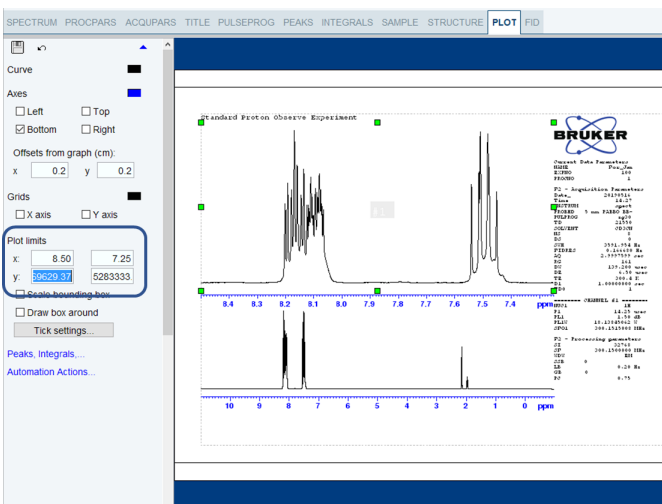
- Process the spectrum you wish to use and then click on the plot tab.



- Click the drop-down arrow to the right of Layout and choose Open. Answer yes to the question about discarding changes and select **1D_H+zoom.xwp** and then choose Open. The displayed spectrum will be duplicated and placed above the first spectrum.

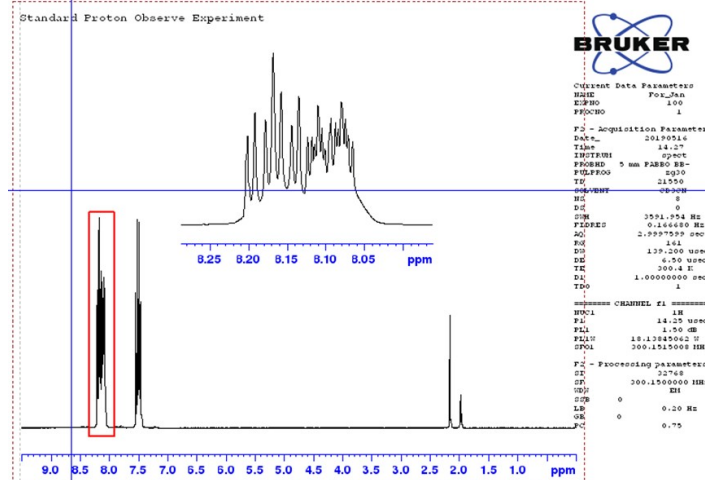
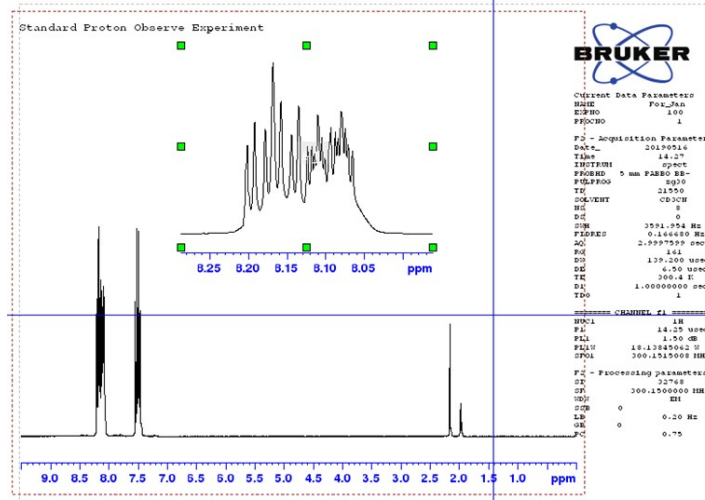
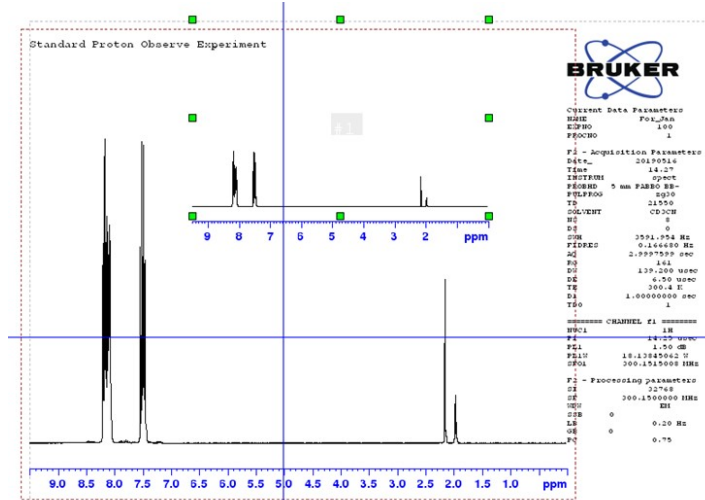
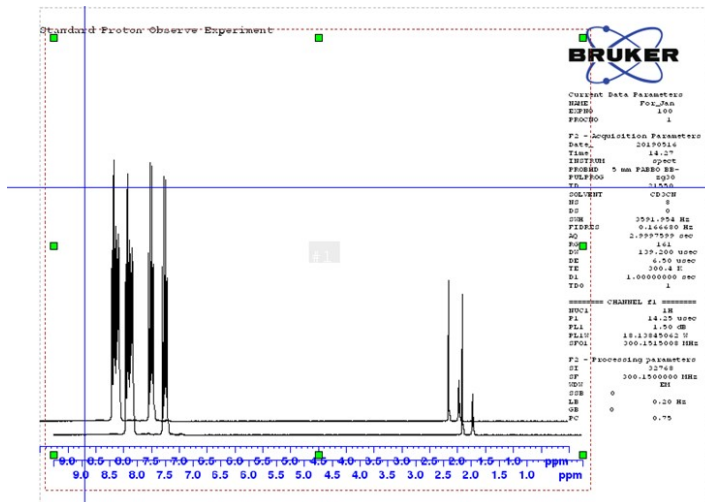


- Mark the top spectrum and then in the left-side menu, choose the “Axes, Grids, Curve...” menu. Specify the chemical shift range that you wish to use in the expansion via the “Plot limits” section. Alternatively, you could right-click over the spectrum, choose “Expand Tool” in the pop-up menu and drag a box over the expansion region.



Method #2 – Duplicate the First Spectrum & Modify

- With the full spectrum displayed in the plot tab, right-click on it and select duplicate in the pop-up menu. This will create a second copy of the full 1D spectrum.
- Drag the second spectrum into position and resize it to your liking by having it marked and dragging the green markers.
- Right-click over the second spectrum and choose “Expand Tool”. Drag a box around the region of the spectrum you wish to expand. You can manually specify the expansion region in the left-hand menu under plot limits. If you prefer to remove the chemical shift axis from the expansion, go to the left side menu with the expansion marked and unclick Axes → Bottom.
- If you’d like to indicate the expanded region in the full spectrum, one can go to the insert menu and under the “Standard” dropdown choose rectangle (or circle). Click and drag a rectangular box over the expansion region. Like other objects, the rectangle can be moved and resized by marking it. Attributes such as line color and thickness can also be changed via the left side menu once it is marked.

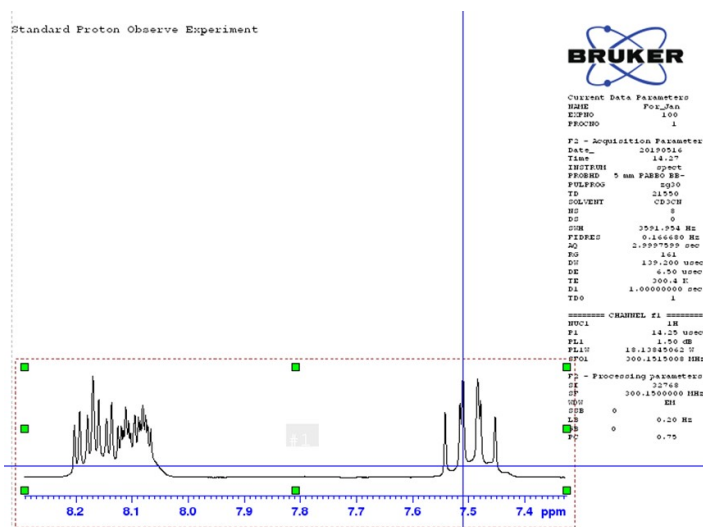


Common Task #2: Creating Stacked Plots

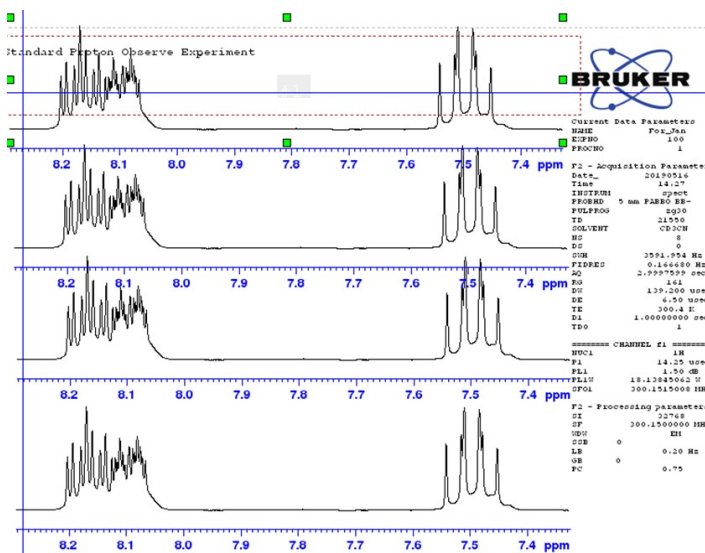
Topspin provides several tools to facilitate the creation of stacked plots. I will outline different approaches to generating these plots; a couple of more glamorous approaches involving the use of pre-defined stacked plot layouts and a robust brute-force method. In the following, we will stack 4 spectra; a highly coupled ^1H spectrum showing numerous J-couplings to ^{19}F nuclei along with a $^1\text{H}\{^{19}\text{F}\}$ experiment and then two ^1H spectra with selective ^{19}F decoupling.

Method 1: Brute-Force Method

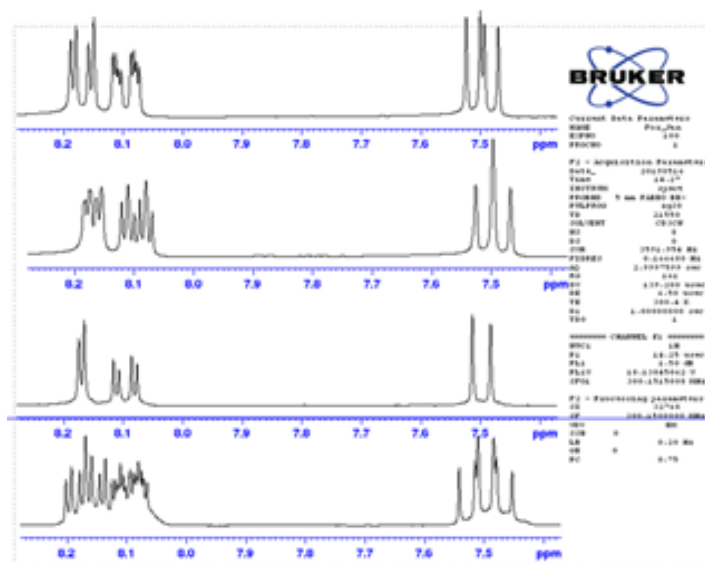
- Go to the Plot tab from the spectrum you want at the bottom of the stack. Expand the spectrum to show the region of interest (right-click and choose Expand Tool) and then reduce its size vertically (by dragging the green markers) to roughly 25% of the full display height (25% since 4 spectra will be stacked)
- Next, populate the plot portfolio with the desired 4 experiments to be stacked. To do this, simply drag the desired experiment numbers from the data browser down into the portfolio.



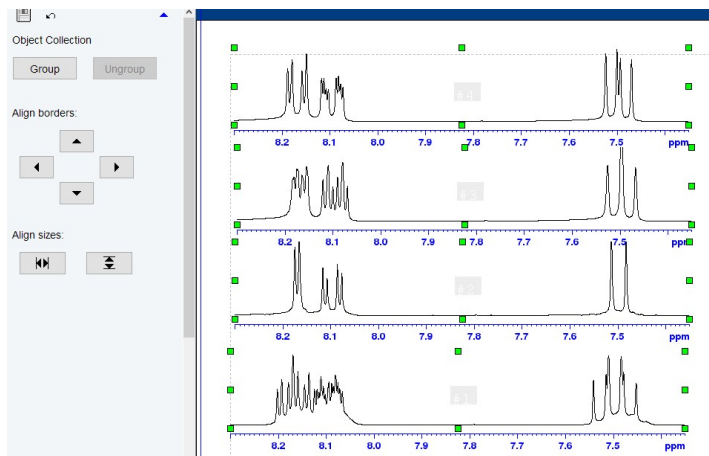
- Right-click anywhere over the spectrum and choose Duplicate. Drag the duplicate into approximate position above the proton. Repeat this step twice more such that you end up with 4 equivalent spectra in a rough stacked plot configuration



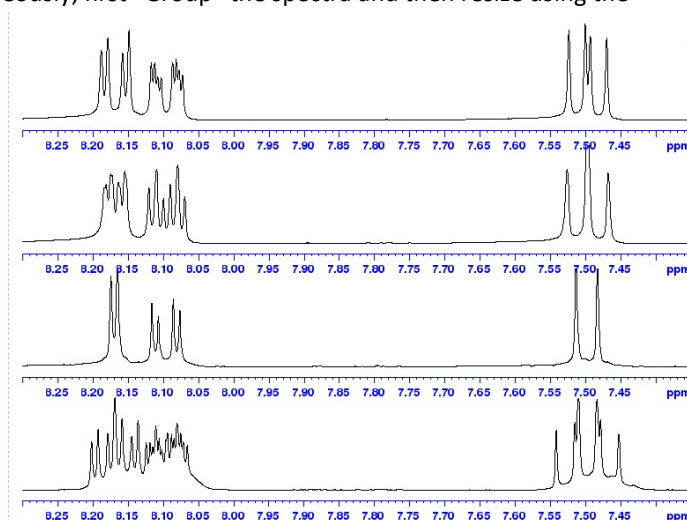
- Update the four spectra to display the desired experimental data. To do this, drag and drop the **experiments from the plot portfolio** over the various 1D spectrum objects - the spectra will be updated accordingly.



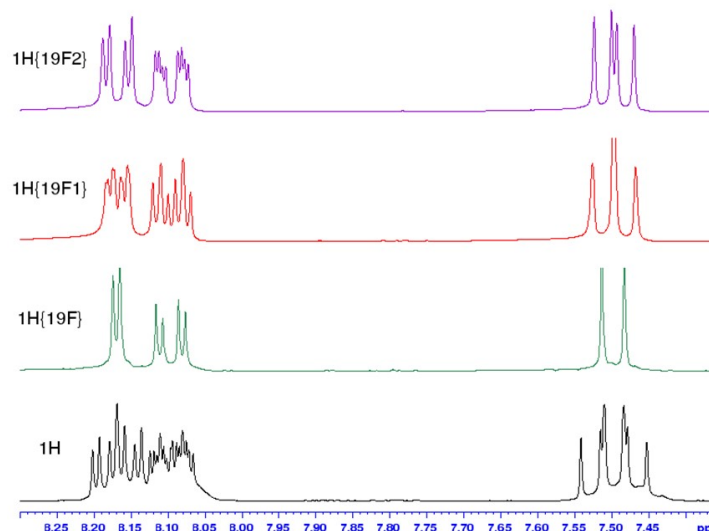
- With the proper spectra loaded into the 1D spectrum objects it only remains to optimize the layout. First, we will (optionally) delete the parameter list and logo (right click over both and choose Delete). Next, select all 4 spectra by holding down the Shift key and selecting each spectrum in turn (all spectra now marked). Note that provided there are no other objects present in the layout, you can alternatively right click somewhere outside of the dotted lines defining the spectra and choose "Mark All". Note in the adjacent figure that the left side menu changes to an "Object Collection" menu whenever more than one object is marked.



- You may now wish to do the following:
 - To change the size of the 4 spectra simultaneously, first "Group" the spectra and then resize using the appropriate green markers. When finished, click Ungroup.
 - To align all spectra horizontally, click either the left arrow or right arrow under "Align borders".
 - If you have been following these instructions, you should not need to "Align sizes". However, if for any reason you changed the size of one or more of your spectra, use "Align sizes" to make them identical.
 - To force a constant vertical offset between the spectra, you should mark the bottom spectrum and in the left menu under Placement, note the y value for Pos (position). To make it easier, consider forcing this number to 1.00. Now mark the remaining spectra individually and make sure there is a constant offset in this y-position between all consecutive spectra.



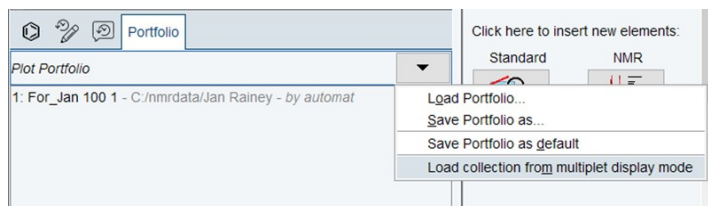
- You may also consider the following:
 - Since all spectra are aligned, you may consider removing the various chemical shift axes except for the bottom one. Mark each spectrum individually and uncheck "Bottom" under the Axes section.
 - To use different colors for each spectrum, select each spectrum and click on the colored rectangle beside "Curve". You may also change the line thickness or type if desired.
 - To label the spectra, start by ensuring nothing is marked. Then in the left side menu at the bottom, choose Standard → Text. Position the mouse roughly where you wish to add the first label, left click, type ^1H , and then left click again. Repeat these steps for each spectrum. Alternatively, with the first label complete, duplicate, drag into position, mark, and then edit.



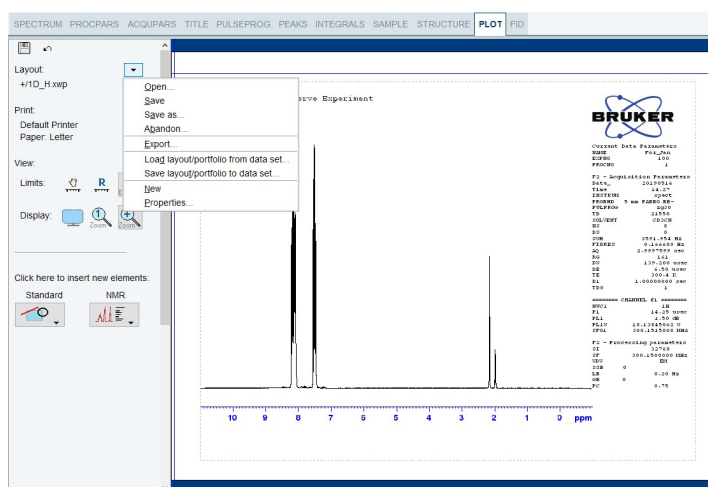
Method 2: Using Pre-Defined “MultiDisp” Layouts

The following approach makes prior use of multiple display mode to stack the spectra, something you likely would want to do anyway before generating the plot. Although not the topic of this document, you can enter multiple display mode by typing “.md” in the command line. For the ultimate purpose of using layouts, it is important to launch multiple display mode from the experiment that you wish to be at the bottom of your stack. Once in this mode, additional spectra can be dragged into the multiple display from the data browser. Order the spectra in the same way you want them ordered in your plot. When you are finished using multiple display mode to examine the spectra, click return to exit that mode and then move to the plot tab. Then proceed as follows:

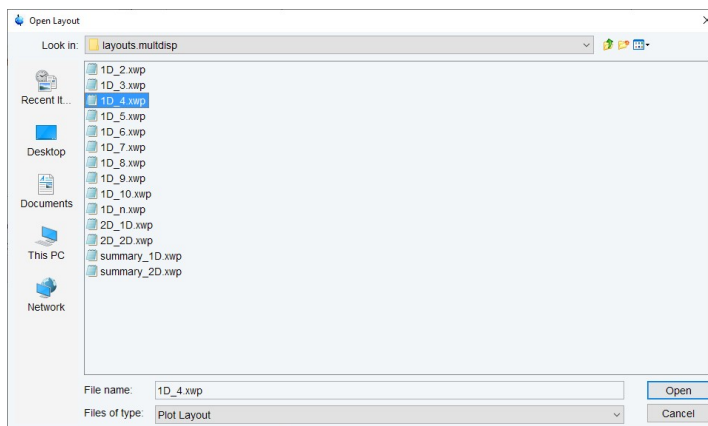
- In the plot portfolio, click the drop-down arrow and choose the bottom option, “Load collection from multiplet display mode”. This should add experiments previously examined in multiple display mode to the portfolio (in that same order).



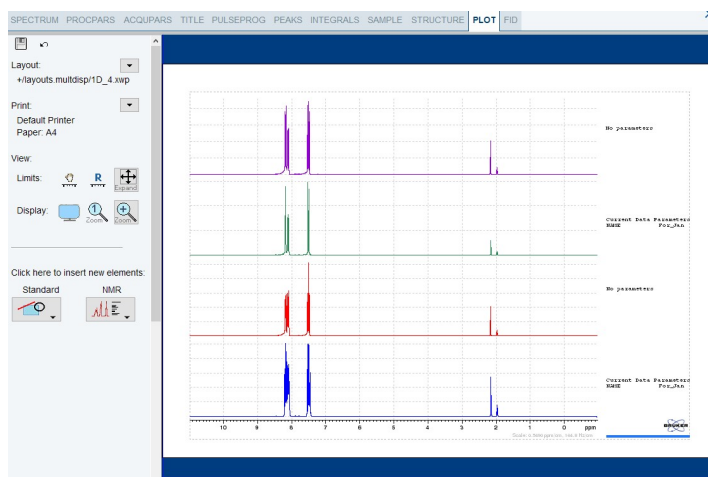
- Ensure no objects in the default layout are marked. Click the down arrow to the right of Layout and choose Open. Click yes when asked about discarding changes.



- In the list of layouts that opens, go to the folder “layouts.multidisp” and choose the appropriate layout (according to the number of spectra you are stacking). In this example, we will choose 1D_4.xwp and click Open.



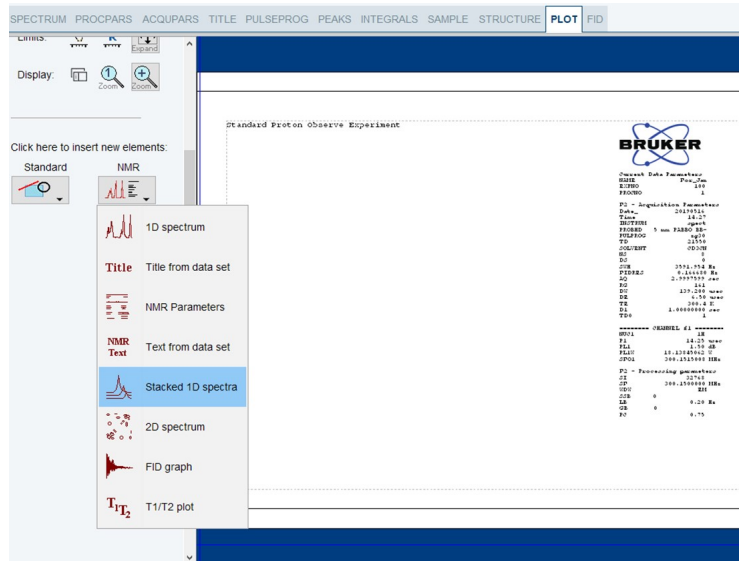
- You should now have a stacked plot in your layout containing the desired 4 spectra in the same order you used in the multiple display mode. You would likely now proceed as in the last bulleted point in the Brute-force method to configure the plot to your satisfaction (resizing, adding text labels, changing colors, etc).



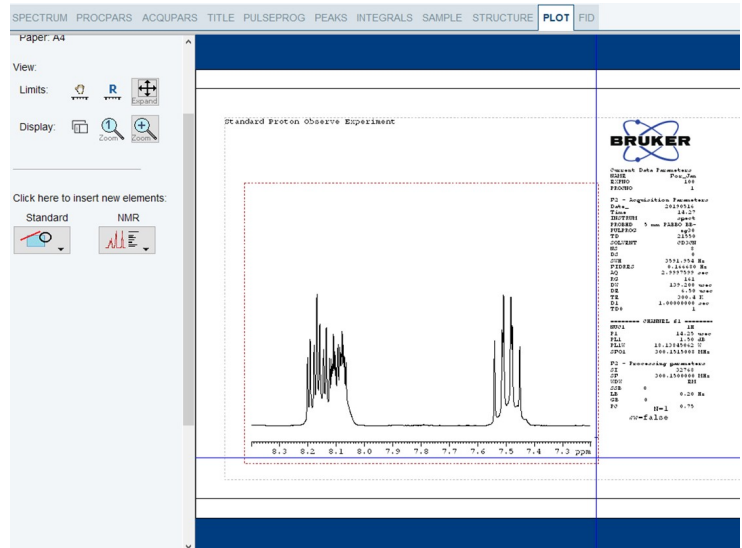
Method 3: Insert a “Stacked 1D Spectrum” Object

As outlined in Method 2, first use multiple display mode to display the spectra you wish to ultimately use in the stacked plot. Then leave multiple display mode, go to the plot tab, and in the plot portfolio use the drop-down arrow to “load the collection from multiplet display mode”. Right-click over the existing spectrum in the display and choose Delete. Then proceed as follows:

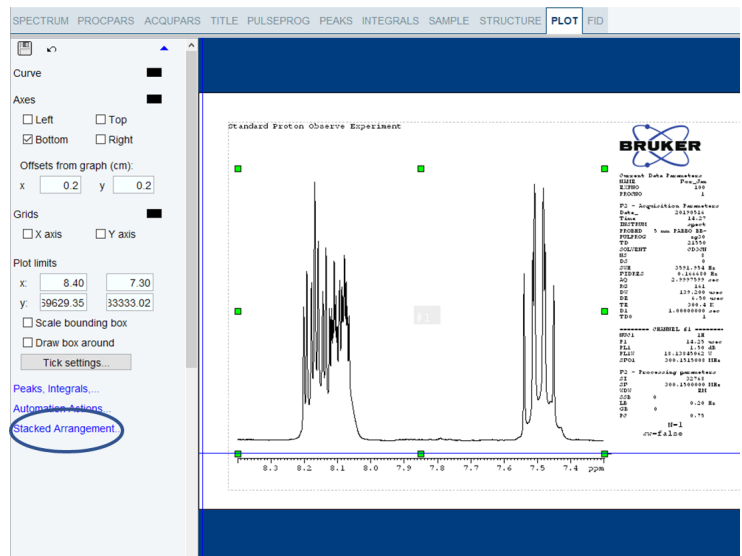
- In the “Insert New Elements” section, click on the NMR dropdown and select “Stacked 1D spectra”.



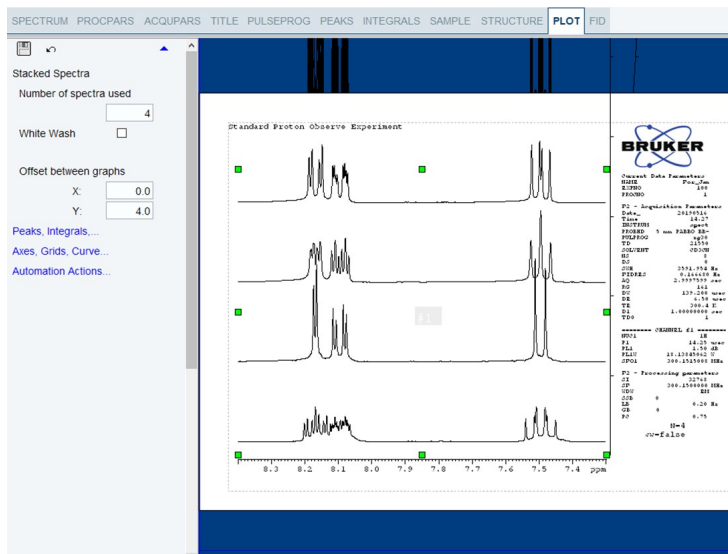
- Click and drag in the layout to define the stacked 1D object. Once the object is created, you can of course mark it to resize and/or drag it to change the position. There will only be a single spectrum at this point containing the first experiment in the Plot Portfolio.



- Mark the stacked 1D object. In the left side menu select the attribute page called “Stacked Arrangement”.



- In the stacked arrangement menu, specify the number of spectra used. In addition, you can add in x- and y-offsets and in addition enable a whitewash effect.



Some additional notes on this method:

- When you mark a “Stacked 1d Object”, green handles appear only for the bottom spectrum. Any changes in position or size that you make to the marked spectrum automatically translate to the others in the stack.
- If you make an expansion to the bottom spectrum, this does NOT automatically carry forward to the other spectra. If you wish to apply the expansion to the other spectra, it is probably easiest to go to the stacked arrangement attributes menu, temporarily make the “number of spectra used” back to 1 and then back again to the desired number.

(5) Information Concerning the “Automation Actions” Interface

Stored within layout files are a series of settings called automation settings which control, among other things, the default appearance of both the horizontal and vertical display of your spectrum. These options are critically important when plotting via automation (ICONNMR or the “autoplot” routine). If the stored settings aren’t appropriate when launching the plot editor, they can be altered via the Automation Actions menu.

Controlling the Default Chemical Shift Range

The figure on the right shows the automation actions interface. The X Plot Limits dropdown allows control of the default horizontal range displayed:

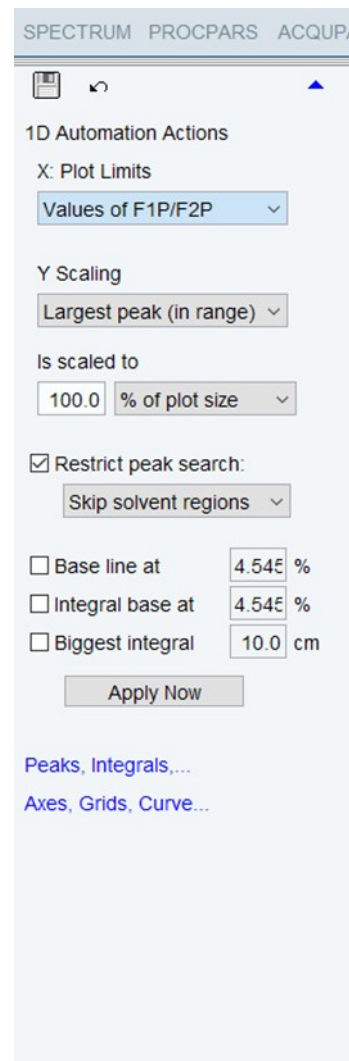
- Use Full Range: use the fully acquired chemical shift range stored in the layout
- Don’t Change: use the limits stored in the layout file
- Values of F1P/F2P: use the values stored in the processing parameters F1P/F2P. These can be readily defined from the spectrum tab by displaying the region desired, right-clicking, choosing “Save Display Region To...” and selecting Parameters F1/2.

Suppose you want a layout file that always displays the region 9.5 to -0.5 ppm. To achieve this, you could either:

1. Update the parameter set on the spectrometer that you use to obtain ^1H NMR spectra and set F1P to 9.5 and F2P to -0.5. When you save your proton layout file, ensure that the “X Plot Limits” setting in the automation actions menu is set to “Values of F1P/F2P”.
2. If you are unable to change the parameter set on the spectrometer, an alternative approach would be to display the region 9.5 to -0.5 ppm in the plot editor. When you save your proton layout file, ensure “X Plot Limits” is set to “Don’t Change”.

Controlling the Default Vertical Scaling

The default vertical scaling is controlled by the three regions of the menu entitled “Y Scaling”, “Is Scaled To” as well as the “Restrict Peak Search Option”. The “Y Scaling” dropdown allows one to choose either the largest peak in the displayed range or the entire spectral range as the reference peak for vertical scaling. With the proper peak specified, the “Is Scaled To” area defines the default height of the reference peak. There are options here to specify height as a percentage of the plot size, directly in cm, or to use the value specified in the processing parameter CY. Lastly, the “Restrict peak search” field, if selected, allows you finer control over your reference peak. Using this option, you can ignore solvent



and reference signals (as defined in the file specified by the SREGLIST parameter), choose only signals that are found within integral regions, or use a REG file (generated via the integration subroutine)

(6) FAQ

1 – Why is it that the positions of objects on the screen change depending upon which experiment I launch the plot editor from?

As mentioned, TopSpin establishes the exact positions and sizes of plot editor objects using layout files. If object attributes are changing as a function of experiment, this likely means that different layout files are being referenced in the different TopSpin datasets you are using.

2 – Why do I have to load the plot editor before making plots? I always use the default layout and seldom make any changes.

In fact, you do not have to load the plot editor first. Rather, you can use the autoplot routine, which will evaluate the layout specified and the dataset portfolio and send the result directly to the plotter. The command “**autoplot**” can be run directly from the TopSpin command line or via the CTRL-P interface by selecting the option “Print with layout – plot directly”.

3 – I would like the plot editor to show a 1D NMR spectrum just like I have it displayed in TopSpin. Is it possible to do this?

It is very easy to do this in the chemical shift dimension. Launch the editor using the CTRL-P command. Provided the “from screen / CY” option is selected in the plot limits section of this interface (which it is by default), the limits displayed in the editor will match those displayed in TopSpin.

In terms of the y-axis (intensities), this is not straightforward. My advice is to not spend your time adjusting intensities within TopSpin when you are doing so in anticipation of creating a figure within the plot editor. Rather, load the data into the plot editor first and then adjust intensities from there.

4 – I spent a lot of time creating my own layout to use in some slides for an upcoming talk. Recently, I wanted to go back and make a few slight modifications. Even though I saved the custom layout with the “Save As...” option and specified it as the layout parameter, it still did not display exactly as I had it originally. Why?

There are a couple of different reasons why things could change when you re-open a layout that was saved using the “Save As...” approach. If the correct experiments are showing in your layout but the chemical shift and/or intensities have changed, it is likely that the automation actions are over-riding your desired display settings. To avoid this, before saving the layout, go to the Automation Actions menu and set both the X Plot Limits and the Y-scaling to “Don’t Change”.

If your layout contains multiple NMR objects which are showing incorrect experimental data, the dataset list is wrong. The easiest solution is when saving your custom layout, rather than using the “Save As...” command, use the “Save Layout/Portfolio to Dataset...” command. This will write the layout file and portfolio directly to the data set rather than to the layout library. If you want to return to this layout in the future, use the “Open Layout/Portfolio from Dataset...” command.

5 – When I make an expansion with the mouse, is there a way I can lock the vertical scale so that I’m just performing a chemical shift expansion?

Yes; when using the expand tool, hold down the shift key when clicking and dragging to define the expansion. This will result in peak intensities remaining fixed. Likewise, if the Control key is pressed when defining the expansion limits, the horizontal scale will remain fixed.

6 – I’d like to add an arrow to my figure. Is there a way to do this?

To add an arrow, go to the “Insert New Elements” area of the main left side menu and click the “Standard” dropdown. Choose the line object and then click and drag within the layout to insert a line. Now mark the line and in the attributes menu, you can adjust the line style and thickness as well as the arrowhead style and width.

7 – I have created a custom-made layout containing some text. My goal was for this text to be the same, regardless of which dataset I opened. However, when I load different datasets, my text is being replaced by the dataset title. Is there a way around this?

When you created your text, you must have used the NMR dropdown to insert a “Title” object. If you want the text to remain independent of dataset, you must use the Standard dropdown and insert a text object.