TopSpin

NMR Data Publishing

User Manual

Version 001

Innovation with Integrity

NMR

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This manual was written by

NMR Software Department

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Contents

1 Introduction

1.1 General

This manual is intended to be a reference guide for plotting and printing NMR related data in TopSpin. It describes the complete TopSpin print functionality, both interactive and automated based on TopSpin 3.5.

The figures shown in this manual are designed to be general and informative and may not represent the specific Bruker model, component or software/firmware version you are working with. Options and accessories may or may not be illustrated in each figure.

For older versions of TopSpin, please refer to the manual supplied at the time.

1.2 System Support

TopSpin runs on Windows, Linux and MacOS operating systems. The elements involved in printing like data sets, portfolios and plot layouts are interchangeable between these platforms. The description and screen shots in this documentation were taken on a Windows computer.

Note that imported WMF graphics in a layout created under Windows, will not be displayed or printed on Linux systems. Vice versa, imported EPSI graphics, in a layout created under Linux, will not be displayed or printed on Windows systems.

1.3 Disclaimer

This guide should only be used for its intended purpose as described in this manual. Use of the manual for any purpose other than that for which it is intended is taken only at the users own risk and invalidates any and all manufacturer warranties.

1.4 Limitation of Liability

All specifications and instructions in this manual have been compiled taking account of applicable standards and regulations, the current state of technology and the experience and insights we have gained over the years.

The manufacturer accepts no liability for damage due to:

- Failure to observe this manual.
- Improper use.
- Deployment of untrained personnel.
- Unauthorized modifications.
- Technical modifications.
- Use of unauthorized spare parts.

The actual scope of supply may differ from the explanations and depictions in this manual in the case of special designs, take-up of additional ordering options, or as a result of the latest technical modifications.

1.5 The Bruker Service

Our customer service division is available to provide technical information. See *Contact [▶ 139]* for contact details.

In addition, our employees are always interested in acquiring new information and experience gained from practical application; such information and experience may help improve our products.

1.6 Conventions

Type of Information	Font	Examples
Shell Command, Commands, "All what you can enter"	Arial bold	Type or enter **fromjdx zg**
Button, Tab, Pane and Menu Names "All what you can click"	Arial bold, initial letters capitalized	Use the **Export To File** button. Click **OK**. Click **Processing**…
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names **Data Path Variables** **Table Column Names** **Field Names (within Dialog Windows)**	Arial Italics	*$tshome/exp/stan/nmr/lists* *expno, procno,*
Parameters	Arial in Capital Letters	VCLIST

Program Code
Pulse and AU Program Names
Macros
Functions
Arguments
Variables
	Courier	`go=2`
		`au_zgte`
		`edmac`
		`CalcExpTime()`
		`XAU(prog, arg)`
		`disk2, user2`

AU Macro	Courier in Capital Letters	`REX` `PNO`

Table 1.1: Font and Format Conventions

2 Publishing Options

2.1 Introduction

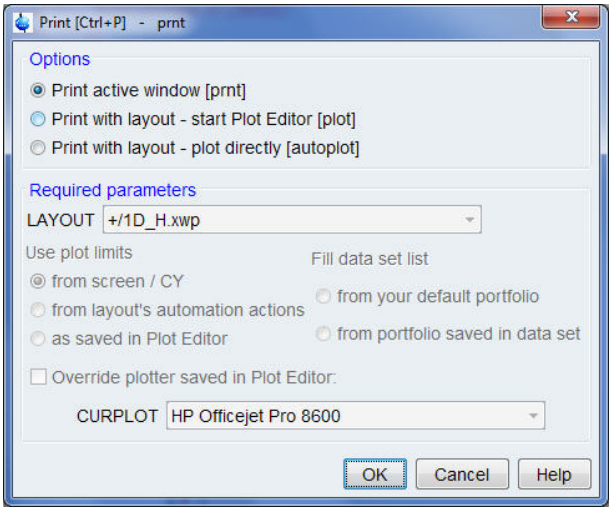
This chapter will guide you through the publishing options of TopSpin. Throughout this guide book, we will focus on using TopSpin icons, if possible, to execute commands or initiate actions. Hot keys or commands will also be mentioned in scenarios where it seems convenient to use them.

2.2 Print Data Displayed in the Active TopSpin Window

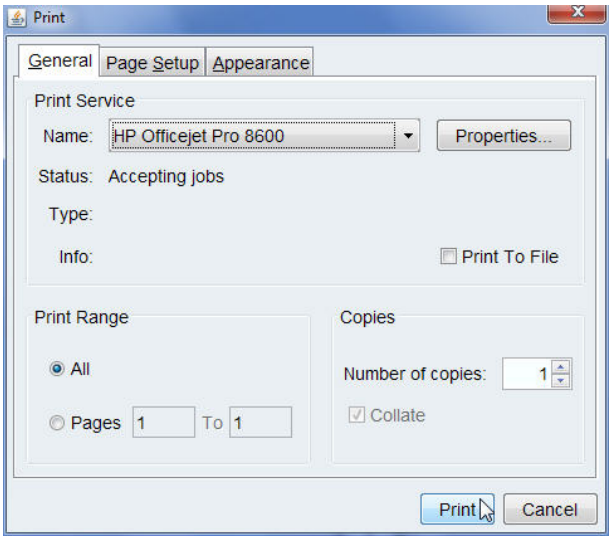
2.2.1 Print Using the Print Icon Tool Bar

- Click on the **Print** icon.

- Select **Print active window [prnt]** option in the Print [Ctrl+P] window.



- Click on the **OK** button inside the Print [Ctrl+P] window.
- Click on the **Print** button inside the Print window.

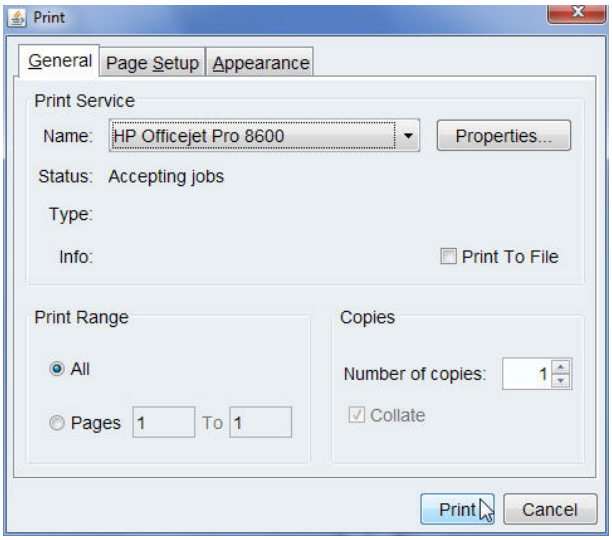


2.2.2 Print Using the Print Button in the Workflow Button Bar

This option is equivalent to Print using the command **prnt** typed in the TopSpin command line in this chapter.

- Click on the **Publish** icon in the Workflow tab bar.

- Click on the **Print** button in the Workflow button bar.

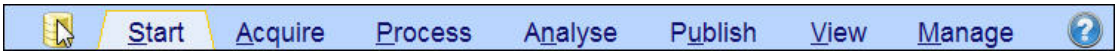


- Click on the **Print** button inside the Print window.

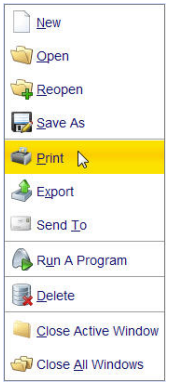
2.2.3 Print Using the Print Command from the File Menu

The step below refers to the **Disk** icon which looks like a stack of old computer tapes. This icon can be replaced by a text button **File**. To make this change, click on the **Man-age** tab in the **Workflow tab bar** and select **Preferences** by clicking on it. In the **Windows setting** section, enable **File menu: Show "File" text rather than icon** and restart TopSpin.

- Click on the **Disk** icon in the Workflow tab bar.



- Select **Print**.



- Click on the **OK** button inside the Print [Ctrl+P] window.
- Click on the **Print** button inside the Print window.

2.2.4 Print Using the Hot Key Ctrl - P

- On the keyboard press the **Ctrl** + **P** keys.
- Select **Print active window [prnt]** option in the Print [Ctrl+P] window.
- Click on the **OK** button inside the Print [Ctrl+P] window.
- Click on the **Print** button inside the Print window.

The Ctrl + p key memorizes the previously selected print option. This means it may show a different plot option than the one explained here when used again in TopSpin.

2.2.5 Print Using the Command Print Typed in the TopSpin Command Line

- Type **print** in the TopSpin command line.
- Click on the **OK** button inside the Print [Ctrl+P] window.
- Click on the **Print** button inside the Print window.

2.2.6 Print Using the Command Prnt Typed in the TopSpin Command Line

- Type **prnt** in the TopSpin command line.
  This option will display the **Print** window and skips the **Print [Ctrl+P]** window.
- Click on the **OK** button inside the Print [Ctrl+P] window.
- Click on the **Print** button inside the Print window.

2.3 Print Data Using Predefined Layouts

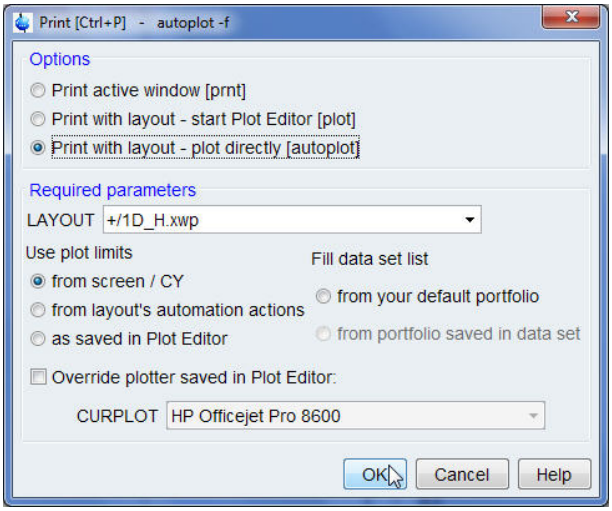
A layout is a template that defines an arrangement of several graphical objects. The graphical objects can be standard graphics such as lines, squares, curves etc. or NMR objects such as Spectrum, FID, Parameters, Title, etc.

One layout can be used for different data sets or a data set can be printed with different layouts. Bruker supplies a large number of predefined layouts within the TopSpin soft-ware and new ones can be easily added.

You can execute the same print commands described in the first four sections in *Print Data Displayed in the Active TopSpin Window [9]*. There will be two options to print the data.

2.3.1 Print Directly Using Autoplot

- On the keyboard press the **Ctrl** + **P** keys.
- Select **Print with layout - plot directly [autoplot]** in the Print [Ctrl+P] window.

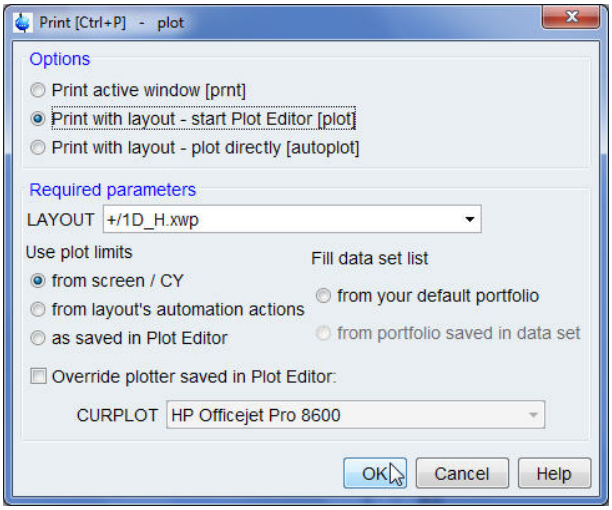


- Click on the **OK** button inside the Print [Ctrl+P] window.

Alternatively you can also use the command **autoplot** typed in the TopSpin command line to access the printer directly.

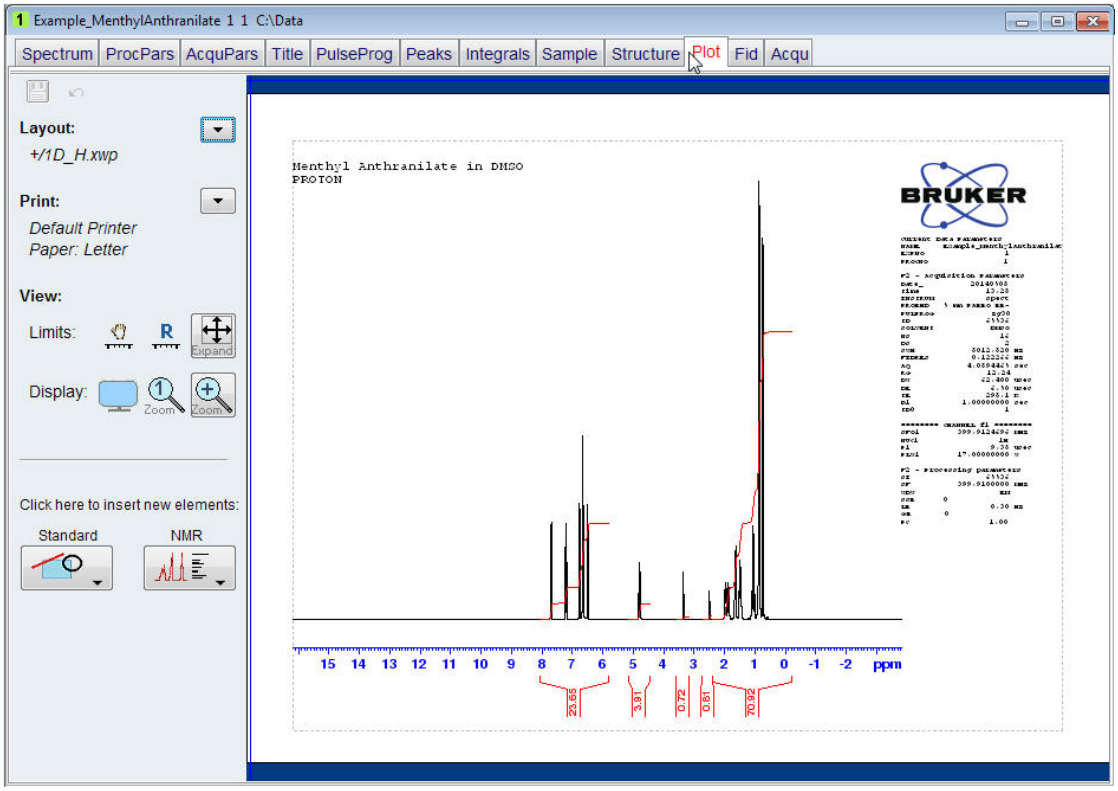
2.3.2 Print Using the Plot Editor

- On the keyboard press the **Ctrl** + **P** keys.
- Select **Print with layout - start Plot Editor [plot]** in the Print [Ctrl+P] window.

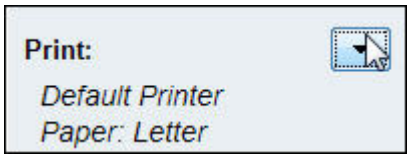


- Click on the **OK** button inside the Print [Ctrl+P] window.

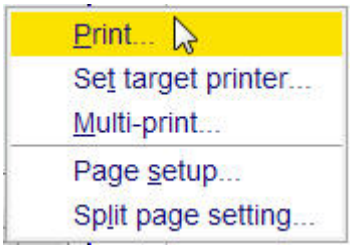
  Alternatively you can also use the command **plot** typed in the TopSpin command line to open the Plot Editor window.



- Click on the **down arrow** next to the **Print** option on the left side of the Plot Editor window.



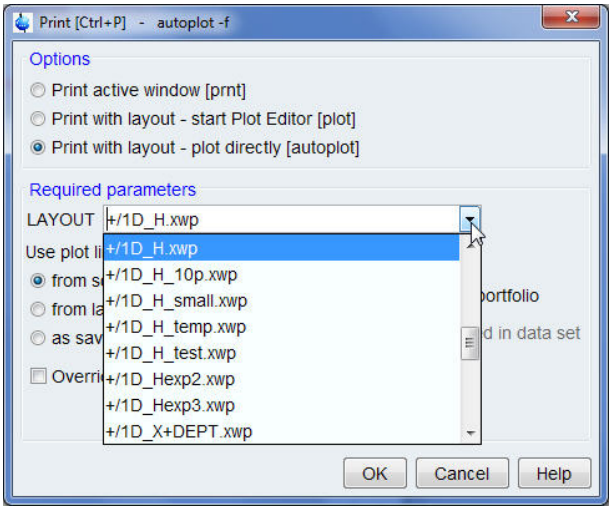
- Select **Print**.



2.4 How to Access the Layout List

2.4.1 Select the Layout from Inside the Print [Ctrl+P] -prnt Window

- Click on the **down arrow** to the right of the **LAYOUT** window.



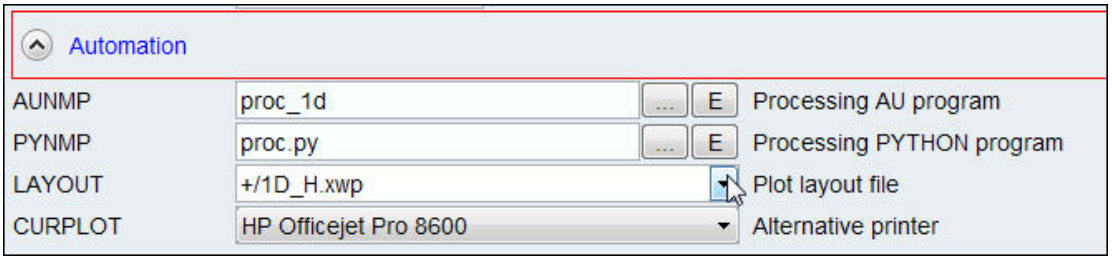
- Select the desired layout.

2.4.2 Select the Layout within the Processing Parameters

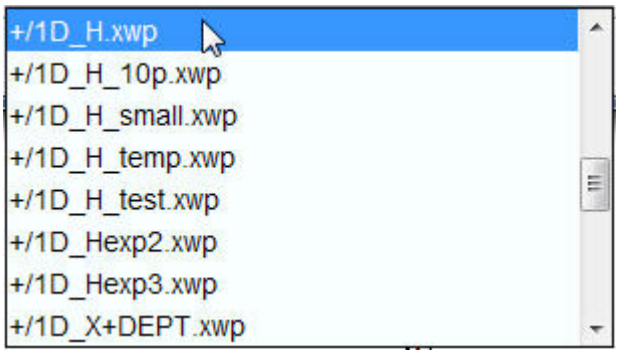
- Display a spectrum.
- Select the **ProcPars** tab in the **Data set tabs** bar.

- Scroll down to the **Automation** section.

- Click on the **down arrow** to the right of the **LAYOUT** window (Plot layout file).

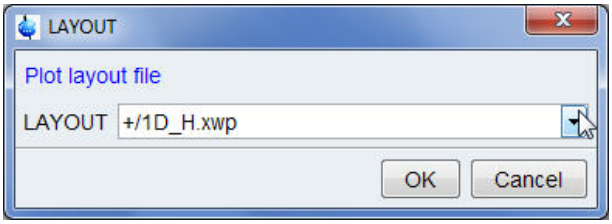


- Select the desired layout.



2.4.3 Typing the Layout Command

- Display a spectrum.
- Type **layout** in the TopSpin command line.
- Click on the down arrow to the right of the **LAYOUT** window.



- Select the desired layout.
- Click on the **OK** button inside the **LAYOUT** window.

2.5 Saving Data as an Image File

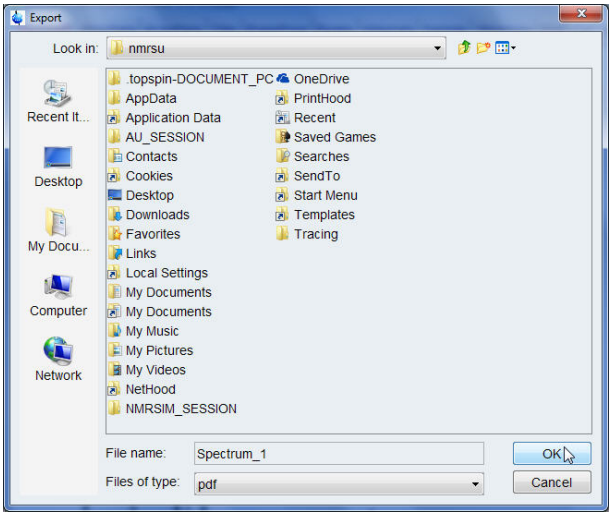
This publishing option lets you save displayed data in TopSpin as an image file of various formats such as pdf, png, jpg, bmp, tif or tiff. The examples below illustrate how to save data as a PDF file, displayed in the TopSpin spectrum, and in the plot editor window.

2.5.1 Save Data Displayed in the Spectrum Window as a PDF File

- Display a spectrum.

- Click on the **Publish** tab in the Workflow tab bar.

- Select the **PDF** button in the Workflow bar.

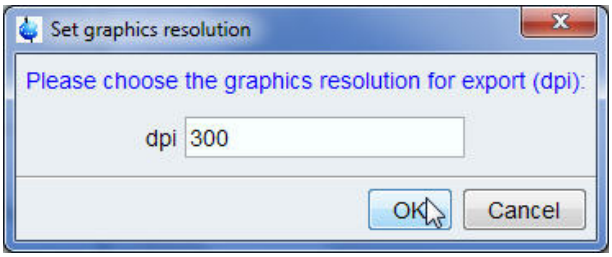


- Select the directory to store the file.
- Type a file name e.g. **Spectrum_1**.
- Click on the **OK** button inside the Export window.

The PDF file is stored as a screen resolution image. Other graphics formats can be chosen when you click on the down arrow inside the **PDF** button in the Workflow bar.

2.5.2 Save Data Displayed in the Plot Editor Window as a PDF File

- Display a spectrum.
- Click on the **Plot** tab in the Data set tab bar to open the Plot Editor.
- Select the **PDF** button in the Workflow bar.
- Select the directory to store the file.
- Type a file name e.g. **Spectrum_1**.
- Click on the **OK** button inside the Export window.
- Choose a graphics resolution e.g. **300**.



- Click on the **OK** button inside the Set graphics resolution window.

The PDF file is stored as an image with the specified resolution. Other graphics formats can be chosen when you click on the down arrow inside the **PDF** button in the Workflow bar.

Here are some hints about choosing the right resolution for publishing spectra. Many scientific journals expect to get a picture for an article in TIFF format with a resolution of a minimum of 600 dpi or better. This does not mean that the image exported from the Plot Editor is required to be at this resolution. The image exported from the Plot Editor will typically be A4 (210 x 297 mm) or Letter (8½ x 11 inches) size. If the final published image is one fourth this size, then an image exported from the Plot Editor at 300 dpi will result in an image at 1200 dpi when scaled to this final publishing size. On the other hand, attempting to export an image from the Plot Editor at 1200 dpi will likely result in various memory overflow error messages because the RGB (24 bit) color image of a letter size picture is 385 MB (not compressed).

Publishing Options

3 Print Data Displayed in the TopSpin Active Window

3.1 Introduction

This chapter will guide you through printing what is shown within the visible TopSpin window. The display options such as colors, parameters, title etc. are con-trolled in the Spectra Display Preferences window. To view the Spectra Display Preferences window, click on the Manage bar in the Workflow tab bar. Click on the **Preferences** button in the Workflow button bar. An easier and faster way to get to the display options is to right click inside the spectrum window and select the Spectra Display Preferences.

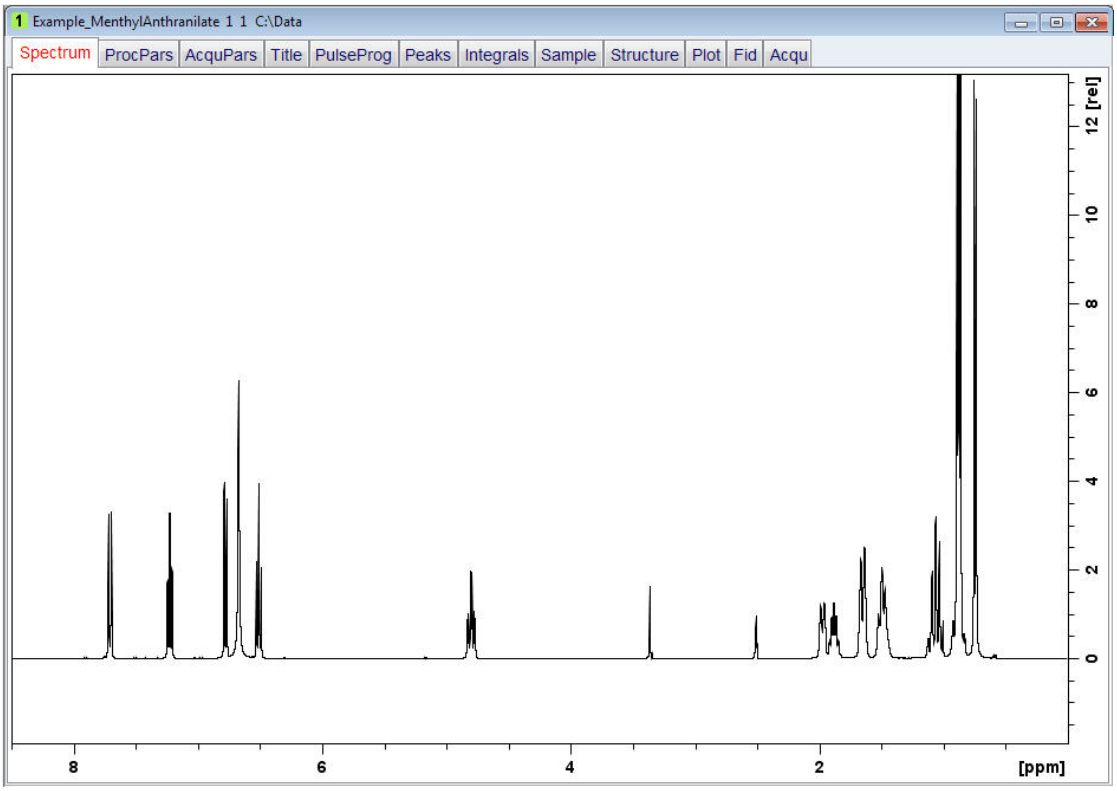
3.2 Print 1D Data Displayed in the TopSpin Window

This section describes how to get a fast print out of a single or multiple1D data sets displayed in the TopSpin window. Due to the many display options which one can select in the **Spectra Display Preferences** window only a few selected examples will be discussed.

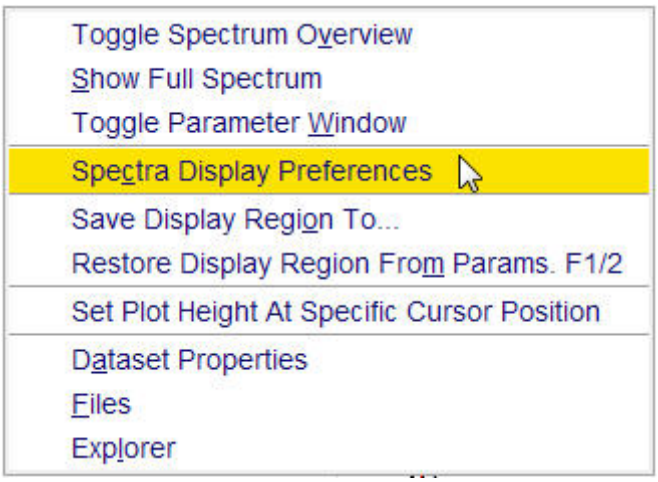
3.2.1 1D Proton Spectrum with Selected Display Options

Run a 1D proton spectrum adding a title and integration of the various peaks. In addition, import or draw the molecular structure of the observed sample.

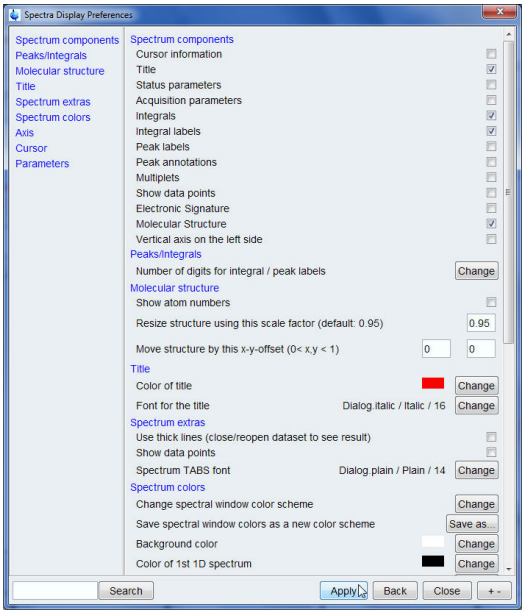
- Display the1D proton spectrum.
- Right click inside the displayed spectrum area.



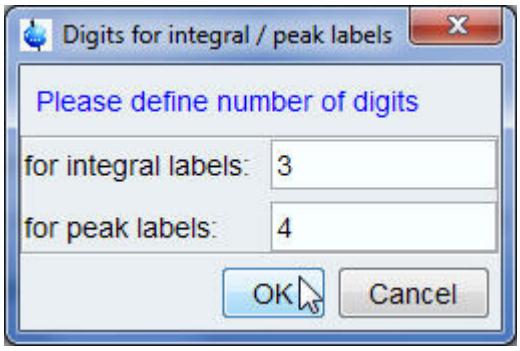
- Select **Spectra Display Preferences**.



- In the **Spectrum components** section enable the following options:
  - Title
  - Integrals
  - Integral labels
  - Molecular Structure

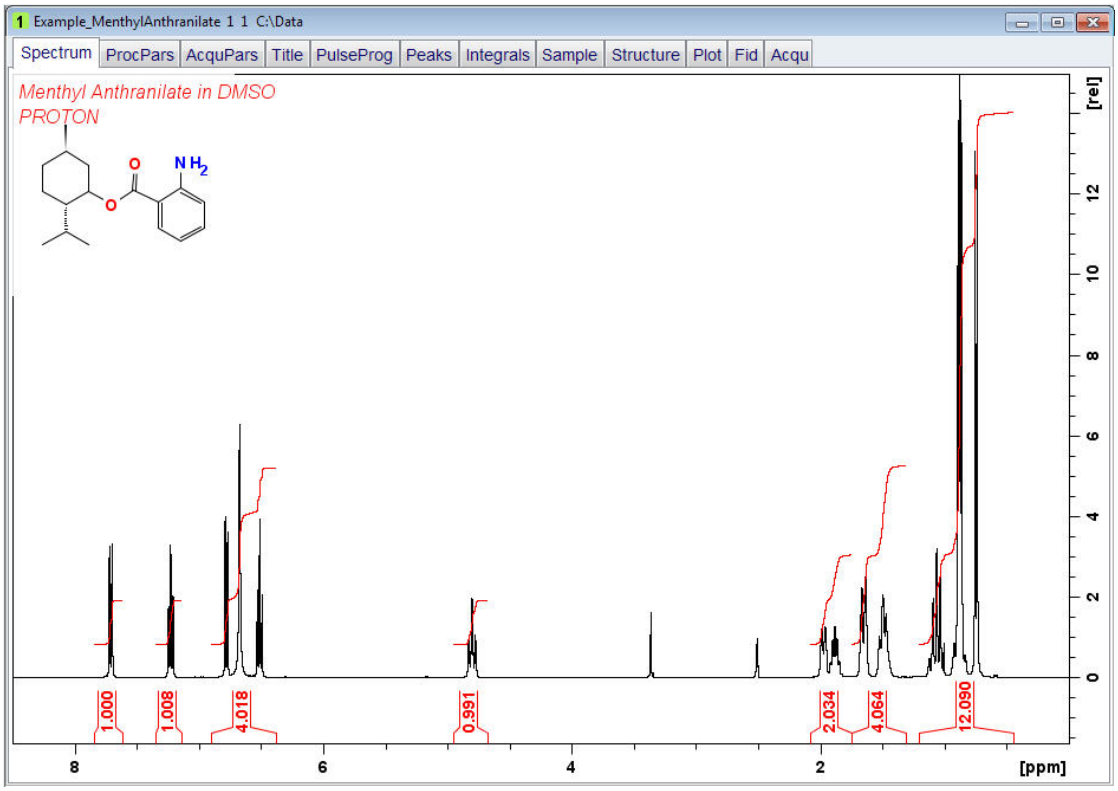


- In the **Peak/Integral** section click on the **Change** button to the right of **Number of digits for integral/peak labels**.
- For the integral labels enter **3**.

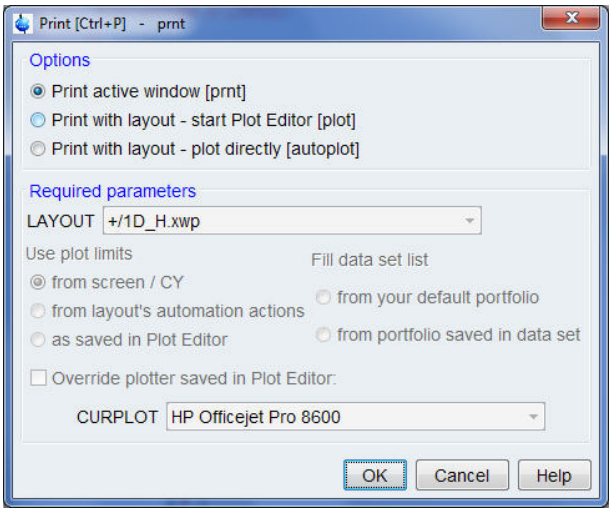


- Click on the **OK** button inside the Digits for integral / peal labels window.
- Click on the **Apply** button inside the Spectra Display Preferences window.

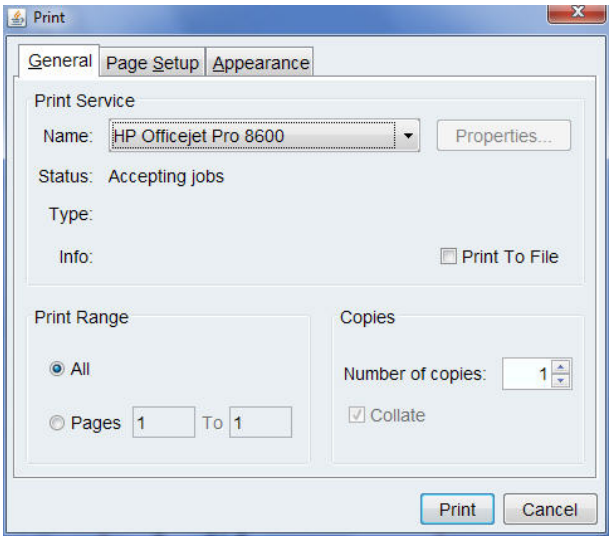
  In the **Molecular structure** section you can move the structure location or resize it. If necessary you can also change the font and color of the title and the spectrum. To apply the changes, you may have to refresh the display.
- Click on the **Close** button inside the Spectra Display Preferences window.



- Click on the **Print** icon in the TopSpin tool bar.
- Select **Print active window [prnt]** inside the Print window.



- Click on the **OK** button inside the Print [Ctrl+P] -prnt window.
- Click on the **Print** button inside the Print window.

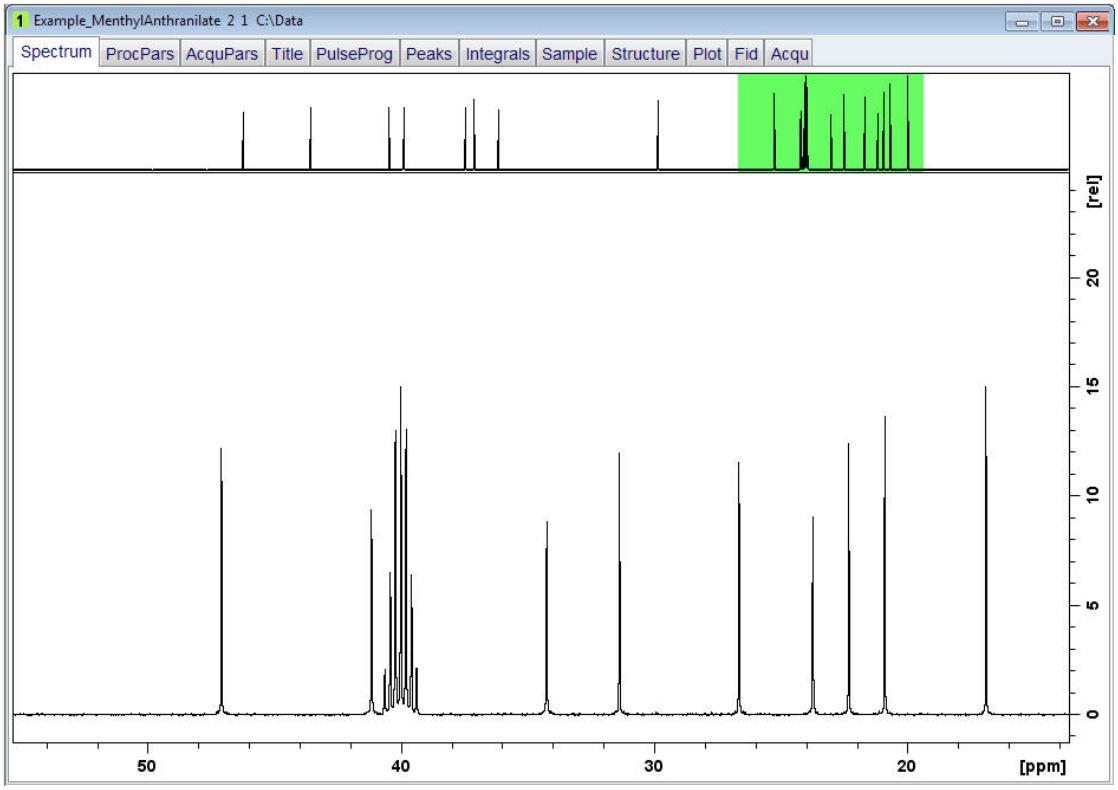


3.2.2 1D Carbon Spectrum with Selected Display Options

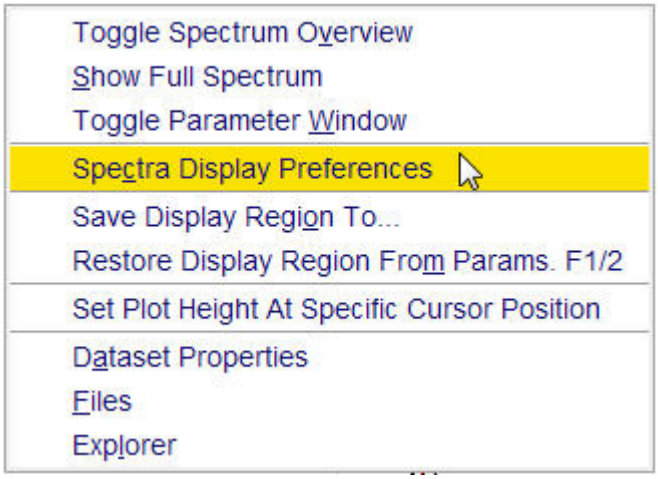
Run a 1D carbon spectrum adding a title and peak picking of the various peaks. Dis-play the spectrum overview and expand a portion of the spectrum. In addition, import or draw the molecular structure of the observed sample.

- Display the 1D carbon spectrum.
- Expand a part of the spectrum (e.g. from 56 ppm to 14 ppm).

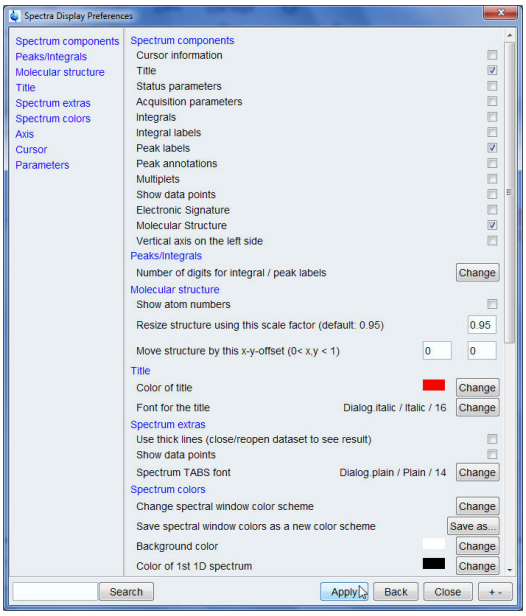
- Click on the **Toggle the display of spectrum overview** button inside the Tool bar.
- Right click inside the displayed spectrum area.



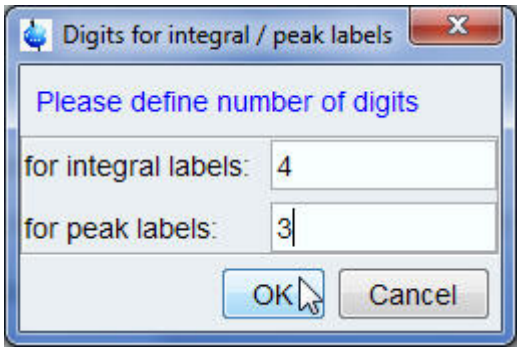
- Select **Spectra Display Preferences**.



- In the **Spectrum components** section enable the following options:
  - Title
  - Peak labels
  - Molecular Structure

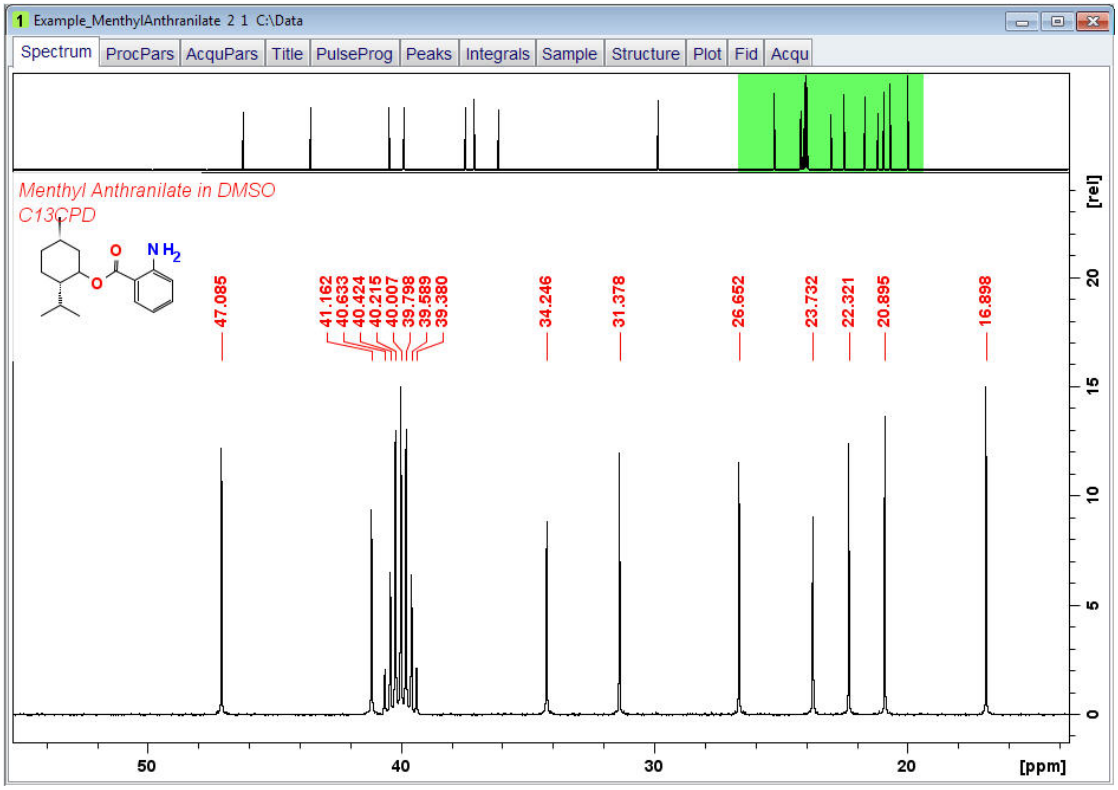


- In the **Peak/Integral** section click on the **Change** button to the right of **Number of digits for integral / peak labels**.
- For the peak labels enter **3**.



- Click on the **OK** button inside the Digits for integral / peal labels window.
- Click on the **Apply** button inside the Spectra Display Preferences window.

  In the **Molecular structure** section you can move the structure location or resize it. If necessary you can also change the font and color of the title and the spectrum colors.
- Click on the **Close** button inside the Spectra Display Preferences window.



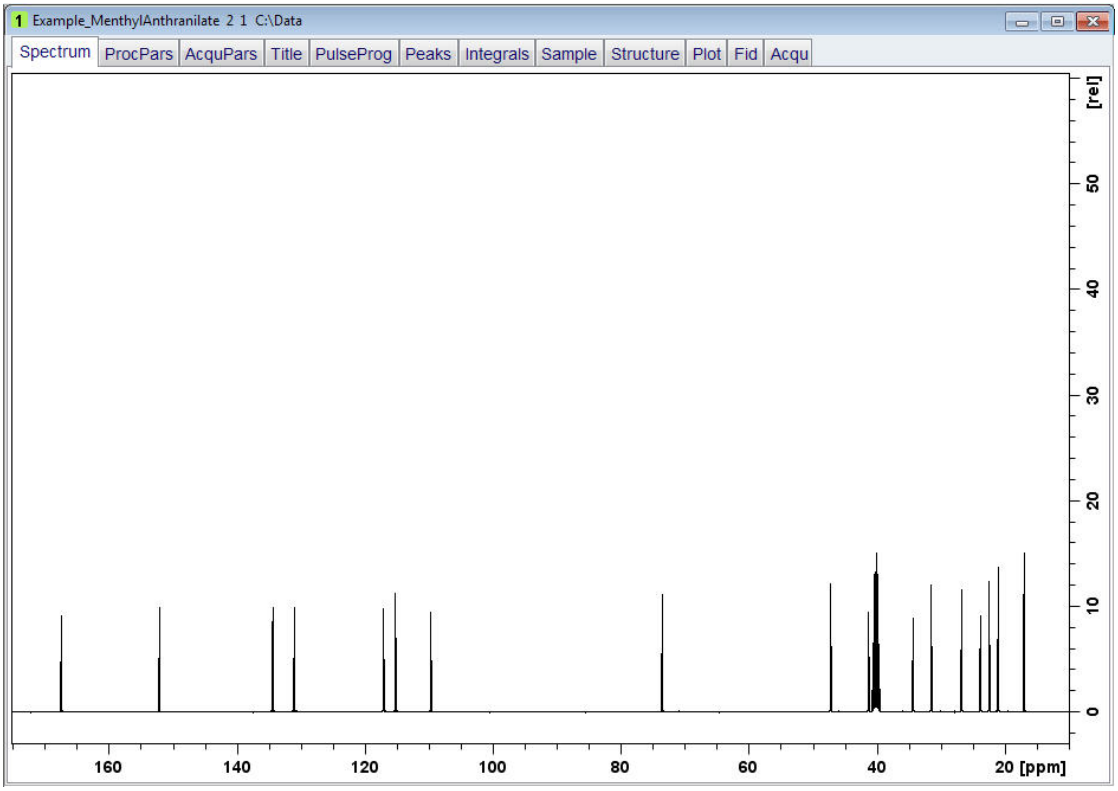
- Use the **Print** icon in the TopSpin tool bar to print the displayed spectrum. For step-by-step instructions see *1D Proton Spectrum with Selected Display Options [▶ 19]*.

3.2.3 Multiple 1D Spectra Displayed in the TopSpin Window

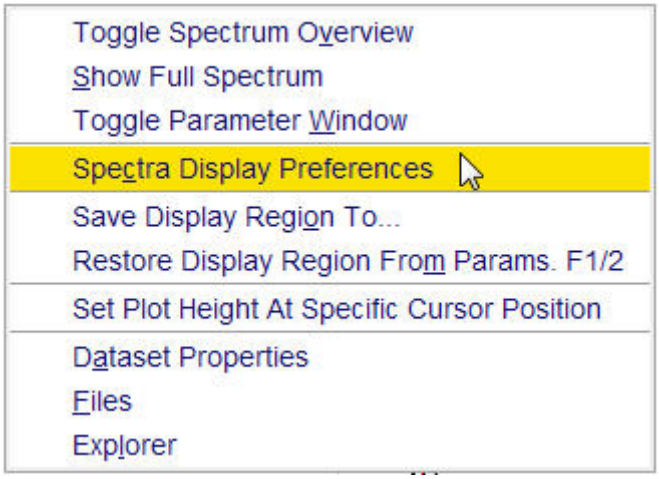
Follow the steps below how to print three spectra displayed in the TopSpin window. The example includes a 1D proton decoupled carbon spectrum along with a 1D carbon DEPT135 and a 1D carbon DEPT90 spectrum.

- Display the1D carbon spectrum.

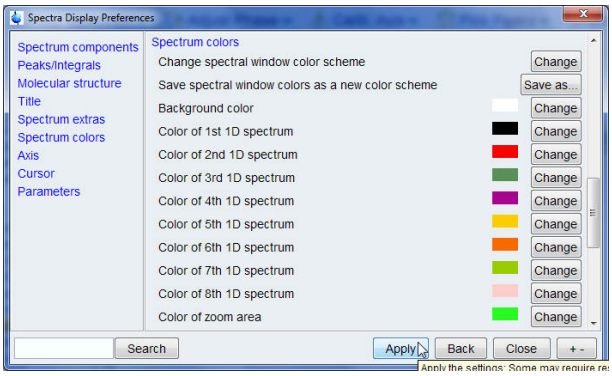
Print Data Displayed in the TopSpin Active Window



- Expand the spectrum to include all peaks of interest.
- Right click inside the displayed spectrum area.
- Select **Spectra Display Preferences**.

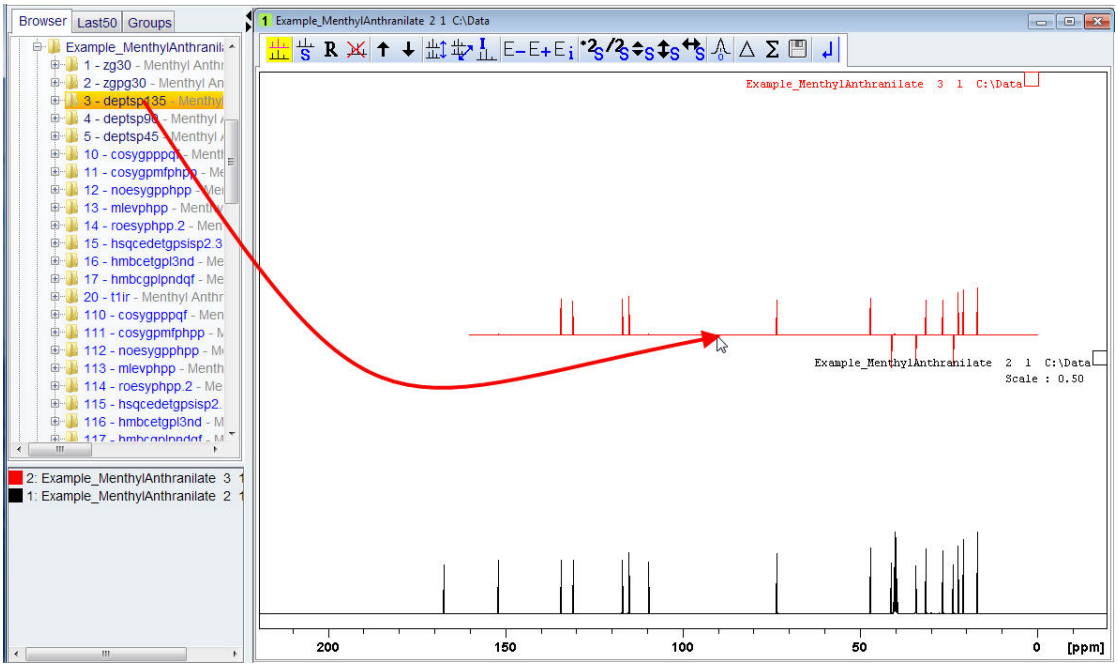


- In the **Spectrum colors** section select the **Colors** for the **1**st (black), **2**nd (red) and **3**rd (green) 1D spectrum.



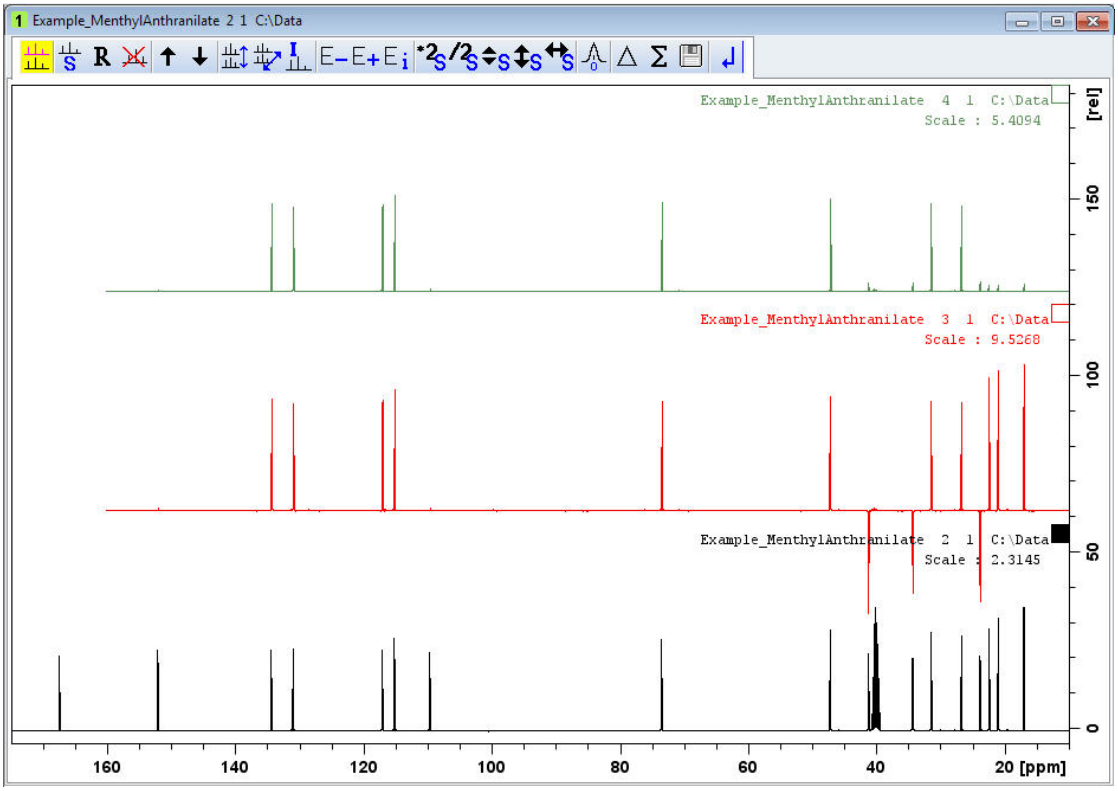
- Click on the **Apply** button inside the Spectra Display Preferences window.
- Click on the **Close** button inside the Spectra Display Preferences window.
- Click on the **Multiple display** button inside the tool bar.

- In the browser window locate the DEPT135 spectrum of the same sample.
- With the left mouse button pressed, drag the DEPT135 spectrum in to the Data display window.



- In the browser window locate the DEPT90 spectrum of the same sample.
- With the left mouse button pressed, drag the DEPT90 spectrum in to the Data display window.

Print Data Displayed in the TopSpin Active Window

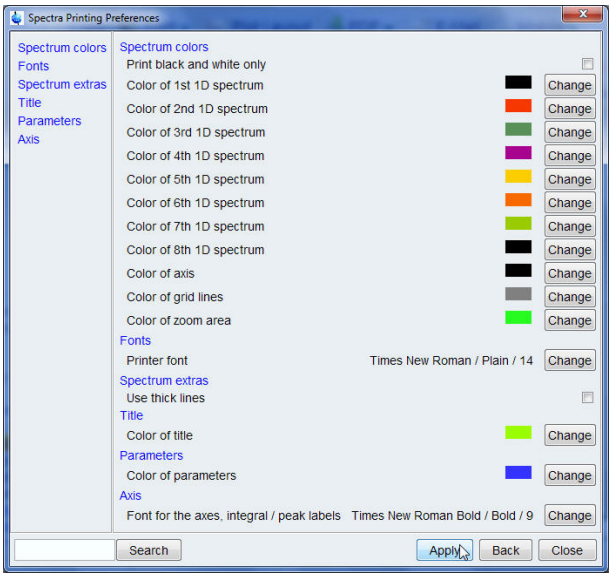


- To adjust the vertical amplitude, click on any of the spectra and use the icons shown below to make the changes.

  To further manipulate all the spectra at once use the general scaling tools. The proton decoupled carbon spectrum was observed with a sweep width of 240 ppm. Both the DEPT135 and the DEPT90 spectra where observed with a sweep width of 160 ppm. This accounts for the missing baseline to the left of the two DEPT spectra.
- Select the **Publish** tab in the Workflow tab bar.

- Click on the **down arrow** inside the **Print button** in the Workflow button bar.
- Select **Change Print Colors/Fonts**.

- Use the same 1D spectrum colors: **1**st (black), **2**nd (red) and **3**rd (green).



Alternatively the **Spectra Printing Preferences** and the **Spectra Display Preferences** window can also be selected within the **Manage tab** in the Workflow tab bar using the **Preferences** button in the Workflow button bar.

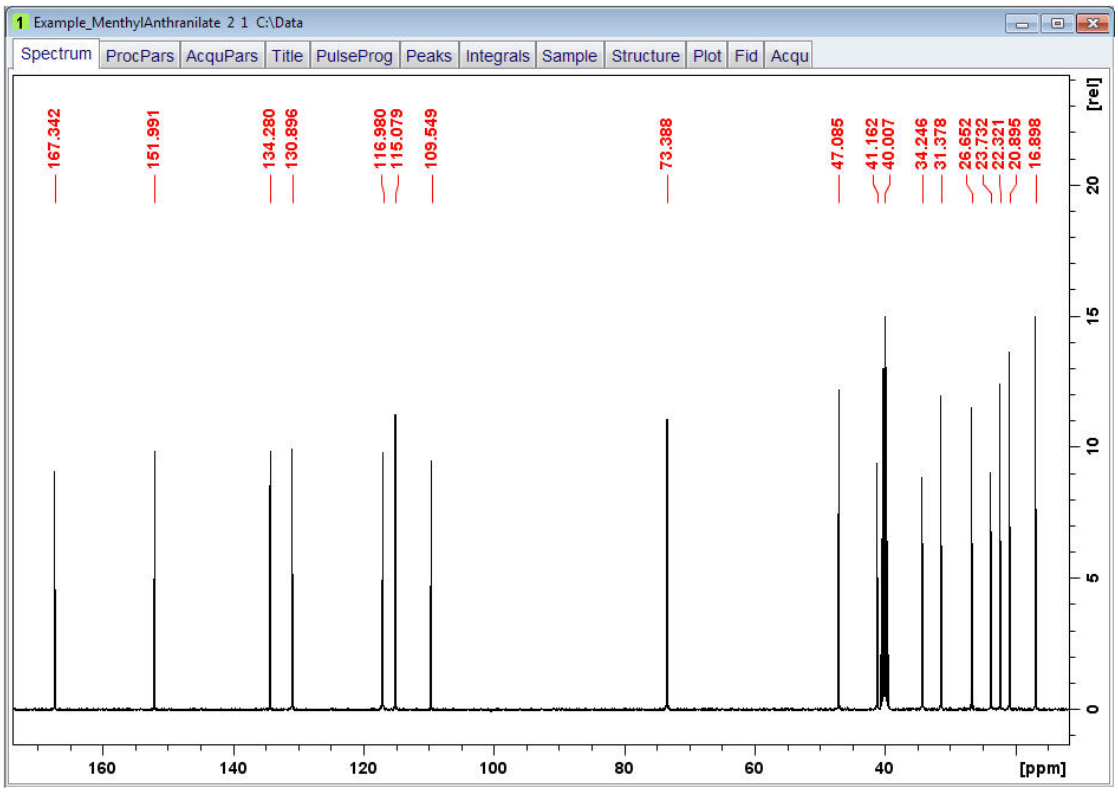
- Click on the **Apply** button inside the Spectra Printing Preferences window.
- Click on the **Close** button inside the Spectra Printing Preferences window.
- Click on the **Print** button in the Workflow button bar or use the **prnt** command.

3.3 Print Lists and Text Displayed in the TopSpin Window

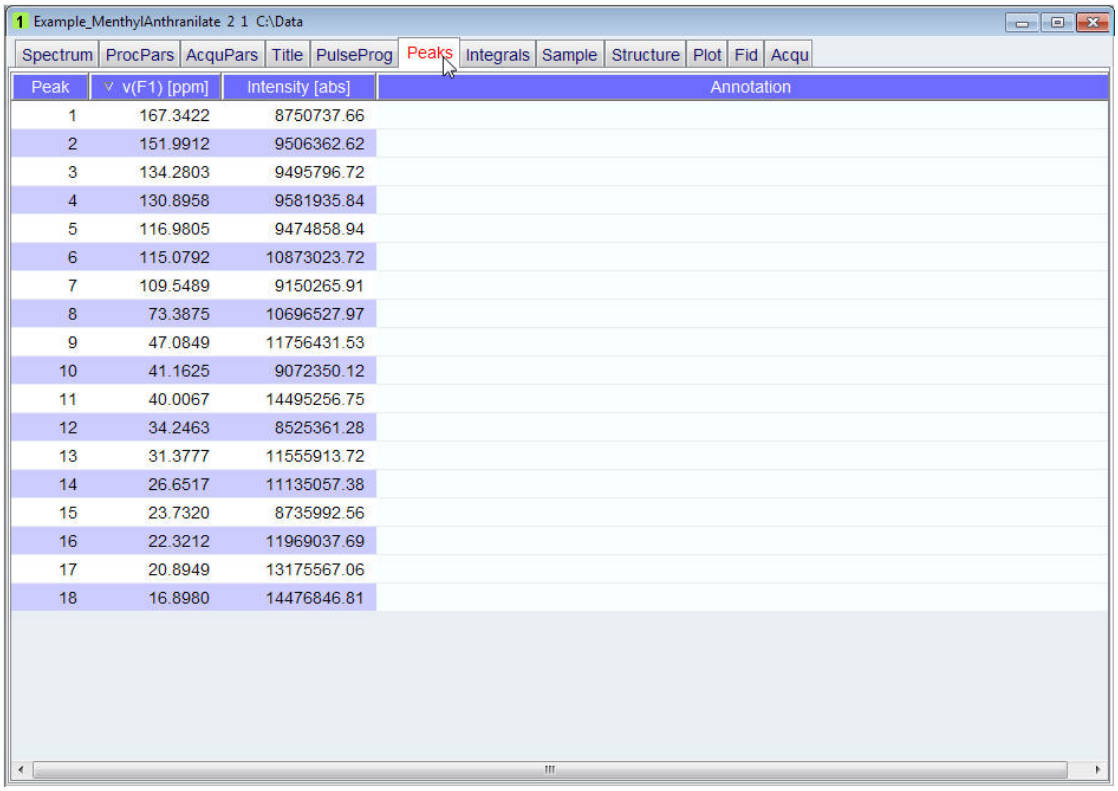
Lists of peaks, integrals, parameters and pulse programs can be displayed in the TopSpin window using the respective tabs in the Data set tabs bar. The example below illustrates how to print a peak list displayed in the TopSpin window. Run a 1D carbon spectrum and peak-pick the spectrum or a part of it.

- Display the 1D carbon spectrum with peak labels.

Print Data Displayed in the TopSpin Active Window



- Select the **Peaks** tab in the Data set tabs bar.



Peak	v(F1) [ppm]	Intensity [abs]	Annotation
1	167.3422	8750737.66	
2	151.9912	9506362.62	
3	134.2803	9495796.72	
4	130.8958	9581935.84	
5	116.9805	9474858.94	
6	115.0792	10873023.72	
7	109.5489	9150265.91	
8	73.3875	10696527.97	
9	47.0849	11756431.53	
10	41.1625	9072350.12	
11	40.0067	14495256.75	
12	34.2463	8525361.28	
13	31.3777	11555913.72	
14	26.6517	11135057.38	
15	23.7320	8735992.56	
16	22.3212	11969037.69	
17	20.8949	13175567.06	
18	16.8980	14476846.81	

- Click on the **Print** icon in the TopSpin tool bar.

- Select **Print active window [prnt]** inside the Print window.
- Click on the **OK** button inside the Print [Ctrl+P] -prnt window.
- Click on the **Print** button inside the Print window.

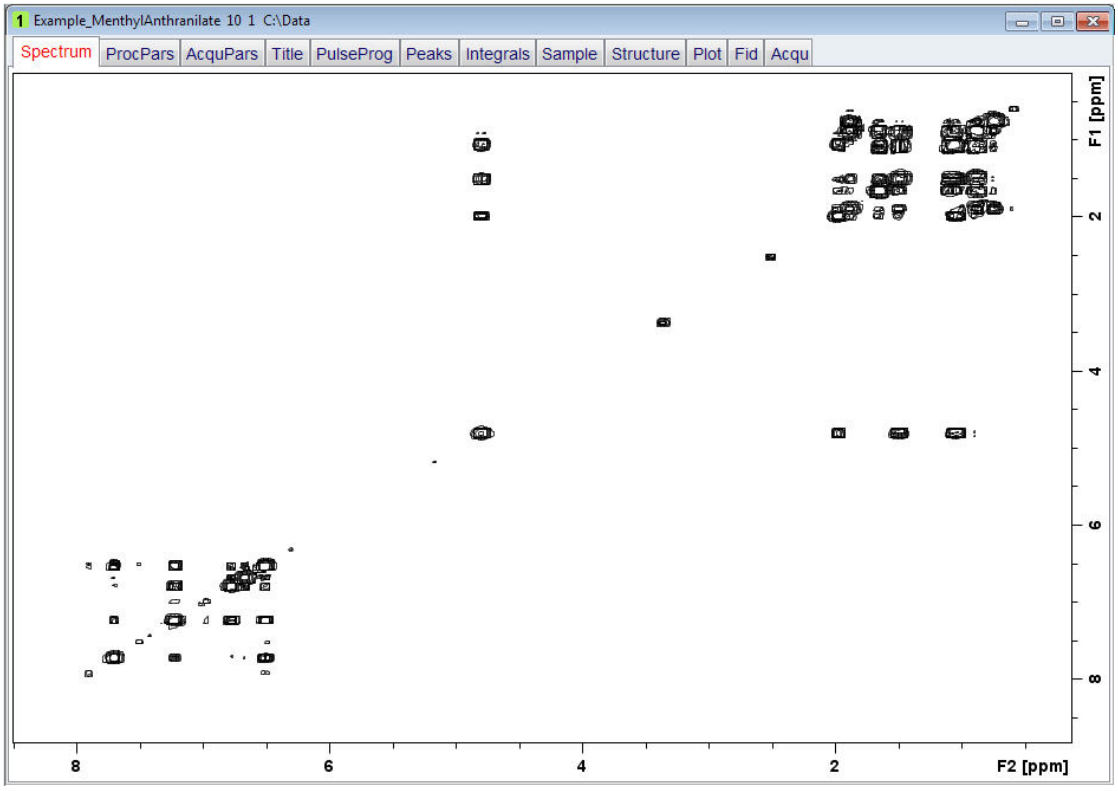
3.4 Print 2D Data Displayed in the TopSpin Window

This section describes how to get a fast print out of a single- or multiple 2D data sets with projections dis-played in the TopSpin window. Due to the many display options which one can select in the **Spectra Display Preferences** window only a few selected examples will be discussed.

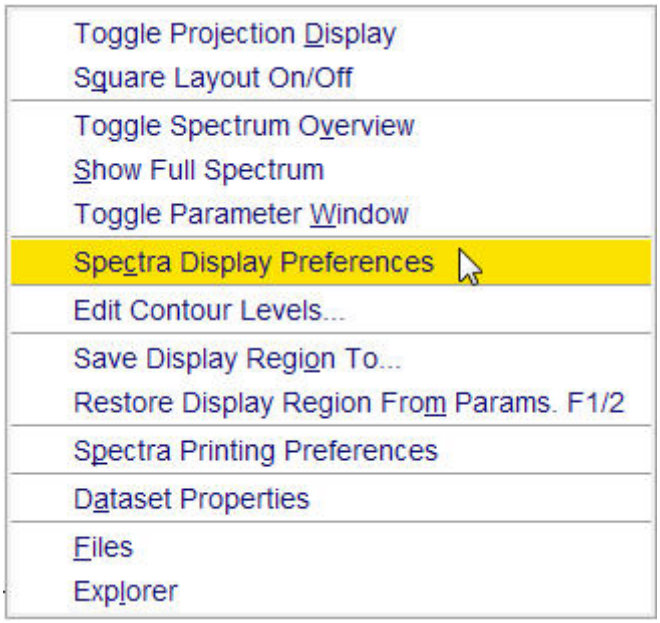
3.4.1 2D Proton COSY Spectrum with Selected Display Options

Run a 2D COSY spectrum, add a title and import or draw the molecular structure of the observed sample. In addition run a 1D Proton spectrum used as projection of the 2D spectrum.

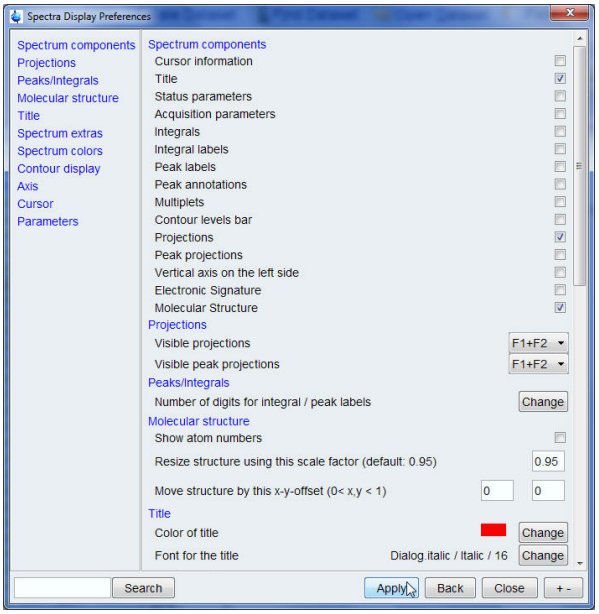
- Display the 2D COSY spectrum.
- Right click inside the displayed spectrum area.



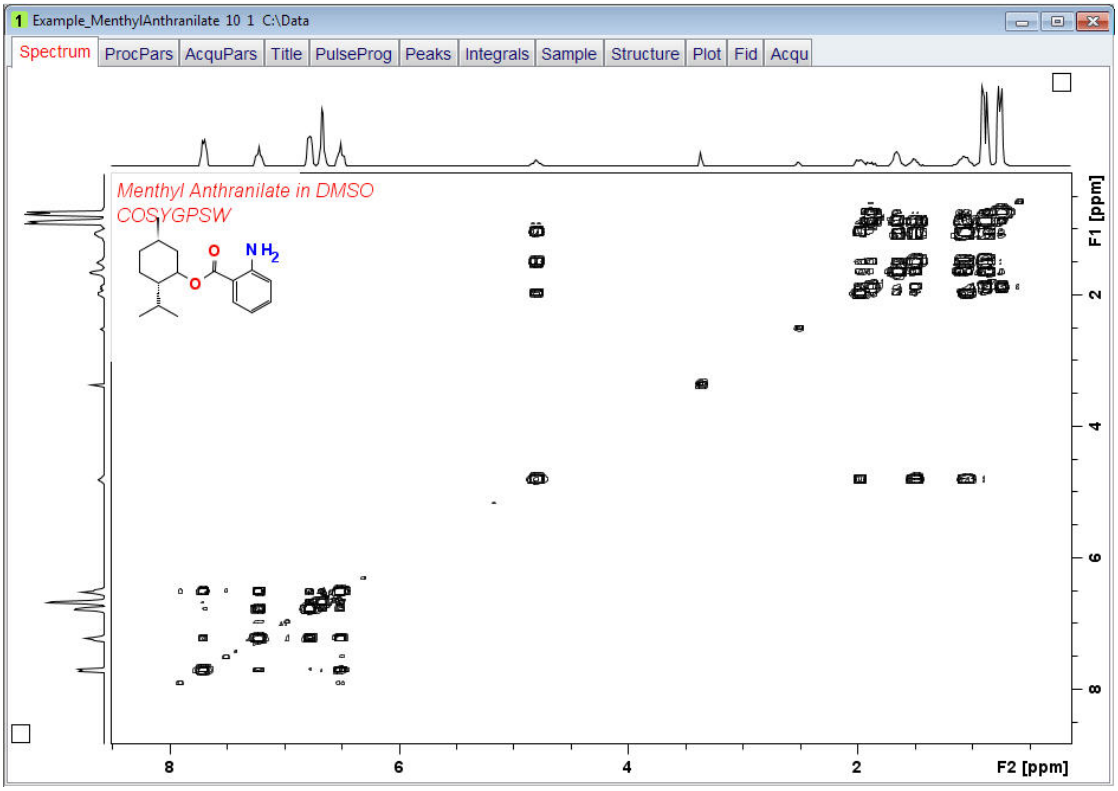
- Select **Spectra Display Preferences**.



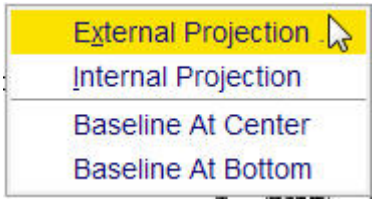
- In the **Spectrum components** section enable the following options:
  - Title
  - Projections
  - Molecular Structure



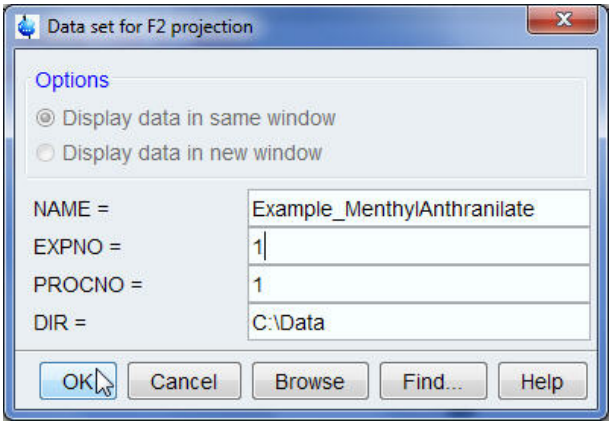
- In the **Projections section** select **F1+F2** for **Visible projections**.
- Click on the **Apply** button inside the Spectra Display Preferences window.
  - In the **Molecular structure** section you can move the structure location or resize it. If necessary you can also change the font and color of the title and the spectrum.
- Click on the **Close** button inside the Spectra Display Preferences window.



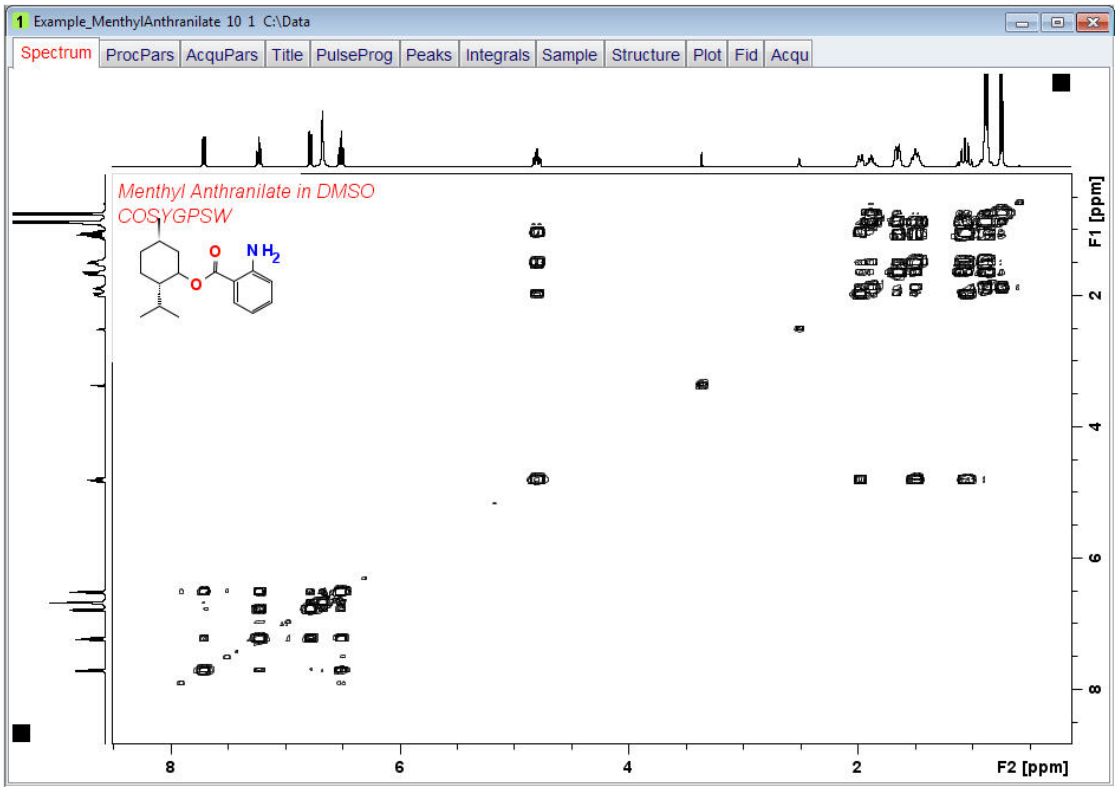
- By default the internal projections are displayed. Follow the steps below to add the external projections which have a better resolution. This requires that a 1D proton spectrum of the same sample has been acquired and stored to the disk.
- Move the cursor inside the **F2** projection display and click the right mouse button.
- Select **External Projection**.



- Enter the **NAME, EXPNO, PROCNO** and **DIR** of the 1D proton experiment.



- Click on the **OK** button inside the F2 projection window.
- Move the cursor inside the **F1** projection display and click the right mouse button.
- Repeat the last three steps to add the **F1** projection.

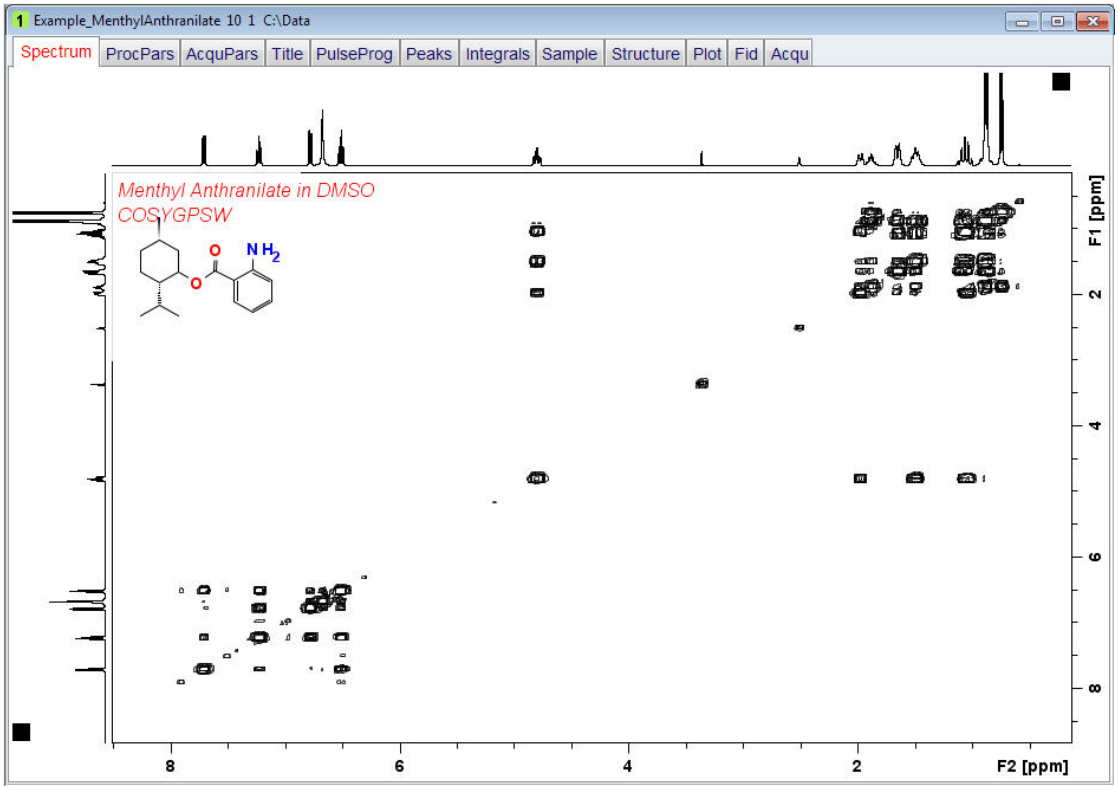


- Click on the **Print** icon in the TopSpin tool bar.
- Select **Print active window [prnt]** inside the Print window.
- Click on the **OK** button inside the Print [Ctrl+P] -prnt window.
- Click on the **Print** button inside the Print window.

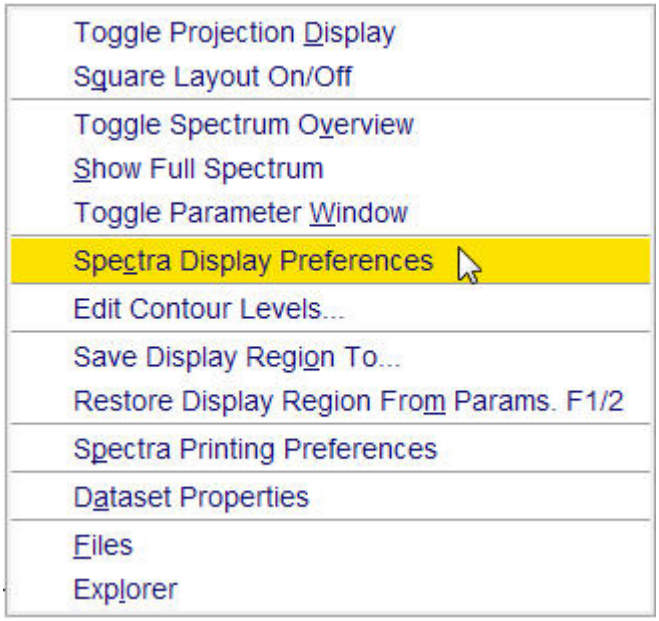
3.4.2 Multiple 2D Spectra Displayed in the TopSpin Window

Follow the steps below how to print two 2D spectra displayed in the TopSpin window. The example includes a 2D COSY- and a 2D NOESY- spectrum.

- Display the 2D COSY spectrum.
- Right click inside the displayed spectrum area.

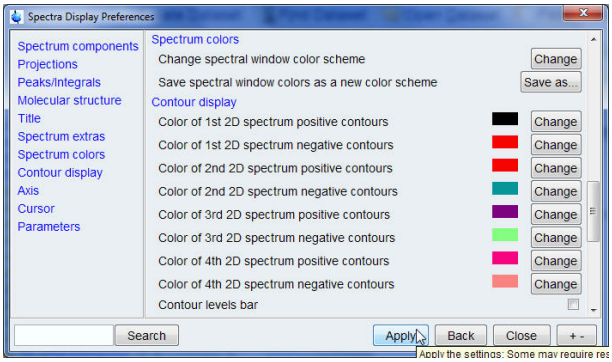


- Select **Spectra Display Preferences**.



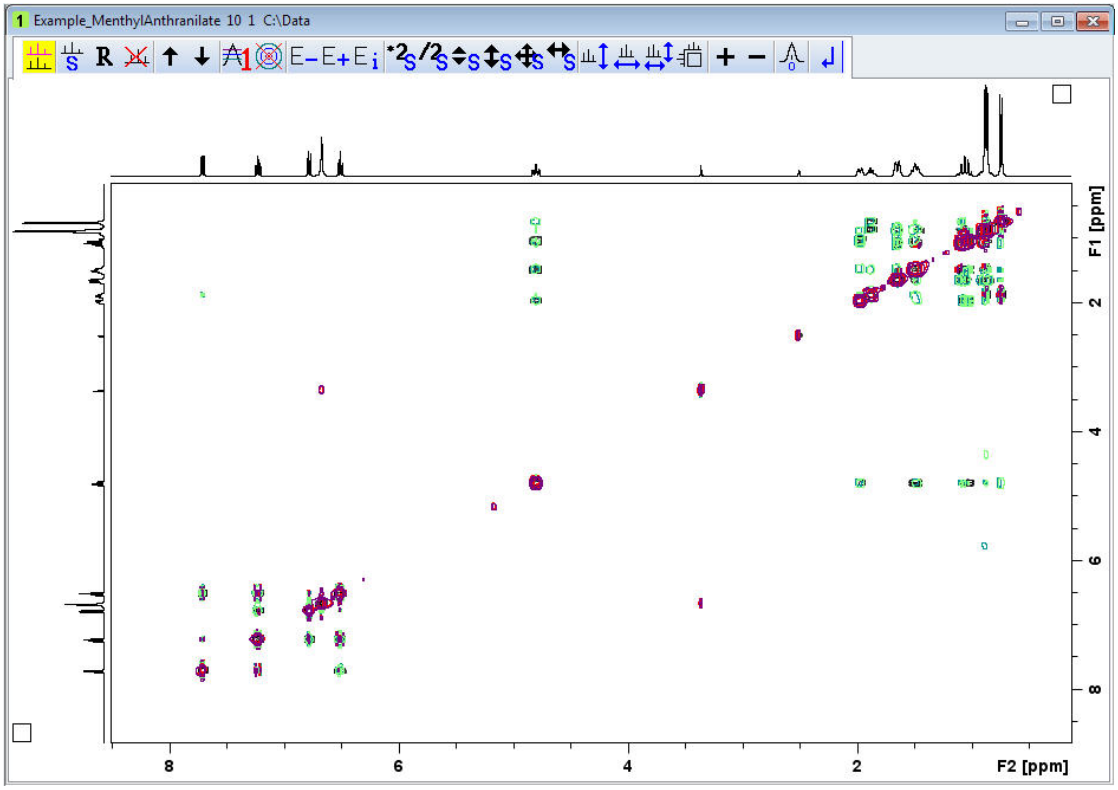
When choosing the colors of the two 2D spectra, keep in mind that the COSY is only showing positive peaks while the NOESY may show positive and negative peaks.

- In the **Contour display** section choose the following colors:
  - Color of 1st 2D spectrum positive contours = black
  - Color of 2nd 2D spectrum positive contours = red
  - Color of 2nd 2D spectrum negative contours = green



- Click on the **Apply** button inside the Spectra Display Preferences window.
- Click on the **Close** button inside the Spectra Display Preferences window.
- Click on the **Multiple display** button inside the Tool bar.

- In the browser window locate the 2D NOESY spectrum of the same sample.
- With the left mouse button pressed, drag the 2D NOESY spectrum in to the Data display window.



- Click on the **Print** icon in the TopSpin tool bar.
- Select **Print active window [prnt]** inside the Print window.

- Click on the **OK** button inside the Print [Ctrl+P] -prnt window.
- Click on the **Print** button inside the Print window.

Print Data Displayed in the TopSpin Active Window

4 Print Data Using Layouts

4.1 Introduction

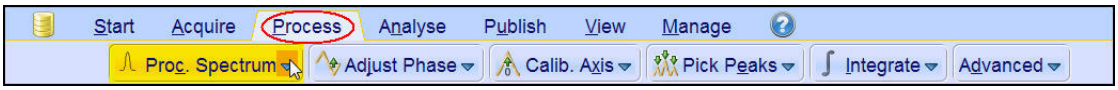
This chapter will guide you through printing using layouts. A layout is a template, which defines a number of graphical objects. It may contain standard graphics, such a lines, squares, curves etc. or NMR objects like Spectrum, FID, Parameters, Titles etc. Each object has its own position, size, attributes and properties. Each NMR object has its own Reset Actions. Layouts can be either standard Bruker or user-defined ones. The print options such as colors, parameters, title etc. are stored and controlled by the selected layout.

4.2 Print Data with a Predefined Layouts

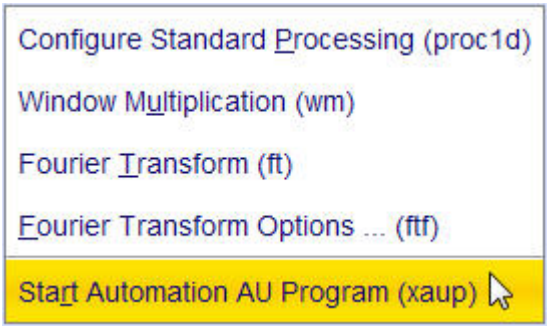
NMR data are often acquired, processed and printed in automation using AU programs or through the use of IconNMR. Printing in automation uses the same layouts and portfolios used by the interactive Plot Editor. Almost all of the Bruker standard parameter sets include a layout and a processing AU program listed in the Automation section of the processing parameters.

4.2.1 Process and Print Using the Automation AU Program

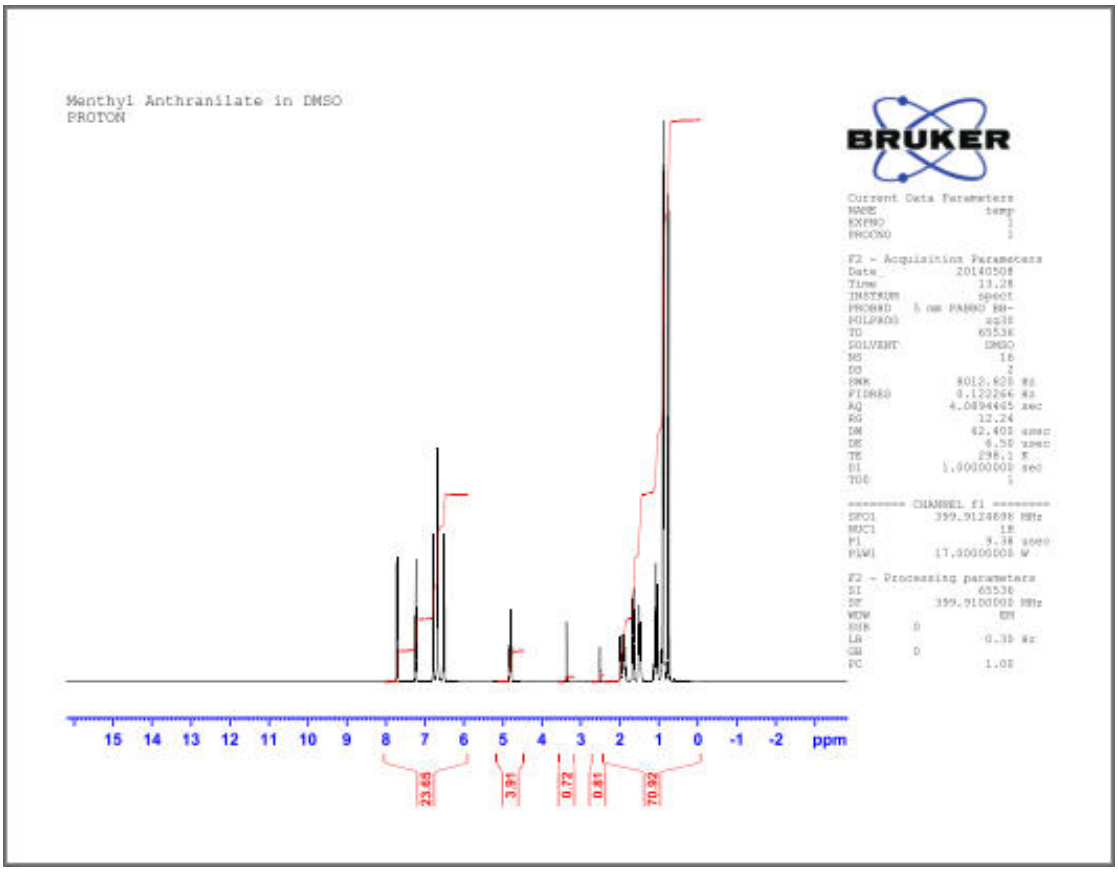
- Run a 1D proton spectrum.
- When the acquisition is finished, click on the **Process** tab in the Workflow tab bar.



- Click on the **down arrow** inside the **Proc Spectrum** button in the Workflow button bar.
- Select **Start Automation AU Program** (xaup).



The command **xaup** will execute the processing AU program of the data set. It includes all processing steps and includes the print command **autoplot**.



The printout shows the full spectrum width. The integration is done during the **abs** command in the processing AU program. By default, the resulting integrals add up to 100 to allow quantification of integral areas based on percentage values.

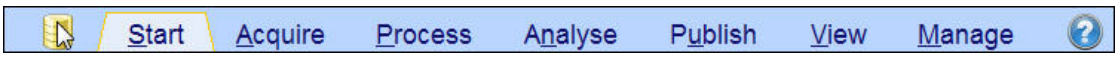
4.2.2 Print Processed Data Using the Predefined Default Layout

This section describes the printing of a processed 1-D proton spectrum using the default predefined layout **+/1D_H.xwp**, which is stored within the processing parameters.

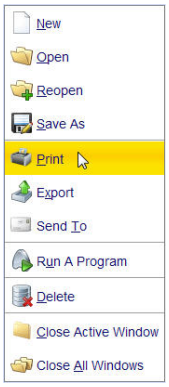
- Run a 1-D proton spectrum.
- Process the data.
- Integrate the peaks and calibrate.

The printout displays the full spectrum width and shows the integration with the calibrated values. Alternatively you can type the command **autoplot** in the Topspin command line to bypass the following steps.

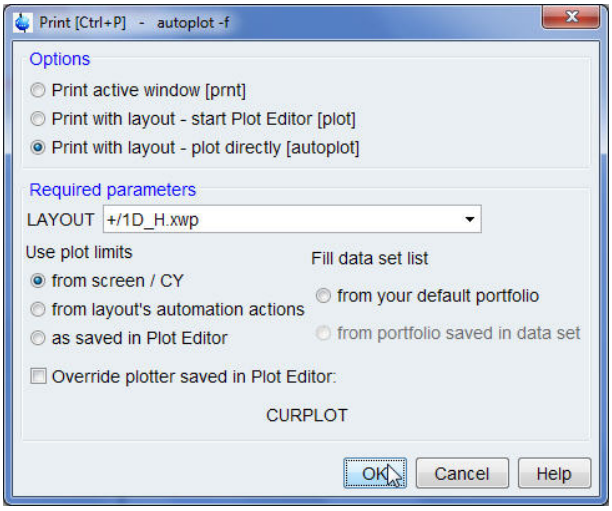
- Click on the **Disk** icon in the Workflow tab bar.



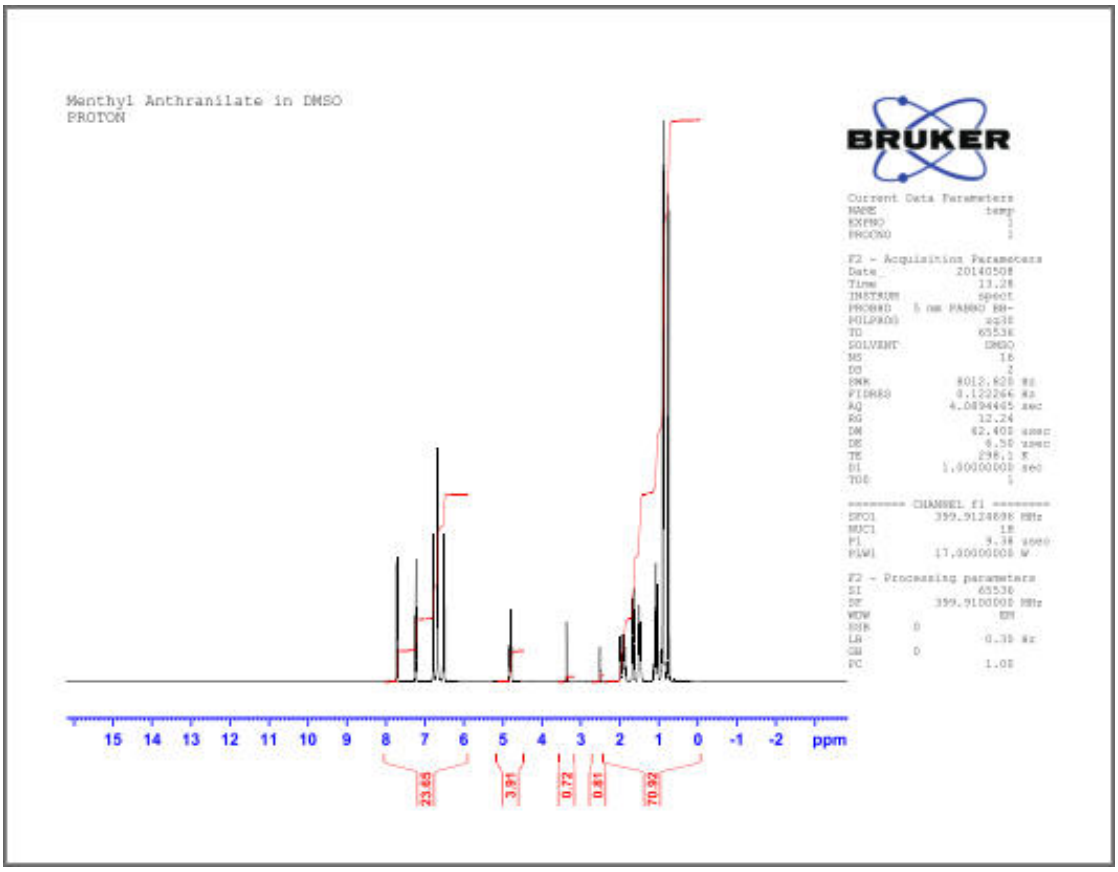
- Select **Print**.



- Select **Print with layout plot directly [autoplot]** in the Print [Ctrl+P] window.



- Click on the **OK** button inside the Print [Ctrl+P] window.



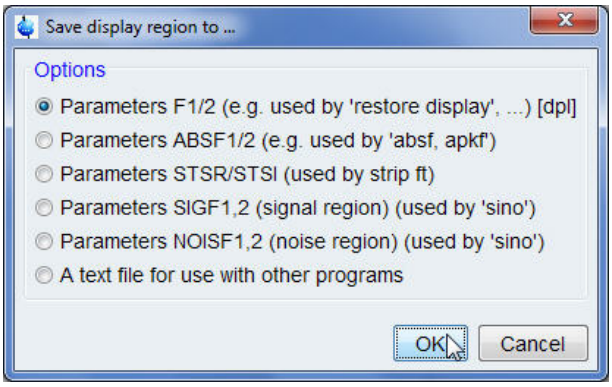
4.2.3 Print Processed Data Using a New Predefined Layout

This section describes the printing of a processed 1-D proton spectrum using a new predefined layout **+/1D_H+zoom.xwp**. The new layout can be selected either within the processing parameters or likewise in the example below from within the Print [Ctrl+P] window.

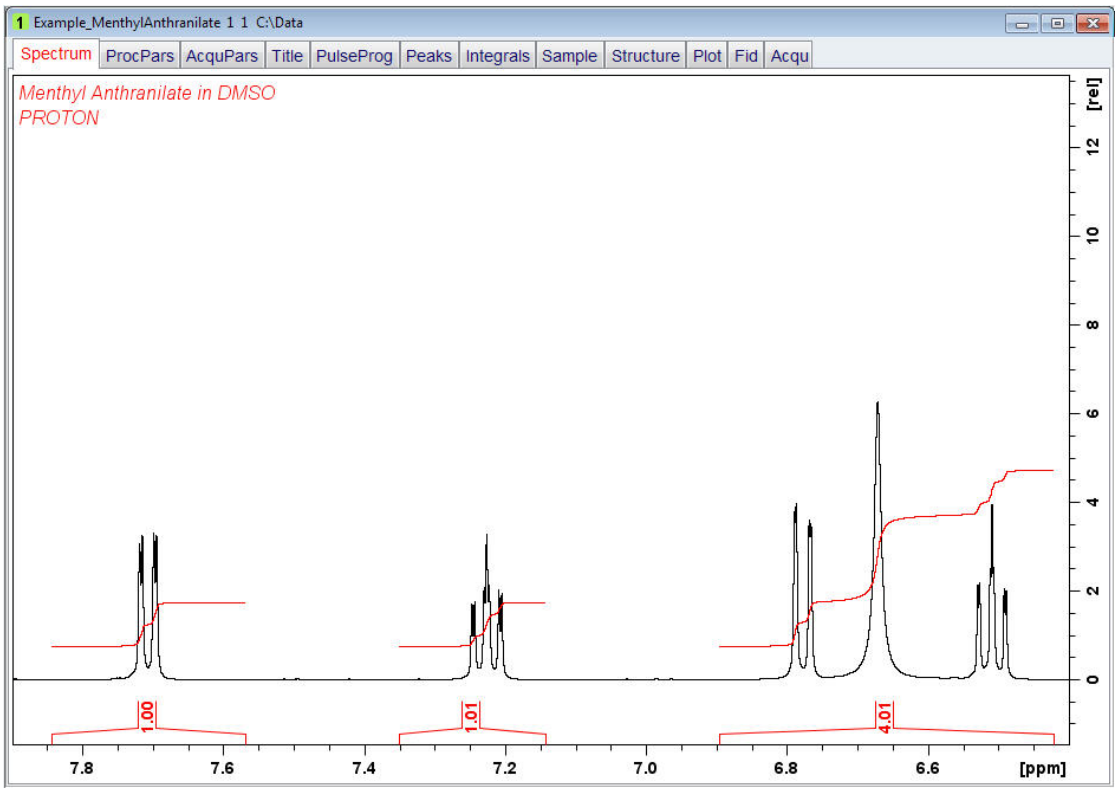
Some layouts may require a different processing AU program to print the data. In the case of selecting a new processing AU program, the changes should be done in the processing parameters and the xaup command should be executed (see *Process and Print Using the Automation AU Program [▷ 39]*).

- Run a 1D proton spectrum.
- Process the data,
- Integrate the peaks and calibrate.
- Display the full spectrum (e.g. **16 ppm** to **-4 ppm**).
- Right click inside the spectrum display window.
- Select **Save Display Region To**.

- Select **Parameters F1/2 (e.g. used by 'restore display')** [dpl1] inside the Save display region to window.

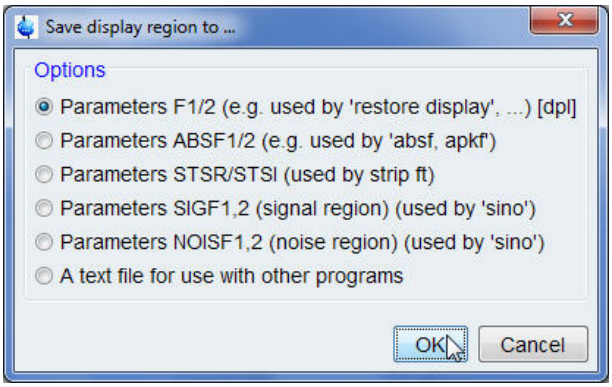


- Click on the **OK** button inside the Save display region to window.
- Expand the region from **7.9 ppm** to **6.4 ppm**.

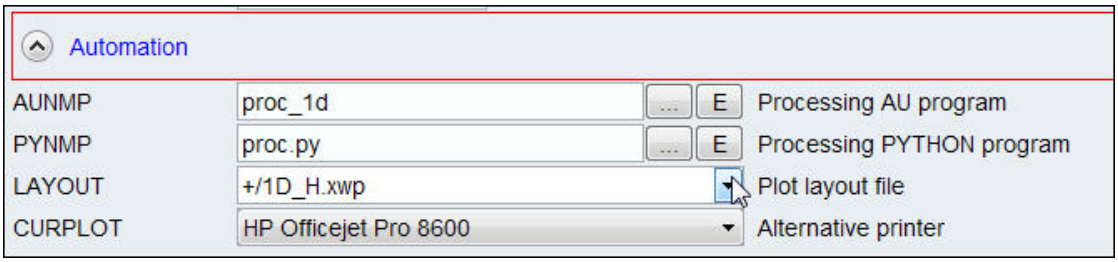


- Right click inside the spectrum display window.
- Select **Save Display Region To**.

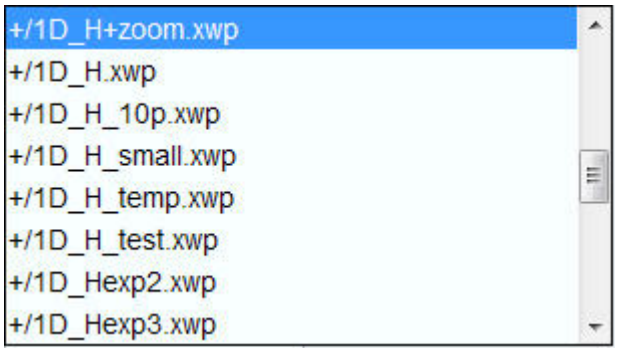
- Select **Parameters F1/2 (e.g. used by 'restore display')** [dpl1] inside the Save display region to window.



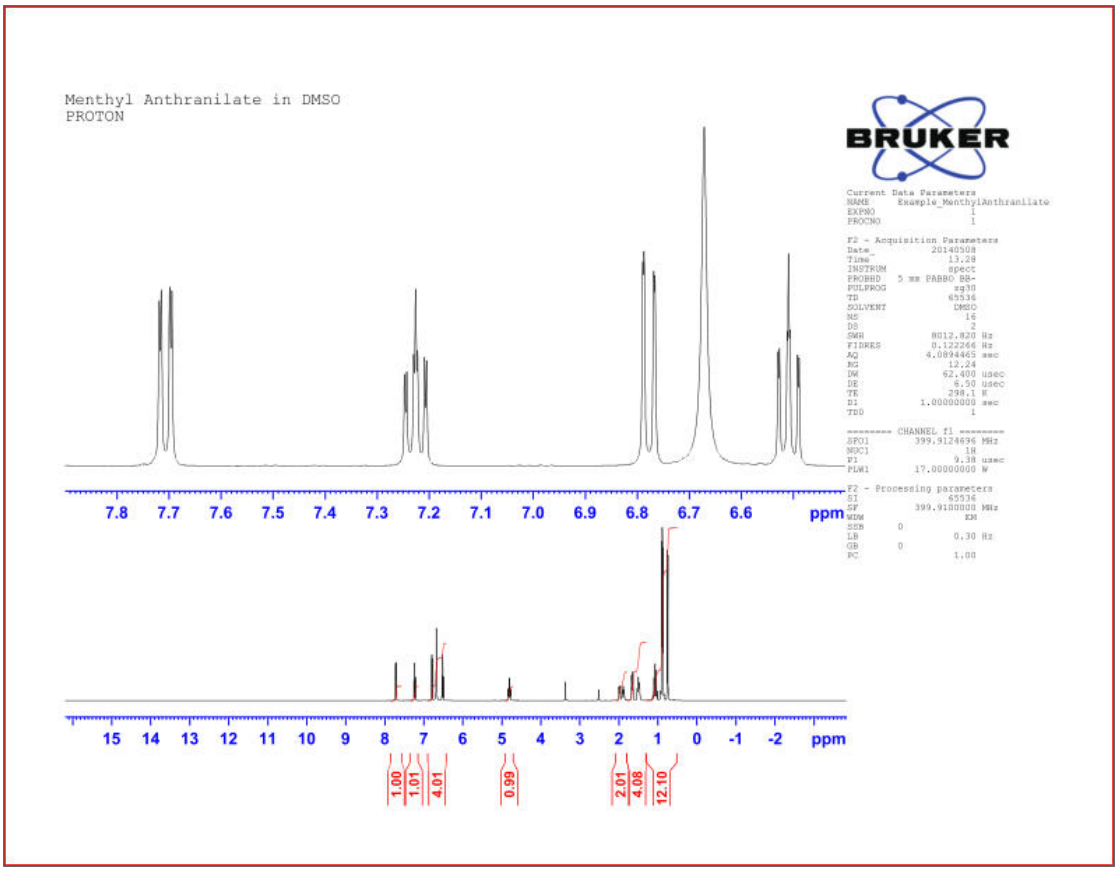
- Click on the **OK** button inside the Save display region to window.
- Select the **ProcPars** tab in the **Data set tabs** bar.
- Scroll down to the **Automation** section.
- Click on the **down arrow** to the right of the **LAYOUT** window (Plot layout file).



- Select the **+/1D_H+zoom.xwp** layout.



- Select the **Spectrum** tab in the Data set tabs bar.
- Type **autoplot** in the TopSpin command line.


Menthyl Anthranilate in DMSO
PROTON
BRUKER
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 ppm
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.00
1.01
4.01
0.99
2.01
4.08
12.10

5 How to Modify Layouts with the Plot Editor

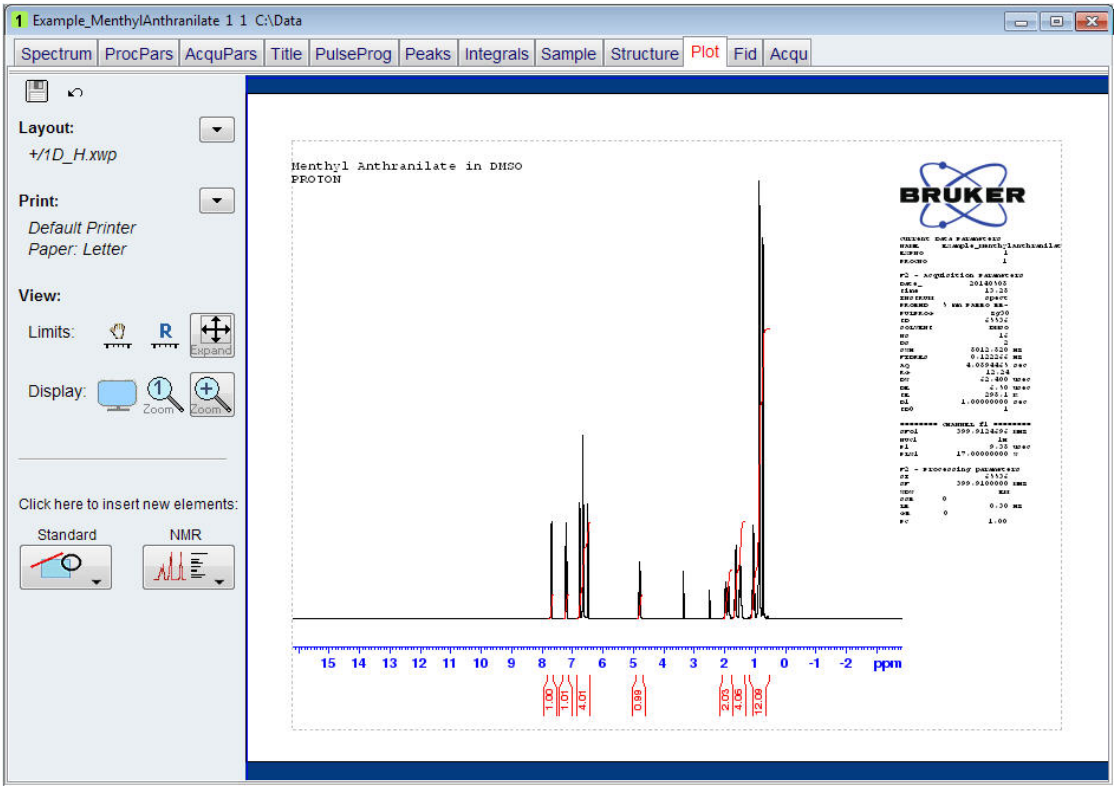
5.1 Introduction

This chapter will guide you through printing using the **Plot Editor** which is included in the TopSpin software. The **Plot Editor** is a fully object-oriented, interactive plot editor for high quality printouts of NMR data. Within this additional software one can modify a pre-defined layout or create a new one to be added to the existing layout library or print without storing the layout.

5.2 Starting the Plot Editor

- Run a 1D proton spectrum.
- Process the data.
- Integrate the peaks and calibrate.
- Click on the **Publish** tab in the Workflow tab bar.
- Select the **Plot Layout** button in the Workflow bar.

You can also click on the **Plot** tab in the **Data set tab** bar to open the **Plot Editor** or type **plot** in the TopSpin command line.



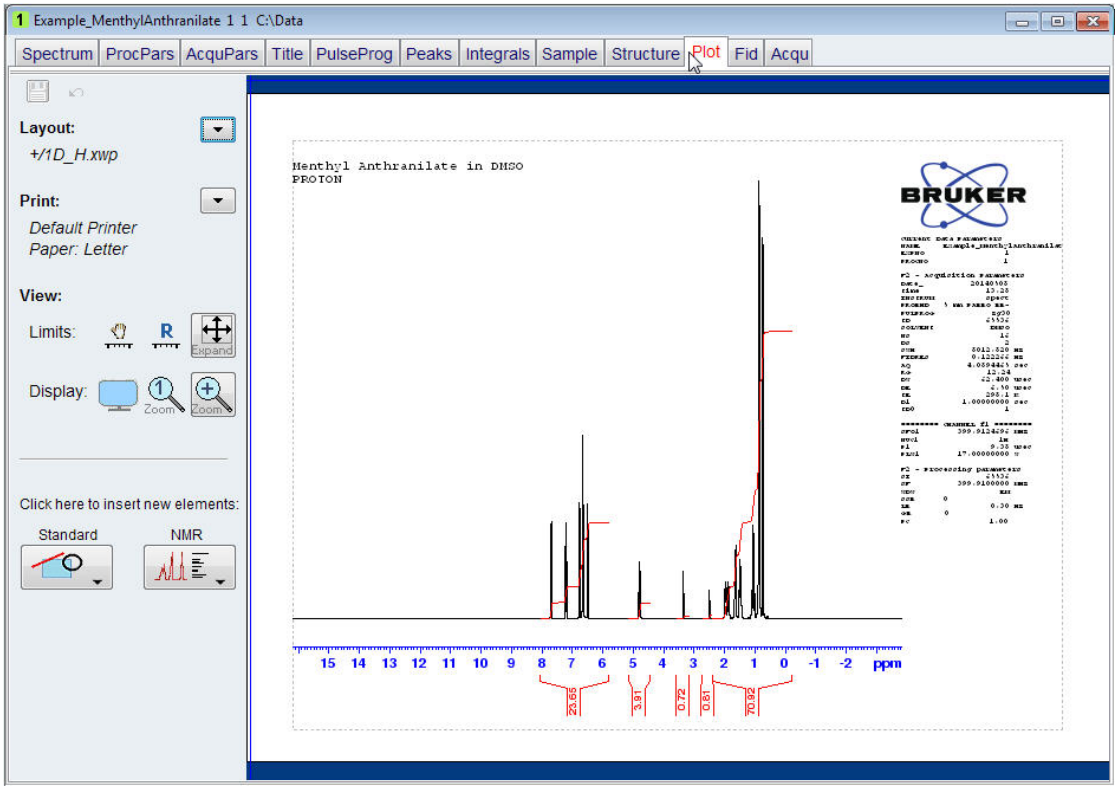
The Plot Editor displays the data using the layout stored in the processing parameters.

5.3 Create a New Layout

5.3.1 Modify the Predefined Layout

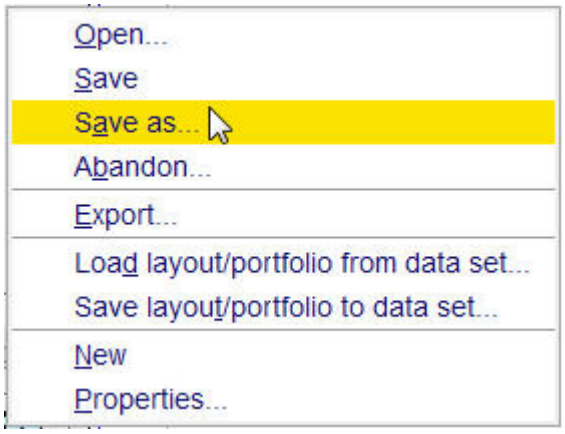
- Display a spectrum.
- Select the **Plot** tab in the **Data set tabs** bar or type **plot** in the TopSpin command line.

- Modify the layout in any way you want.

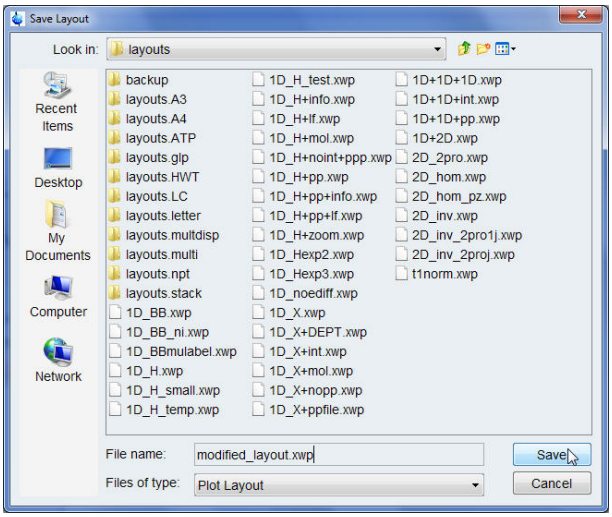


- In the tool menu on the left of the plot display, click on the **down arrow** next to the **Layout** option.

- Select **Save as**.



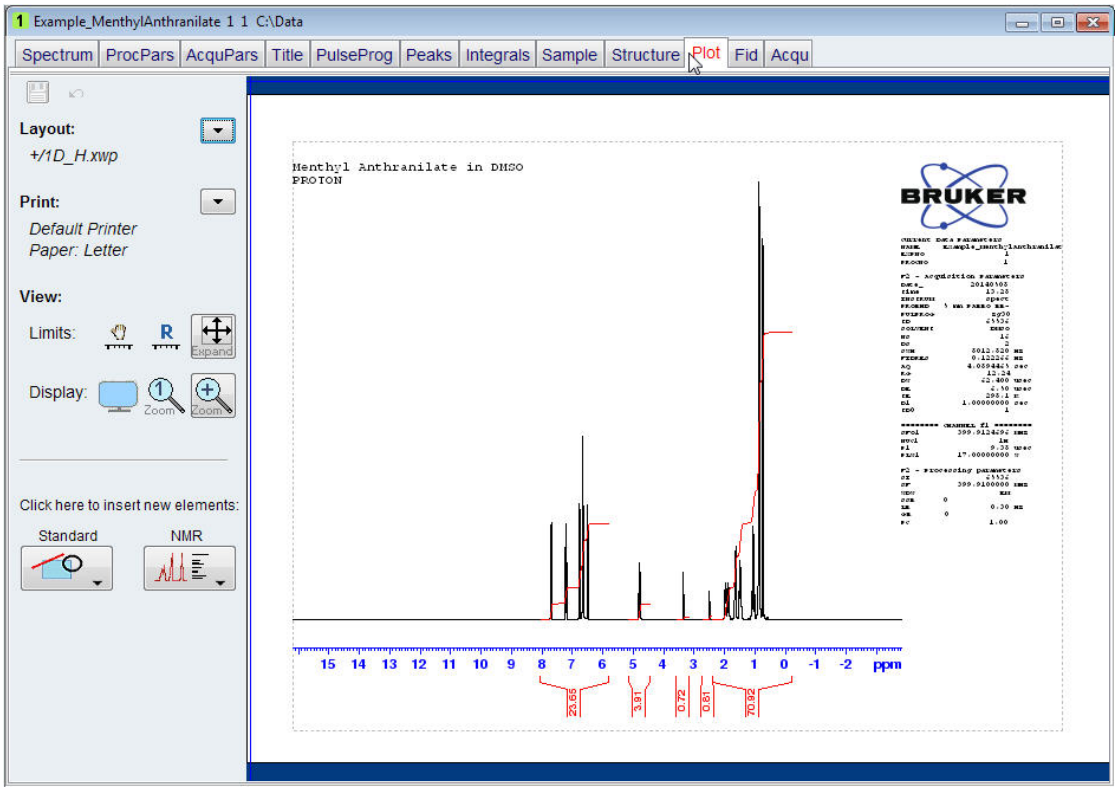
- Enter a new File name inside the Save Layout window.



- Click on the **Save** button inside the Save Layout window.

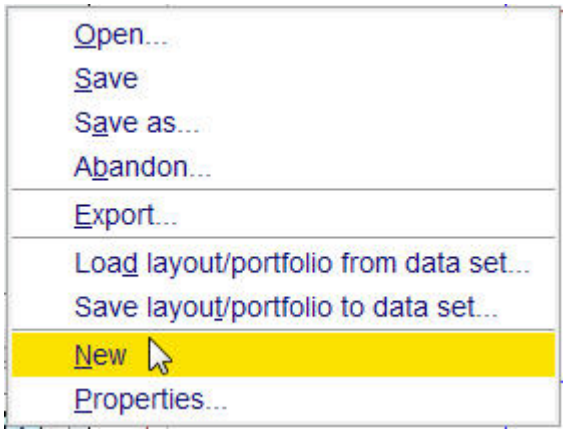
5.3.2 Start with an Empty Layout

- Display a spectrum.
- Select the **Plot** tab in the Data set tabs bar.

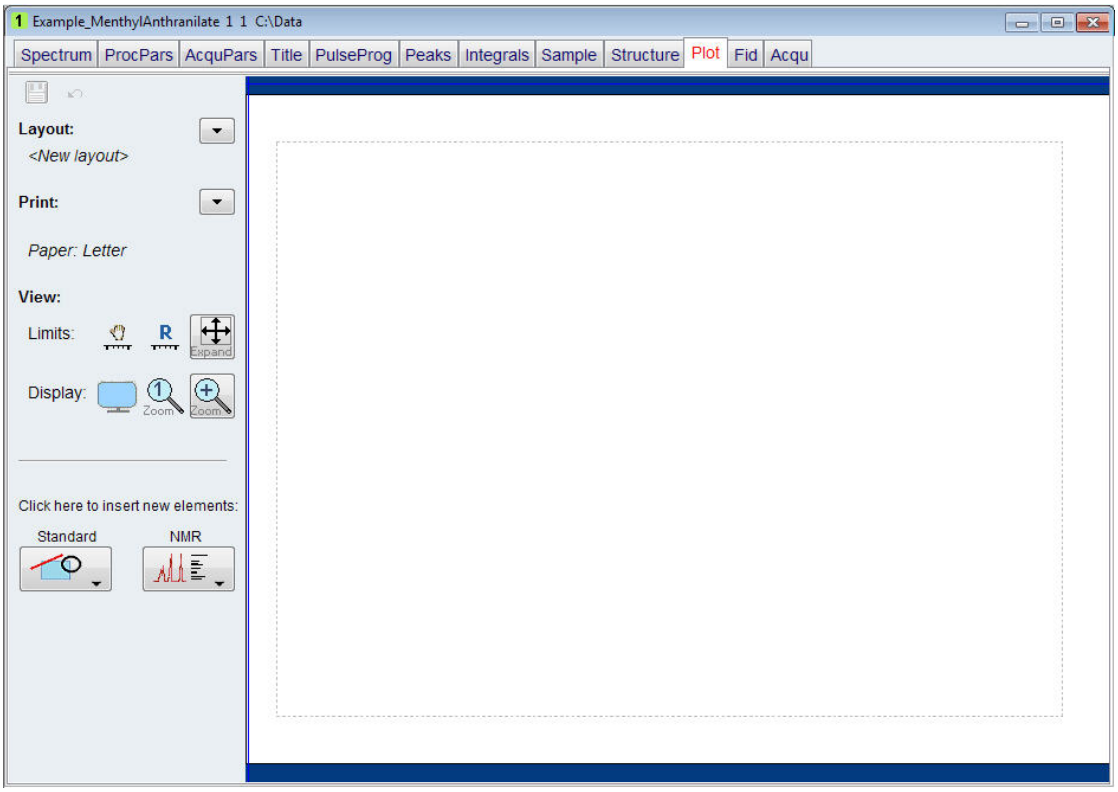


- In the tool menu on the left of the plot display, click on the **down arrow** next to the **Layout** option.

- Select **New**.

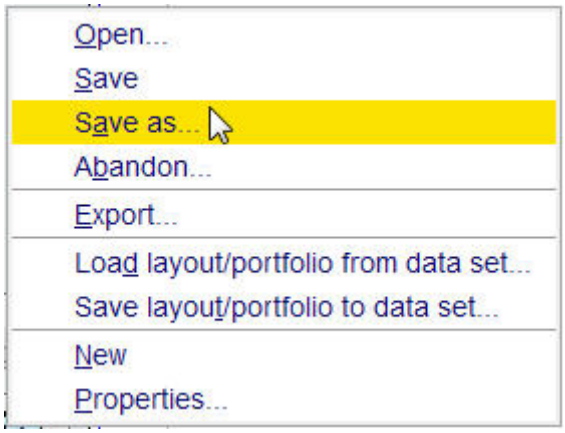


- Add graphical objects to the layout and manipulate the content of the graphical objects as you wish.

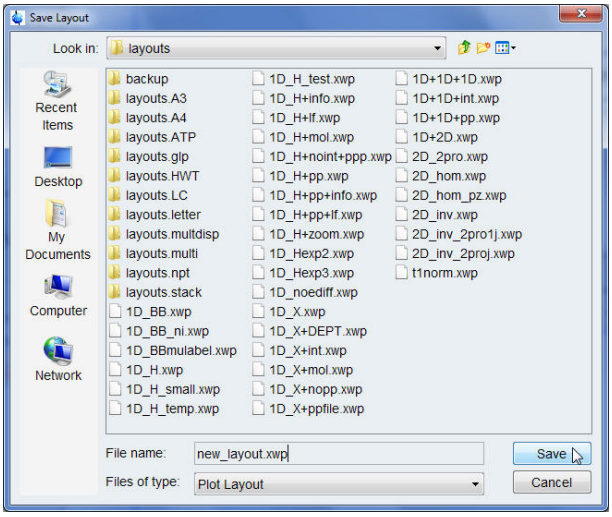


- In the tool menu on the left of the plot display, click on the **down arrow** next to the **Layout** option.

- Select **Save as**.



- Enter a new file name inside the Save Layout window.



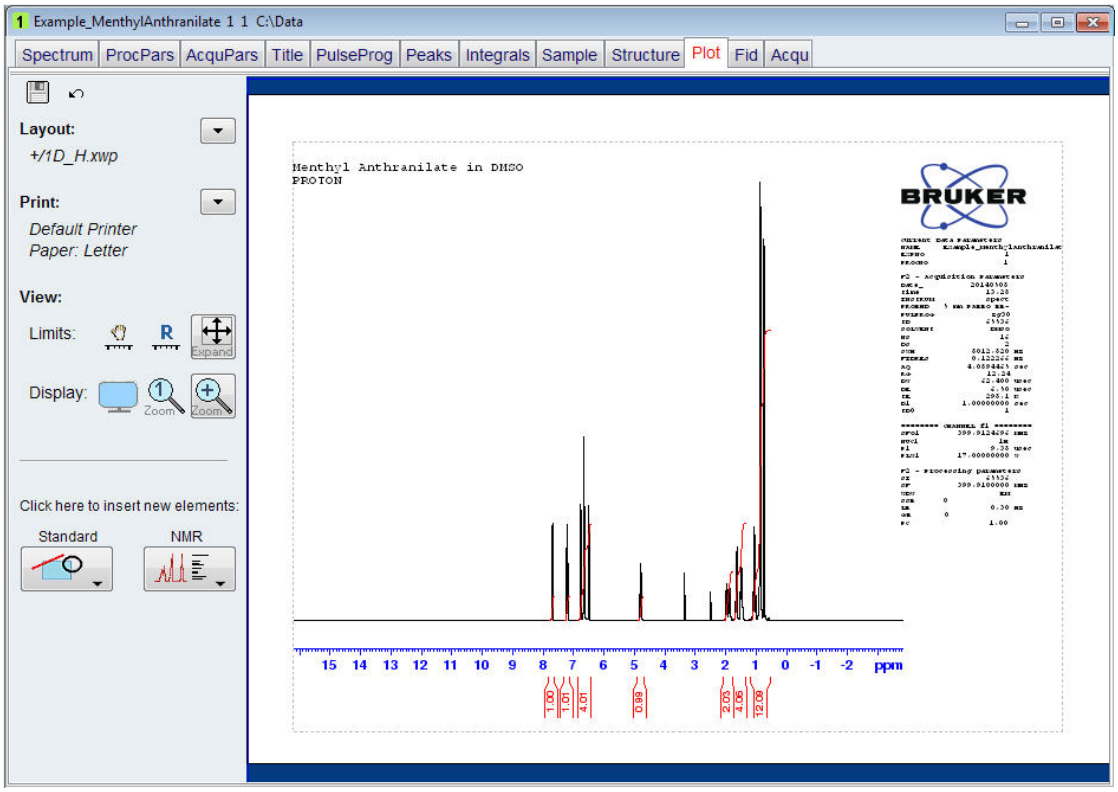
- Click on the **Save** button inside the Save Layout window.

How to modify the different graphical objects will be explained in *Printing 1D Data after Modifying the Layout [▷ 52]*, below in this chapter.

5.4 Printing 1D Data after Modifying the Layout

This section will guide you through the various functionality of the plot editor while modifying the layout of a 1D proton spectrum. The steps below can be applied to any 1D spectrum, also of other nuclei.

- Follow the instructions in *Starting the Plot Editor [▶ 47]*.

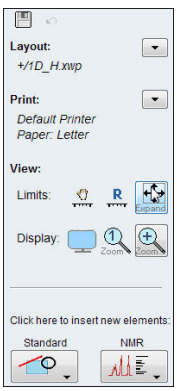


Before you start to modify a layout, you should plan ahead what you would like to change or add to the layout by making a list of the changes.

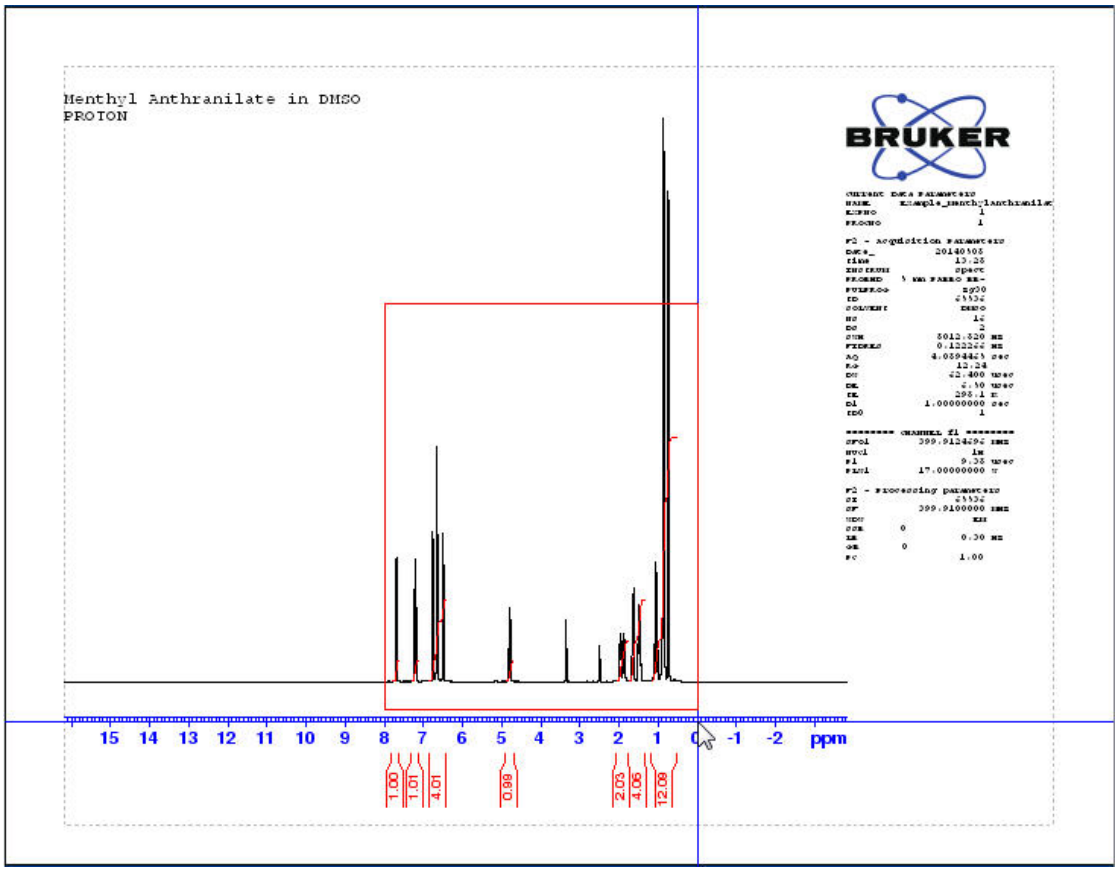
- Make a list of the changes to the layout like the example below.
  - Change the spectrum limits and its scaling.
  - Insert a peak expansion.
  - Mark the location of the peak expansion in the full spectrum.
  - Add a molecule structure.

5.4.1 Changing the Spectrum Limits and its Scaling

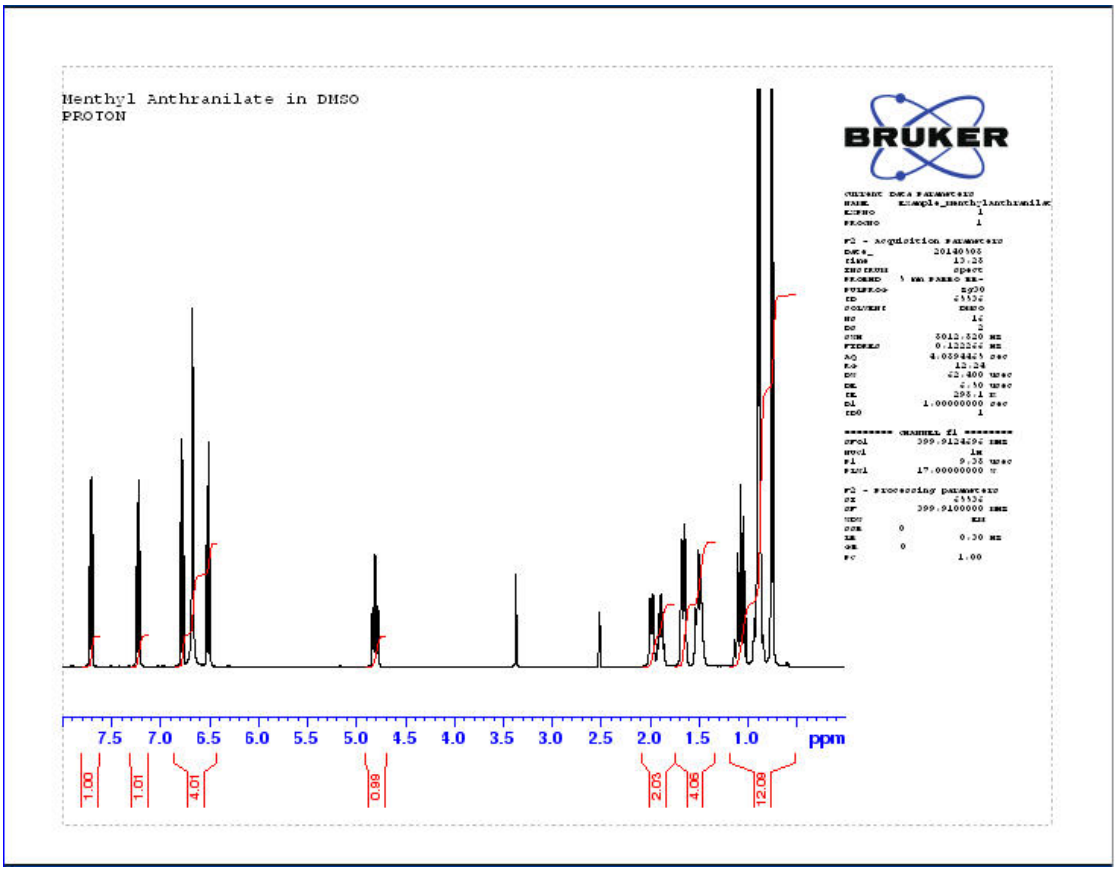
- Click on the **Expand** icon in the **View** options on the left side of the Plot Editor window.



- Left click starting at the left of the spectrum and while keeping the mouse button pressed, draw a rectangular area inside the spectrum object to change its limits.

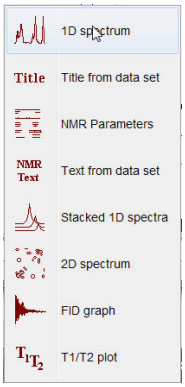


If for any reason you are not satisfied with the expansion, click on the **undo** icon on the left side of the Plot Editor window and start over again.

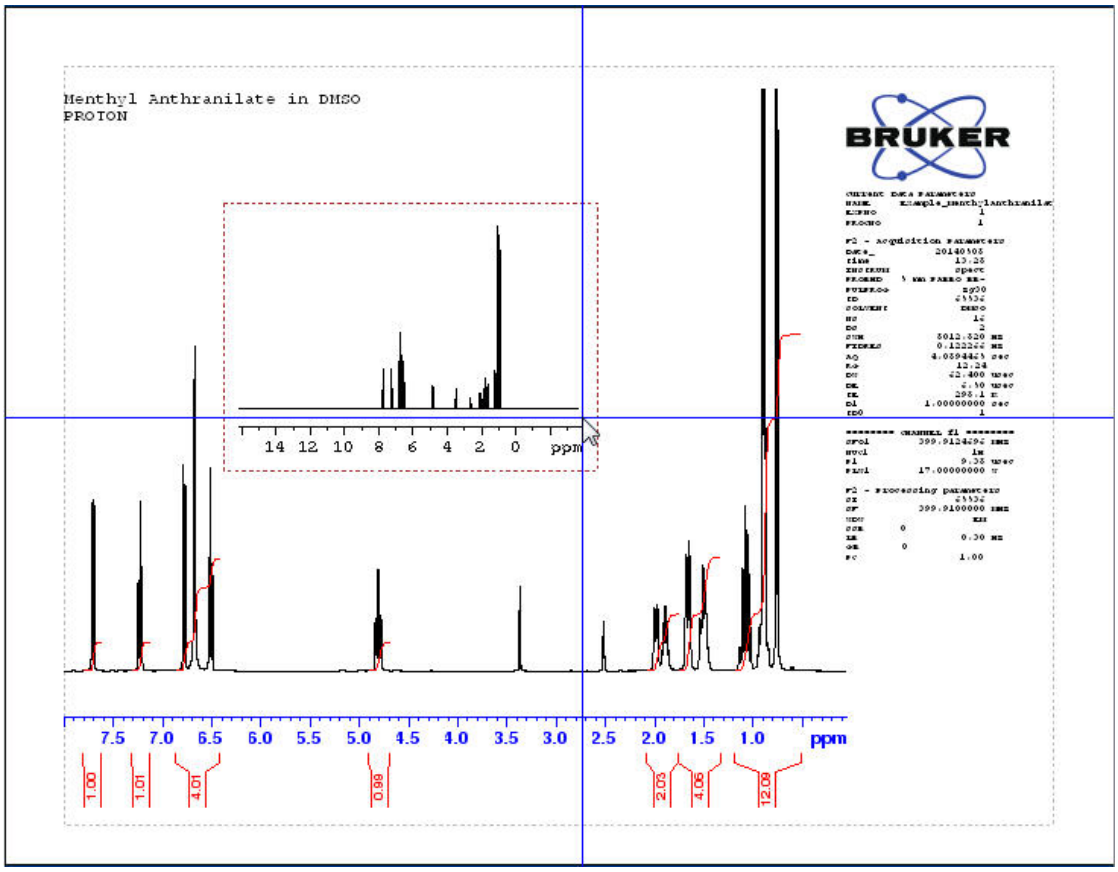


5.4.2 Inserting a Peak Expansion

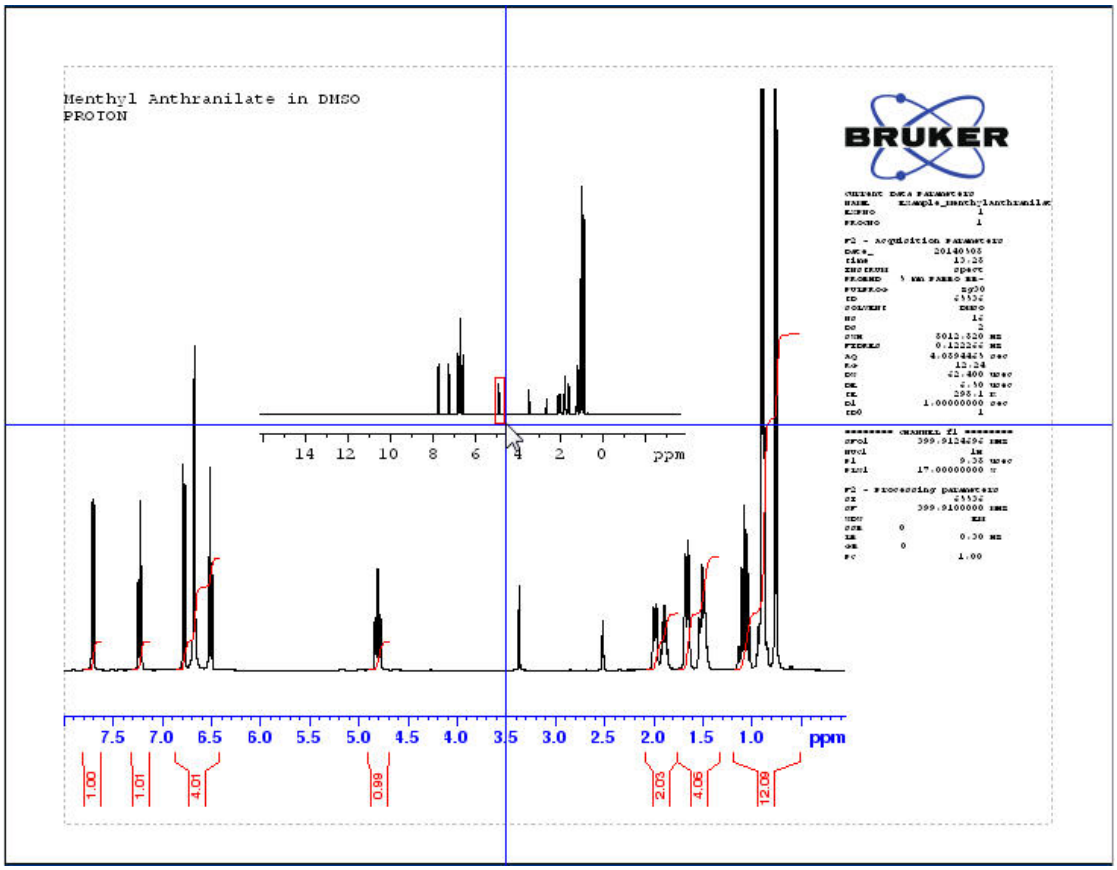
- Click on the **NMR** icon in the **Click here to insert new elements** options on the left side of the Plot Editor window.
- Select **1D spectrum**.



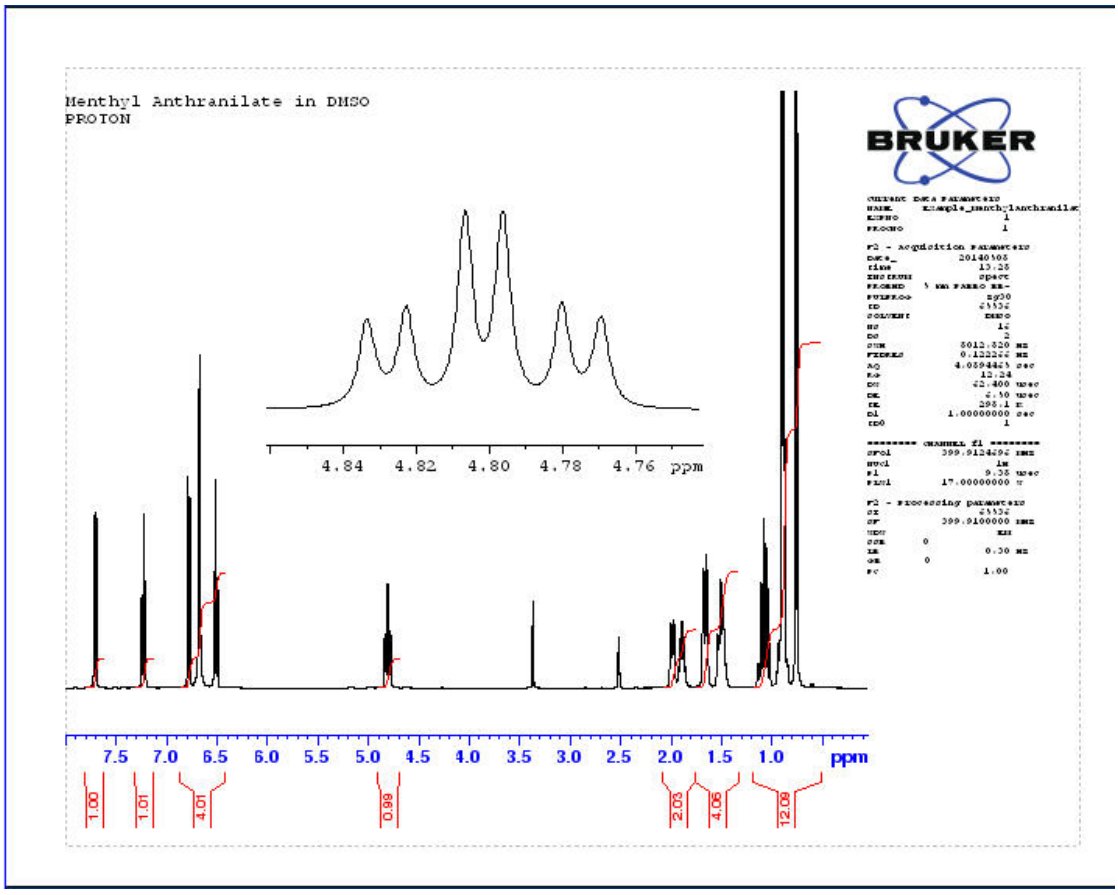
- In an empty area of the displayed spectrum, left click starting at the left and while keeping the mouse button pressed, draw a rectangular box with the original 1D spectrum displayed.



- Click on the **Expand** icon in the **View** options on the left side of the Plot Editor window.
- Left click starting at the left of the area to be expanded (e.g. the peaks at 4.5 ppm) and while keeping the mouse button pressed, draw a rectangular box around the peaks.

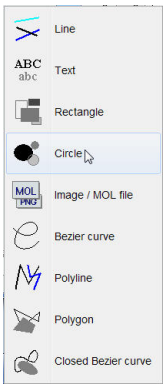


If for any reason you are not satisfied with the expansion, click on the **undo** icon on the left side of the Plot Editor window and start over again. Clicking on the expanded spectrum will mark it with small green boxes that allow you to reposition and resize the insert.



5.4.3 Marking the Location of the Peak Expansion in the Full Spectrum

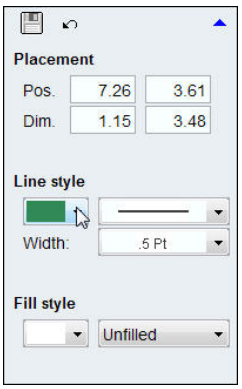
- Click on the **Standard** icon in the **Click here to insert new elements** options on the left side of the Plot Editor window.
- Select **Circle**.

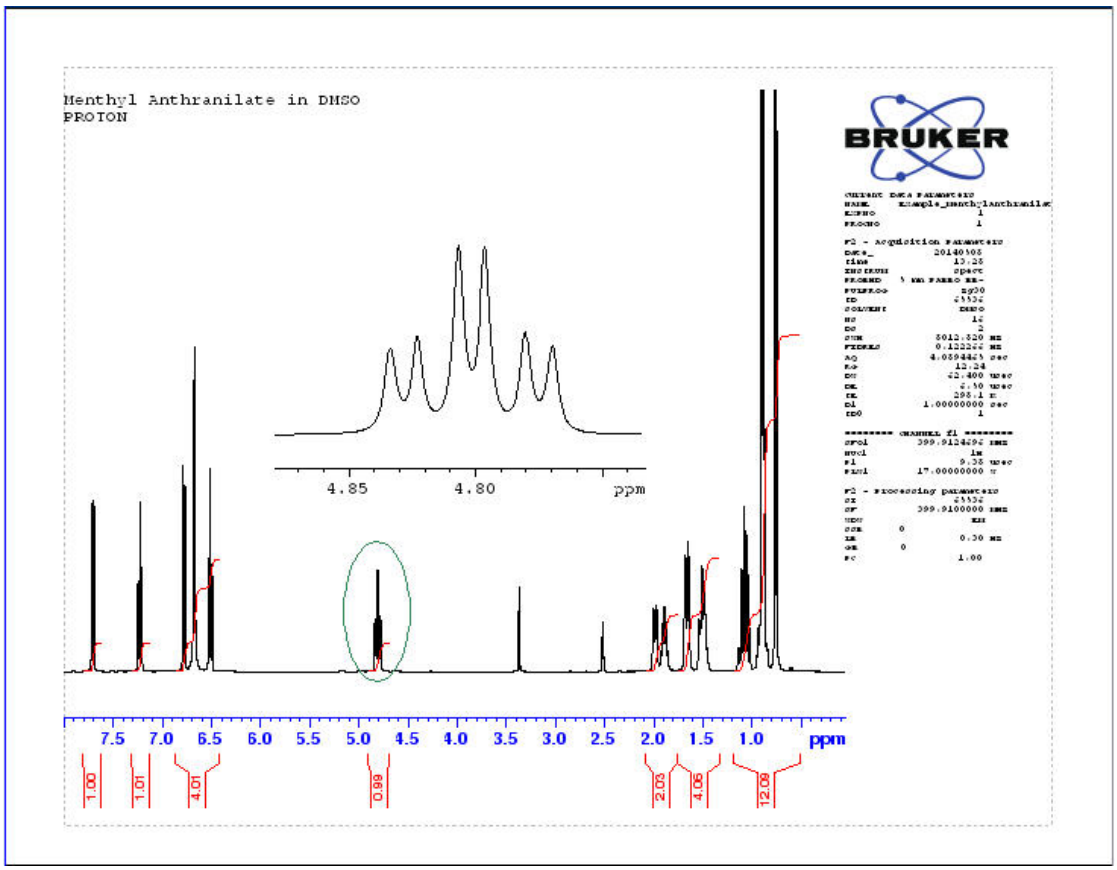


- Left click starting at the left of the peaks in the full spectrum (e.g. the peaks at 4.5 ppm) and while keeping the mouse button pressed, draw an oval figure around the peaks.

  If for any reason you are not satisfied with the figure, click on the **undo** icon on the left side of the Plot Editor window and start over again. Clicking on the oval figure you can reposition and resize the figure.

- To change the outline color of the oval figure, click on the oval figure to display the configuration handles.
- Click on the **down arrow** next to the color selection in the **Line style** options on the left side of the Plot Editor window.
- Select (e.g. green) from the color bar.

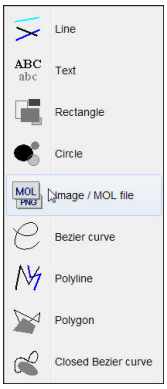




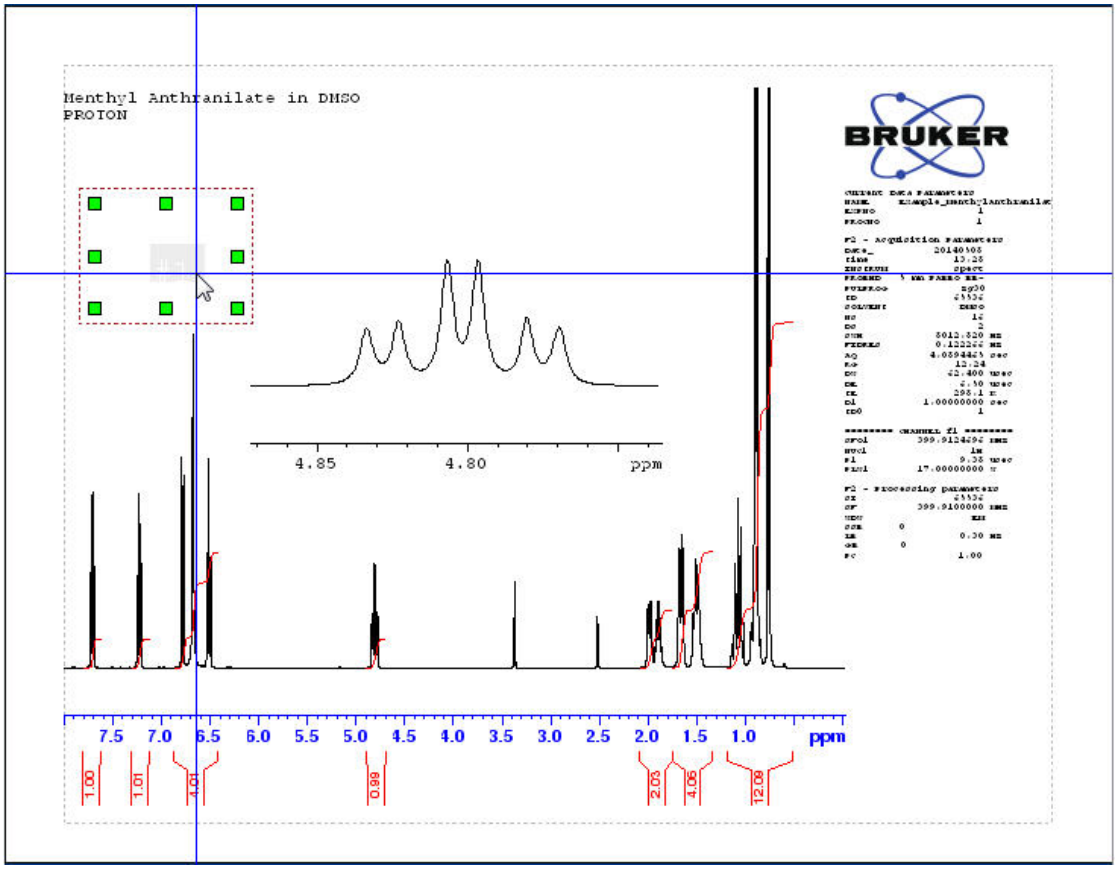
5.4.4 Adding a Molecule Structure

- To add the molecular structure, a MOL file of the sample has to be stored on the disk, preferably one level above the acquisition directory of the data set. The advantage of using this location is that the same MOL file can be used in all plots of all experiments in this data set.

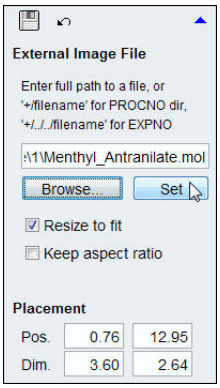
- Click on the **Standard** icon in the **Click here to insert new elements** options on the left side of the Plot Editor window.
- Select **Image / MOL** file.



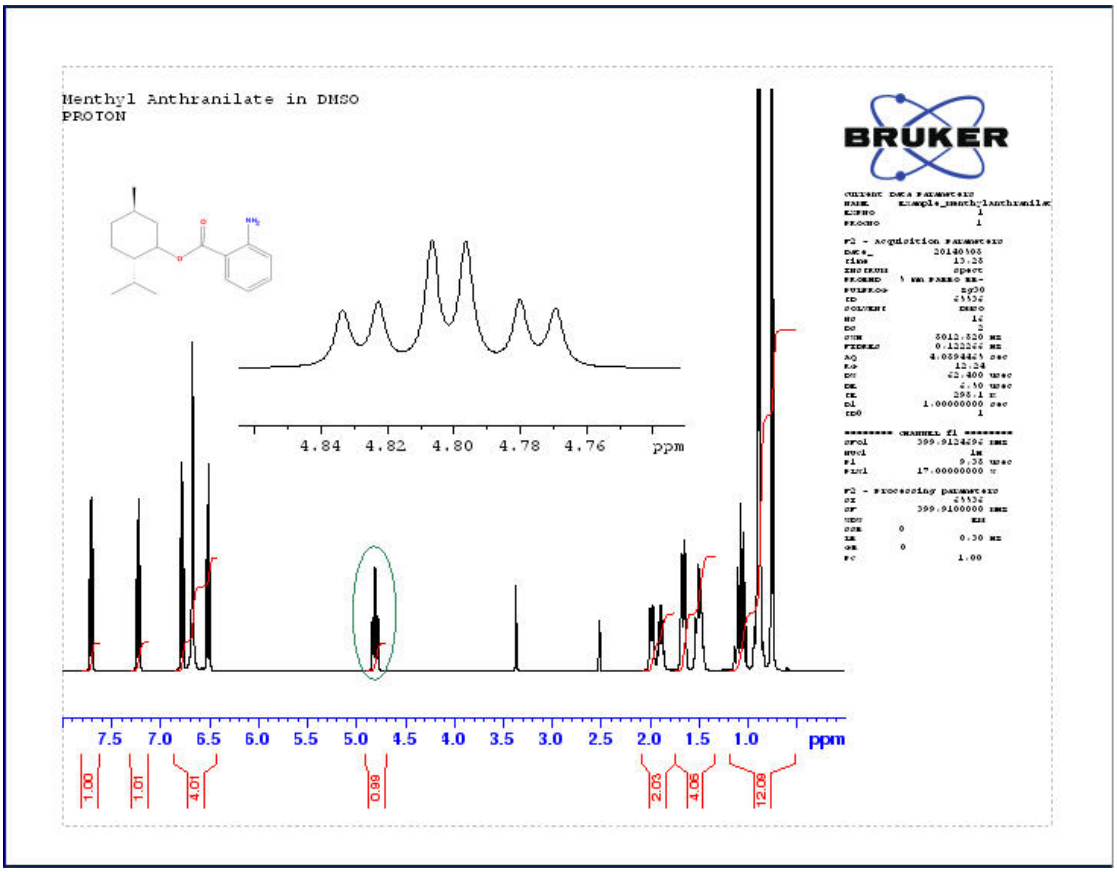
- In an empty area of the displayed spectrum, left click starting at the left and while keeping the mouse button pressed, draw a rectangular box.
- Double click inside the rectangular box.



- Click on the **Browse** button on the left side of the Plot Editor window to locate the MOL file. You can also type the full path to locate the file.

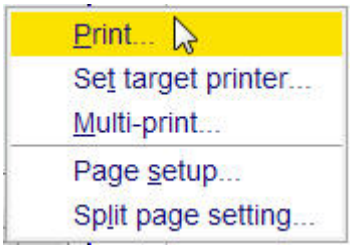


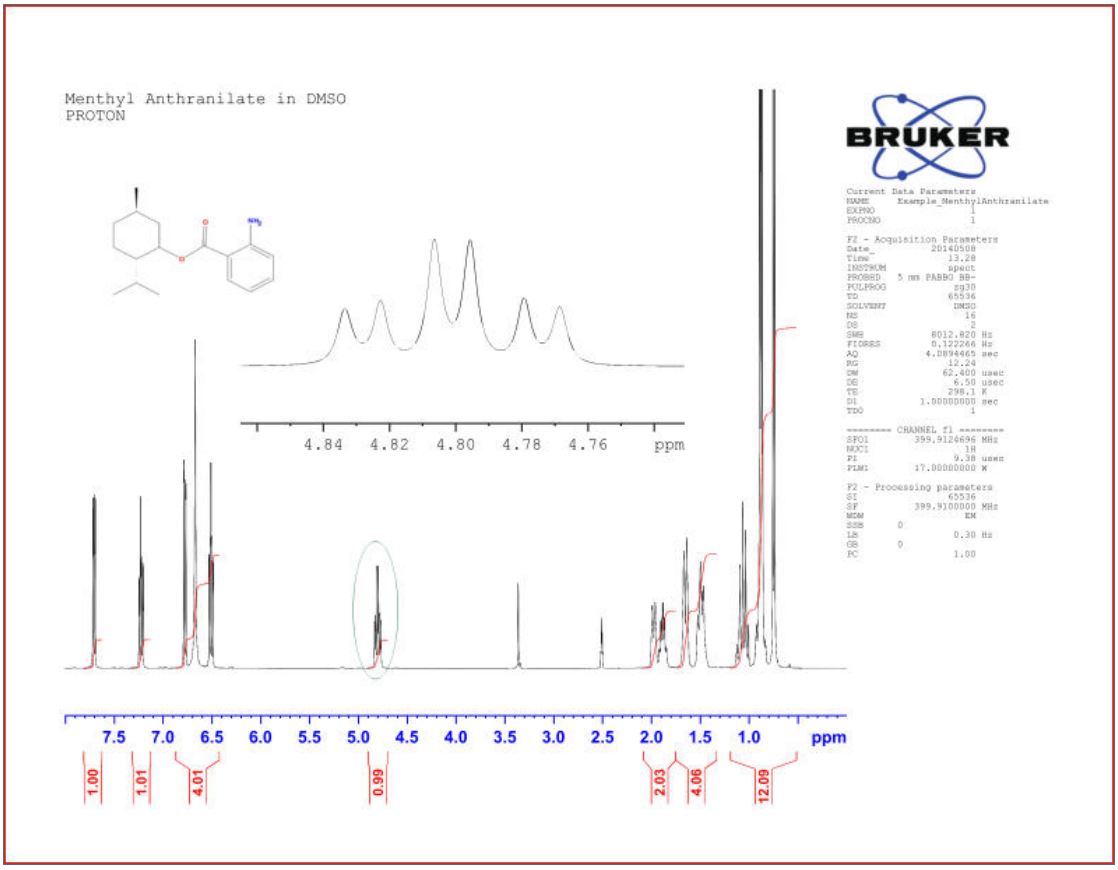
- If needed, adjust the size of the rectangular box using the handles around it or move it to a different place.



- To print this newly created layout, click on the **down arrow** next to the **Print** option on the left side of the Plot Editor window.

Then select **Print**.





To save the layout for future use e.g. automated or repeated printout of the same layout, refer to the chapter *Automation [▶ 107]*.

5.5 Multiple 1D Spectra

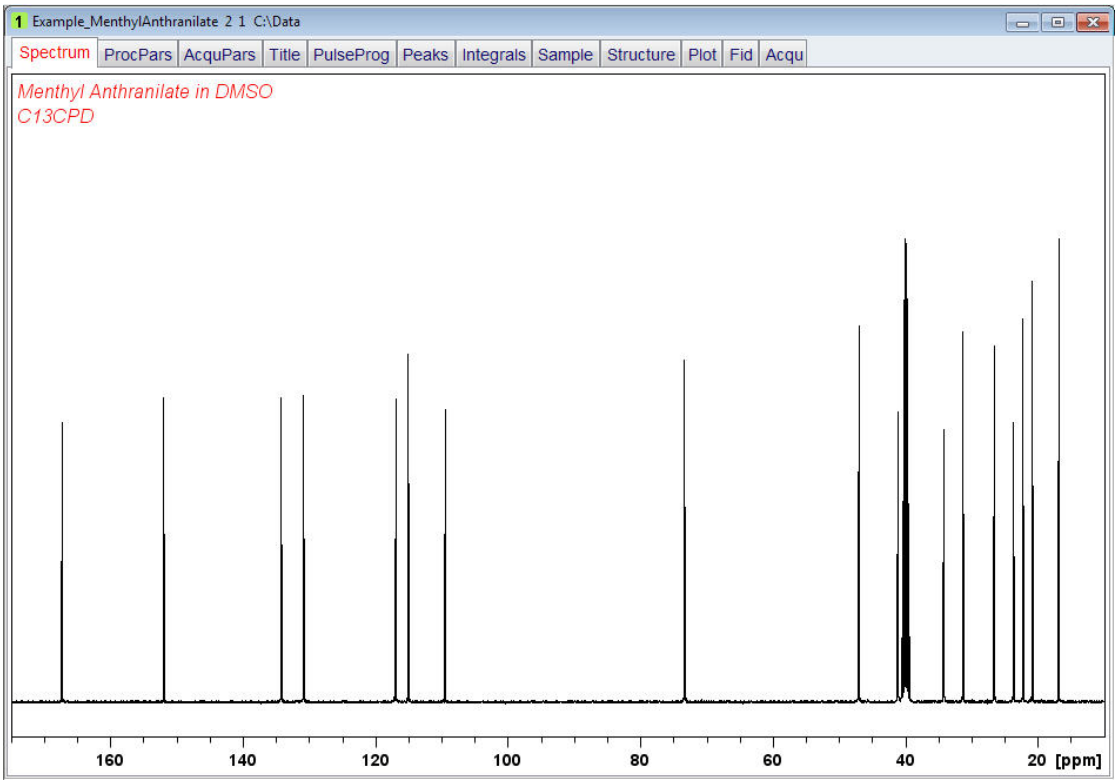
This section describes the setup for printing multiple 1D spectra using the Plot Editor. There are two options to display and print the multiple spectra using the Plot Editor. In both cases the initial setup is done with in the TopSpin display window. The multiple 1D spectra are stored in a portfolio. A portfolio consists of a list of available data directories and a list of separate data sets in those directories. The current portfolio can be made the default and it can be stored with the current data set.

5.5.1 Using edc2 in TopSpin to Add Files to the Portfolio

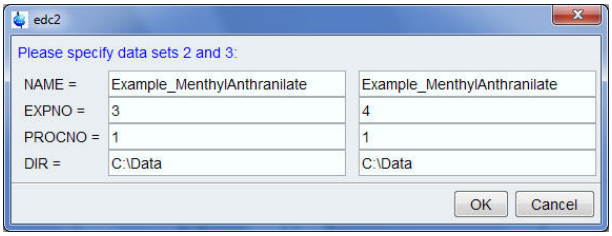
This option can only display and print up to three spectra. In this example the layout +/1D+1D +1D.xwp is used to display and print a C13, DEPT135 and DEPT90 spectrum. The preference how to present the three spectra depends on which spectrum you like to have at the bottom, the middle and on the top of the display. The spectrum on the top has to be displayed first in TopSpin, than the other spectra have to be selected using edc2. In this example we are displaying the C13 spectrum in TopSpin which will appear on the top of the plot editor display. The DEPT135 will be in the middle and the DEPT90 spectrum will be at the bottom.

5.5.1.1 Select the Layout

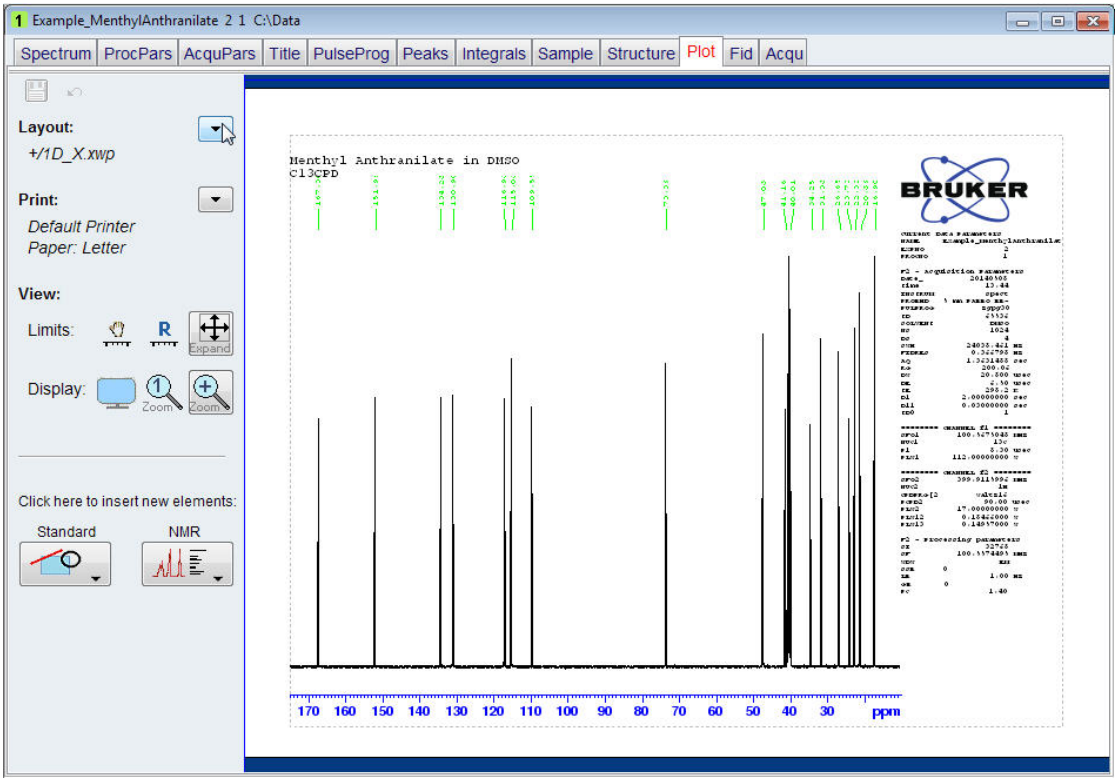
- Run a **C13CPD**, **C13DEPT135** and a **C13DEPT90** spectrum using the default Bruker parameter sets.
- Display the **C13CPD** spectrum.
- Expand the spectrum to include all peaks (e.g. **174 ppm - 1 ppm**).



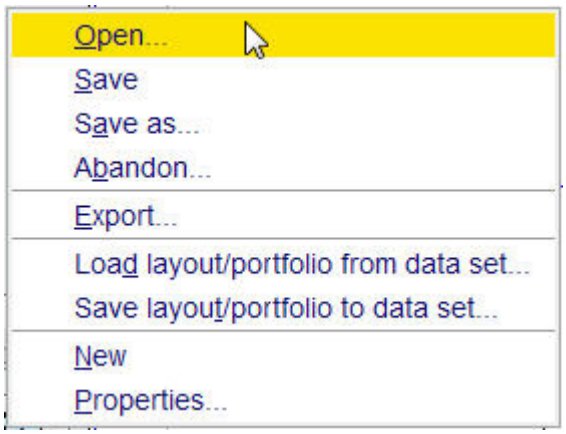
- Type **edc2** on the TopSpin command line.
- Change the following parameters:
  - Data set 2
  - **EXPNO = 3** (C13DEPT135)
  - PROCNO = **1**
  - Data set 3
  - **EXPNO = 4** (C13DEPT90)
  - PROCNO = **1**



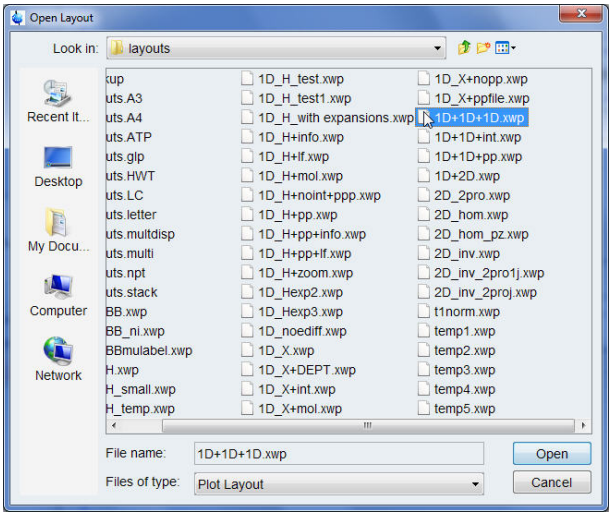
- Click on the **OK** button inside the **edc2** window.
- Click on the **Plot** tab in the Data set tab bar to open the **Plot Editor.**



- Click on the **down arrow** button to the right of the **Layout** option on the left side of the plot editor window.
- Select **Open**.

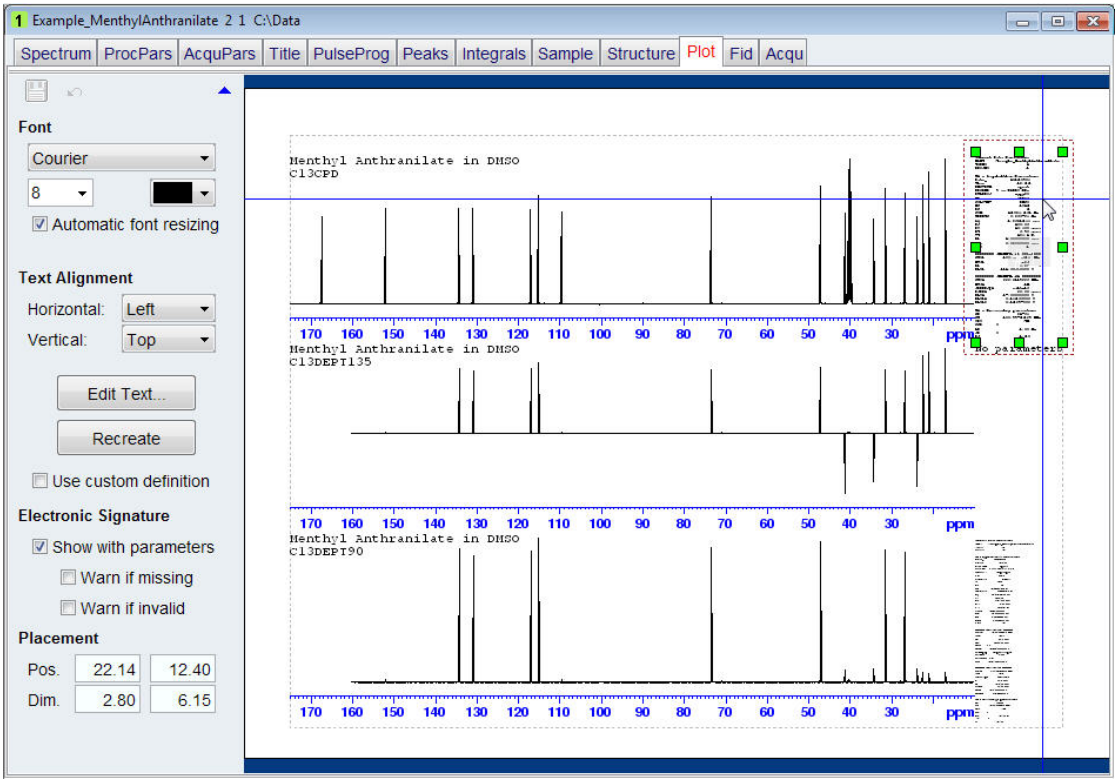


- Select **1D+1D+1D.xwp** inside the Open Layout window.
- Click on the **Open** button inside the Open Layout window.

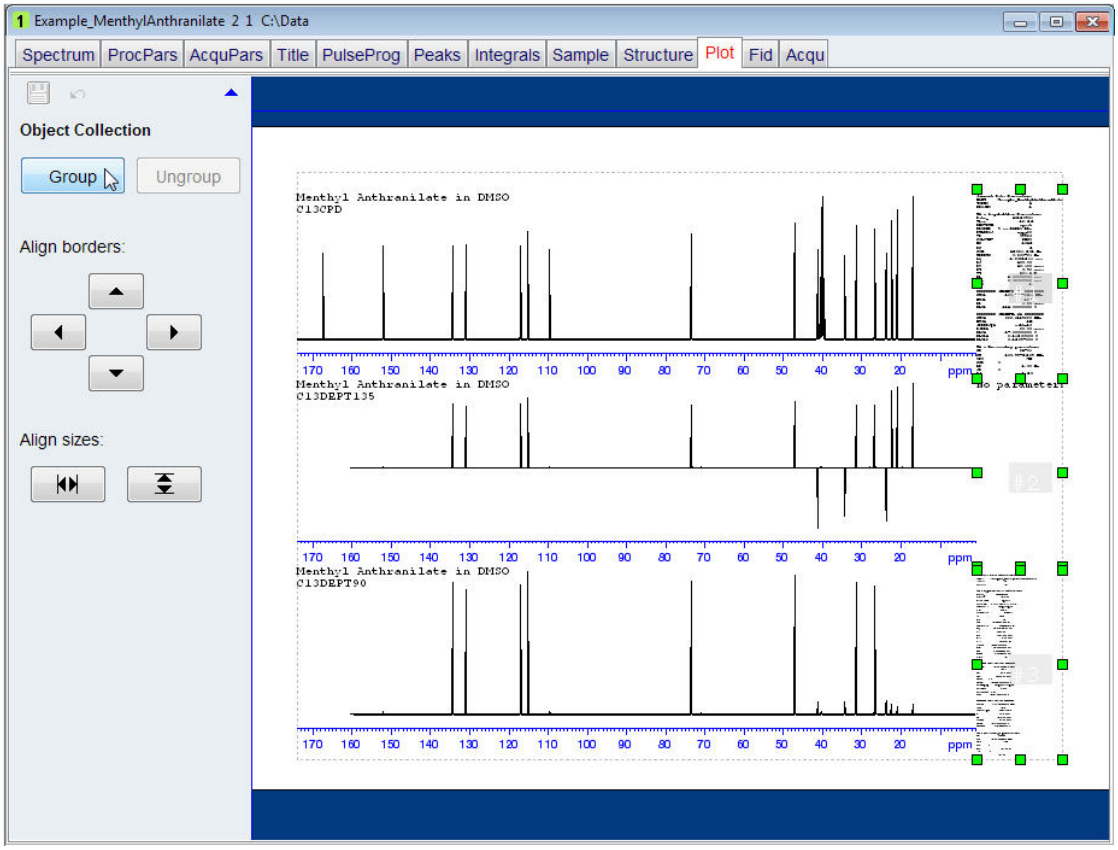


5.5.1.2 Optimizing the Layout

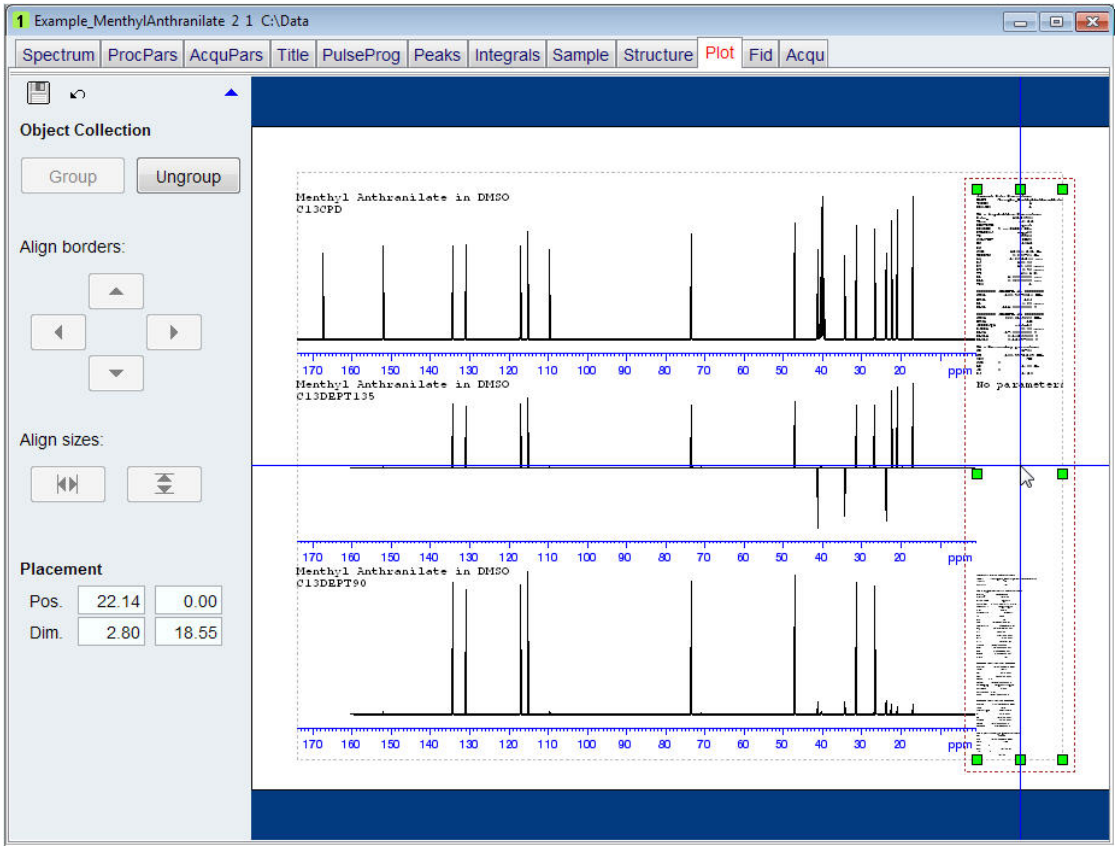
- Left click inside the parameters of the C13CPD spectrum at the top.



- With the **Ctrl** key pressed, left click on the parameters of the C13DEPT135 in the middle and the C13DEPT90 spectrum at the bottom.
- Click on the **Group** button in the **Object Collection** option on the left side of the plot editor window.

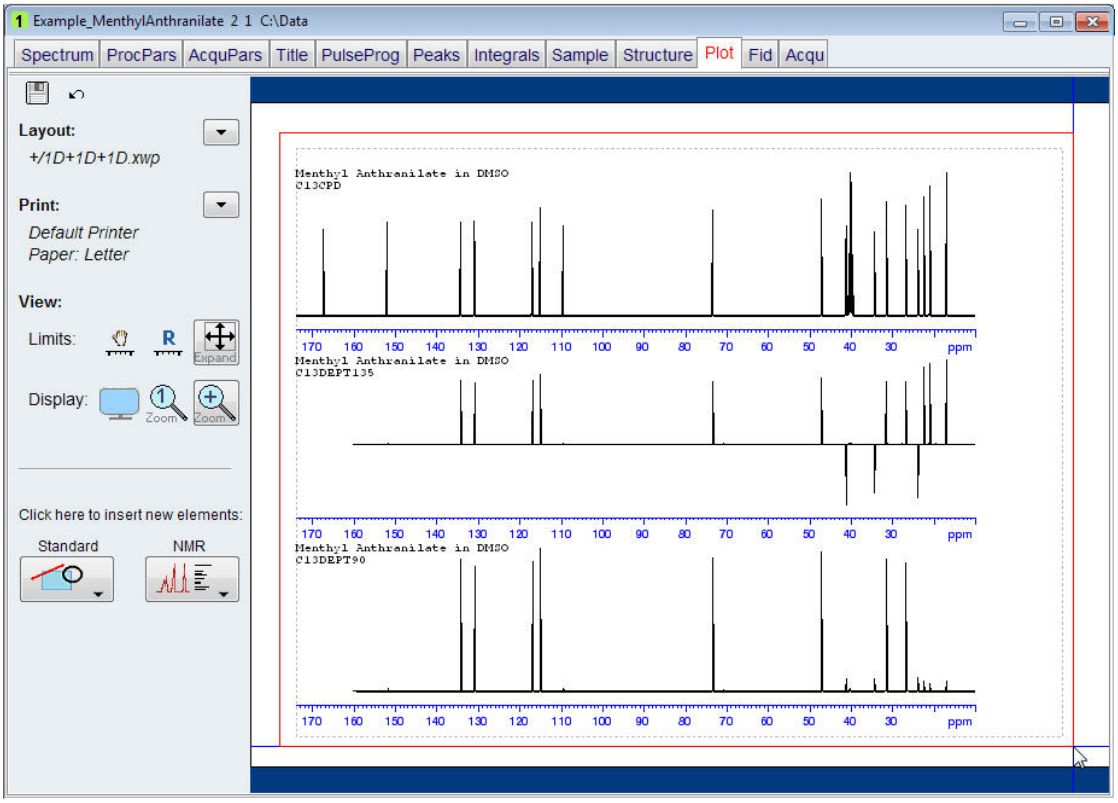


- Right click inside the grouped parameters.



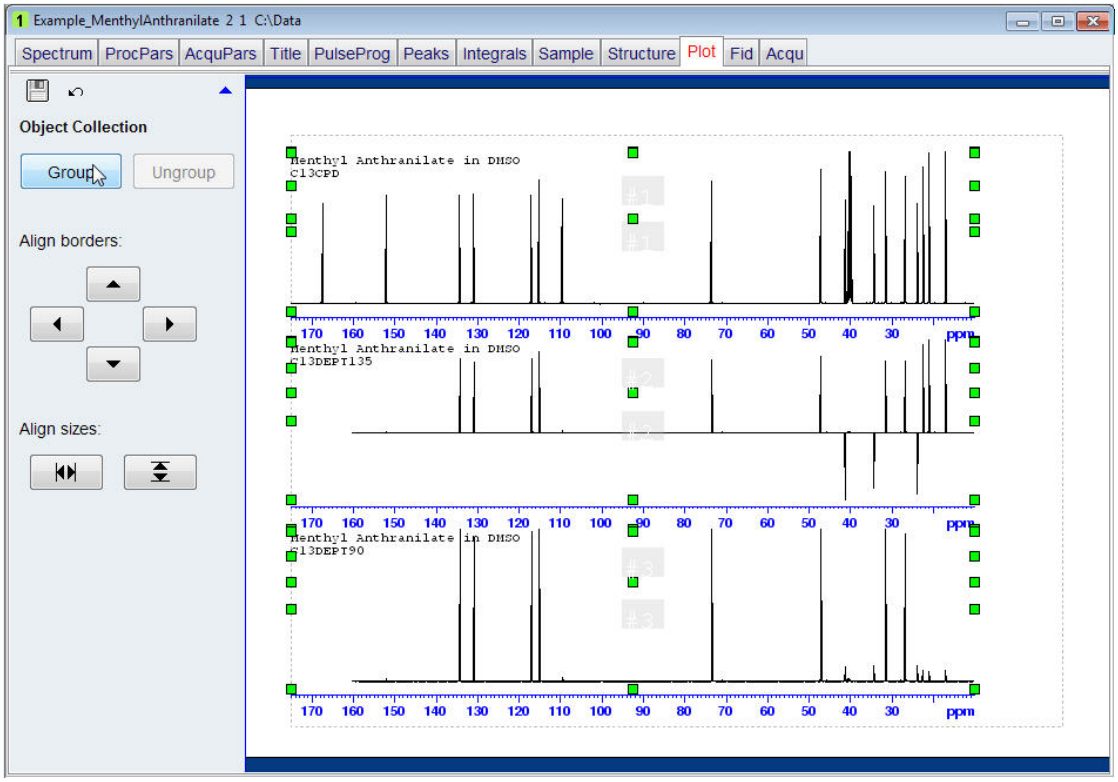
- Select **Delete**.

- Click in the left upper corner of the displayed spectra, but outside of the dotted line bordering the spectra.

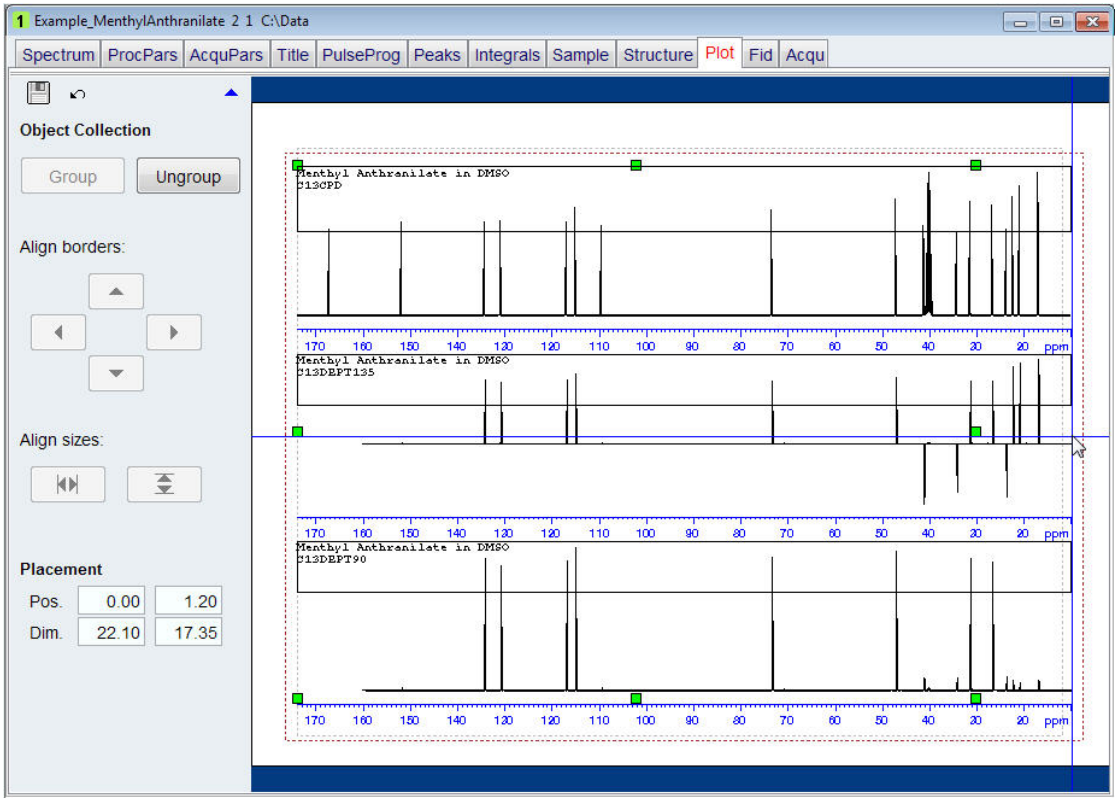


- With the left mouse pressed, draw a box around the three spectra placing it outside the dotted line bordering the spectra.

  Green handles will mark each of the spectra.
- Click on the **Group** button in the **Object Collection** option on the left side of the plot editor window.

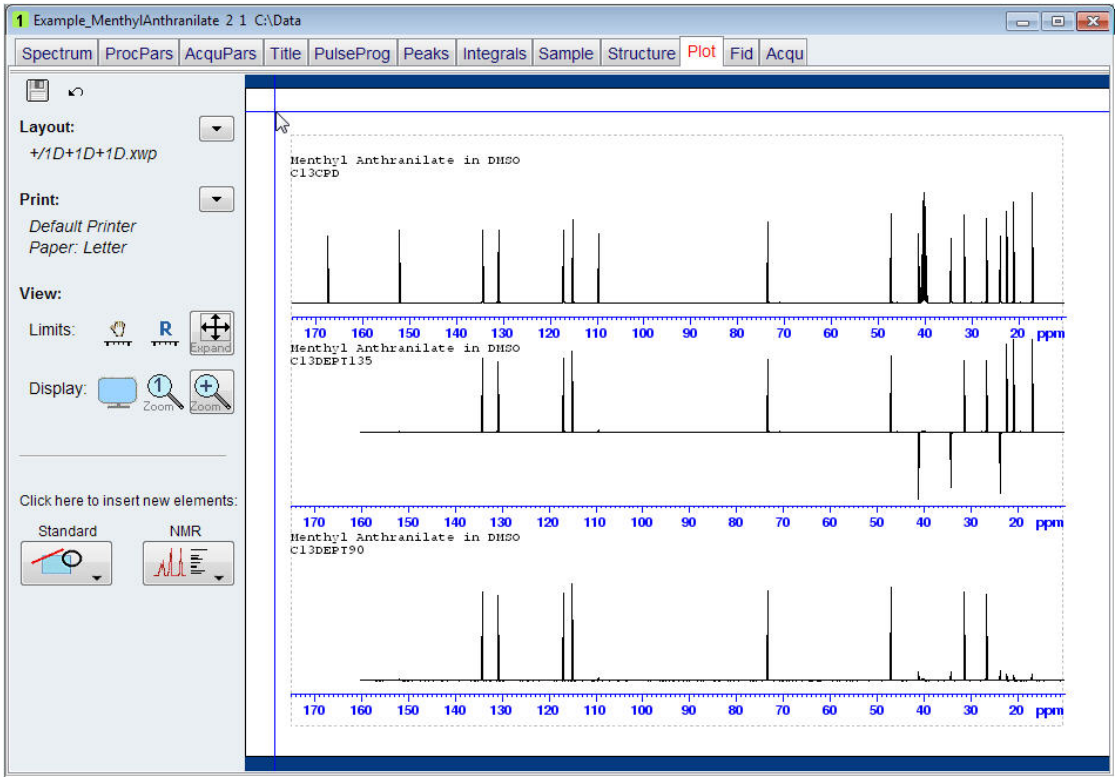


- Click on the green handle on the right side of the C13DEPT135 spectrum.
- With the left mouse button pressed move the green handle just outside of the dotted line on the right.



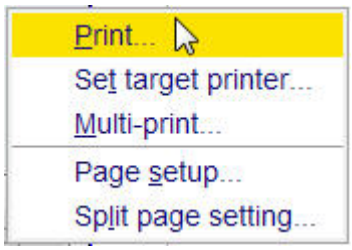
- Click on the **Ungroup** bottom in the **Object Collection** option on the left side of the plot editor window.

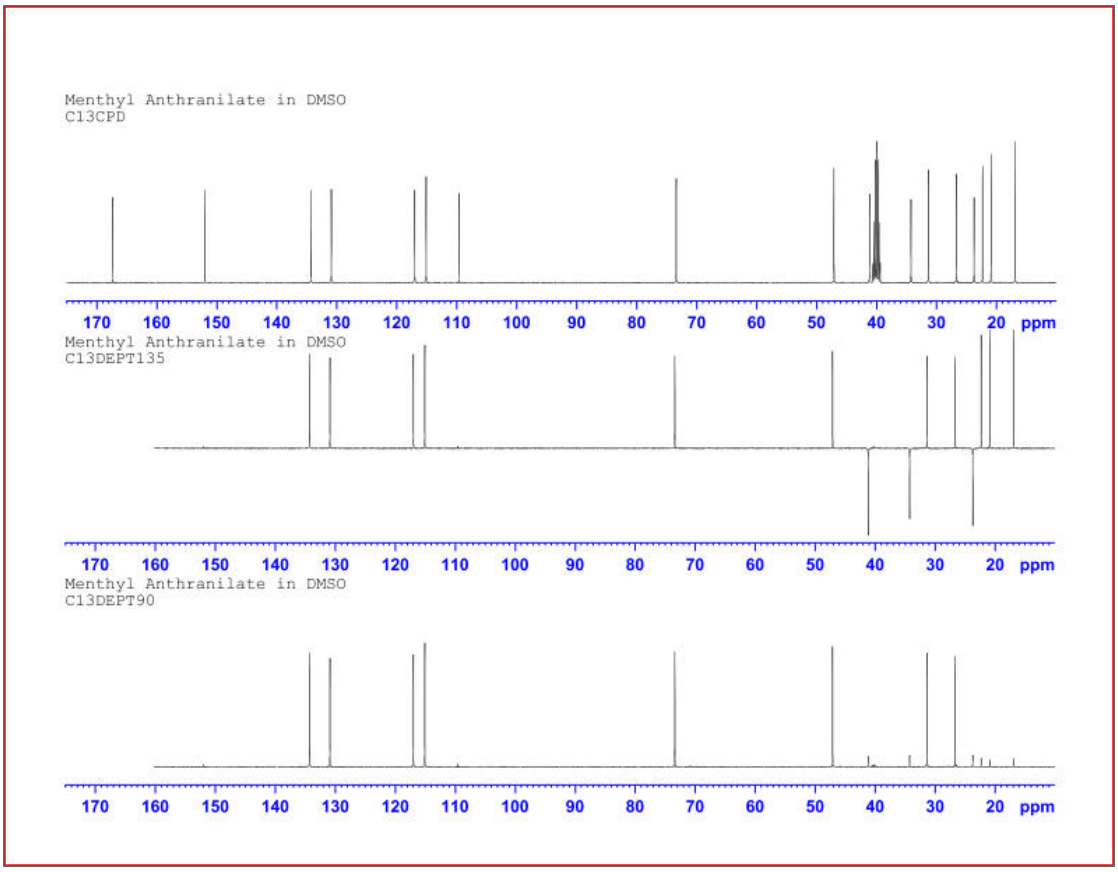
  Each spectrum can now be individually adjusted to the desired vertical scale by clicking on the spectrum and use the mouse wheel.
- Click anywhere outside the dotted line bordering the 3 spectra.



- To print this newly created layout, click on the **down arrow** next to the **Print** option on the left side of the Plot Editor window.

Then select **Print**.





To save the layout for future use e.g. automated or repeated printout of the same layout, refer to the chapter *Automation [▷ 107]***.**

5.5.2 Using the Multiple Display in TopSpin to Add Files to the Portfolio

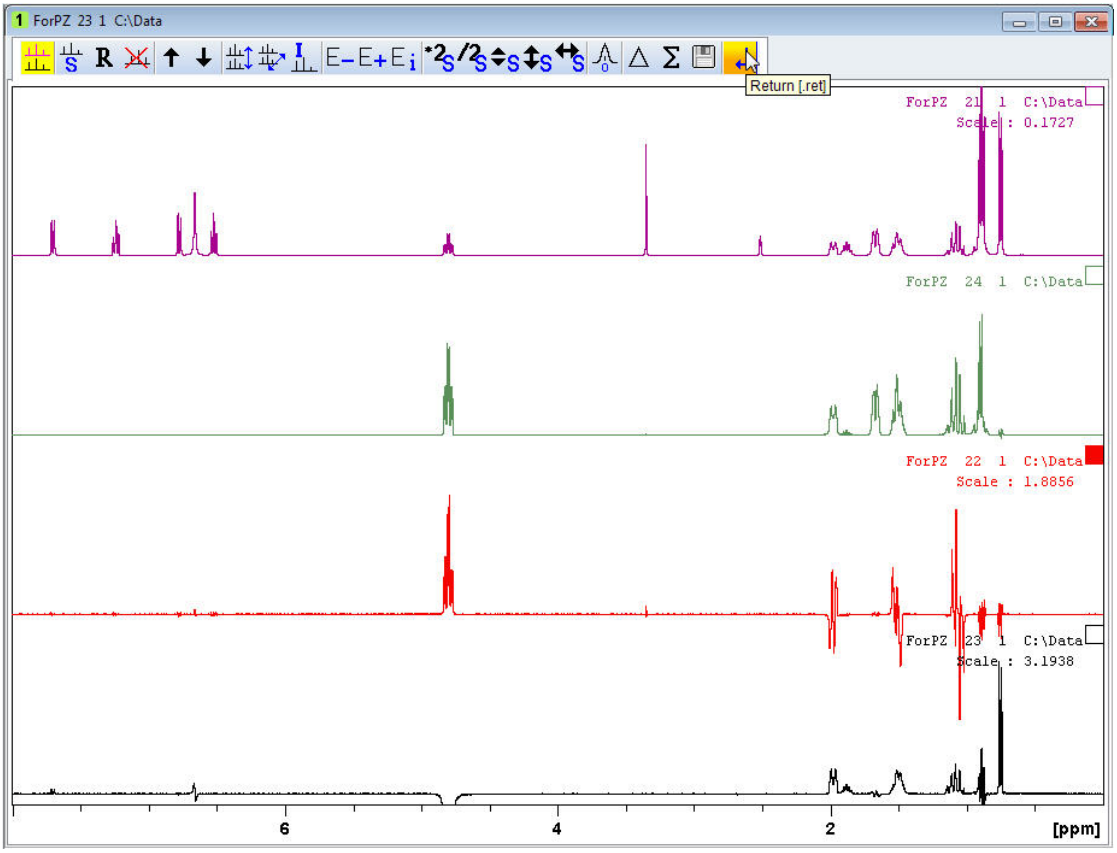
This option can display and print multiple 1D spectra. In this example the multiple display option in TopSpin is used to display and print any number of spectra. The preference how to present the multiple spectra depends on the order you would like to see the spectra printed.

5.5.2.1 Selecting the Layout

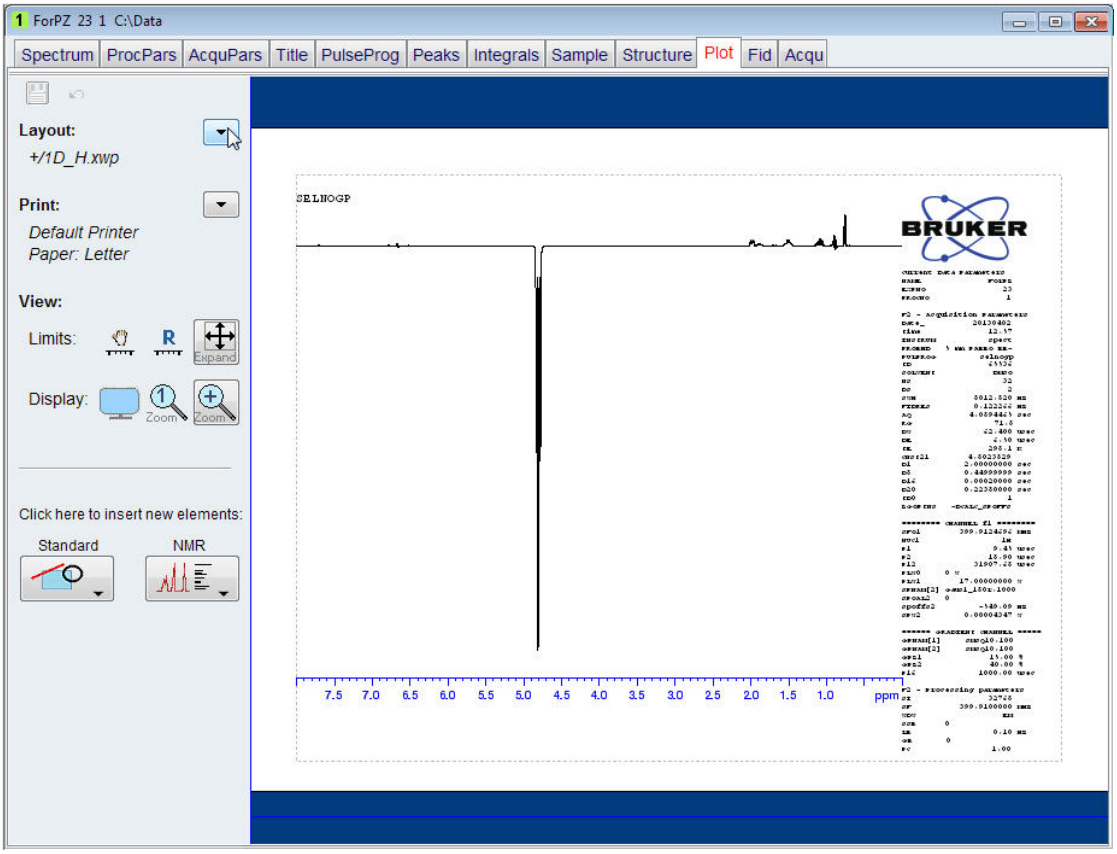
- Run a **1D PROTON, SELCOGP, SELNOGP**, and a **SELMLGP** spectrum using the default Bruker parameter sets.
- Display the **SELNOGP** spectrum.
- Expand the spectrum from **8 ppm** to **0 ppm**.
- Click on the **Multiple display** button inside the Toolbar.

- In the Browser window locate the **SELCOGP** spectrum of the same sample.
- With the left mouse button pressed, drag the **SELCOGP** spectrum in to the Data display window.

- Repeat the last two steps for the **SELMLGP** and the original **Proton** spectra of the same sample.
- Click on the **Return** button inside the Multiple display toolbar.



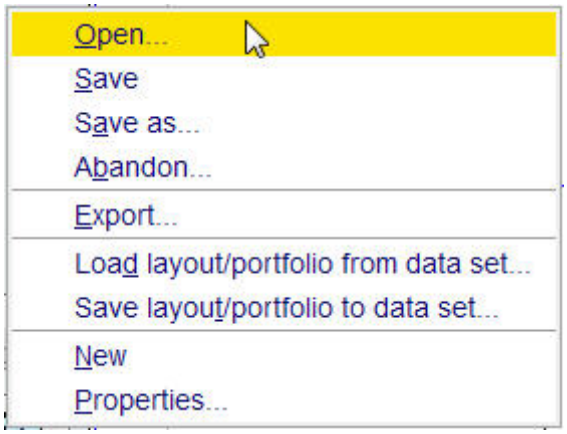
- Click on the **Plot** tab inside the Data set tabs bar.



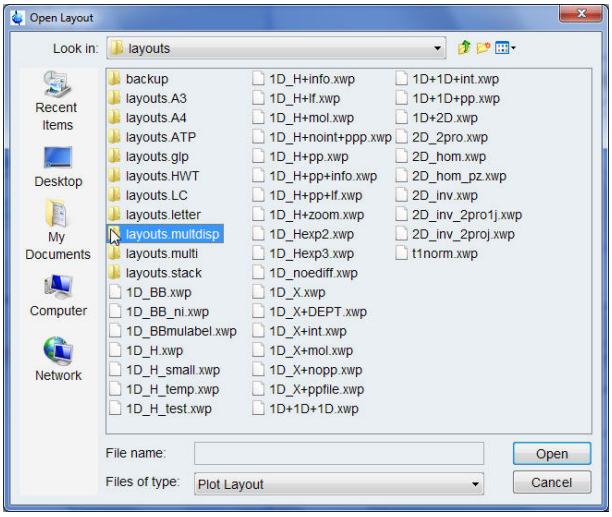
Make sure that the basic display options are shown as in the picture above. If you have clicked inside the display area in the plot editor a new option window will be displayed on the left side of the plot editor. In this case, click on the up pointed arrow in the upper right corner of the plot editor option window (see picture below) or click anywhere inside the blue area at the top or bottom of the plot editor display.

- Click on the **down arrow** button to the right of the **Layout** option.

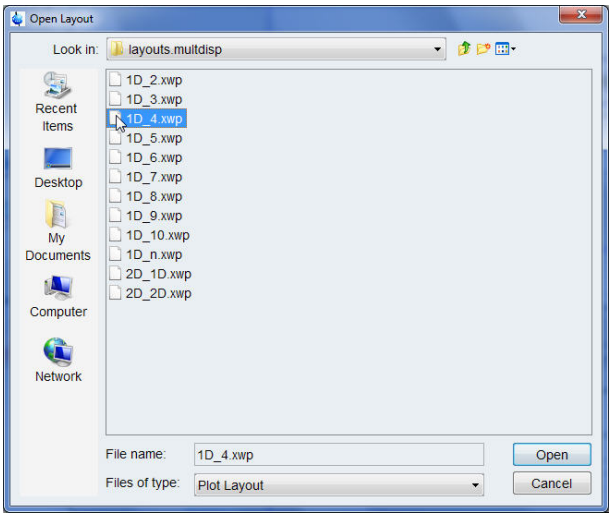
- Select **Open**.



- Double click on the **layouts.multdisp** folder.

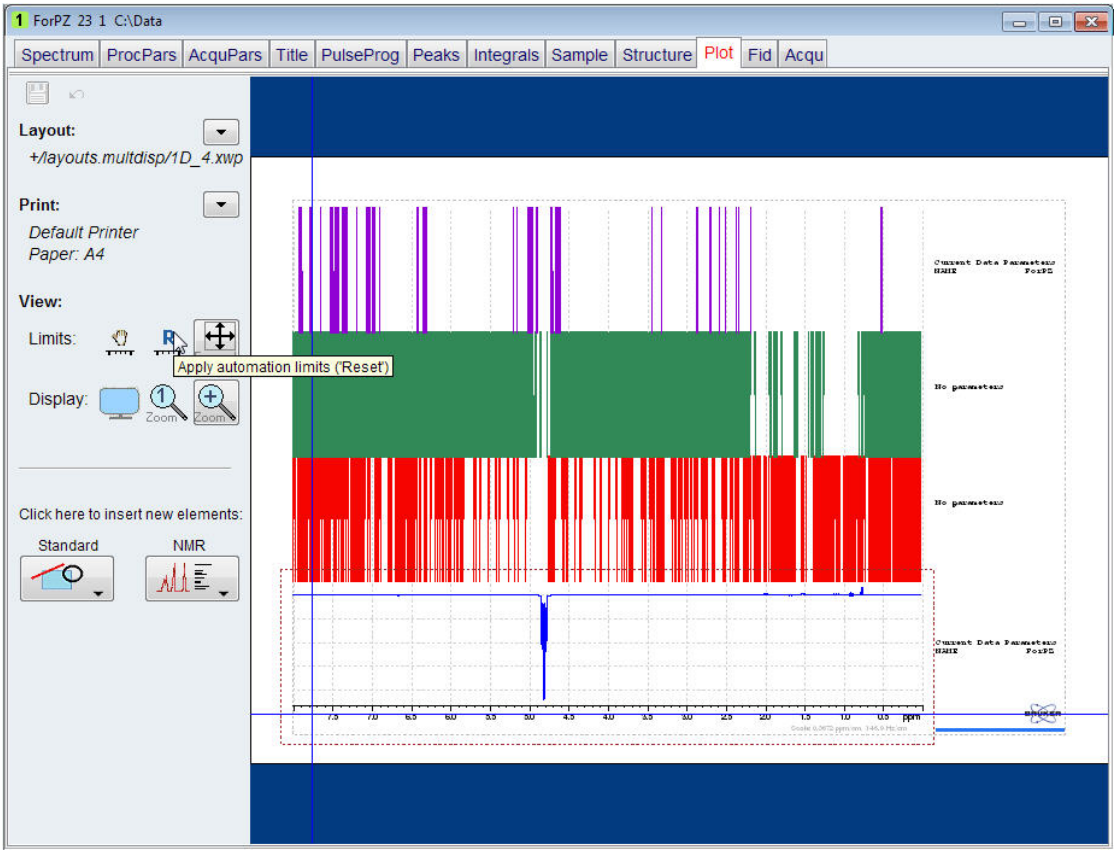


- Select **1D_4.xwp** inside the Open Layout window.



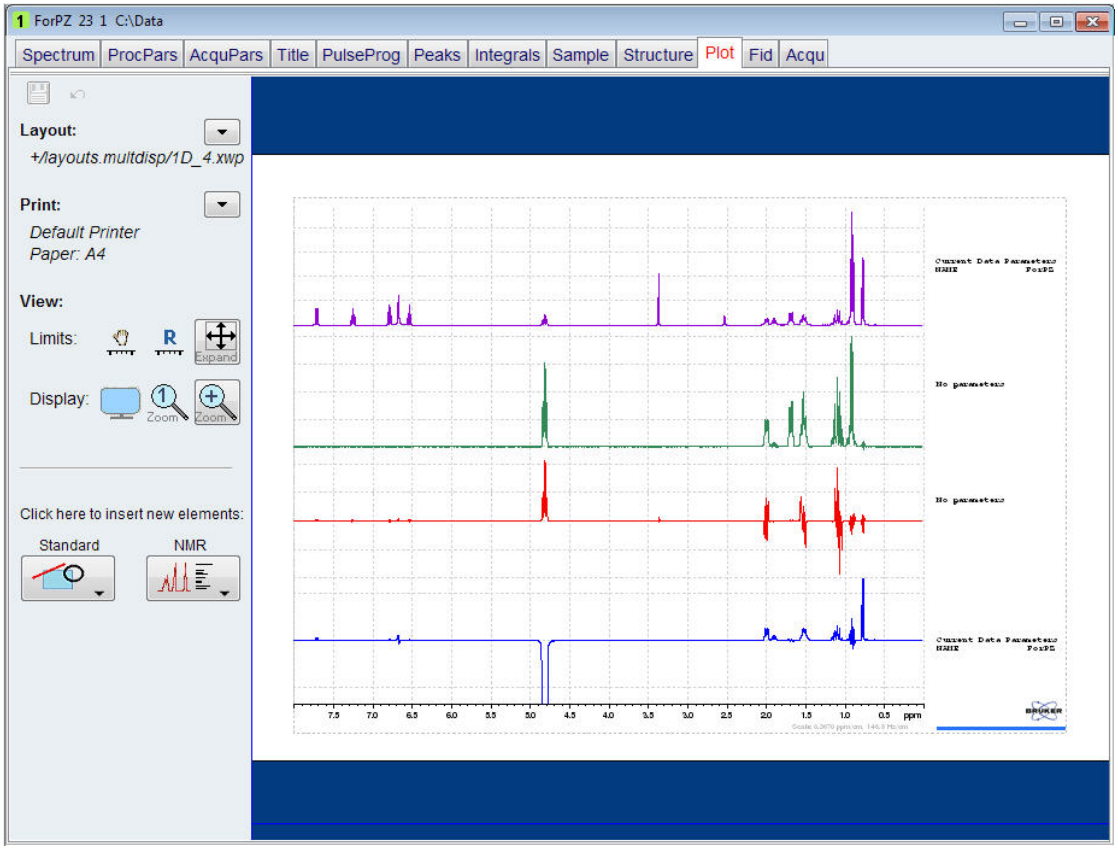
- Click on the **Open** button inside the Open Layout window.
- Click on the **down arrow** next to the **Plot Portfolio** option below the Browser window.

- Select **Load collection from multiple display mode**.

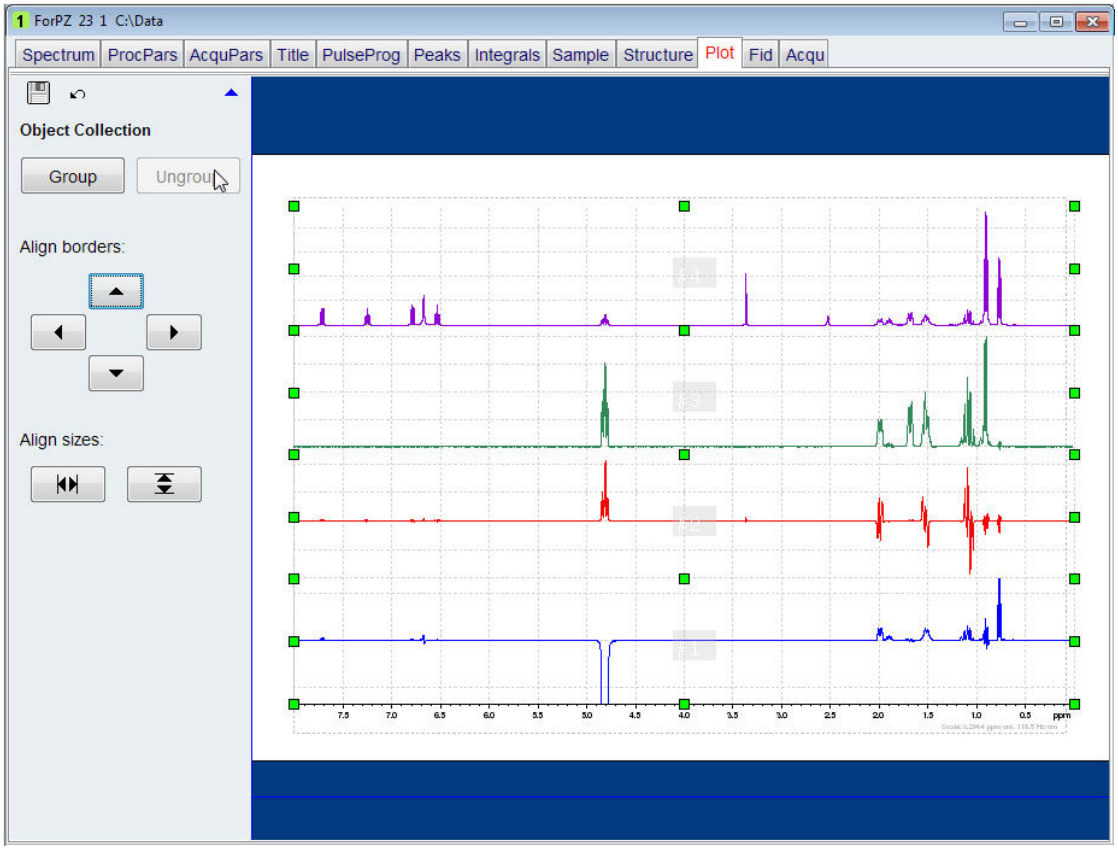


5.5.2.2 Modifying the Layout

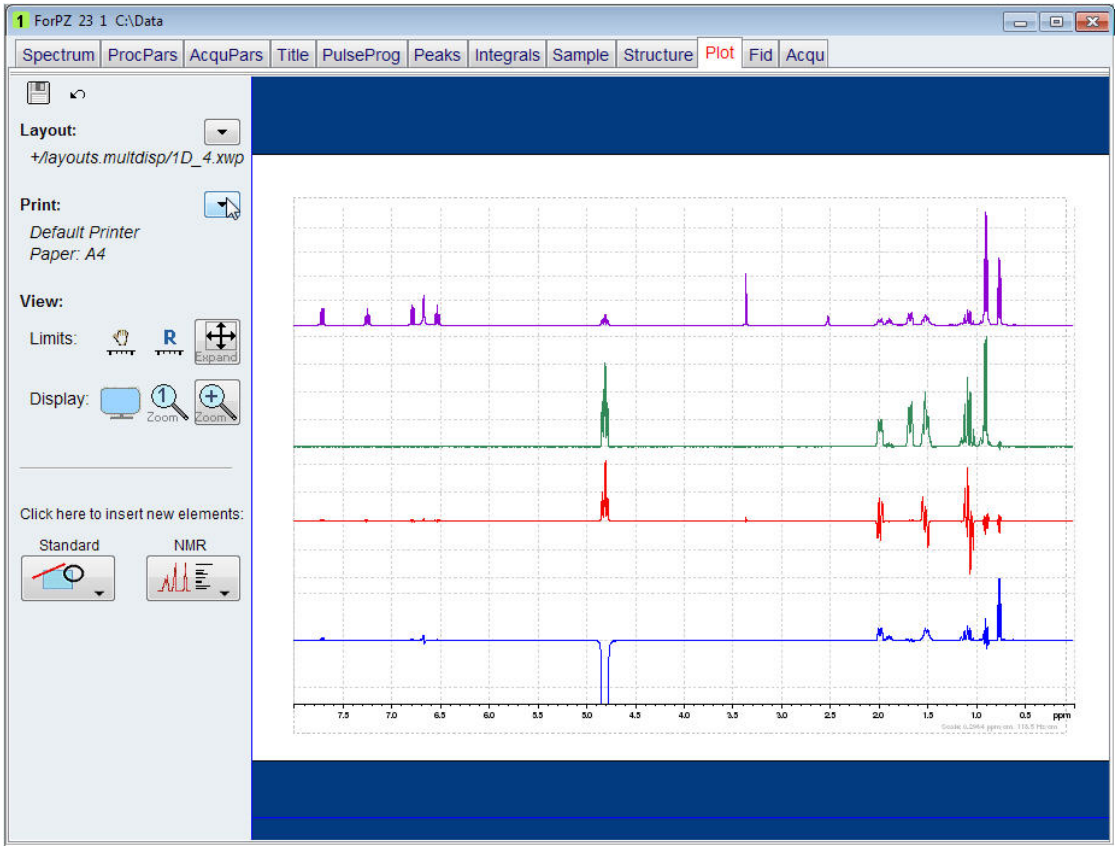
- Click on the **R** button in the **View** section on the left side of the plot editor window.



- Group all the parameter listing including the Bruker logo on the right side of the display window and delete them following the first six steps in *Optimizing the Layout [▶ 65]*.
- Group all the spectra and expand them following the first six steps in *Optimizing the Layout [▶ 65]*.
- Ungroup all the spectra.



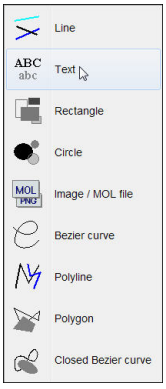
Each spectrum can now be individually controlled to the desired vertical scale and base line adjustment by clicking on the spectrum and use the adjust buttons of the TopSpin toolbar.



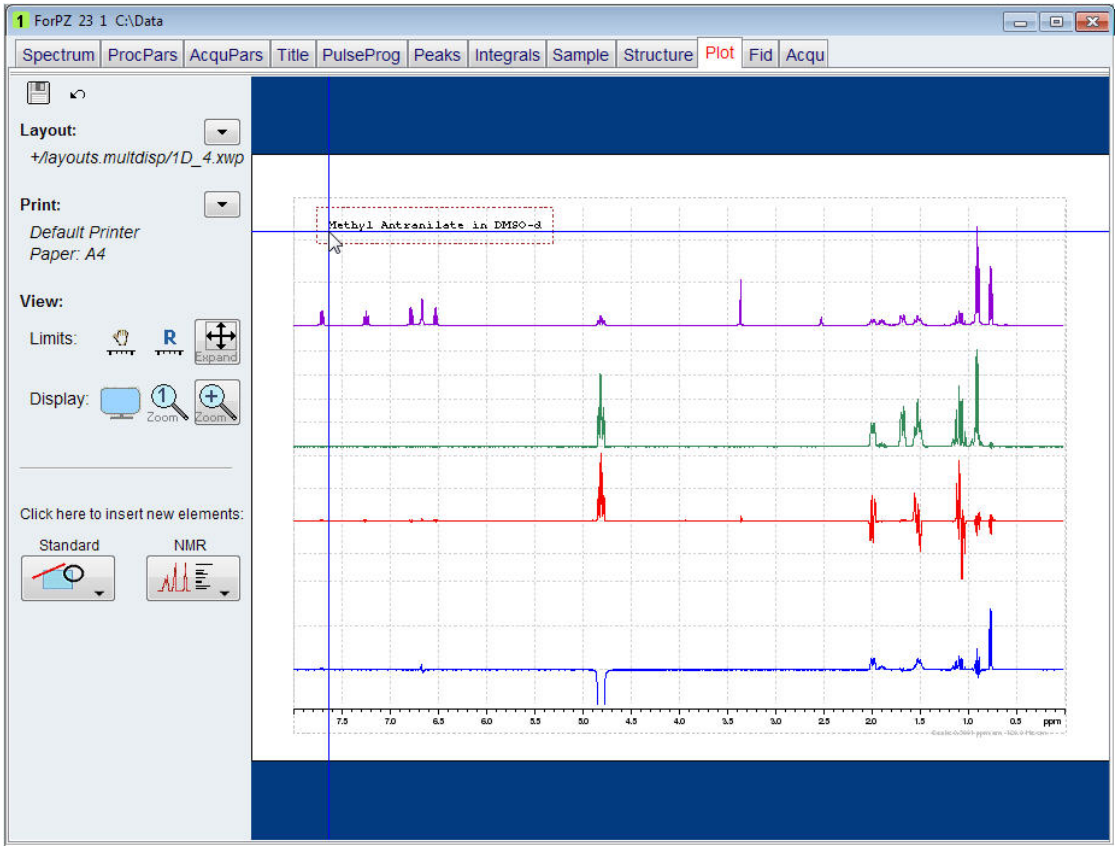
Click anywhere outside the dotted line bordering the four spectra.

5.5.2.3 Adding Text to the Layout

- Click on the **Standard** icon in the **Click here to insert new elements** options on the left side of the Plot Editor window.
- Select **Text**.

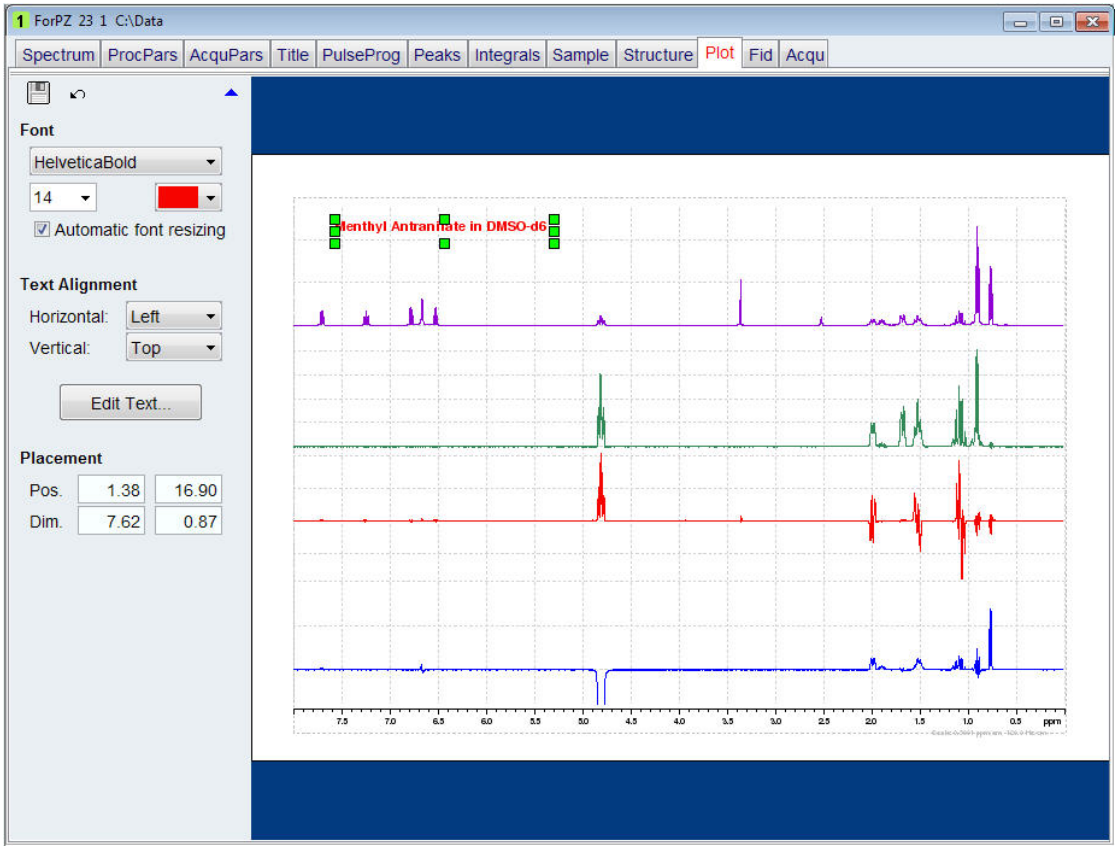


Move the cursor in to the left upper corner of the proton spectrum and click the left mouse button.

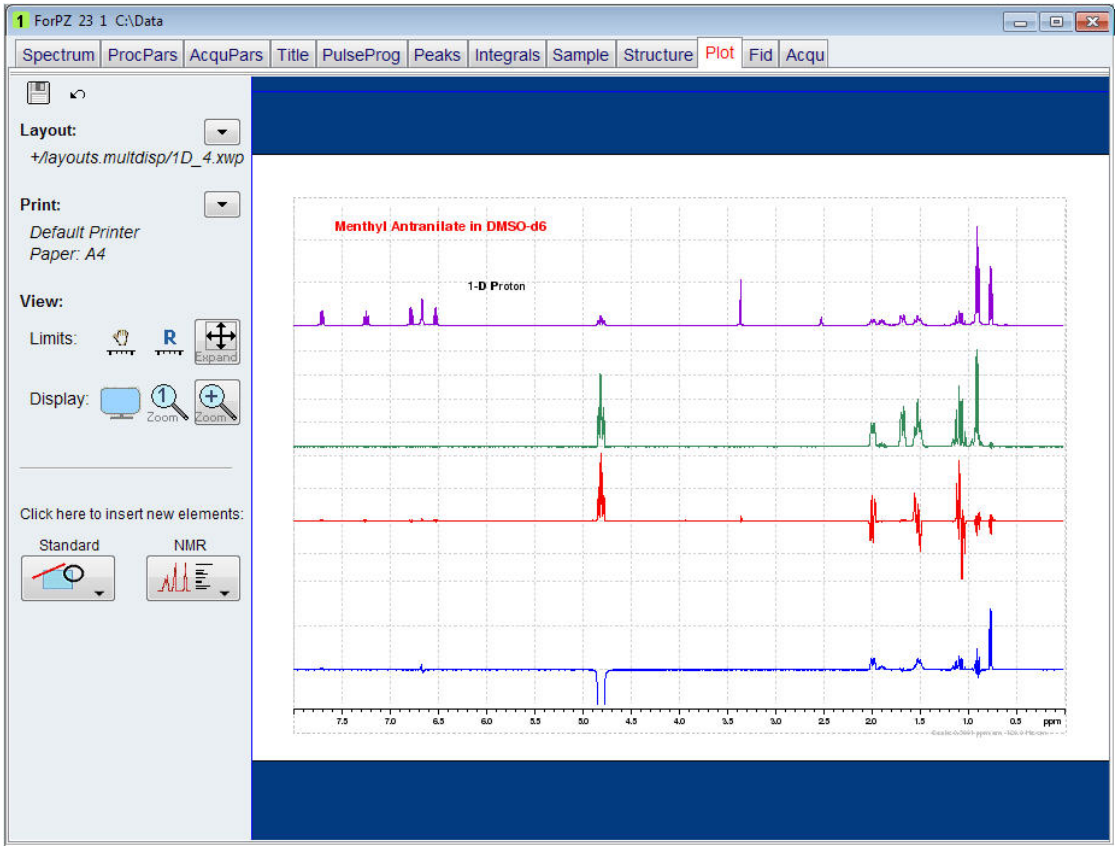


- Type **Menthyl Antranilate in DMSO-d6**.
- Hit the **Return** key.
- Click the left mouse button.

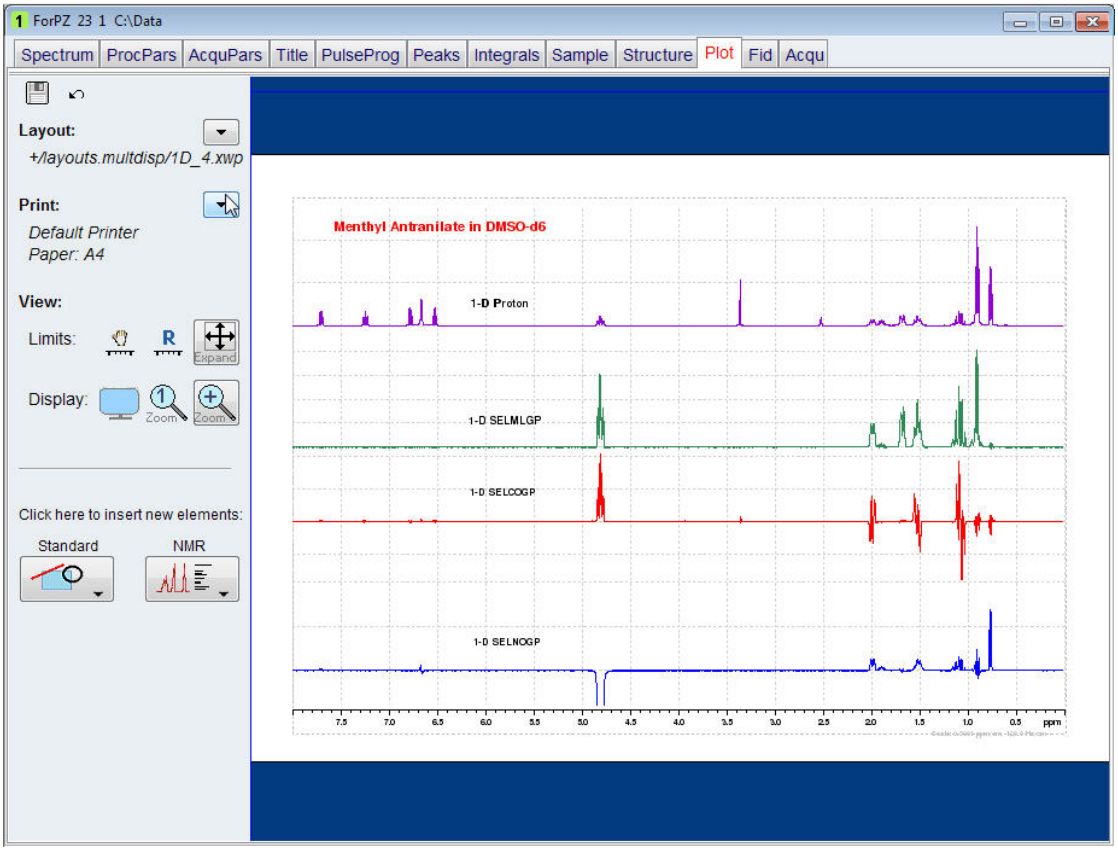
  To change the font, size, style or color of the text, left click on the text box to display the green handles. The options are displayed on the left side of the plot editor window. The example below illustrates how to change the settings to the Font **Helvetia Bold**, the Size to **14** and the Color to **red**.



- Click anywhere outside the dotted line bordering the 4 spectra.
- Click on the **Standard** icon in the **Click here to insert new elements** options on the left side of the Plot Editor window.
- Select **Text**.
- Move the cursor above the baseline of the proton spectrum and click the left mouse button. Choose a section of the spectrum which does not contain any peaks.
- Type **1D Proton**.
- Click the left mouse button.
- Change the Font to e.g. **Helvetia Bold** the Size to **12** and the Color to **black**.

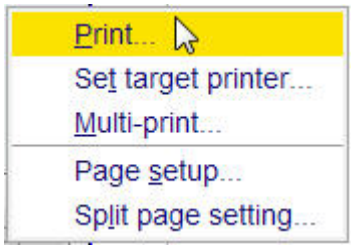


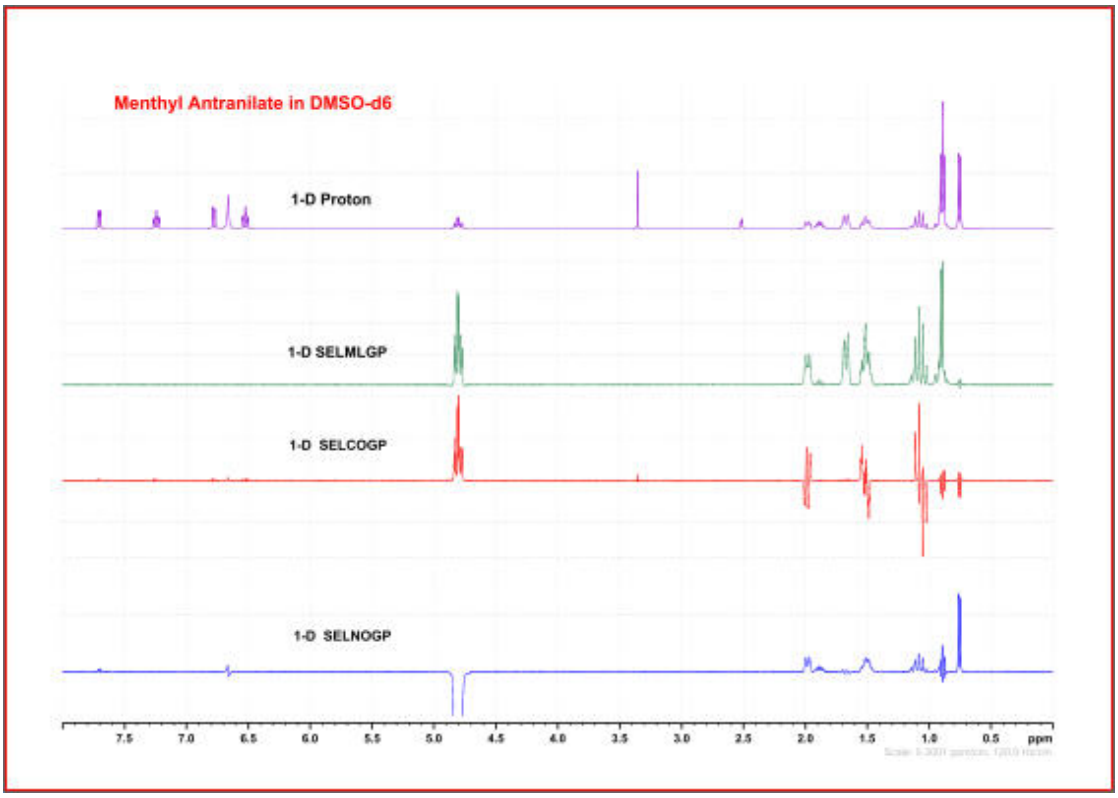
- Repeat the last five steps for the other spectra, adding the text **1D SELMLGP**, **1D SELCOGP** and **1D SELNOGP**.



- To print this newly created layout, click on the **down arrow** next to the **Print** option on the left side of the Plot Editor window.

Then select **Print**.





5.6 Printing 2D Data

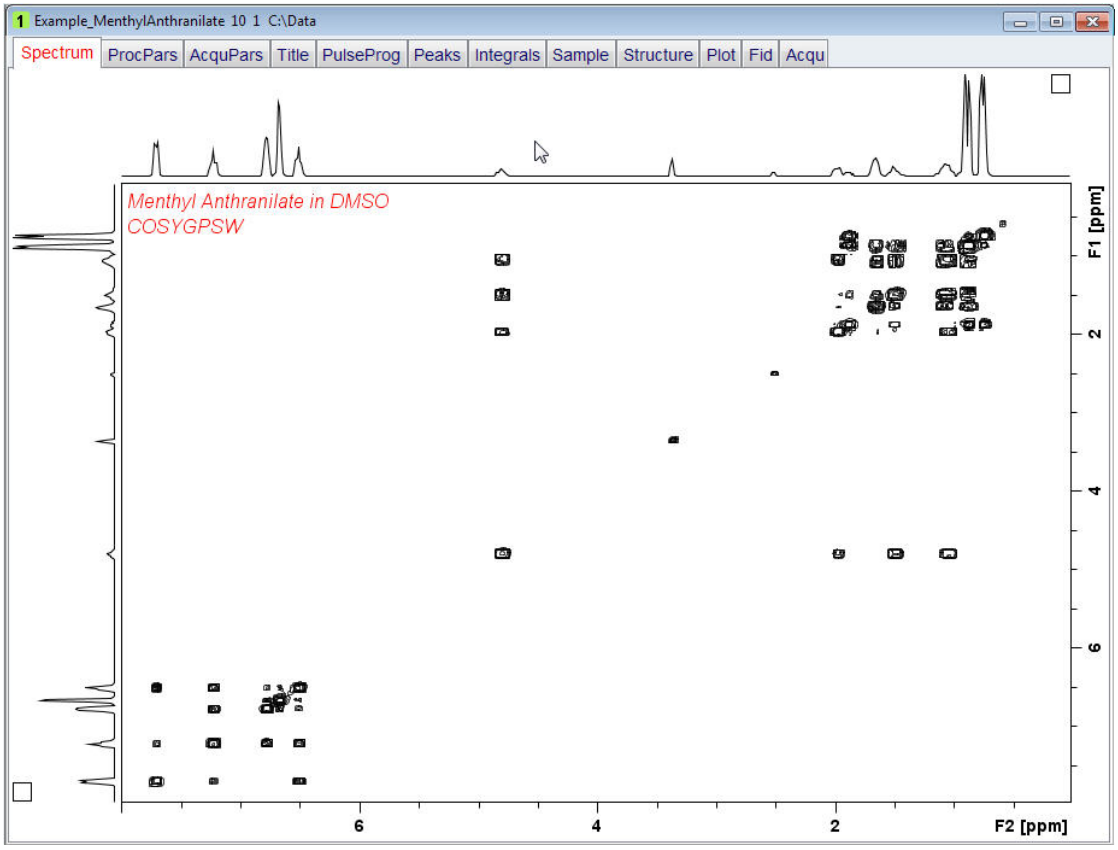
To properly print 2D data it is necessary to observe 1D spectra of the same sample first and then use the **Set Limits** button to assign an optimized Sweep width in the F2 and F1 dimensions. Using the **Set Limits** will also copy the SR (Solvent Reference) values in to the 2D data. The 1D data sets are used to add high resolution spectra for the projections. If the 1D and the 2D data sets were observed without the aid of the **Set Limits** option then it is very important to calibrate the spectra and copy the **SR** values manually to the 2D data set. If no reference substance has been added to the sample, such as TMS or TSP, then use **0** (zero) for the **SR** values in both the 1D and the 2D data. To avoid peak shifts, record the 1D and the 2D data at the same temperature and within a short time frame.

5.6.1 Printing Homonuclear 2D Data

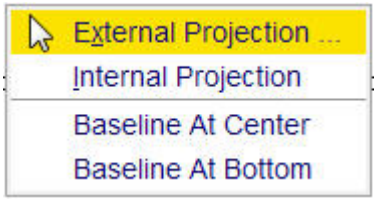
Homonuclear 2D data sets use only one 1D spectrum for both the F2 and F1 projection. The example below illustrates the printing of a 2D COSY experiment.

- Run a 1D Proton spectrum followed by a 2D COSY setting the limits manually.
- Process the data.

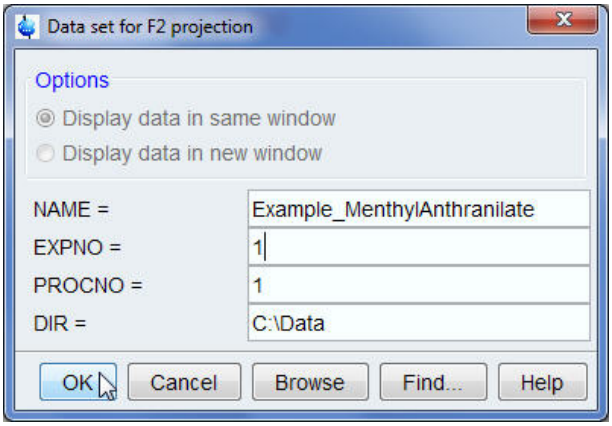
  The 2D spectrum displays the internal projections which usually have reduced resolution. When using the **Set Limits** button in TopSpin to set up the 2D COSY, the external projections with the better resolution are displayed.



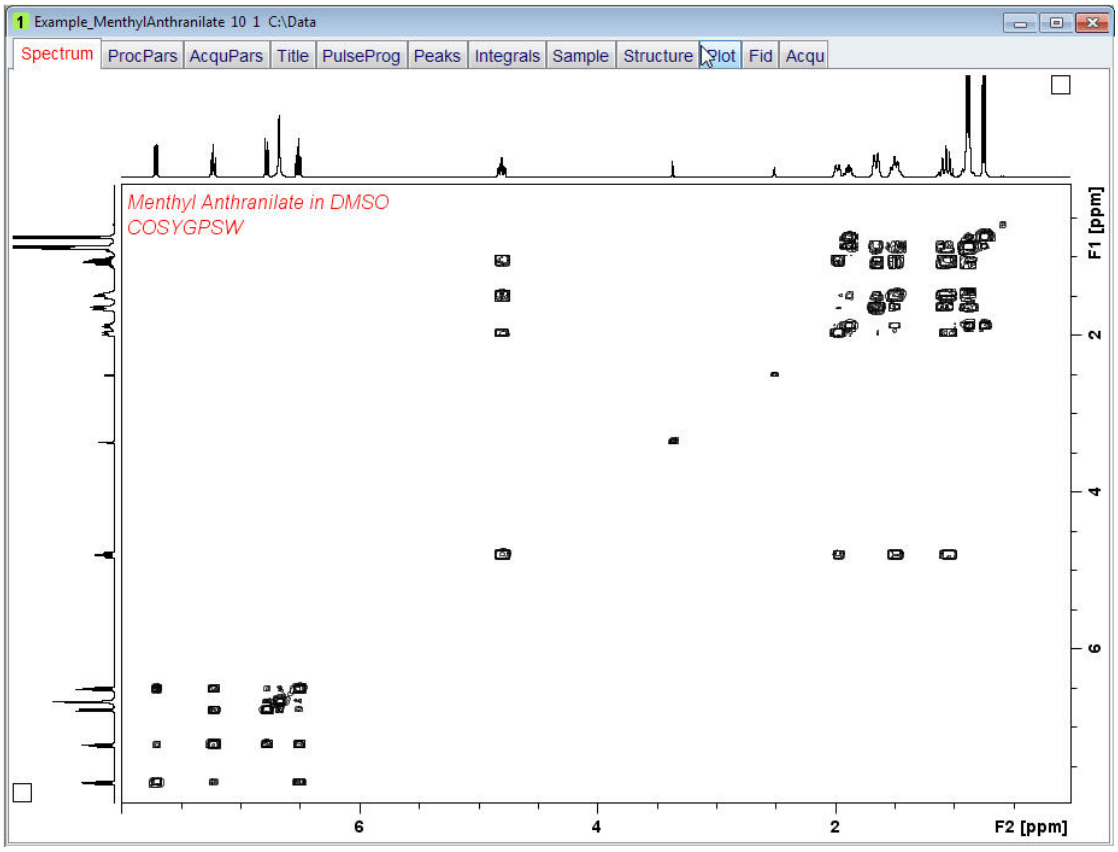
- Right click inside the **F2** projection window.
- Select **External Projection**.



- Enter the **EXPNO** and **PROCNO** of the 1D proton spectrum inside the data set for **F2** projection window.

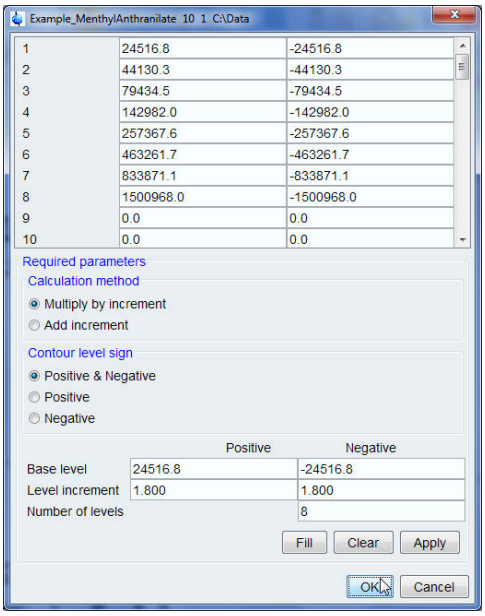


- Click on the **OK** button inside the data set for **F2** projection window.
- Right click inside the **F1** projection window.
- Repeat the last three steps to add the **F1** high resolution projection.
- Adjust the contour level of the 2D display.

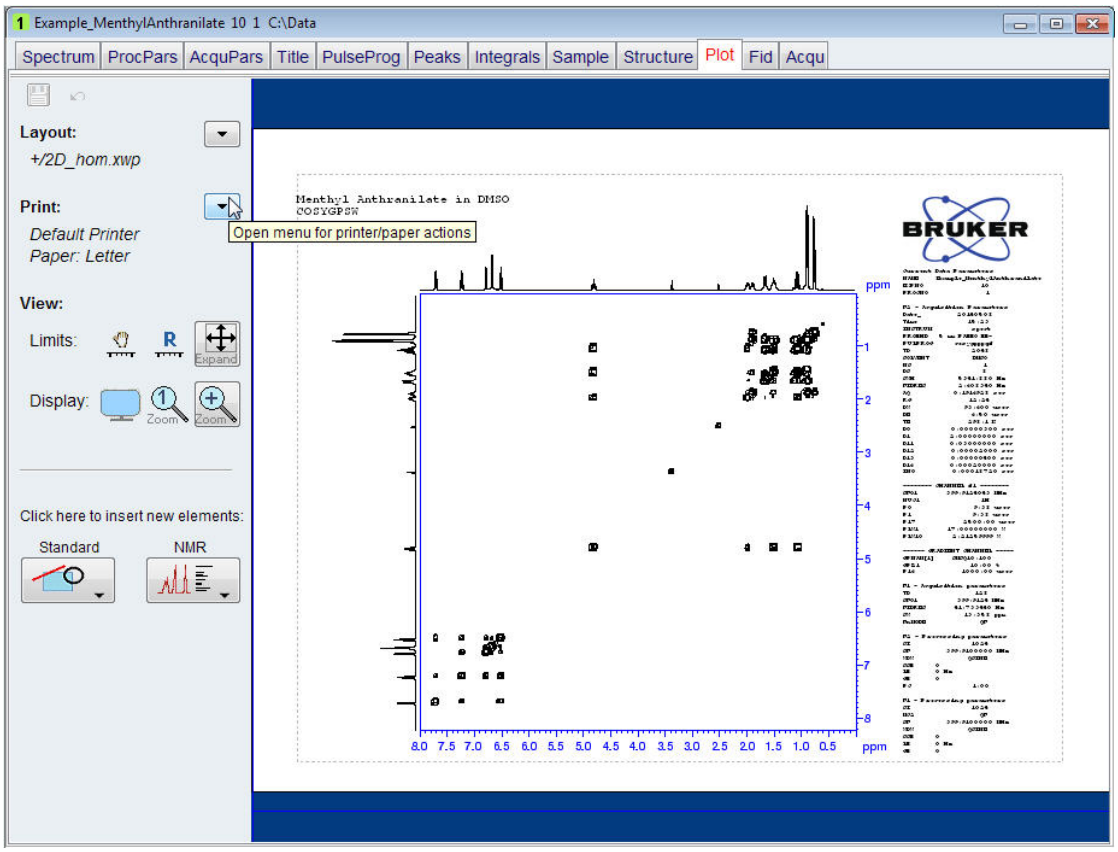


- Right click inside the 2D display window.
- Select **Edit Contour Levels** by clicking on it.

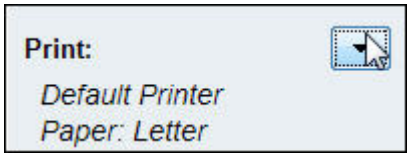
- Click on the **OK** button inside the level adjustment window.



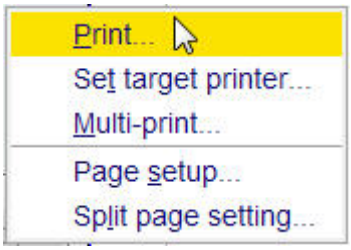
- Click on the **Plot** tab inside the Data set tabs bar.

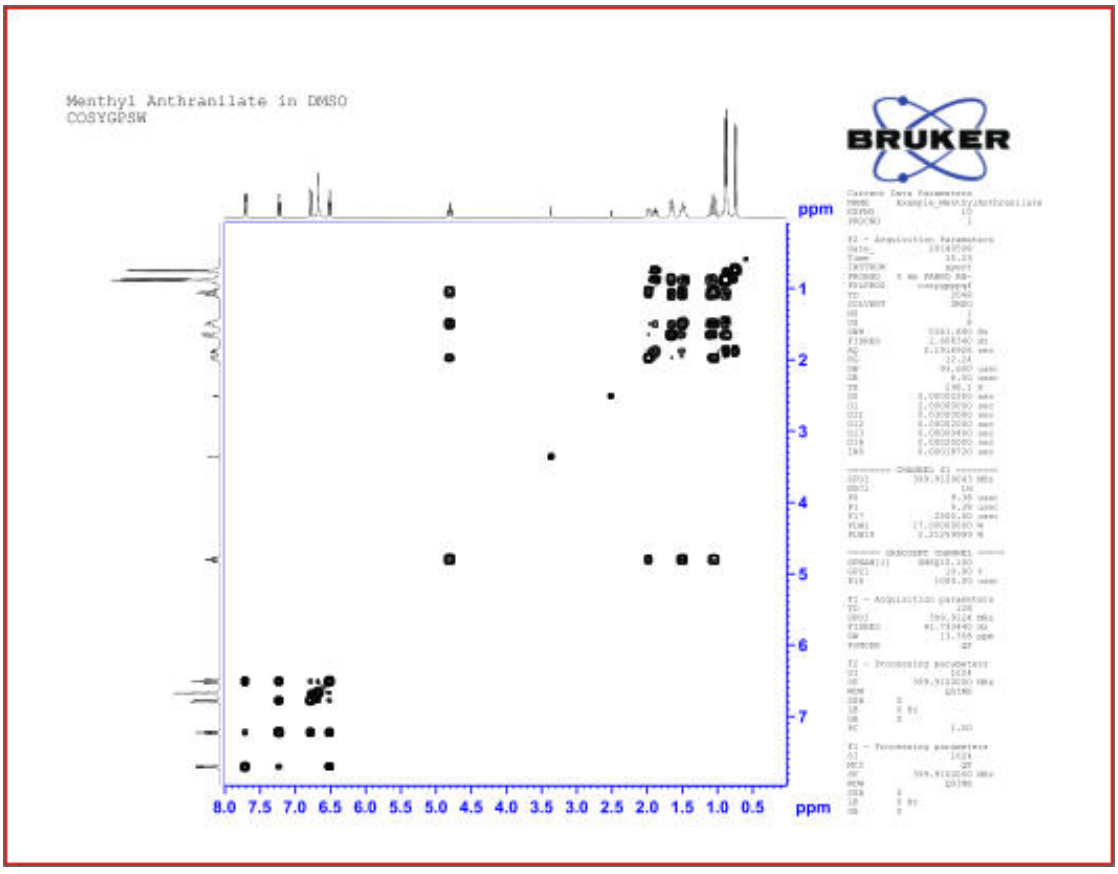


- To print this newly created layout, click on the **down arrow** next to the **Print** option on the left side of the Plot Editor window.



Then select **Print**.



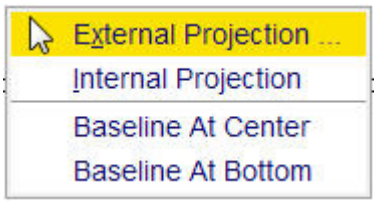


5.6.2 Printing Heteronuclear 2D Data

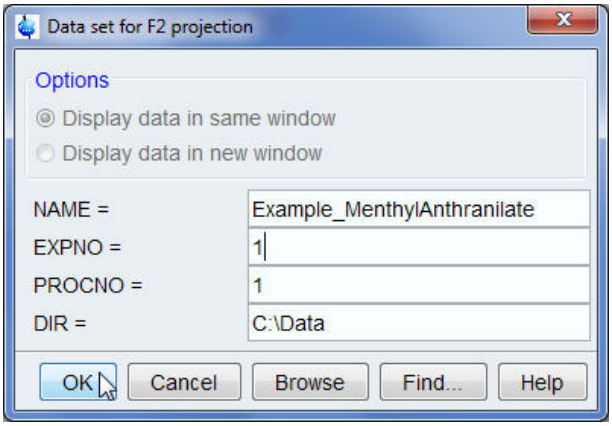
Most of the 2D Heteronuclear data are observed in inverse mode such as HSQC and HMBC type of experiments. Inverse spectroscopy was developed to study insensitive nuclei such as 13C or 15N from a high-sensitive nucleus, typically 1H. For that reason it is assumed that an insensitive nuclei would take too many scans to observe a 1D spectrum with a reasonable S/N. All of the Bruker inverse experiment parameter sets have therefore a fixed SW in the F1 dimension. The layout for printing such data will only show the F2 projection and not the F1. The example below shows how to print an HMBC spectrum using the default parameters and layout.

- Run a 1D proton spectrum followed by a 2D gradient HMBC experiment setting the limits manually.
- Process the data.

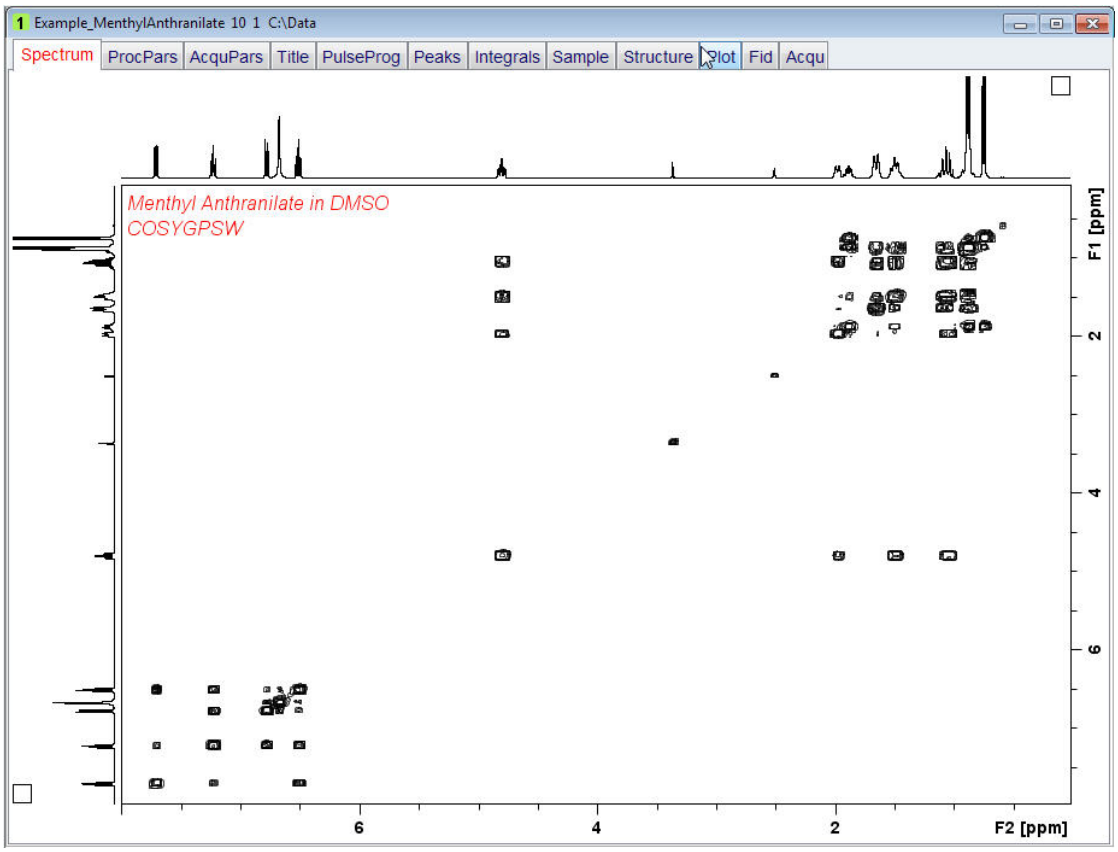
  The 2D spectrum displays the internal projection of the proton spectrum which usually has reduced resolution. When using the **Set Limits** button in TopSpin to set up the 2D HMBC, the external 1D proton projection with the better resolution is displayed.
- Right click inside the **F2** projection window.
- Select **External Projection**.



- Enter the **EXPNO** and **PROCNO** of the 1D proton spectrum inside the data set for **F2** projection window.



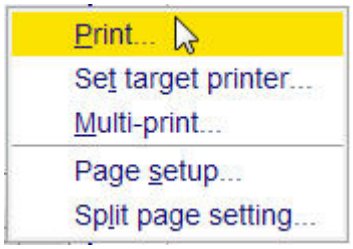
- Click on the **OK** button inside the data set for **F2** projection window.
- Right click inside the **F1** projection window.
- Repeat the last three steps to add the **F1** high resolution projection.
- Adjust the contour level of the 2D display.

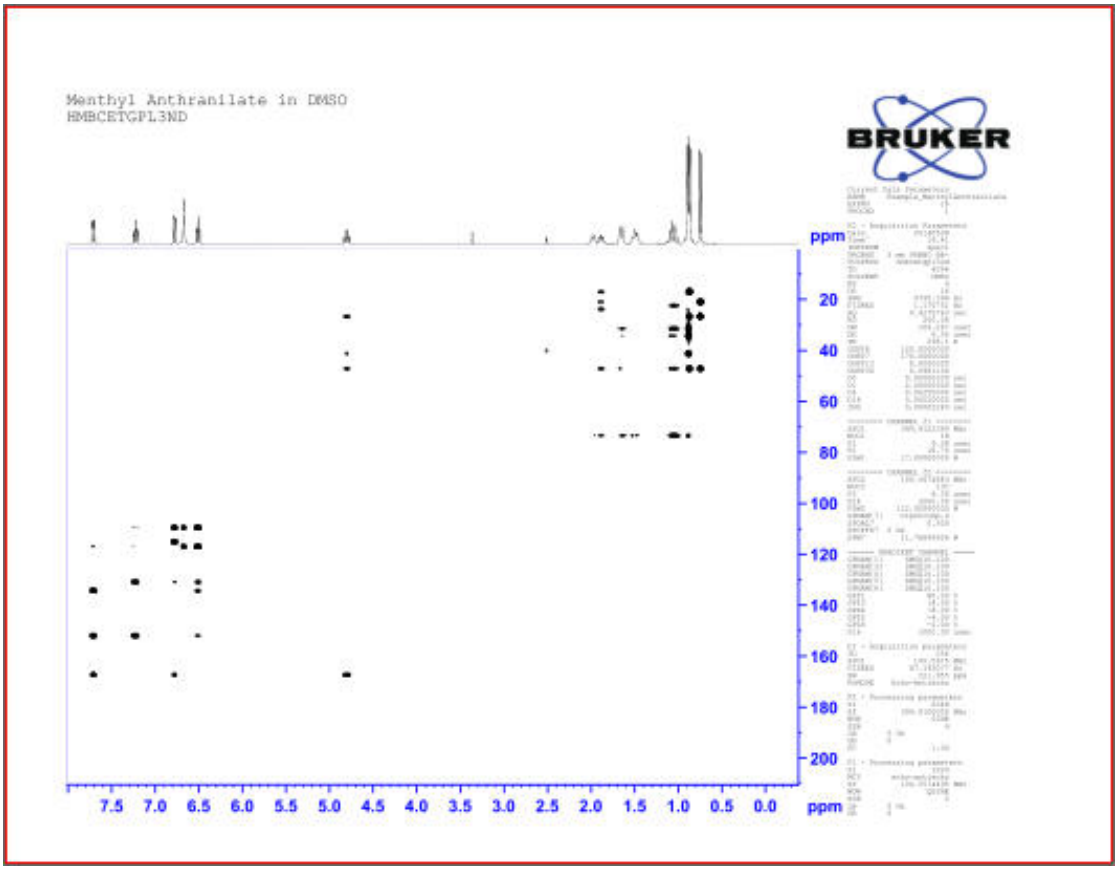


- Right click inside the 2D display window.
- Select **Edit Contour Levels** by clicking on it.

- Click on the **OK** button inside the level adjustment window.
- Click on the **Plot** tab inside the data set tabs bar.
- To print this newly created layout, click on the **down arrow** next to the **Print** option on the left side of the Plot Editor window.

Then select **Print**.





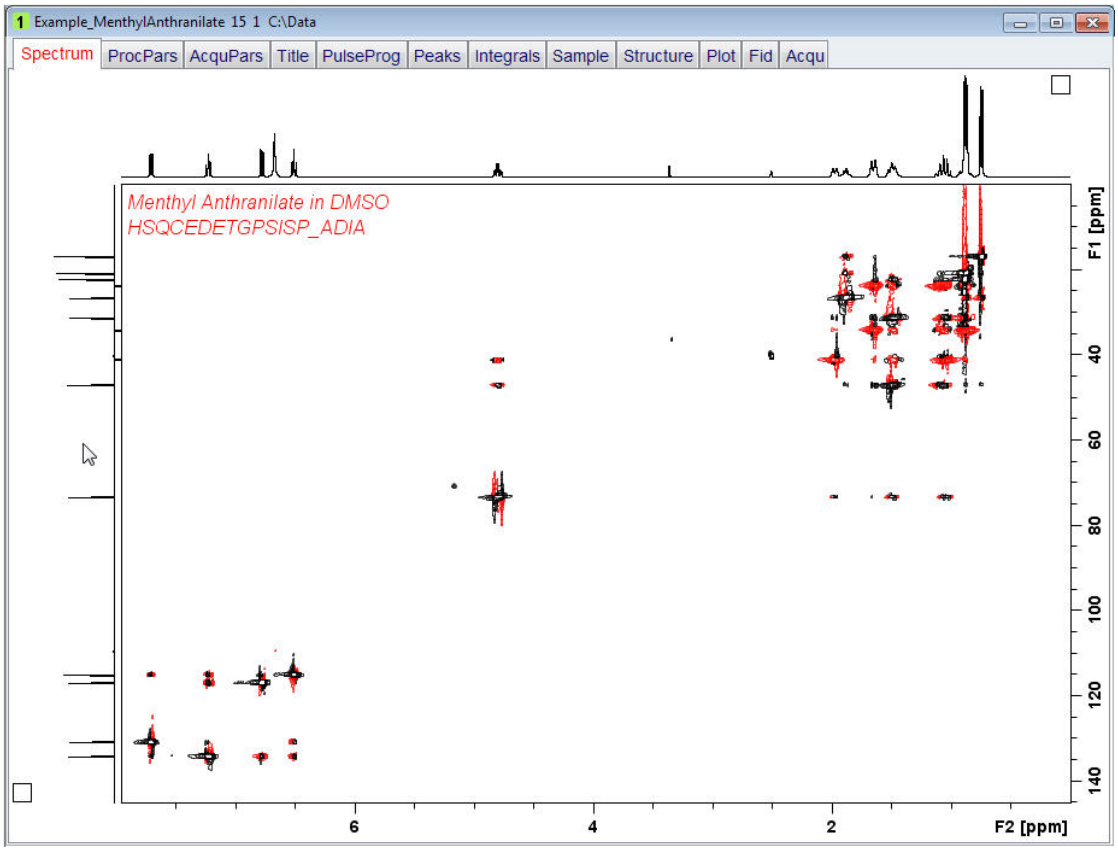
5.6.3 Printing Heteronuclear 2D Data after Modifying the Layout

With the increase in S/N performance of the modern probes, it is possible to observe a 1D X-nucleus spectrum in a reasonable amount of time. This will allow the SW to be reduced to gain increased digital resolution and the 1D spectrum can be added as a projection to the 2D data set.

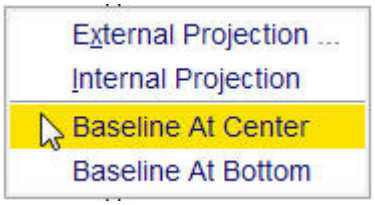
5.6.3.1 Selecting the Layout

- Run a 1D Proton and a 1D DEPT135 spectrum followed by a 2D edited gradient HSQC experiment using the **Set Limits** button in TopSpin.

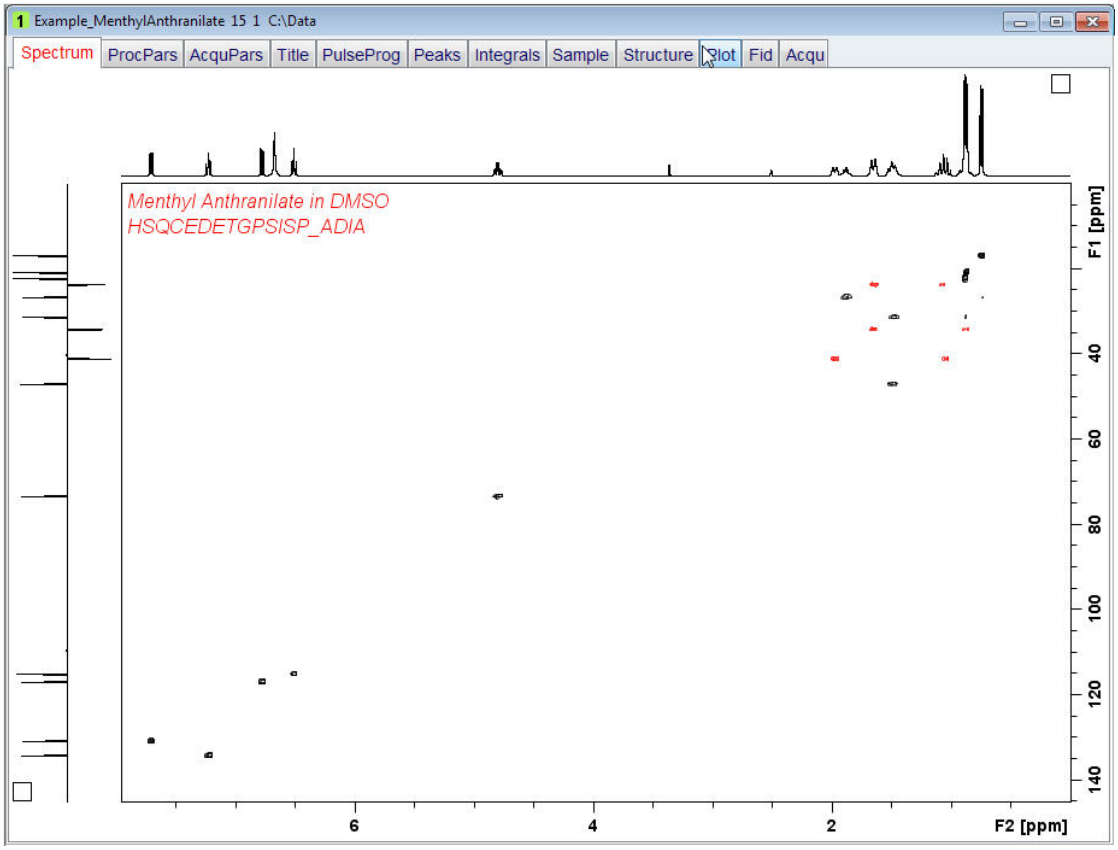
- Process the data.



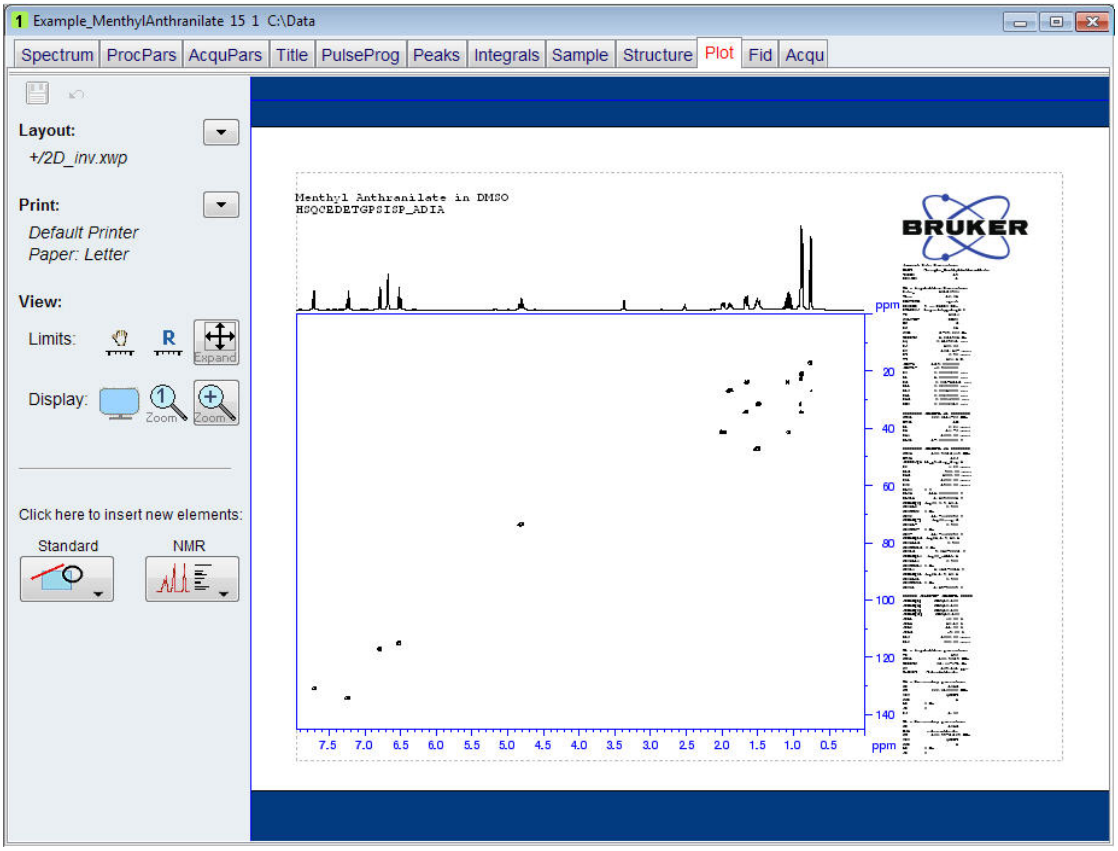
- Right click inside the **F1** projection window.
- Select **Baseline At Center**.



- Adjust the contour level of the 2D display.



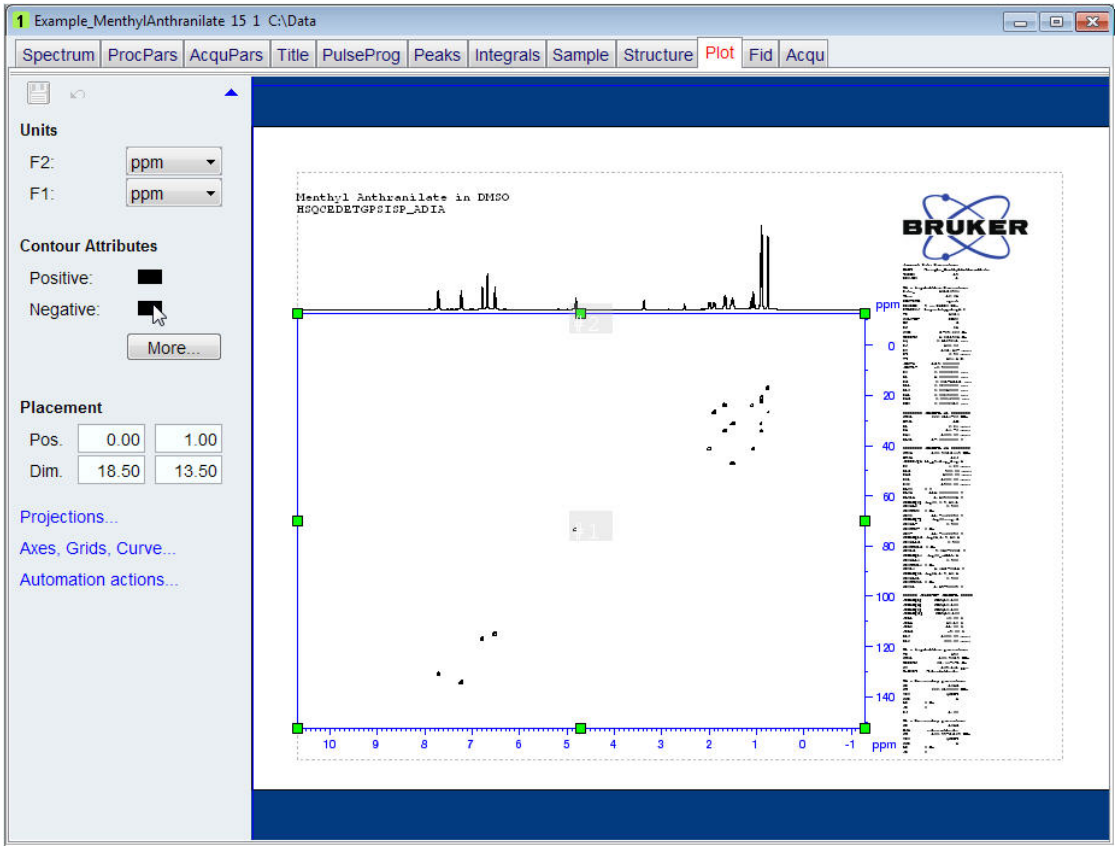
- Right click inside the 2D display window.
- Select **Edit Contour Levels** by clicking on it.
- Click on the **OK** button inside the level adjustment window.
- Click on the **Plot** tab inside the Data set tabs bar.



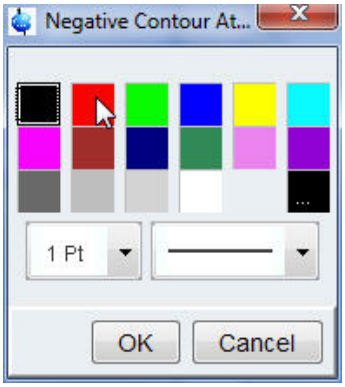
By default the positive and negative peaks of the HSQC spectrum have the same color black. Follow the steps in the next section to change the negative peak color to red.

5.6.3.2 Modifying the Layout

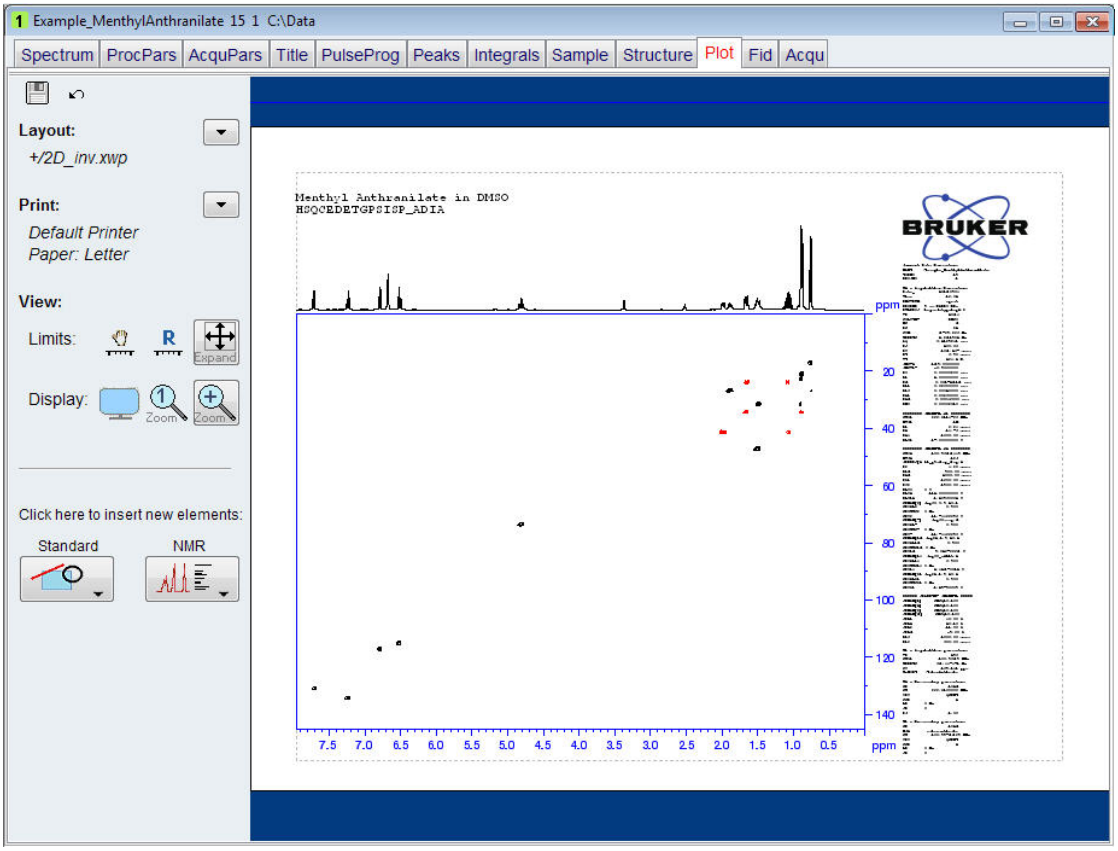
- Click inside the HSQC spectrum in the plot editor window.



- Click on the **Negative color square** in the **Contour Attributes** section on the left side of the plot editor window.
- Select the **red** color by clicking on it inside the **Negative Contour Attributes** window.

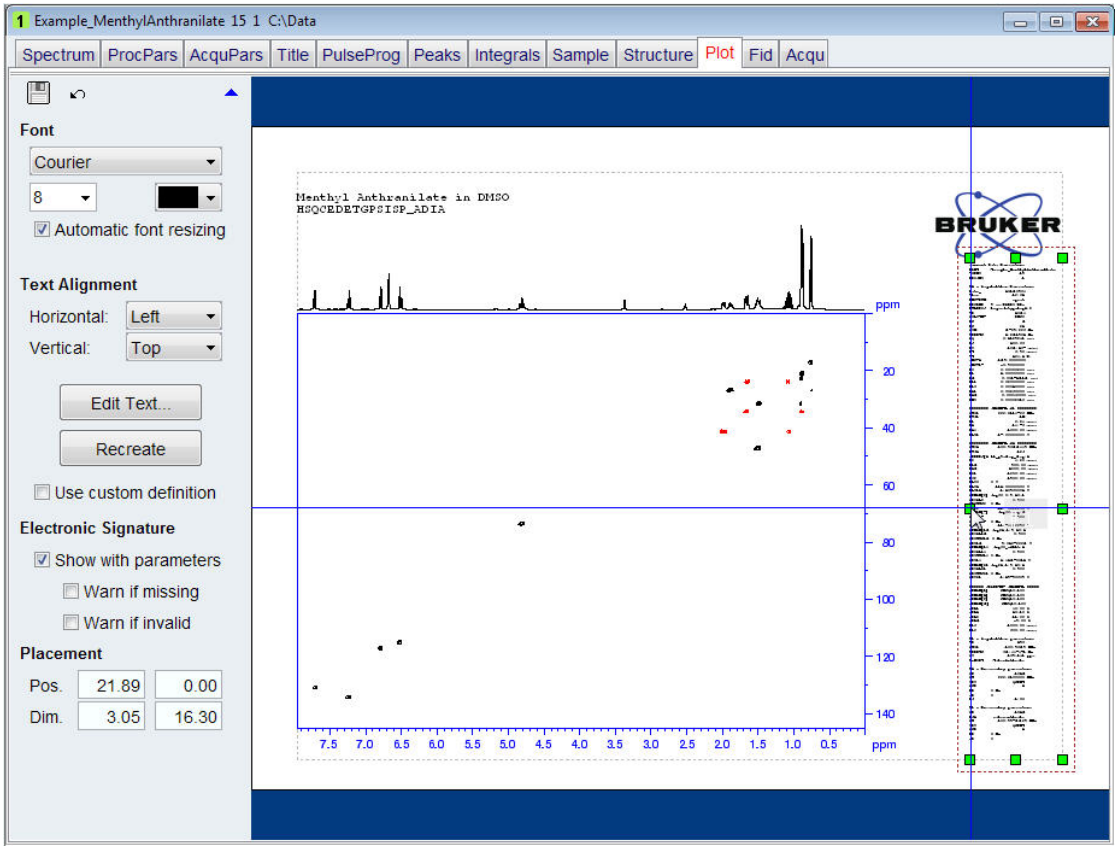


- Click on the **OK** button inside the **Negative Contour Attributes** window.
- Click inside the parameters on the right side of the plot editor window.

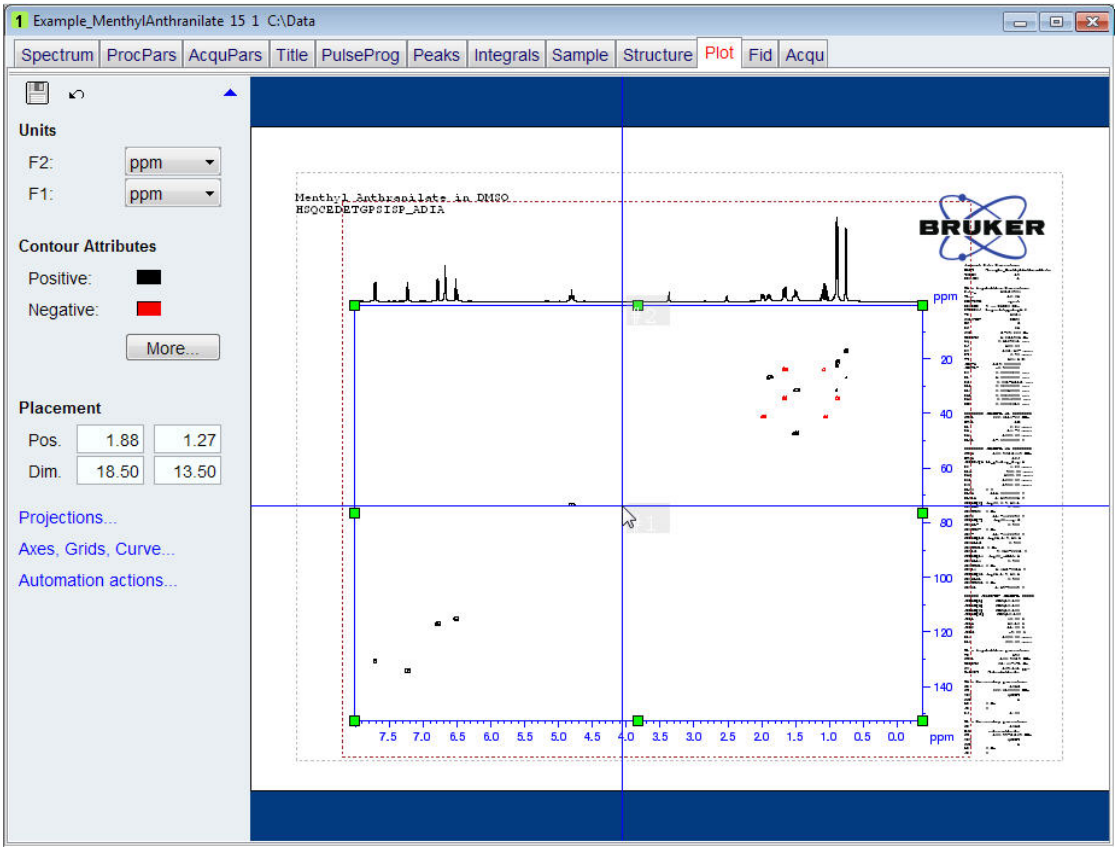


- With the left mouse pressed, move the parameters to the right edge of the display window.

  Make sure not to clip some of the parameters. You may also have to move the Bruker logo to the right.

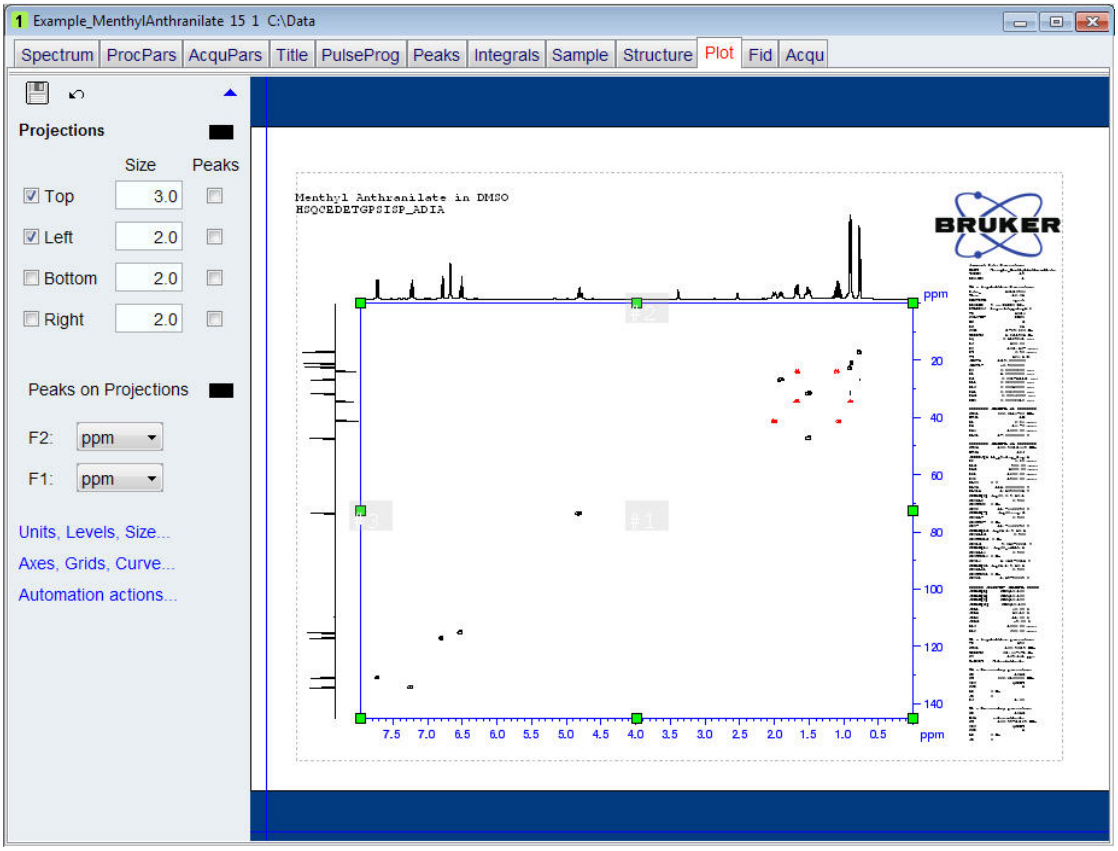


- Click inside the spectrum in the plot editor window.

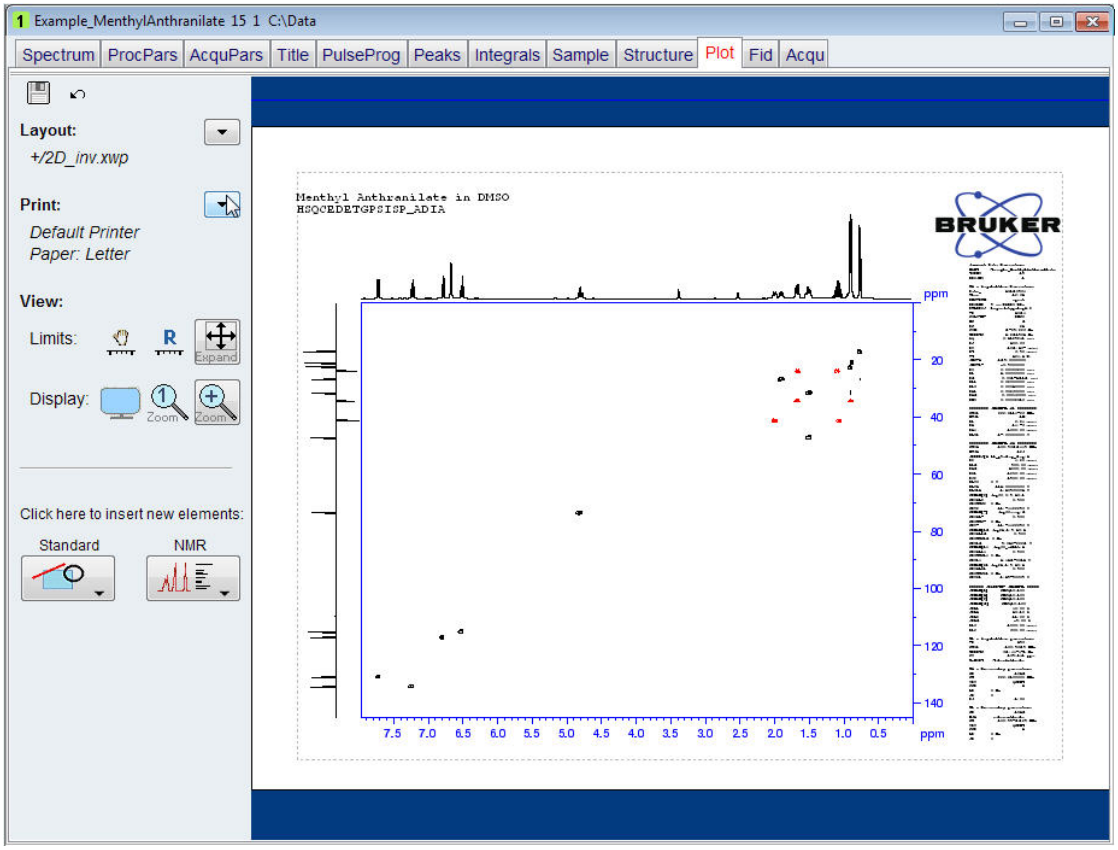


- With the left mouse button pressed, move the spectrum window to the right.

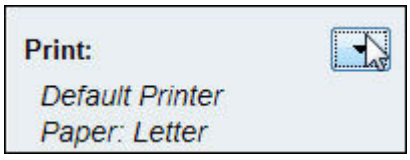
  Make sure that the vertical ppm scale numbers are clearly visible and not overlapping with the parameters.
- Click on the **Projections** option on the left side of the plot editor window.
- Enable the **Left** button and select **2.0** for the size in the **Projections** section of the plot editor window.



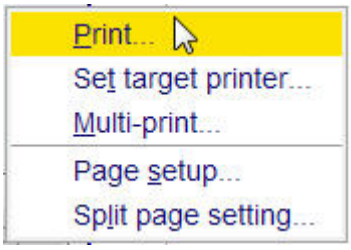
- Click anywhere outside the dotted line bordering the 2D spectrum to display the basic display options.

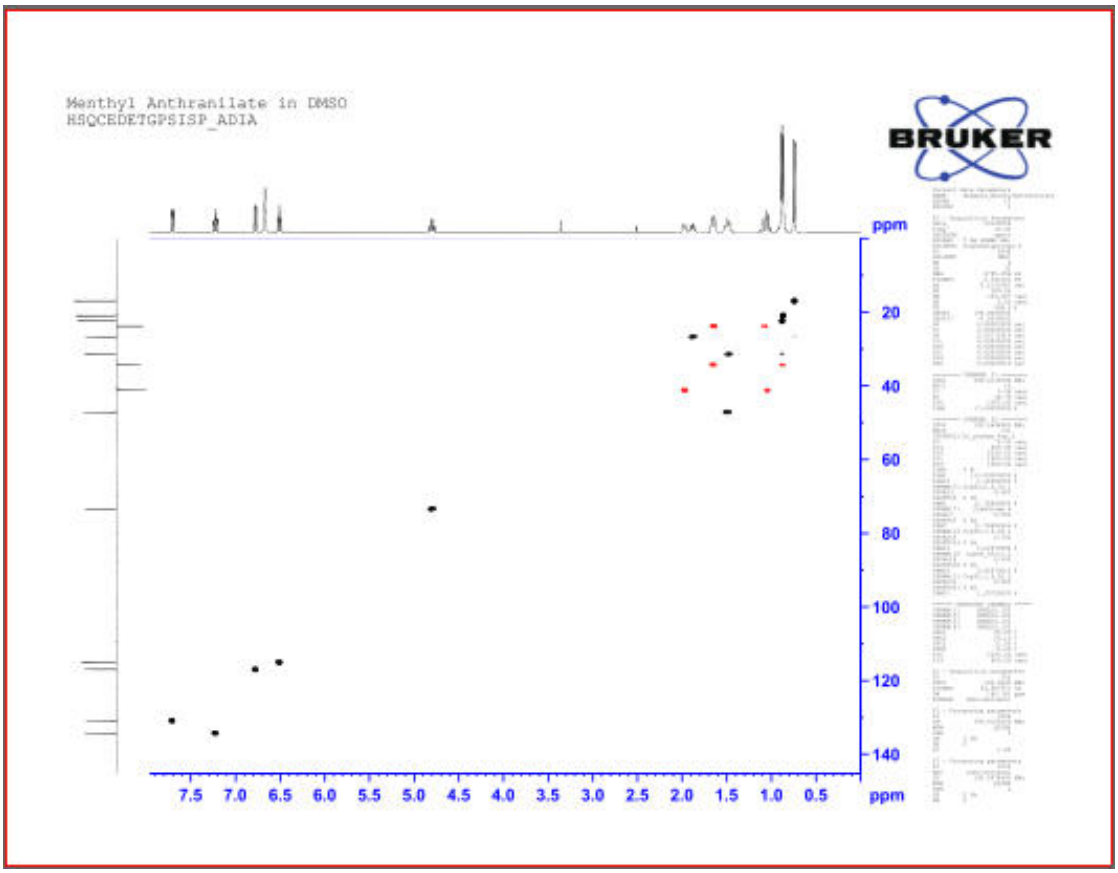


- To print this newly created layout, click on the **down arrow** next to the **Print** option on the left side of the Plot Editor window.



Then select **Print**.



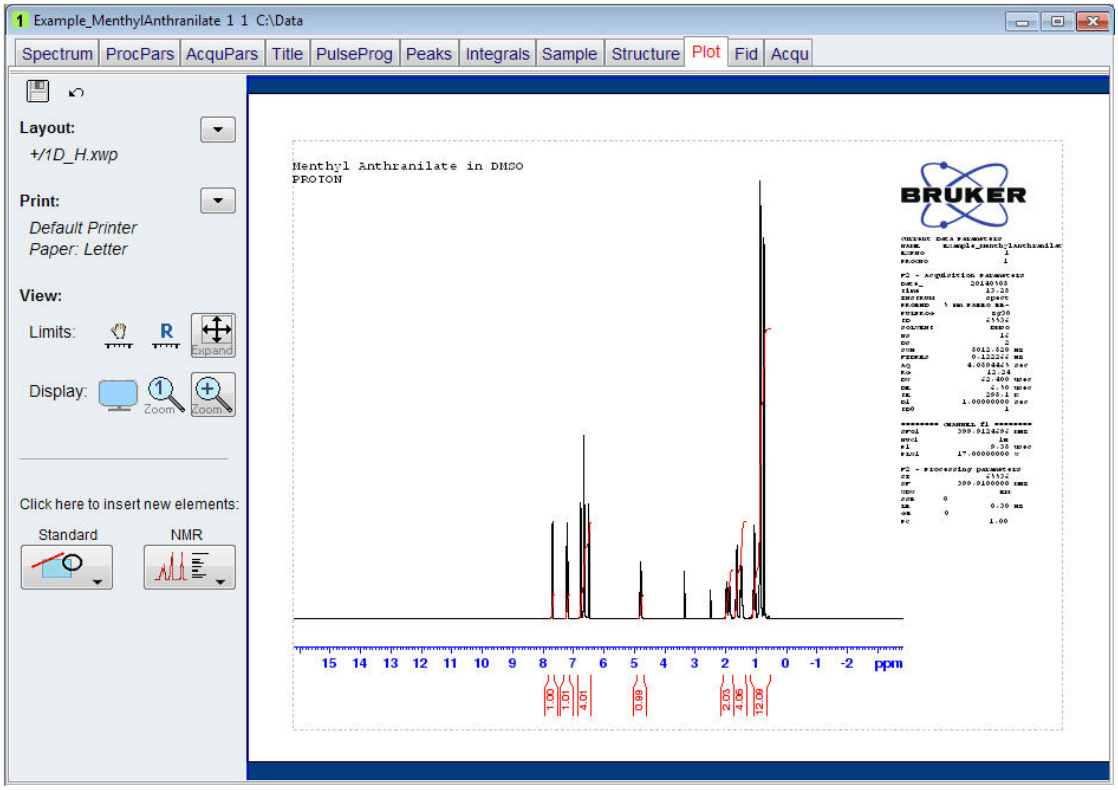


To save the layout for future use e.g. automated or repeated printout of the same layout, refer to the chapter *Automation [▶ 107]*.

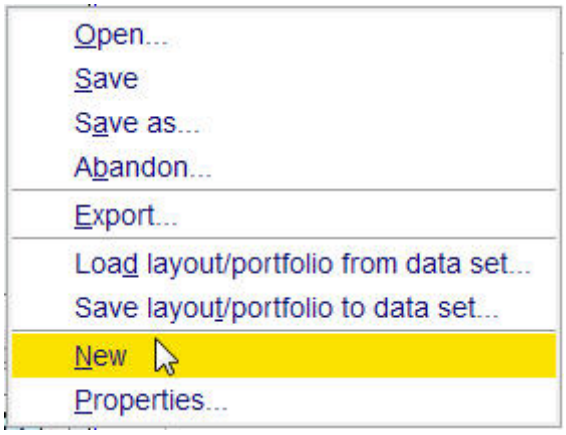
5.7 Printing 1D and 2D Data Combined in a New Layout

This section will guide you through an example of combining 1D and 2D data in to a new created layout.

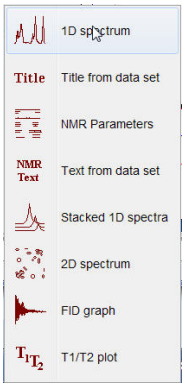
- Run a 1D proton, 2D HSQC and a 2D COSY spectrum of the same sample.
- Display the 1D proton spectrum.
- Click on the **Plot** tab to open up the Plot Editor.



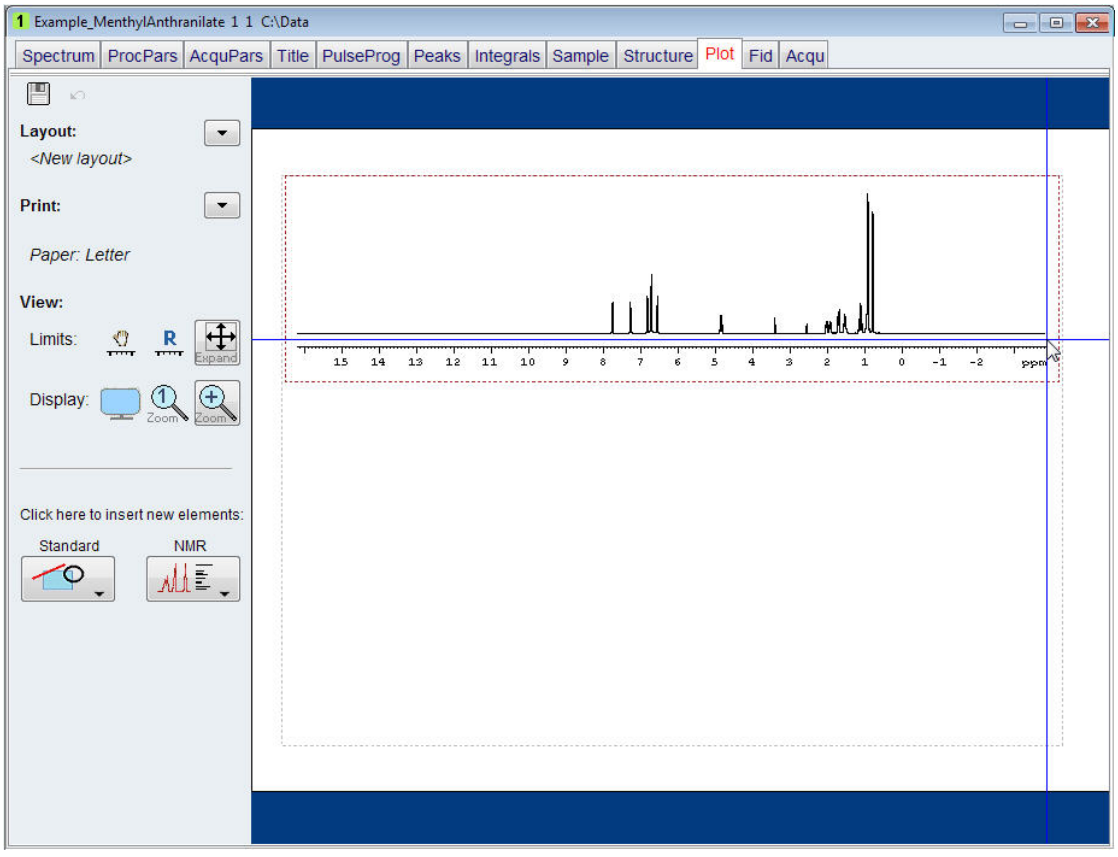
- Click on the **down arrow** button to the right of the **Layout** option on the left side of the plot editor window.
- Select **New**.



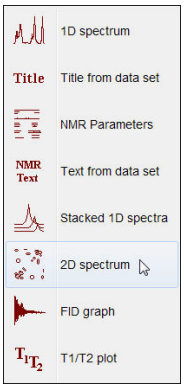
- Click on the **NMR** icon in the **Click here to insert new elements** options on the left side of the Plot Editor window.
- Select **1D spectrum**.



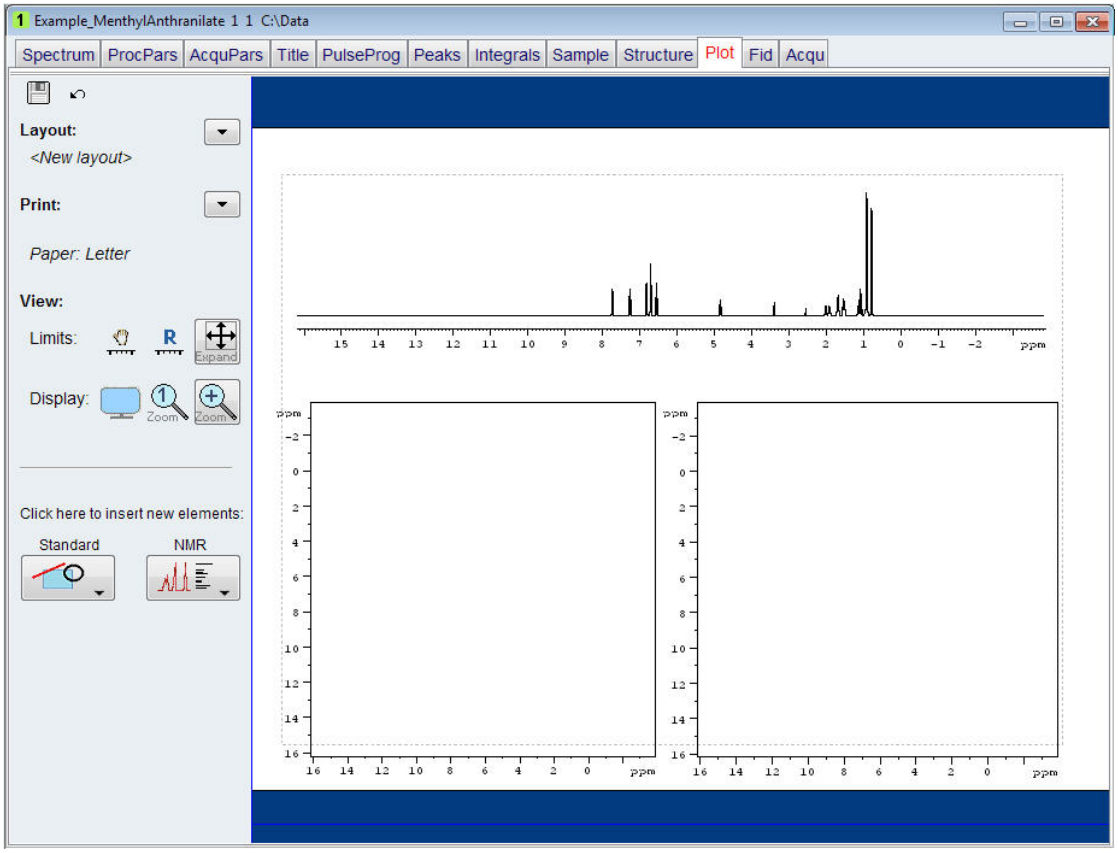
- Add the 1D spectrum object to the layout by left-clicking at the top left of the desired location and while keeping the mouse button pressed, drag the rectangular box with the 1D spectrum to the bottom right.
- Click on the **NMR** icon in the **Click here to insert new elements** options to the left side of the Plot Editor window.



- Select **2D spectrum**.

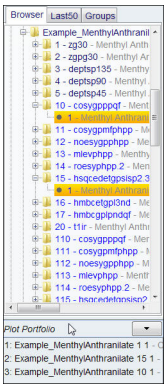


- Add the 2D object to the layout by left-clicking at the top left of the desired location and while keeping the mouse button pressed, drag the rectangular box with the 2D object to the bottom right.
- Repeat the steps to display a second 2D object.
- In the Browser window on the left, select the HSQC processed data and drag it in to the portfolio window on the bottom of the Browser window.



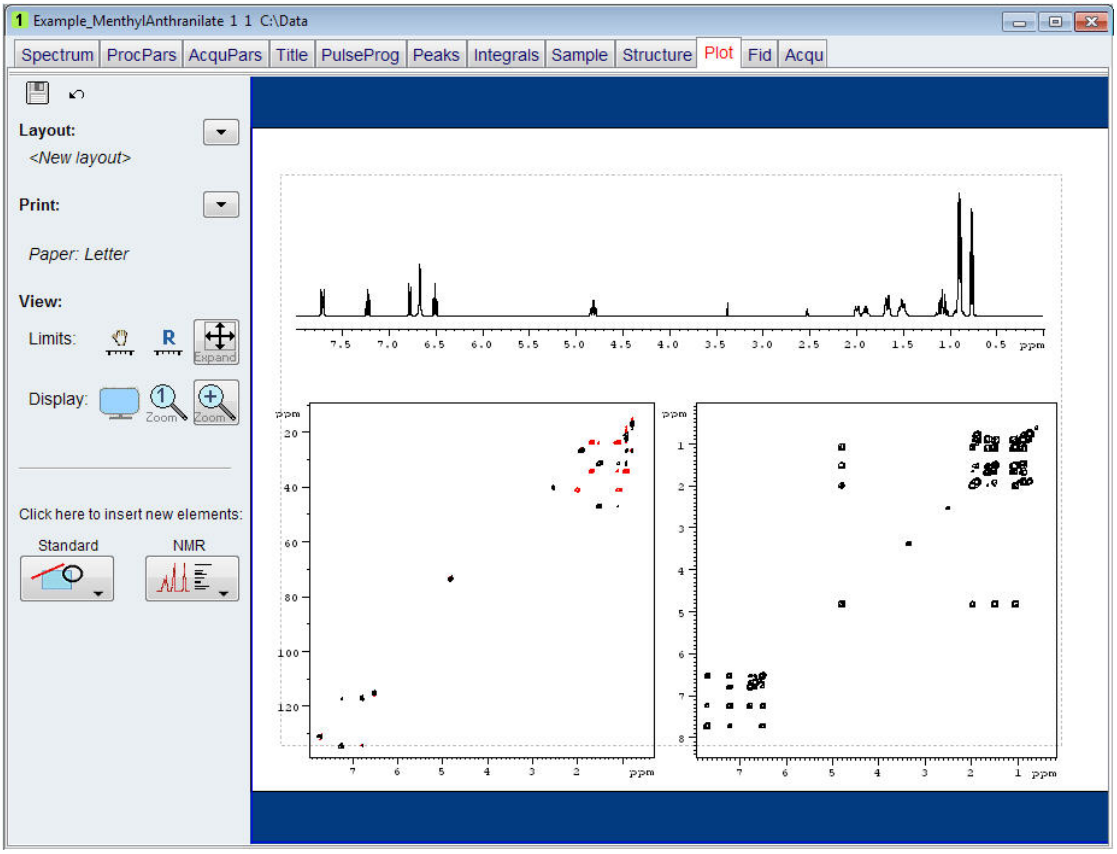
Only processed data can be dragged in to the Portfolio window.

- Repeat the steps for the processed COSY data.
- With the left mouse pressed, drag the HSQC data from the Portfolio window in to the left 2D object square.

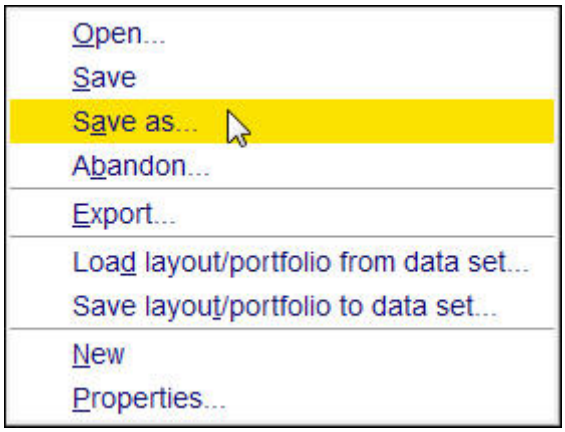


- With the left mouse pressed, drag the COSY data from the Portfolio window in to the right 2D object square.
- With a spectrum object selected in the layout, use the toolbar TopSpin icons to adjust the display limits, color and scaling of the spectra.

- Click on the **down arrow** button to the right of the **Layout** option on the left side of the plot editor window.



- Select **Save as** to use this layout for other data sets.



6 Automation

6.1 Introduction

NMR data are often acquired, processed and printed in automation, with AU programs or with the use of IconNMR. Printing in automation uses the same plot layouts and portfolios used by the interactive Plot Editor. Layouts can be standard Bruker or user-defined layouts.

6.2 Printing in IconNMR

IconNMR is a standard program for automated spectroscopy. It uses predefined experiments (Parameter sets) to obtain data of various samples. Furthermore, it uses AU programs to acquire process and print the results of the experiments. Processing and printing are executed by the same AU program. An example of such an AU program is **proc_1d**, which is used in many 1D experiments. AU programs print data by executing plot macros, the main one being **AUTOPLOT**. This macro executes the **auto-plot** command which prints the current data set according to the current plot layout.

6.3 Automation Actions

Automation actions, also called Reset actions are a set of rules, which controls the appearance of individual spectrum or FID objects, by either using or overruling experiment parameters. They influence:

- The X and Y limits of the displayed region.
- The intensity scaling.
- The spectrum and integral baseline positions.

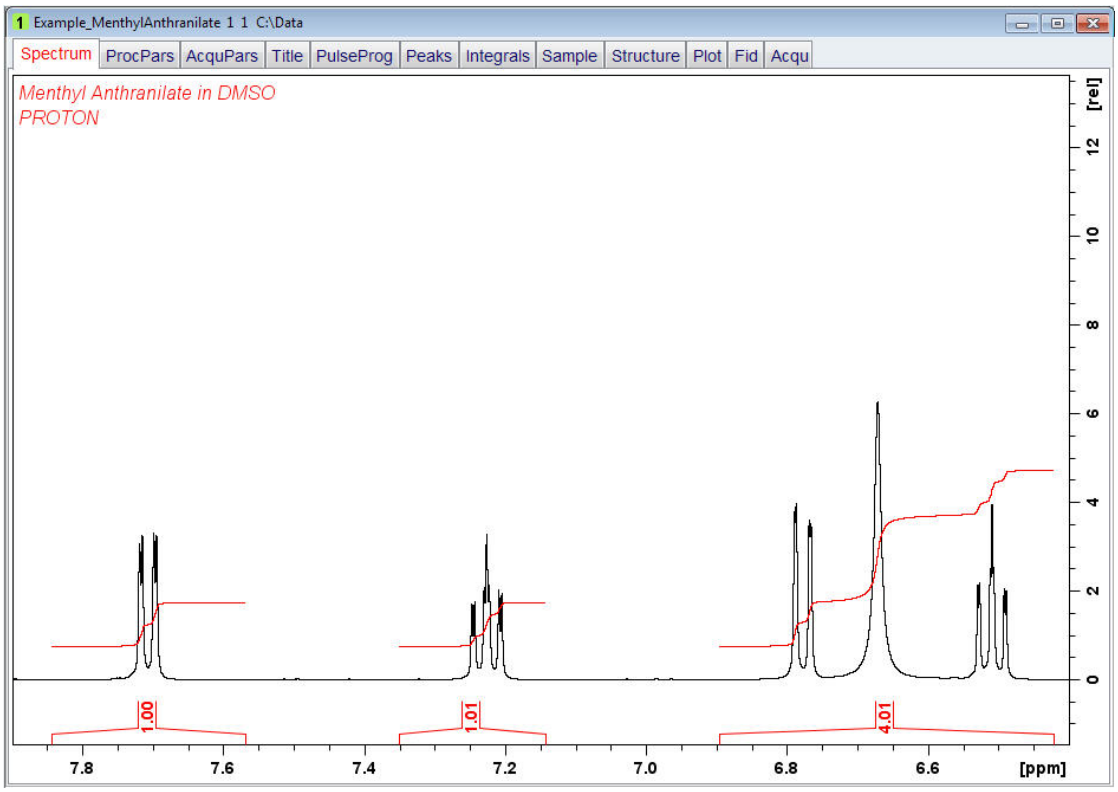
Automation actions are object specific and stored in the layout.

6.4 Automation Actions on 1D Spectra

The following examples will guide you through the various settings of the automation actions for a 1D spectrum using the Plot Editor.

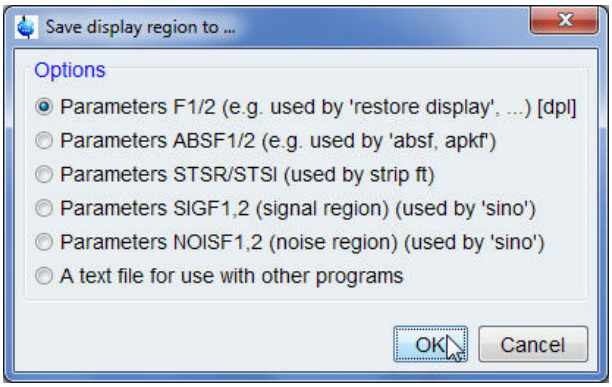
6.4.1 X Plot Limits

- Observe or open a 1D Proton spectrum with calibrated integrals.
- Expand the region from **7.9 ppm** to **6.4 ppm**.
- Right click inside the spectrum display window.

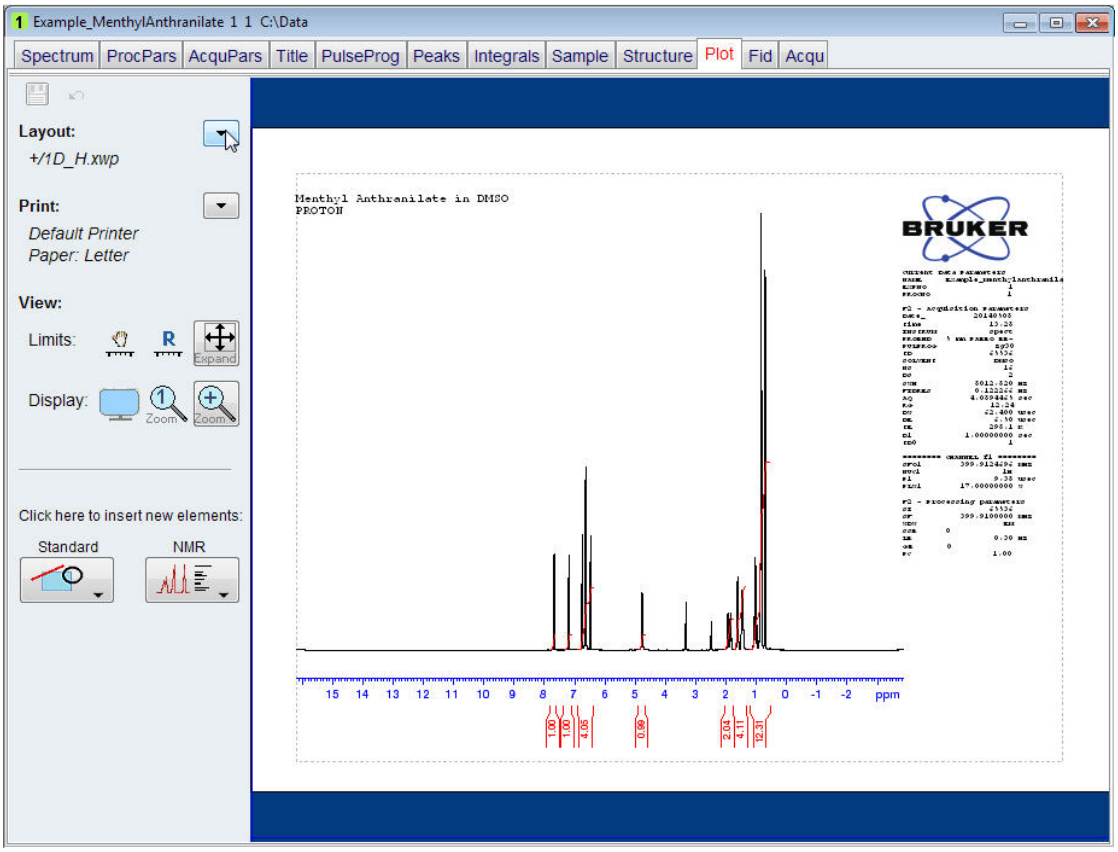


- Select **Save Display Region To**.

- Select **Parameters F1/2 (e.g. used by** '**restore display**') **[dpl1]** inside the Save display region to window.

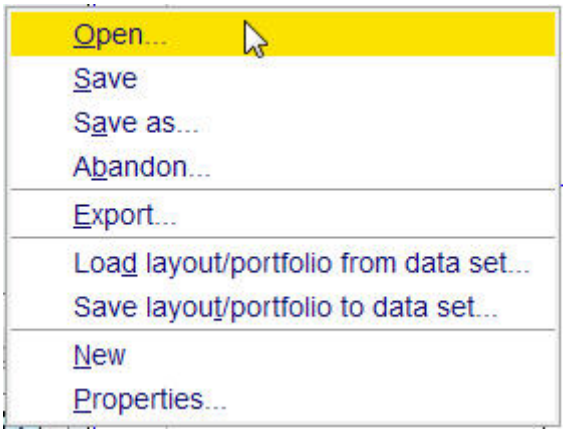


- Click on the **OK** button inside the Save display region to window.
- Click on the **Plot** tab in the **Data set tab** bar to open the Plot Editor.

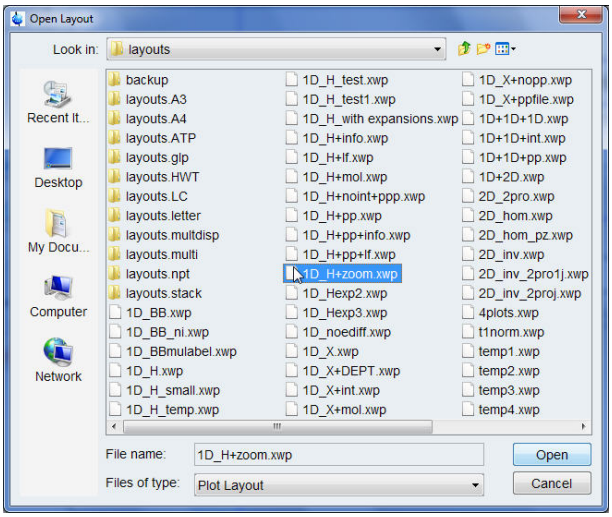


Depending on the automation settings of the predefined layout of the data set, the spectrum will be displayed with the limits defined in the layout or with the limits set in the steps mentioned above.

- Click on the **down arrow** button to the right of the Layout option on the left side of the plot editor window.
- Select **Open**.



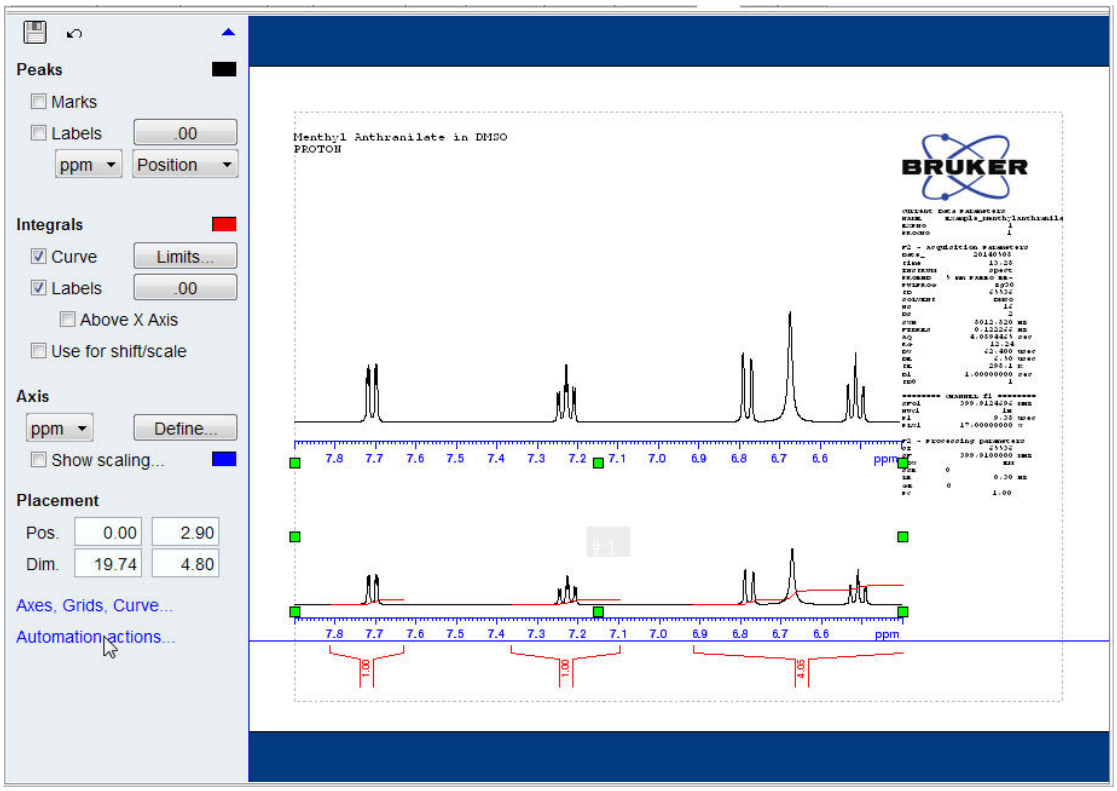
- Select **1D_H+zoom.xwp** inside the Open Layout window.



- Click on the **Open** button inside the Open Layout window

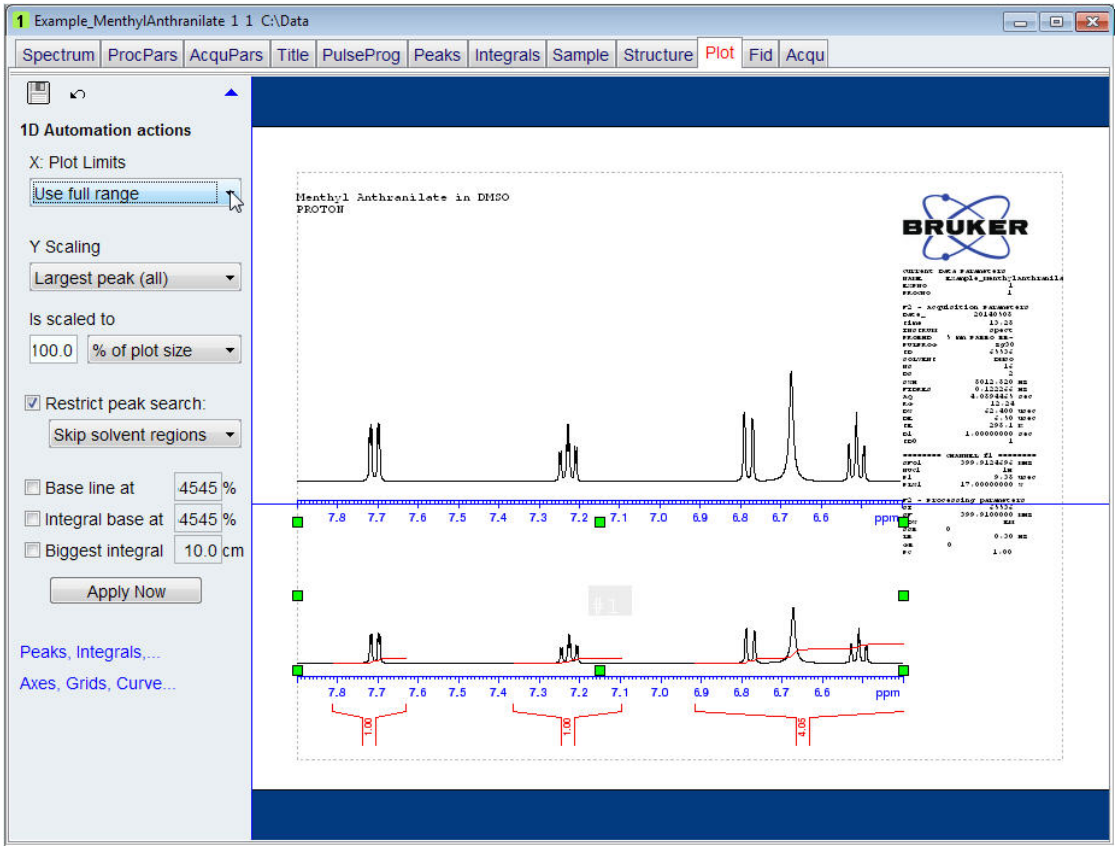
  Two spectra are displayed with the same peak expansion in the Plot Editor window. The bottom spectrum is the original spectrum, while the top one is the zoomed spectrum.
- Click inside the bottom spectrum.

  Green handles will mark the spectrum and on the left side of the Plot Editor window the spectrum options are displayed.

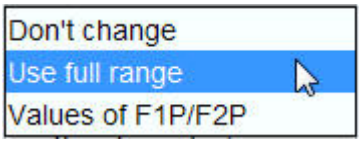


- Click on the **Automation actions** inside the Spectrum options window on the left side of the Plot Editor window.

  Green handles are still marking the spectrum and on the left side of the Plot Editor window the **1D Automation actions** options are displayed.
- Click on the down arrow of the **X Plot Limits** option inside the **Automation actions** window on the left side of the Plot Editor window.

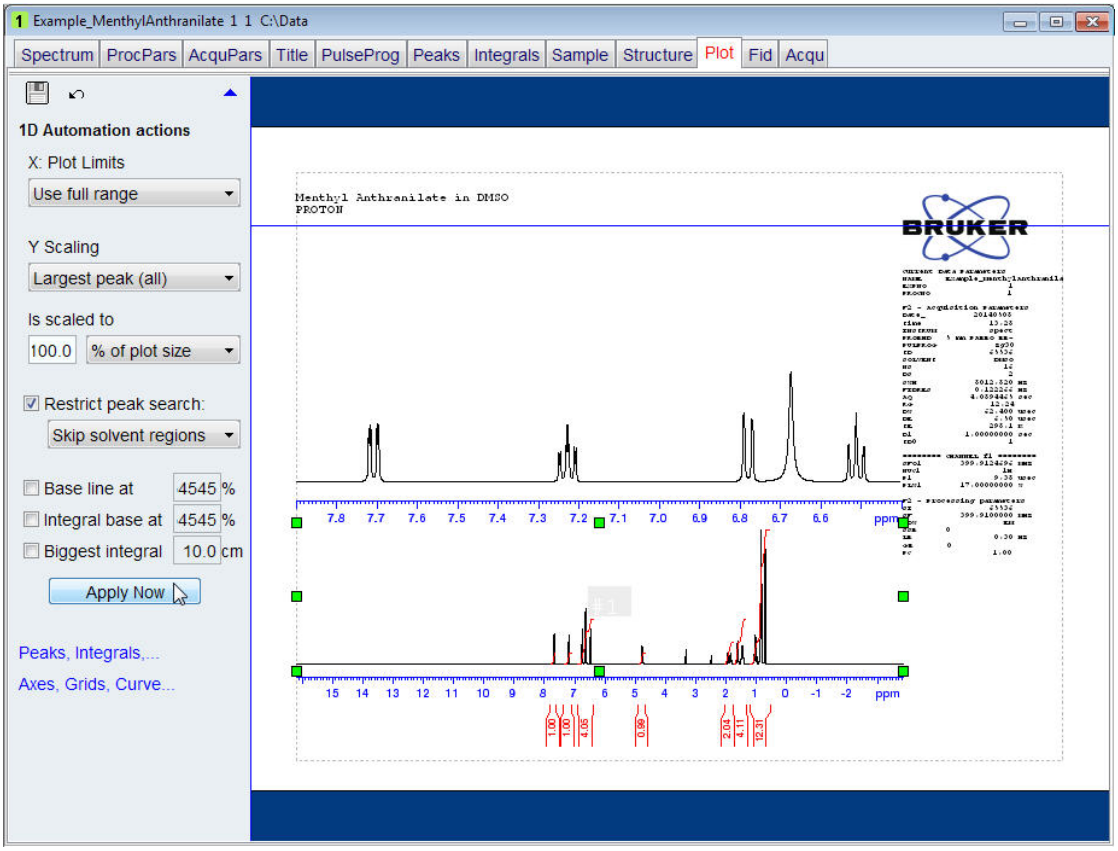


- Select **Use full range** from the pull down window.



  The full ppm range which has been acquired will be displayed. If the **Don't change** option is selected, then it will keep the X Limits defined in the layout. Useful for e.g. proton spectra with fixed plot limits (e.g. 9 ppm to -1 ppm).

- Click on the **Apply Now** button inside the Automation actions window on the left side of the Plot Editor window.



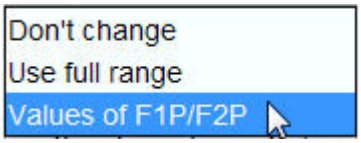
The bottom spectrum displays the full observed sweep width with all the integrals.

- Click inside the top spectrum.

  Green handles will mark the spectrum and on the left side of the Plot Editor window the Automation Actions window is displayed.

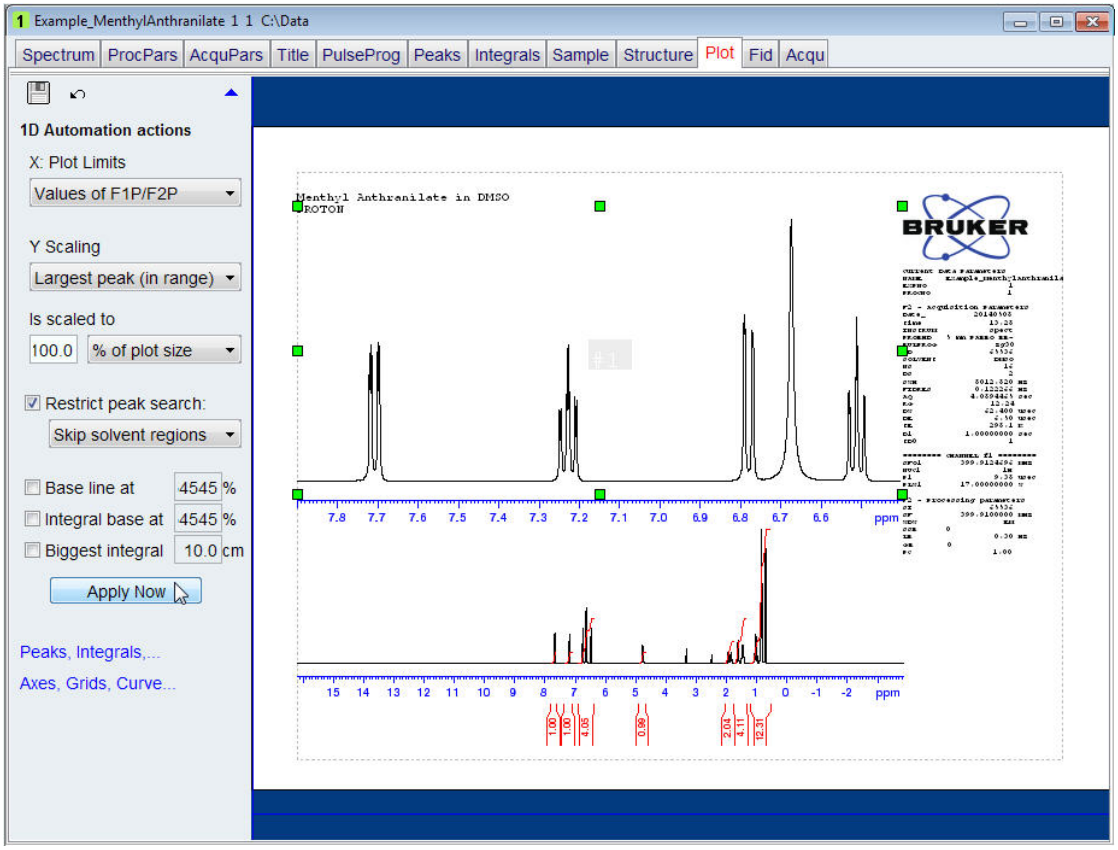
- Click on the down arrow of the **X Plot Limits** option inside the Automation actions window on the left side of the Plot Editor window.

- Select **Values of F1P/F2P.**



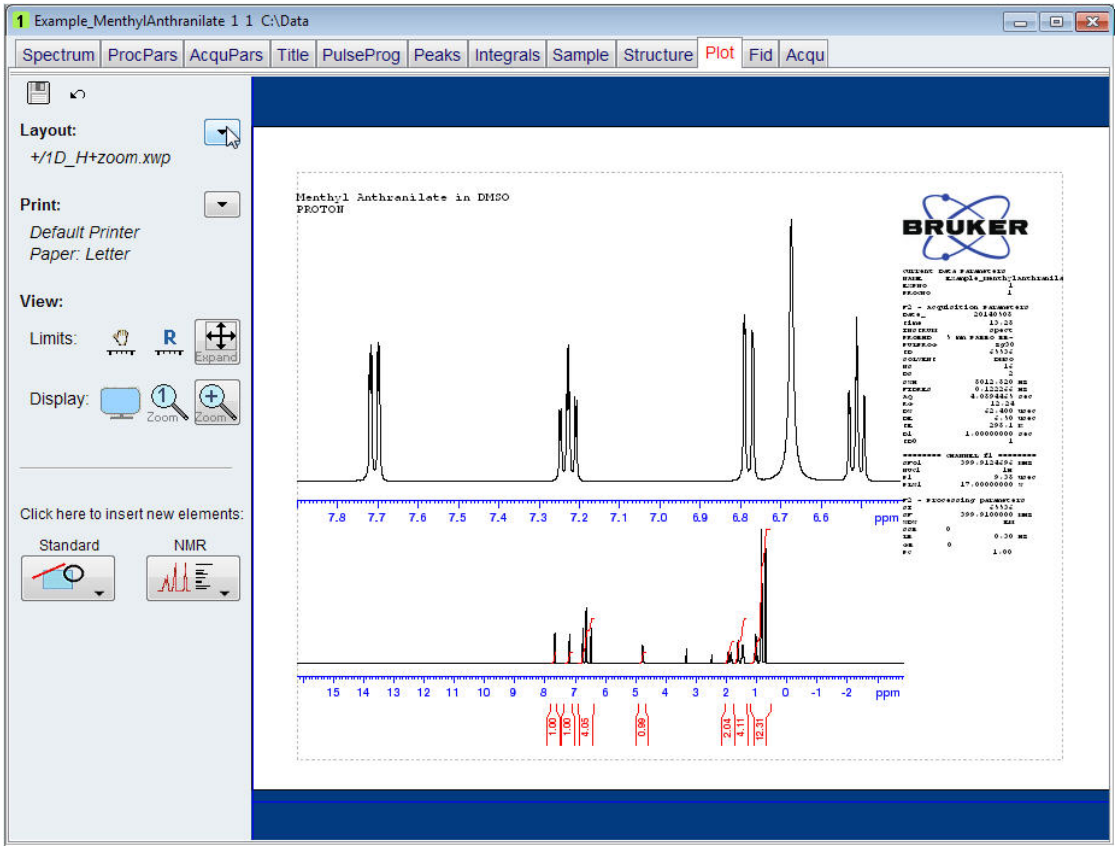
  F1P/F2P are parameters which can be set manually in TopSpin from the command line, in the processing parameter list, define plot region or within an AU program.

- Click on the **Apply Now** button inside the Automation actions window on the left side of the Plot Editor window.

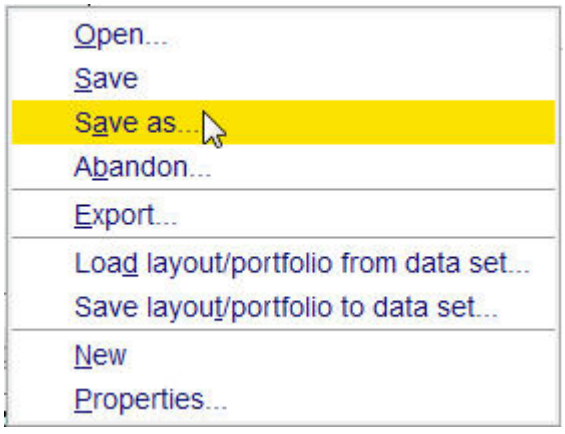


The top spectrum displays the expansion set in TopSpin.

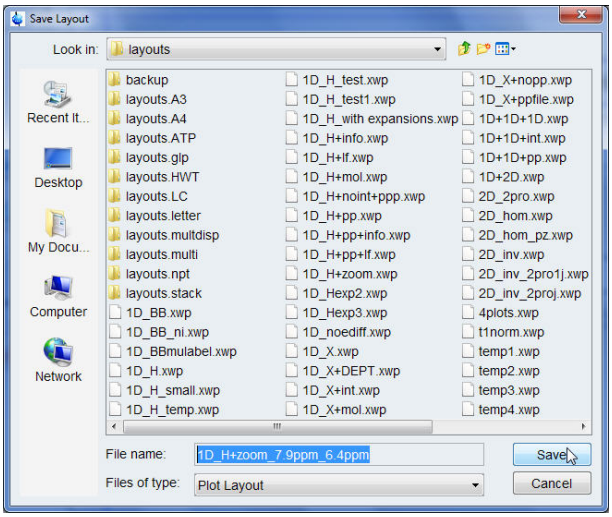
- Click on the up arrow in the upper right of the 1D Automation actions window or click anywhere inside the blue border of the Plot Editor display window.
- Click on the **down arrow** button to the right of the Layout option on the left side of the plot editor window.



- Select **Save as**.



- Type e.g. **1D_H+zoom_7.9ppm_6.4pp** in to the File name window.



- Click on the **Save** button inside the Save Layout window

This new layout can now be used in Automation by adding it to any 1D proton dataset that has peaks in the region between 7.9 ppm and 6.4 ppm. The auto-plot command will send the layout with the spectra directly to the printer. The command plot -r will open the Plot Editor displaying the layout with the two spectra.

6.4.2 Y Scaling

A spectrum of **Ethylbenzene** in **CDCl3** and **TMS** as a reference is used in examples to explain the various functions of the Y-scaling reset options. Each of the examples or combinations of them can be stored as new layout. The **auto-plot** command will send the new layout directly to the printer. The command **plot -r** will open the Plot Editor displaying the layout

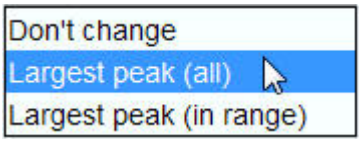
6.4.2.1 Example 1

- Observe or open a 1D proton spectrum.
- Process the data.
- Click on the **ProcPars** tab in the data set bars.
- Scroll down to the **Peak picking / plotting** section and change the **SREGLST** to the **reg** file associated with the lock solvent used. In this case it is **1H.CDCL3**.
- Type **sref** inside the command line to calibrate the spectrum.

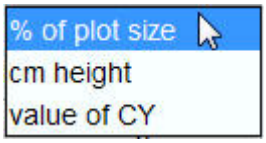
  If no reference substance has been added to the sample, an independent calibration is per-formed using the lock solvent as a reference.
- Integrate and calibrate all but the solvent and reference peak.
- Expand the spectrum from **8.5 ppm** to **-1 ppm** and store the display region.
- Click on the **Plot** tab in the **Data set tab** bar to open the Plot Editor.
- Click on the spectrum displayed inside the Plot Editor window.

  Green handles will mark the spectrum and on the left side of the Plot Editor window the spectrum options are displayed.
- Click on the **Automation actions** inside the Spectrum options window on the left side of the Plot Editor window.

- Click on the down arrow of the **Y Scaling** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **Largest peak (all)**.

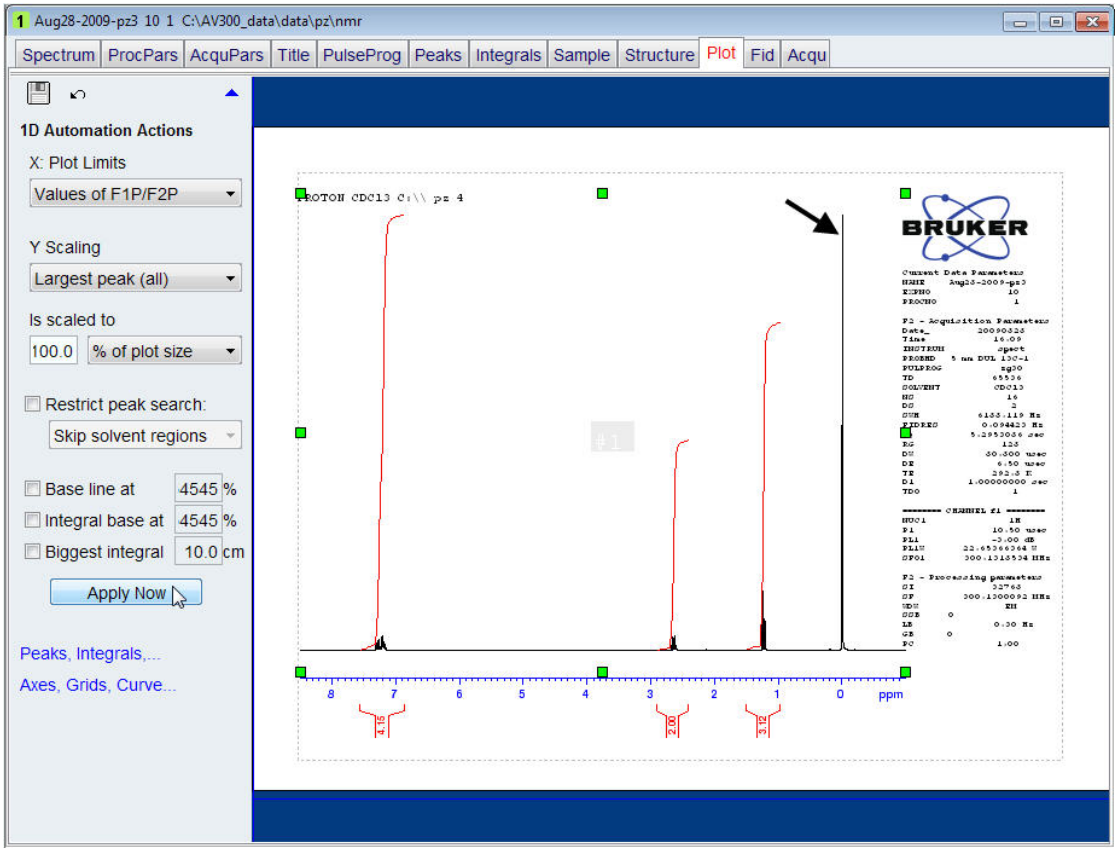


- Click on the down arrow of the **Is scaled to** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **% of plot size** and enter **100.0** as a value.



- This setting defines the size of the biggest peak in the spectrum set by the element size. Other settings are available such as **cm height** which can be entered in numbers and **value of CY** which is taken from entry defined in the processing parameters.
- Disable the **Restrict peak search** option inside the Automation actions window on the left side of the Plot Editor window.
- Click on the **Apply Now** button inside the Automation actions window on the left side of the Plot Editor window.

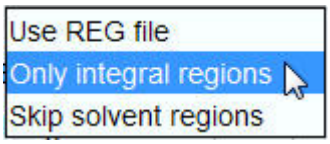
  The **Largest peak (all)** option scales the signals relative to the biggest signal in the whole spectrum, which in this case is the reference peak **TMS**.



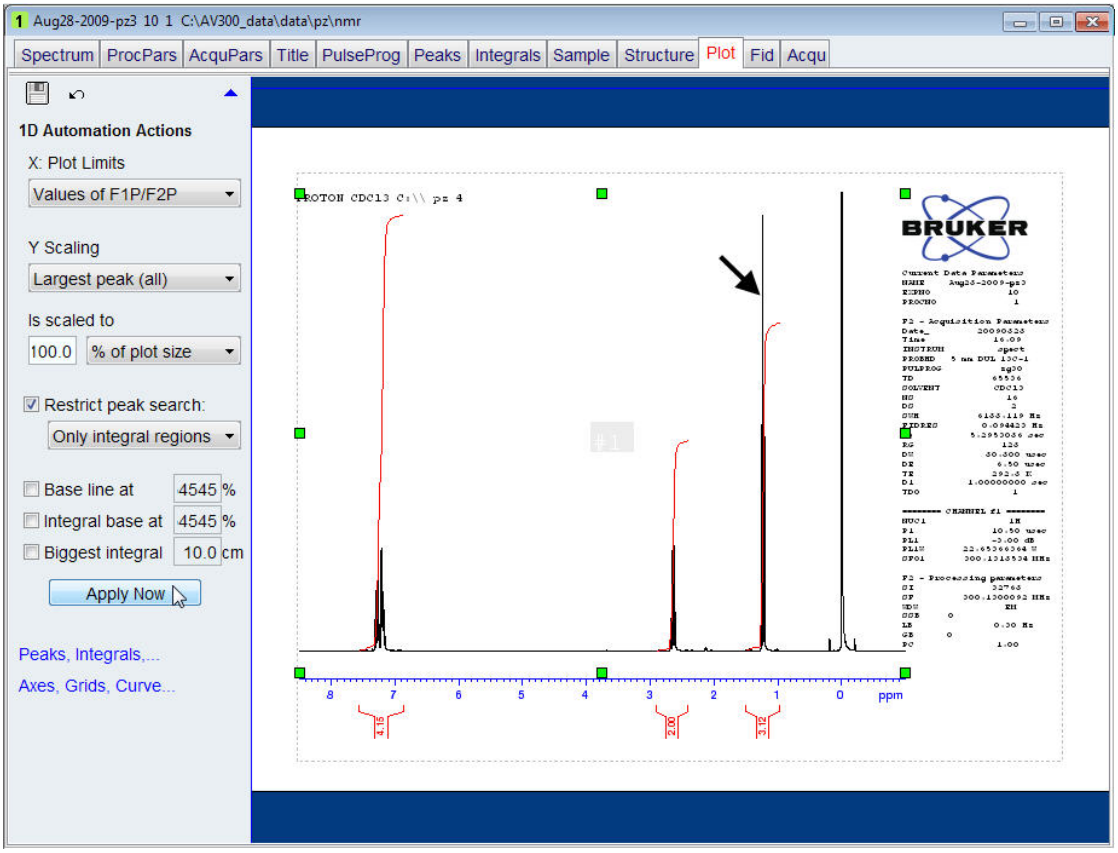
6.4.2.2 Example 2

- Observe or open a 1D proton spectrum.
- Process the data.
- Type **sref** inside the command line to calibrate the spectrum.
- Integrate and calibrate all but the solvent and reference peak.
- Expand the spectrum from **8.5 ppm** to **-1 ppm** and store the display region.
- Click on the **Plot** tab in the **Data set tab** bar to open the Plot Editor.
- Click on the spectrum displayed inside the Plot Editor window.

  Green handles will mark the spectrum and on the left side of the Plot Editor window the spectrum options are displayed.
- Click on the **Automation actions** inside the Spectrum options window on the left side of the Plot Editor window.
- Click on the down arrow of the **Y Scaling** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **Largest peak (all)**.
- Click on the down arrow of the **Is scaled to** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **% of plot size** and enter **100.0** as a value.
- Enable the **Restrict peak search** option inside the Automation actions window on the left side of the Plot Editor window.
- Click on the down arrow of the **Restrict peak search** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **Only integral regions**.



- Click on the **Apply Now** button inside the Automation actions window on the left side of the Plot Editor window.



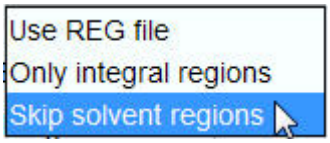
The **Only integral regions** option scales the signals relative to the biggest signal defined by the integral regions, which in this case is the peak at **1.24 ppm**. Since the **TMS** reference peak was not integrated it will be off scale.

6.4.2.3 Example 3

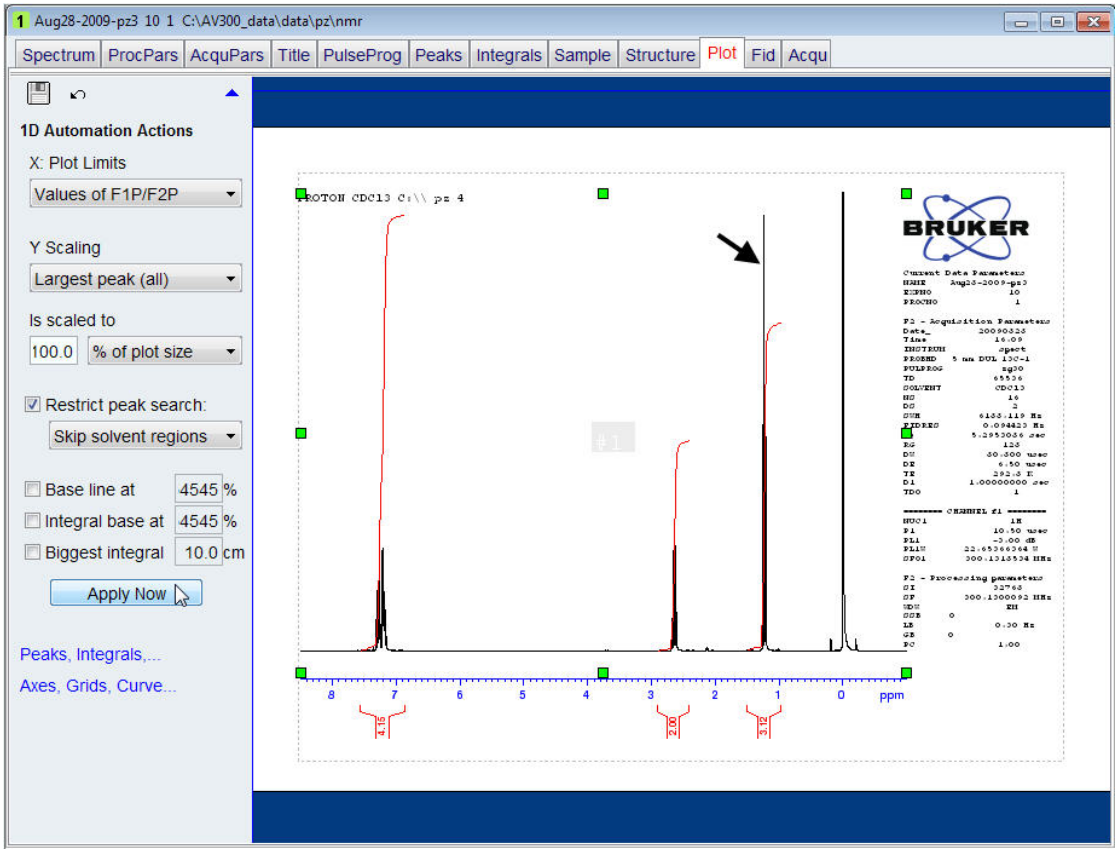
- Observe or open a 1D proton spectrum.
- Process the data.
- Type **sref** inside the command line to calibrate the spectrum.
- Integrate and calibrate all but the solvent and reference peak.
- Expand the spectrum from **8.5 ppm** to **-1 ppm** and store the display region.
- Click on the **Plot** tab in the **Data set tab** bar to open the Plot Editor.
- Click on the spectrum displayed inside the Plot Editor window.

  Green handles will mark the spectrum and on the left side of the Plot Editor window the spectrum options are displayed.

- Click on the **Automation actions** inside the Spectrum options window on the left side of the Plot Editor window.
- Click on the down arrow of the **Y Scaling** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **Largest peak (all)**.
- Click on the down arrow of the **Is scaled to** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **% of plot size** and enter **100.0** as a value.
- Enable the **Restrict peak search** option inside the Automation actions window on the left side of the Plot Editor window.
- Click on the down arrow of the **Restrict peak search** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **Skip solvent region**.



- Click on the **Apply Now** button inside the Automation actions window on the left side of the Plot Editor window.

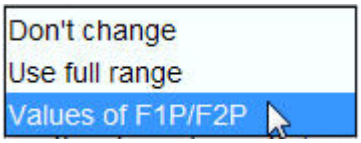


The **Skip solvent regions** option scales the signals relative to the biggest signal in the spectrum, excluding the solvent / reference peaks defined in the SREGLST parameter (for this sample 1H.CDCl3). In this case the peak at **1.24 ppm** is scaled to the full height. Since the **TMS** reference peak was excluded from the region it will be off scale.

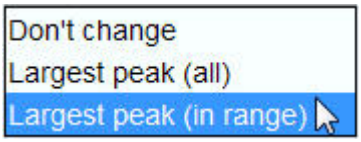
6.4.2.4 Example 4

- Observe or open a 1D proton spectrum.
- Process the data.
- Type **sref** inside the command line to calibrate the spectrum.
- Integrate only the peak at **2.65 ppm** and **Save Region To reg**.
- Expand the spectrum from **8.5 ppm** to **-1 ppm** and store the display region.
- Click on the **Plot** tab in the **Data set tab** bar to open the Plot Editor**.**
- Click on the spectrum displayed inside the Plot Editor window.

  Green handles will mark the spectrum and on the left side of the Plot Editor window the spectrum options are displayed.
- Click on the **Automation actions** inside the Spectrum options window on the left side of the Plot Editor window.
- Click on the down arrow of the **X Plot Limits** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **Values of F1P/F2P**.

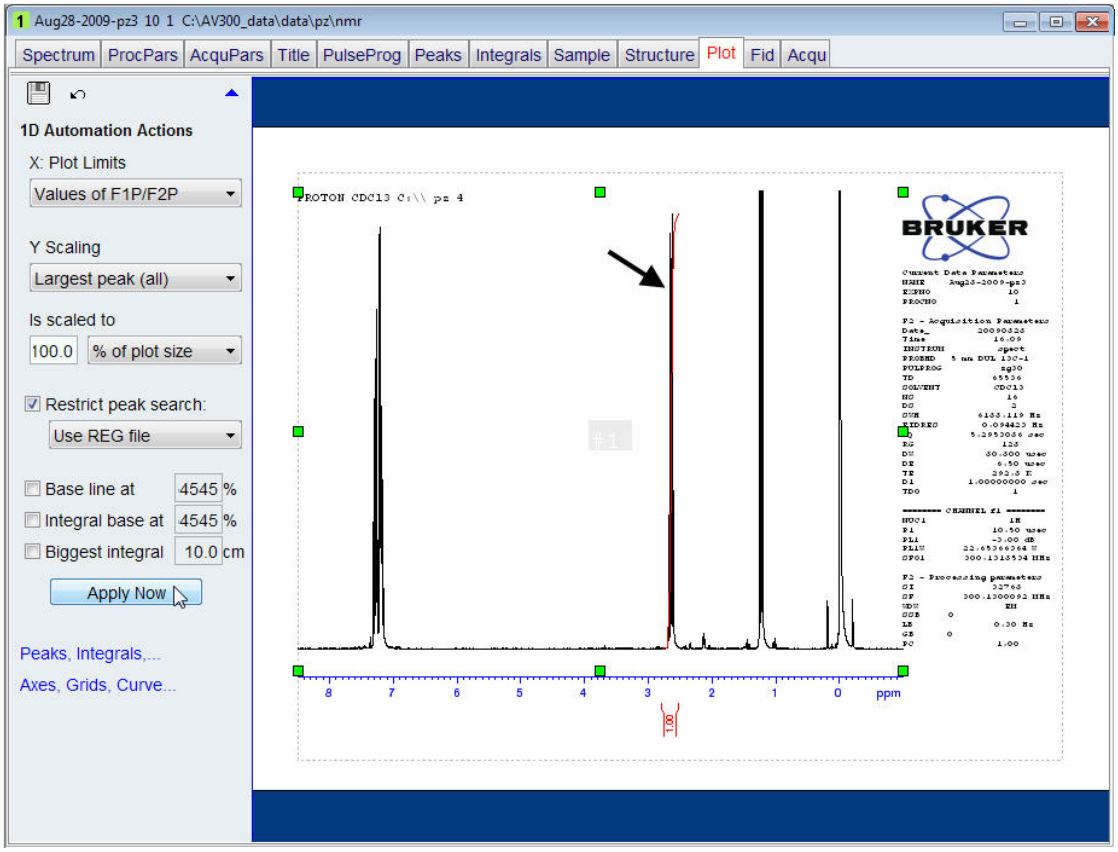


- Click on the down arrow of the **Y Scaling** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **Largest peak (in range)**.



- Enable the **Restrict peak search** option inside the Automation actions window on the left side of the Plot Editor window.
- Click on the down arrow of the **Restrict peak search** option inside the **Automation actions** window on the left side of the Plot Editor window.
- Select **Use REG file**.

- Click on the **Apply Now** button inside the Automation actions window on the left side of the Plot Editor window.

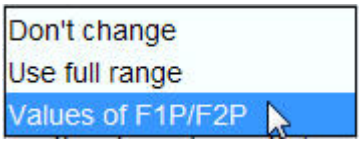


The **Use REG file** option scales the signals relative to the biggest signal defined by the region file and saved using the integration, which in this case is the peak at **12.65 ppm**. All other peaks will be off scale.

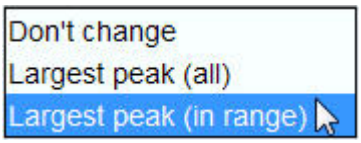
6.4.2.5 Example 5

- Observe or open a 1D proton spectrum.
- Process the data.
- Type **sref** inside the command line to calibrate the spectrum.
- Integrate and calibrate all but the solvent and reference peak.
- Expand the spectrum from **8.5 ppm** to **2 ppm** and store the display region.
- Click on the **Plot** tab in the **Data set tab** bar to open the Plot Editor.
- Click on the spectrum displayed inside the Plot Editor window.

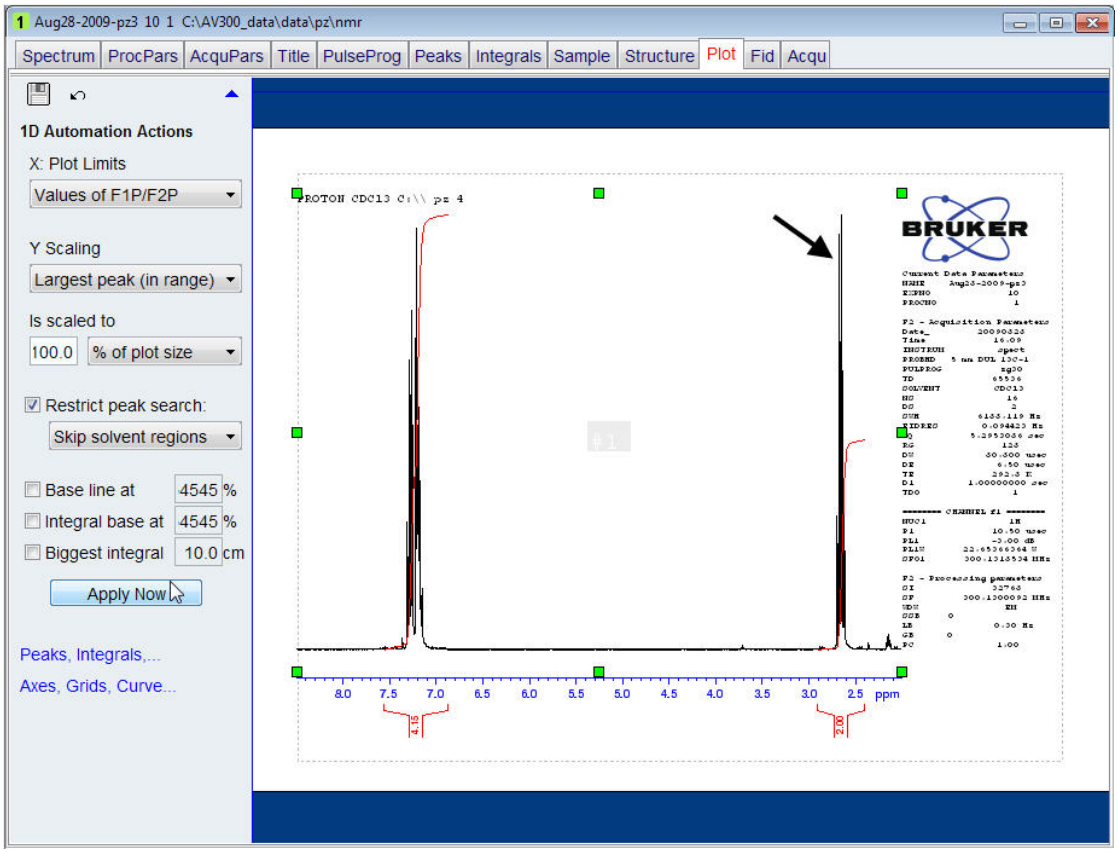
  Green handles will mark the spectrum and on the left side of the Plot Editor window the spectrum options are displayed.
- Click on the **Automation actions** inside the Spectrum options window on the left side of the Plot Editor window.
- Click on the down arrow of the **X Plot Limits** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **Values of F1P/F2P**.



- Click on the down arrow of the **Y Scaling** option inside the Automation actions window on the left side of the Plot Editor window.
- Select **Largest peak (in range)**.



- Disable the **Restrict peak search** option inside the Automation actions window on the left side of the Plot Editor window.
- Click on the **Apply Now** button inside the Automation actions window on the left side of the Plot Editor window.



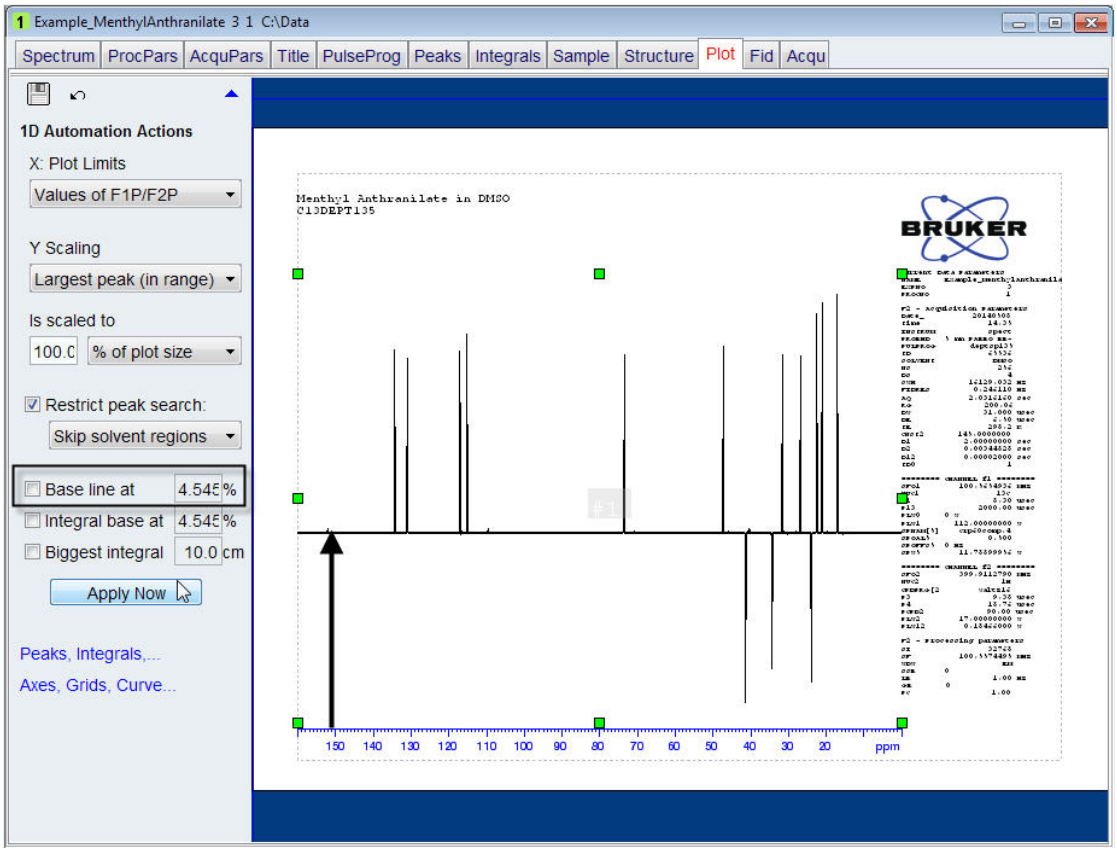
The **Largest peak (in range)** option scales the signals relative to the biggest signal in the expanded spectrum, which in this case is the quartet at **2.65 ppm**.

6.4.3 Additional Automation Actions

In this section some automation actions settings for the base line and integrals are discussed.

6.4.3.1 Base line at

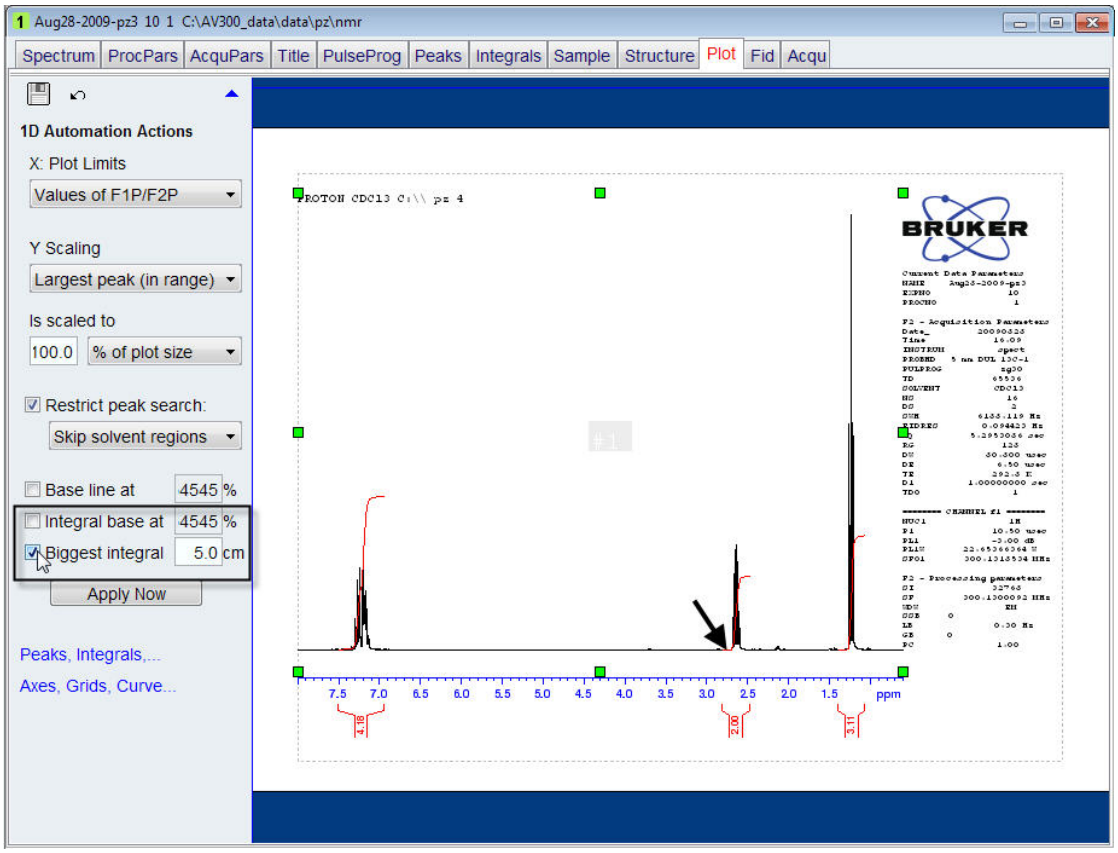
By default the setting for **Base line at** is disabled (unchecked) and the base line of the spectrum is placed in such a way that all positive and negative peaks are visible (see the example below of a DEPT135 spectrum).



If the setting for the **Base line at** is enabled (checked) it will place the base line at the position entered as a value in percent (the default value is **4.545 %**). Keeping the base line at a fixed value is useful for noisy spectra (see the example below of a carbon spectrum with low signal to noise ratio).

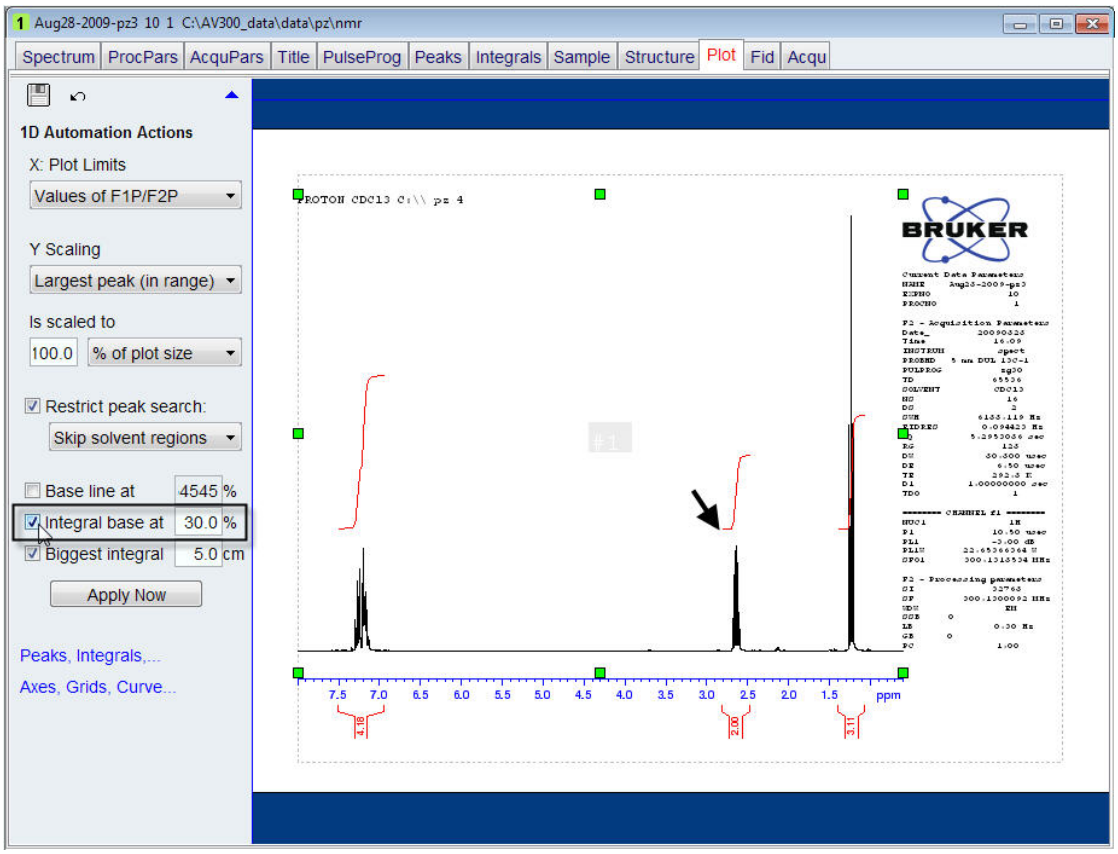
6.4.3.2 Biggest integral

By default the **Biggest integral** setting is disabled (unchecked) and the biggest integral is printed a little bit smaller than the biggest signal in the spectrum. If the **Biggest integral** setting is enabled (checked) the biggest integral is scaled to the value entered. Also note that the **Integral base at** is disabled (unchecked). The spectrum below shows the integrals scaled to the biggest integral at **5 cm** starting at the base of the spectrum.



6.4.3.3 Integral base at

By default the **Integral base at** setting is disabled (unchecked) and the left side of the integral starts at the base line of the spectrum. If the **Integral base at** setting is enabled (checked) the left side of the integral starts at the value in percent entered. This makes it easier to measure integrals with a ruler. The spectrum below shows the integrals moved up **30 %** from the base line where the biggest integral is still scaled to **5 cm**.


Aug28-2009-pz3 10 1 C:\AV300_data\data\pz\nmr
Spectrum
ProcPars
AcquPars
Title
PulseProg
Peaks
Integrals
Sample
Structure
Plot
Fid
Acqu
1D Automation Actions
X: Plot Limits
Values of F1P/F2P
Y Scaling
Largest peak (in range)
Is scaled to
100.0
% of plot size
Restrict peak search:
Skip solvent regions
Base line at
4545 %
Integral base at
30.0 %
Biggest integral
5.0 cm
Apply Now
Peaks, Integrals,...
Axes, Grids, Curve...
PROTON CDCl3 C:\\ pz 4
BRUKER
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.16
2.00
3.11

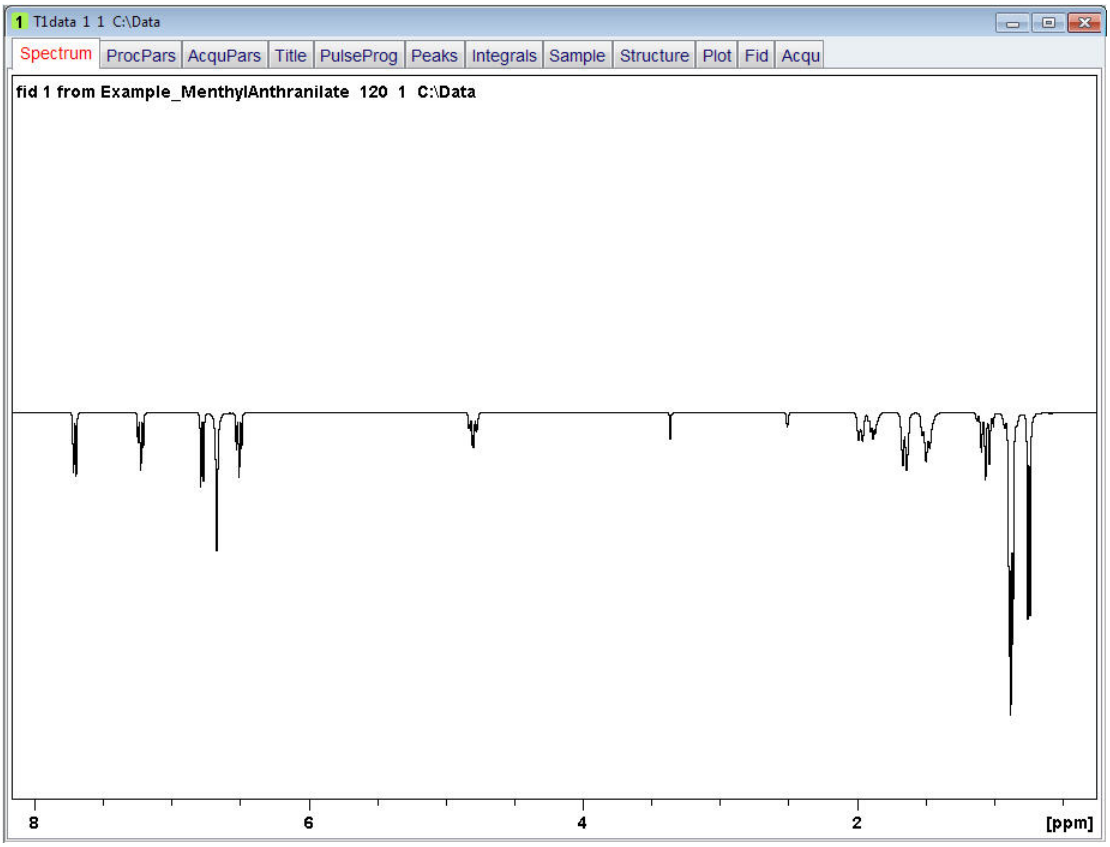
7 Additional Printing Options

7.1 Introduction

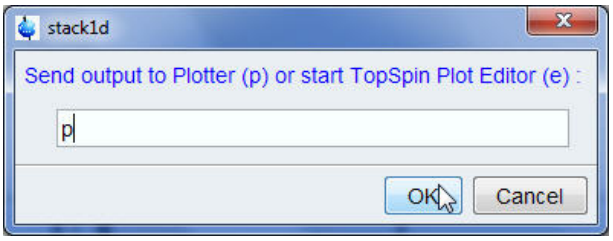
Printing NMR data can also be executed using AU programs such as stack1d. The list of parameters on the printout can be edited and lists of integration-, peak- values can be printed which will be discussed in this chapter.

7.2 Printing T1 Data

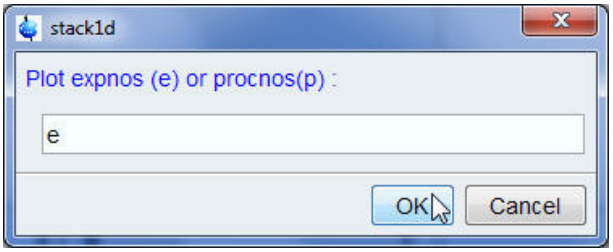
- In TopSpin observe a T1 experiment using e.g. 6 increasing variable delays, starting with the shortest Tau value first.
- Extract the 1D data using the AU program splitser.
- Process the 1D data.
- Display the first data set.



- Type **stack1d** inside the TopSpin command line followed by a return.
- Type **p** inside the stack1d window to select the plotter option.

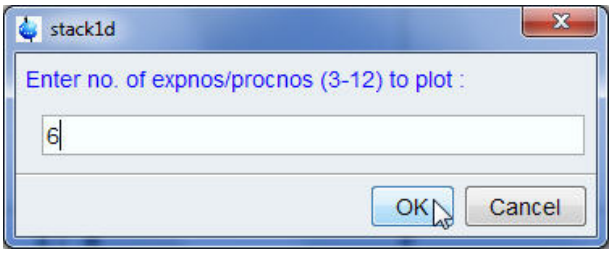


- Click on the **OK** button inside the stack1d window.
- Type **e** inside the stack1d window to select the experiment number.

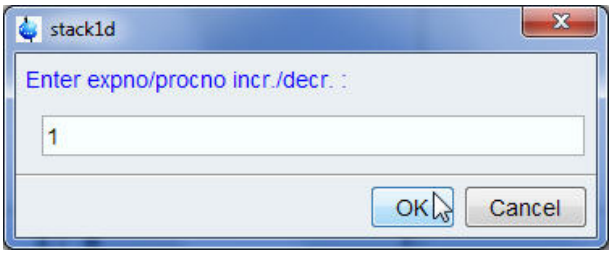


- Click on the **OK** button inside the stack1d window.
- Type **1** inside the stack1d window to select the first experiment number.

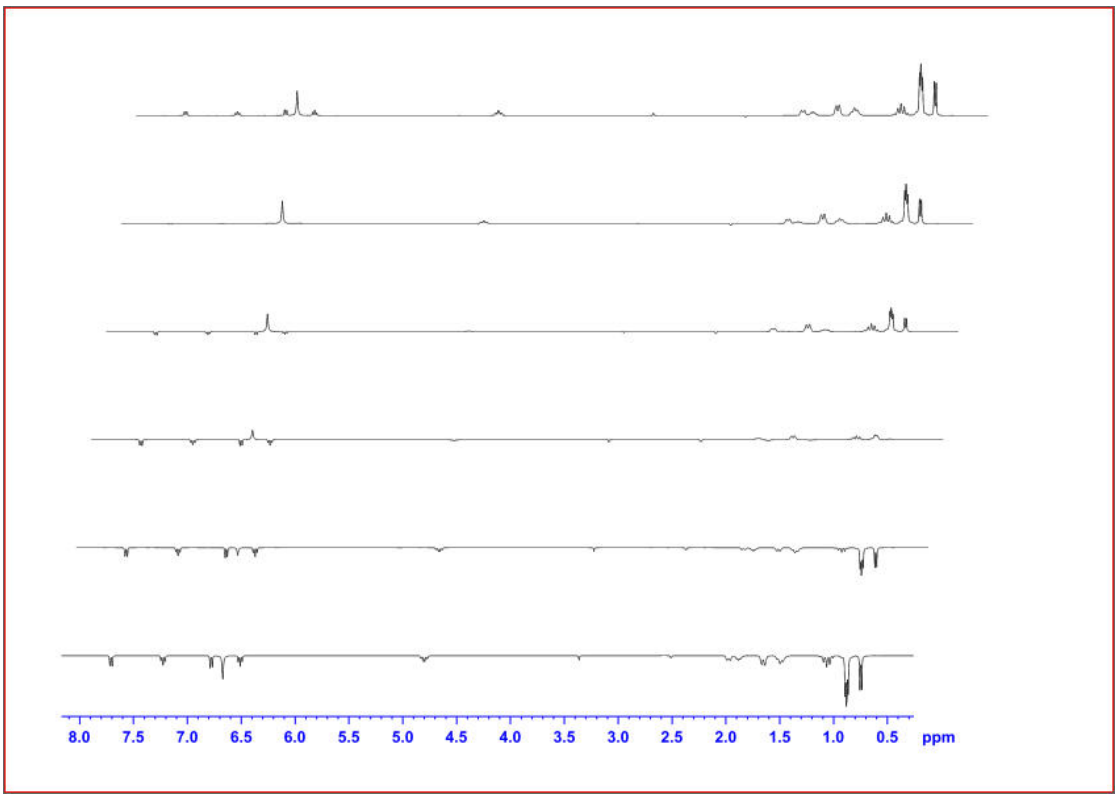
- Click on the **OK** button inside the stack1d window.
- Type **6** inside the stack1d window to select the number of experiments.



- Click on the **OK** button inside the stack1d window.
- Type **1** inside the stack1d window to select experiment number increase.



- Click on the **OK** button inside the stack1d window.
  It will take a few seconds to calculate and print out the T1 data.



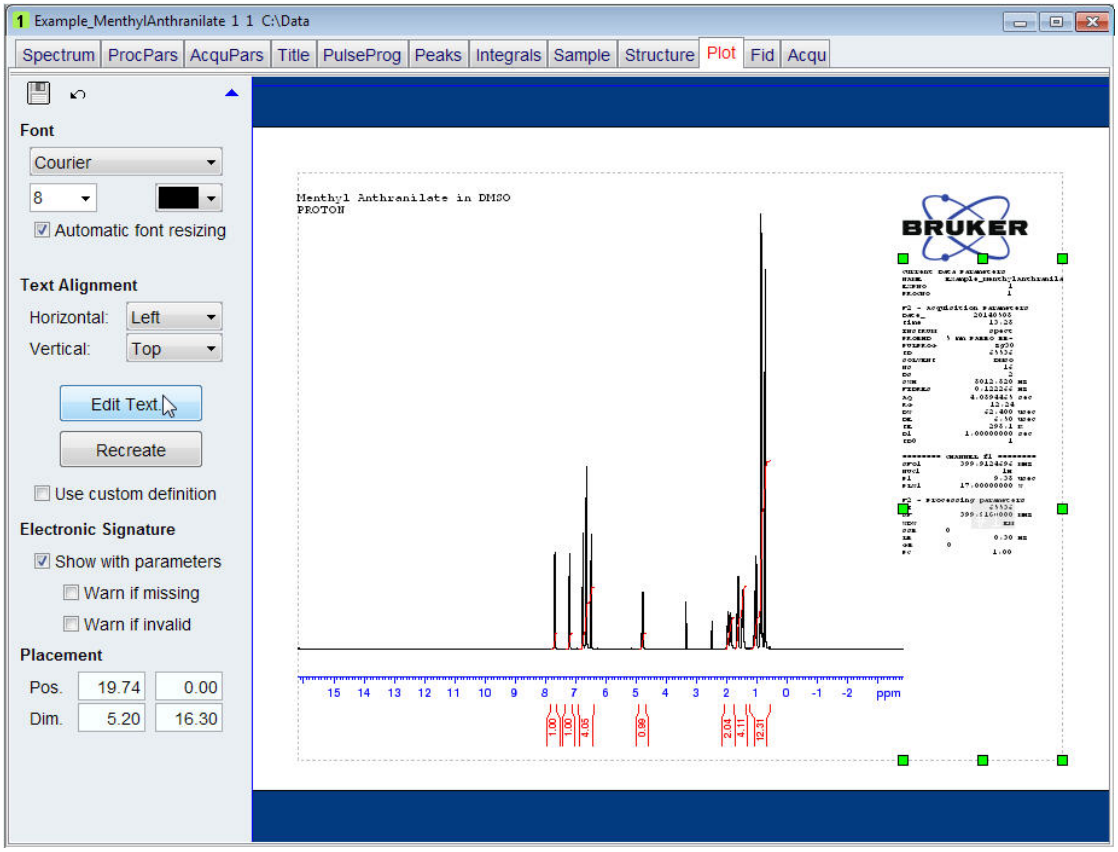
7.3 Modifying Parameters on Printout

A global TopSpin configuration for a 1D or 2D data sets defines which parameters appear on a printout. There are two ways to modify the parameters on the printout.

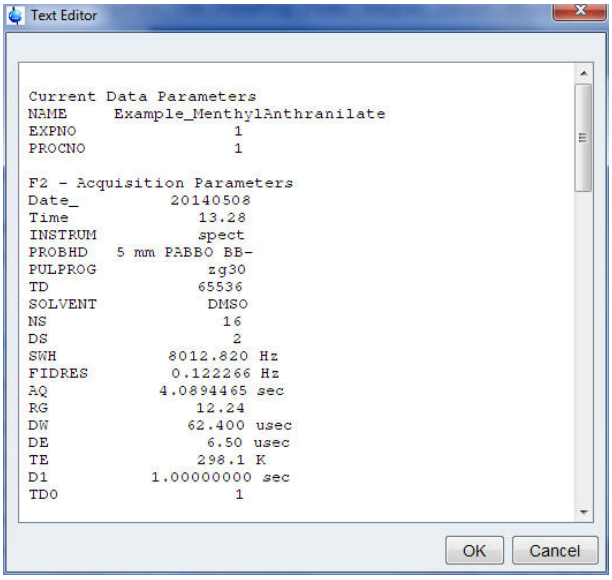
7.3.1 Modifying Parameters Using the Plot Editor Option

This option of modifying parameters will only effect the current printout and cannot be stored as a layout. The example below will only printout the edited parameters.

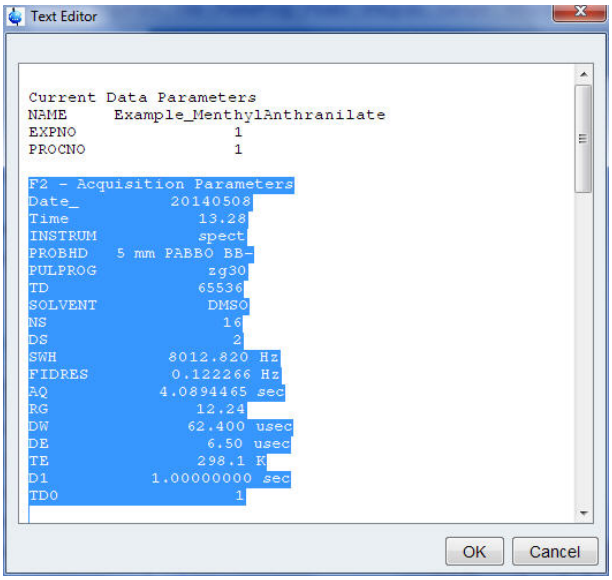
- In TopSpin observe a 1D Proton experiment, process and open the plot editor.
- Click inside the listed parameters.
  Green handles will mark the parameter list window.



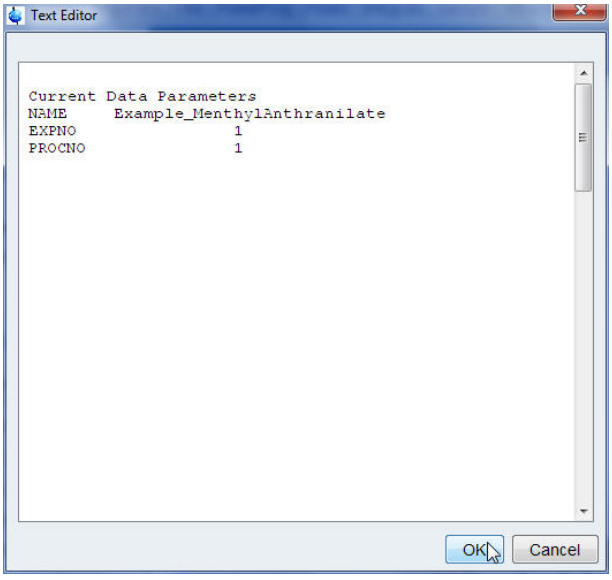
- Click on the **Edit Text** button inside the left side of the plot editor window.



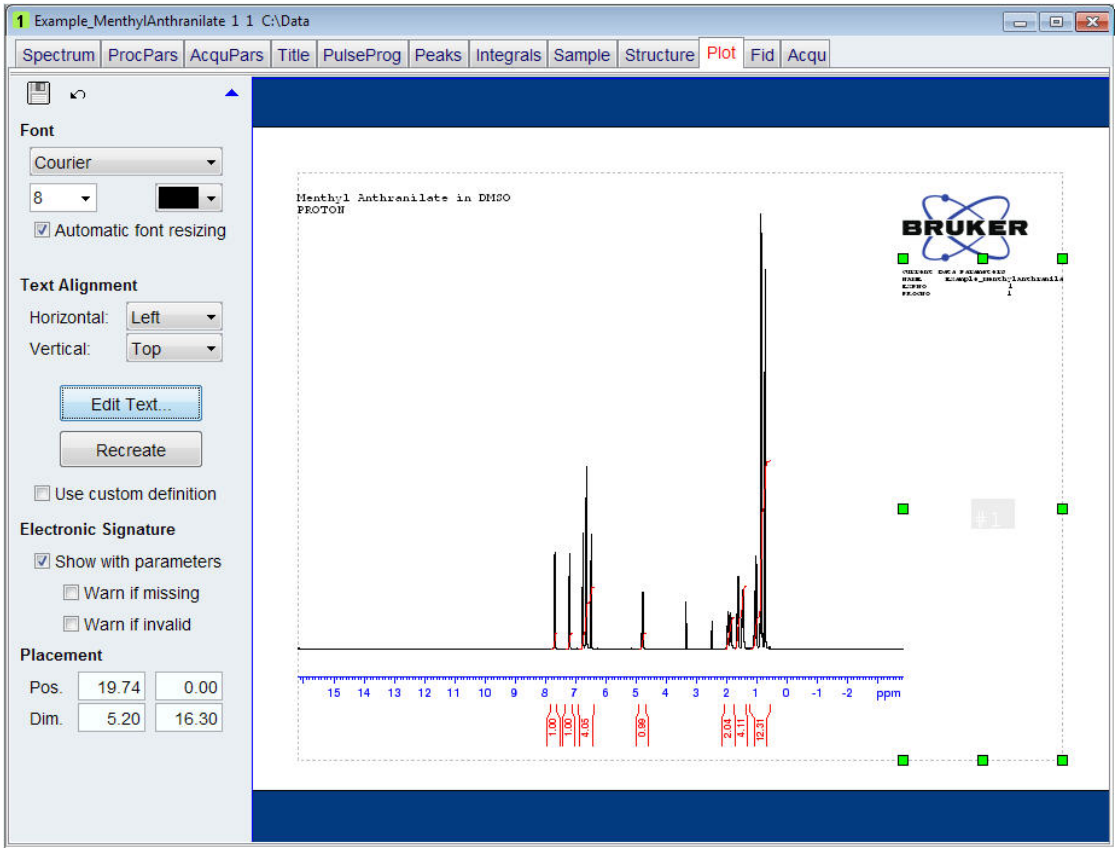
- While holding the left mouse button pressed, highlight all the text below **PROCNO 1**.



- Hit the **Delete** key on the keyboard.



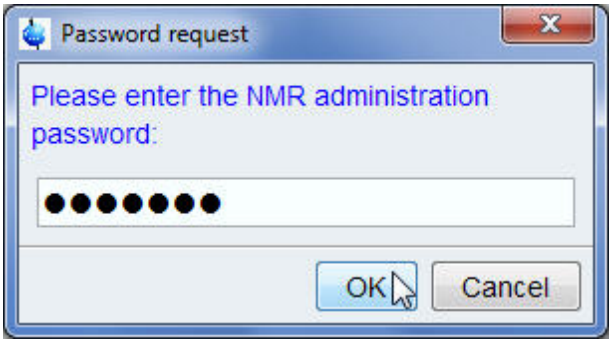
- Click on the **OK** button inside the Text Editor window.



7.3.2 Modifying Parameters Using the TopSpin Parplot Option

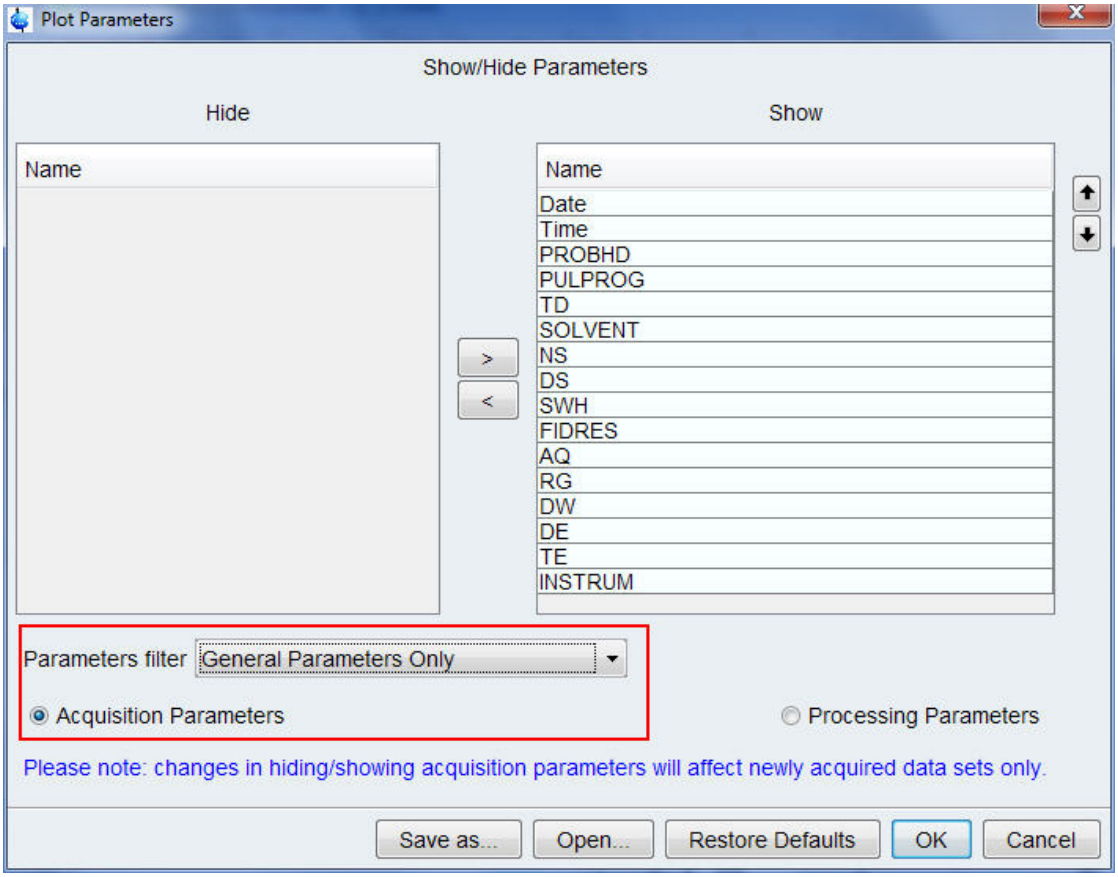
A global TopSpin configuration defines which parameters appear on a spectrum printout. Using the **parplot** command for modifying parameters will affect the parameter list print-out of all data sets acquired from this point on. The example below will only print-out the edited parameters.

- In TopSpin observe a 1D proton experiment, process and open the plot editor.
- Type **parplot** on the TopSpin command line.
- Type the NMR administrator password into the Password request window.

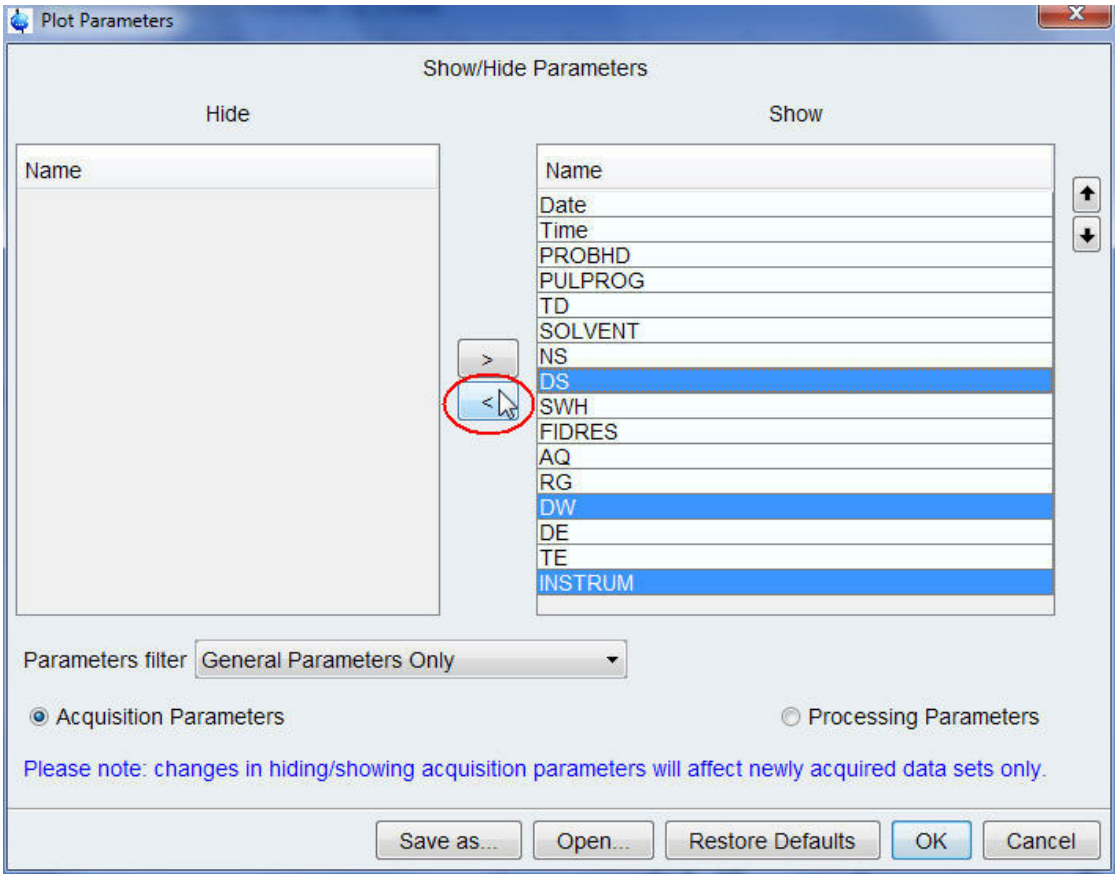


- Click on the **OK** button in the Password request window.

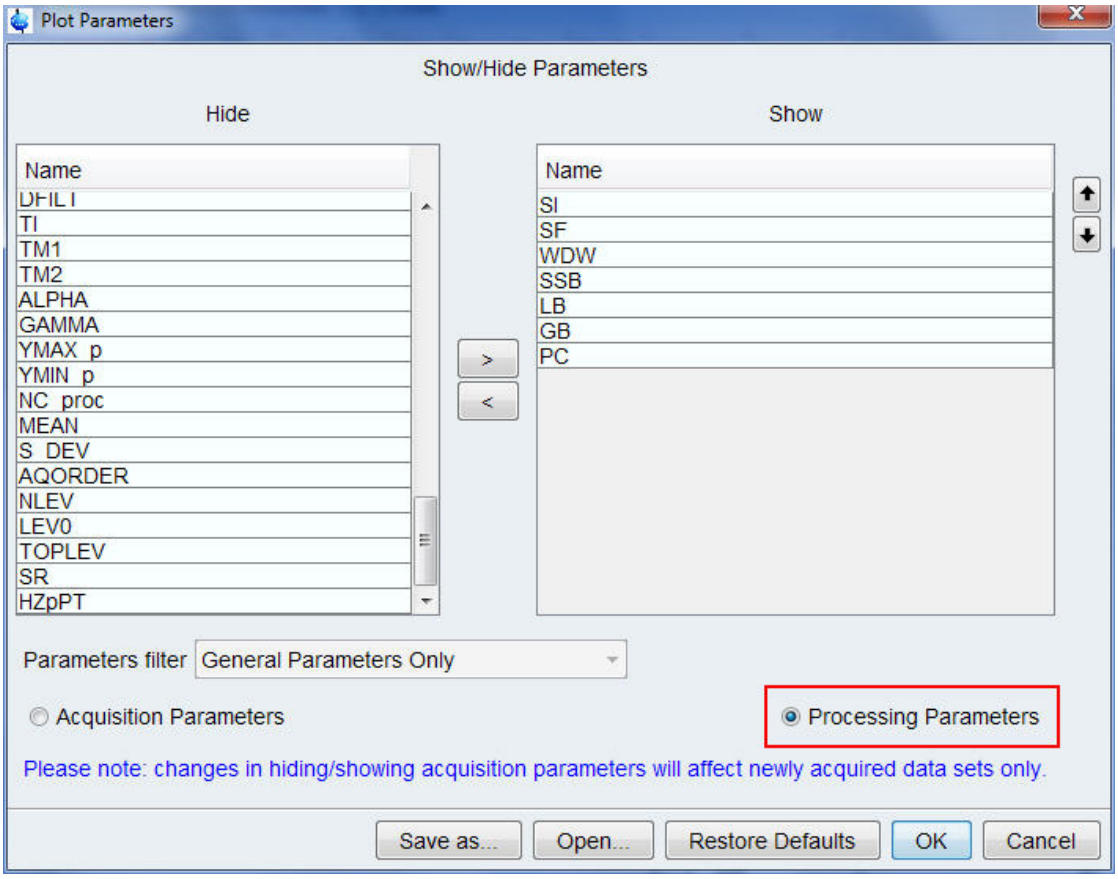
  The window displays parameters you can show or hide in the parameter printout. By default the **General Parameters Only** are displayed and the **Acquisition Parameters** option is enabled. Below are examples how to hide or show parameters.



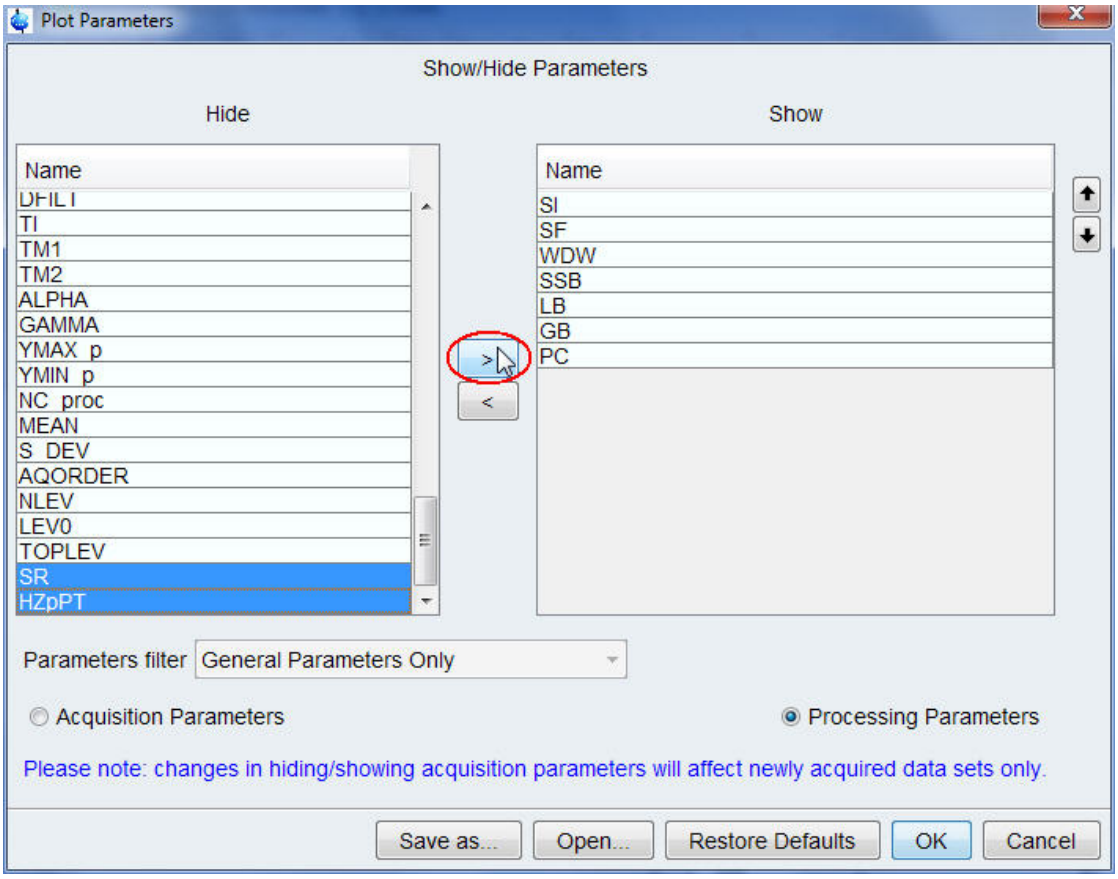
- Highlight the parameters: **DS, DW** and **INSTRUM** using the **Ctrl** keyboard key.
- Click on the **left arrow** button which points to the Hide window.



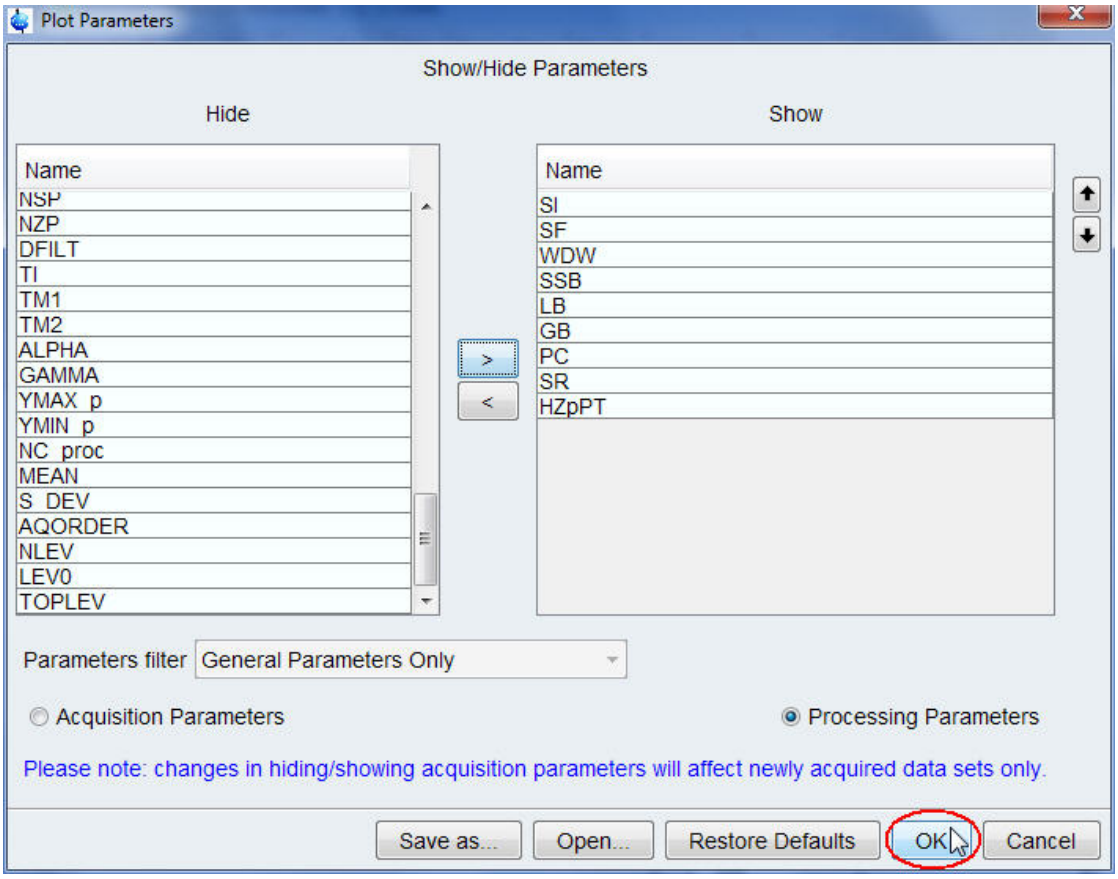
- Click on the **Processing Parameter** button inside the Plot Parameters window.



- Highlight the parameters: **SR** and **HZpPT** using the **Ctrl** keyboard key.
- Click on the **right arrow** button which points to the **Show** window.



- Click on the **OK** button inside the Plot Parameters window to save the selection.



- Other options that can be selected using the buttons inside the Plot Parameters window are listed below:
  - **Save as:** Save the current selection under a user defined name.
  - **Open:** Open a user defined selection.
  - **Restore Defaults:** Restore the TopSpin default selection.
  - **OK:** Save the current selection.
  - **Cancel:** Close the Plot Parameters window.

The **parplot** modifications take effect only on newly acquired data sets. Already existing data sets will show the previous parameter list on each print out.

Additional Printing Options

8 Contact

Manufacturer

Bruker BioSpin GmbH
Silberstreifen 4
D-76287 Rheinstetten
Germany
http://www.bruker.com

WEEE DE43181702

NMR Hotlines

Contact our NMR service centers.

Bruker BioSpin NMR provides dedicated hotlines and service centers, so that our specialists can respond as quickly as possible to all your service requests, applications questions, software or technical needs.

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