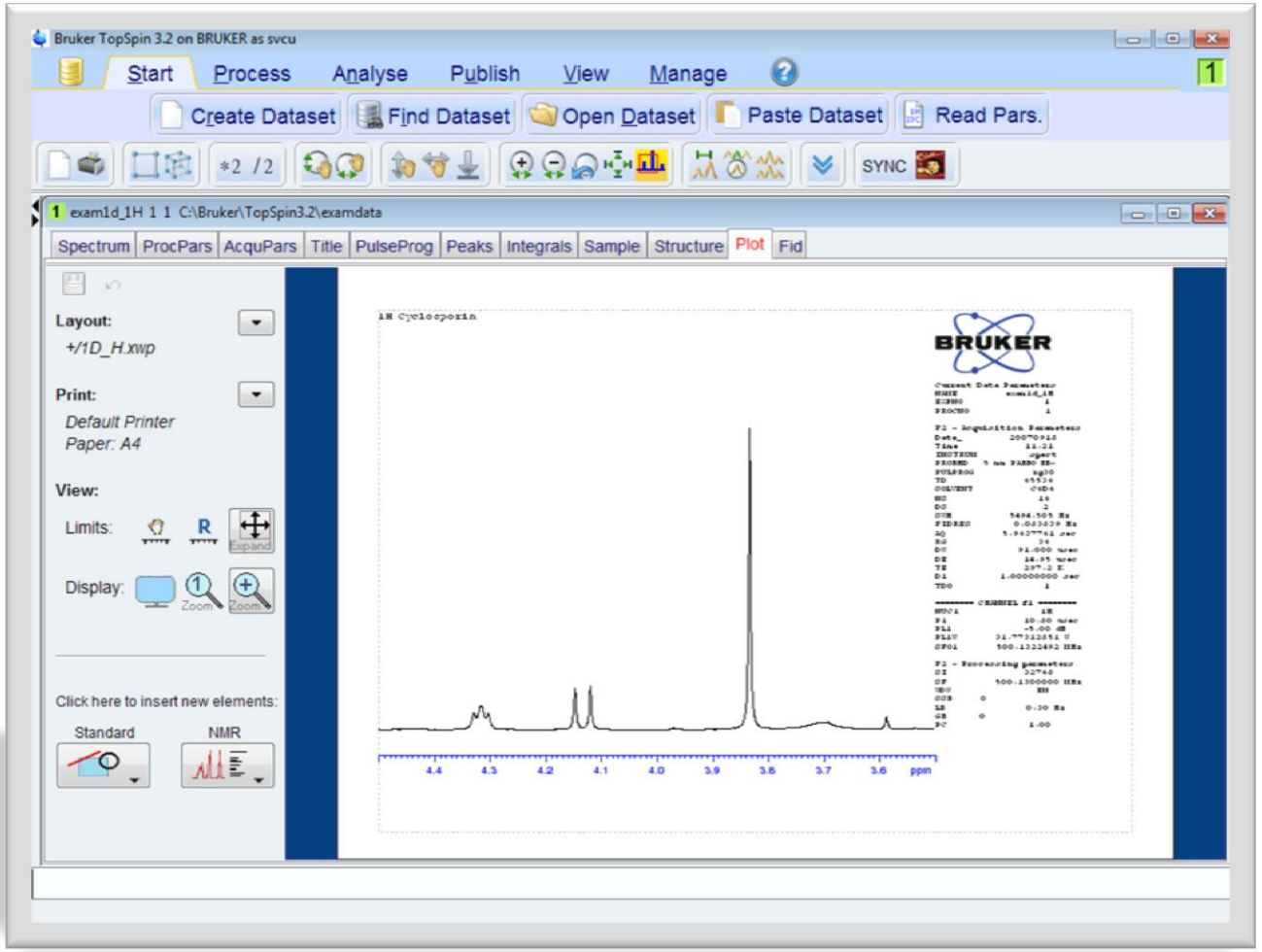
How to plot in TopSpin

Basic introduction



Different situations = different solutions
→ 1 tool

Situation 1

- I just want to easily print what I see in TopSpin

Situation 2

- I want to easily print my own layout

Situation 3

- I would like to optimize my print-out for individual datasets

Situation 4

- I would like to get nice print-outs for all samples of my automation run

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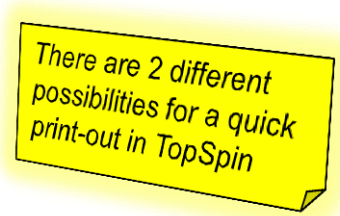
Different situations = different solutions → 1 tool

Situation 1

- I just want to easily print what I see in TopSpin
  - Fast print-out – without anything else
  - Fast print-out – with predefined layouts



Situation 2

- I want to easily print my own layout

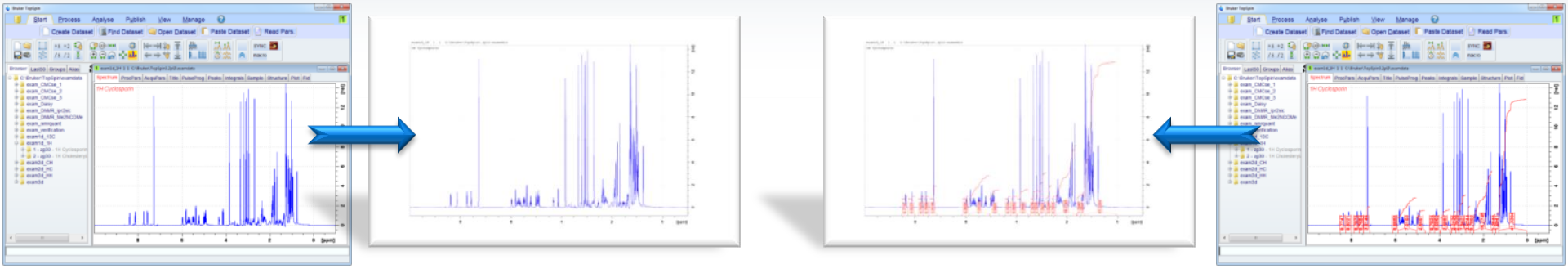
Situation 3

- I would like to optimize my print-out for individual datasets

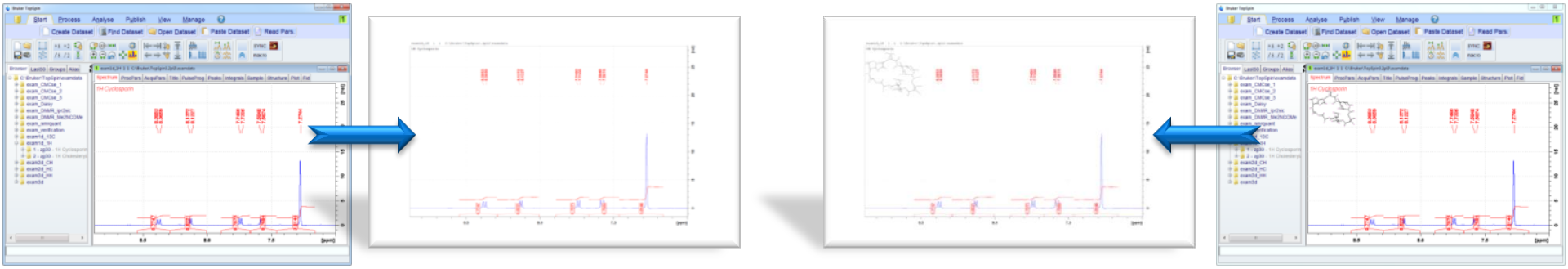
Situation 4

- I would like to get nice print-outs for all samples of my automation run

I just want to easily print what I see in TopSpin – without anything else



just use the command:
prnt



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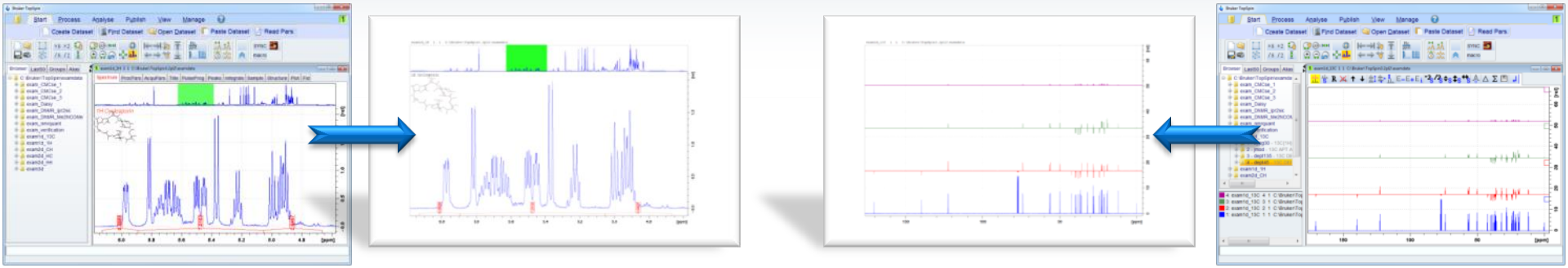
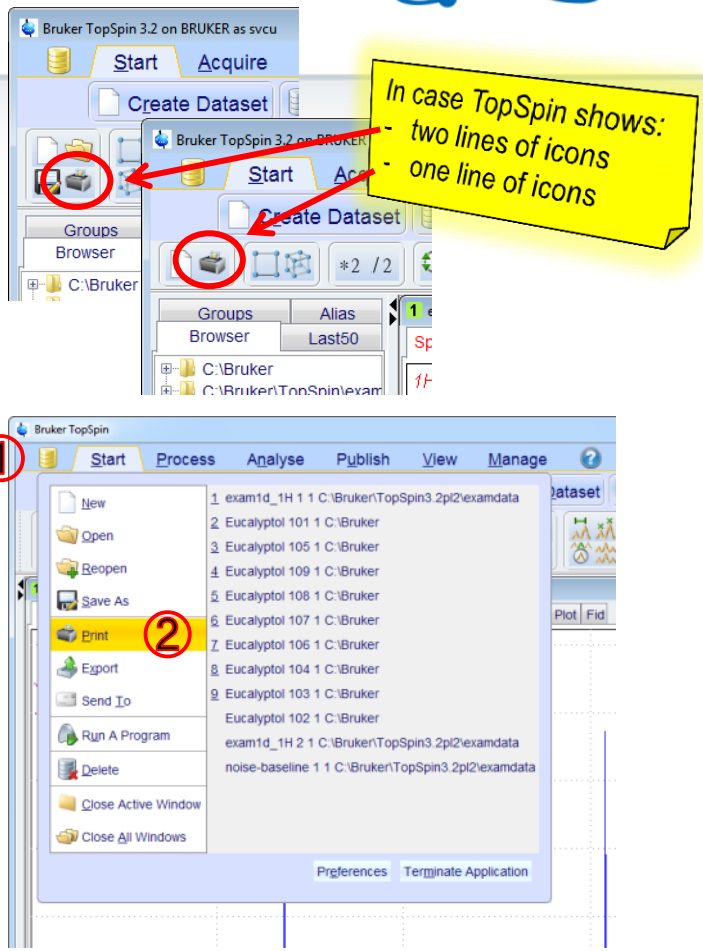


just use the command:
prnt

I just want to easily print what I see in TopSpin – without anything else

Instead of typing in the command **prnt** you can also:

- press **Ctrl-p**
- or enter the command **print**
- or click on the printer icon: 
- or click on the TopSpin disk icon ①
  and select **Print** ②



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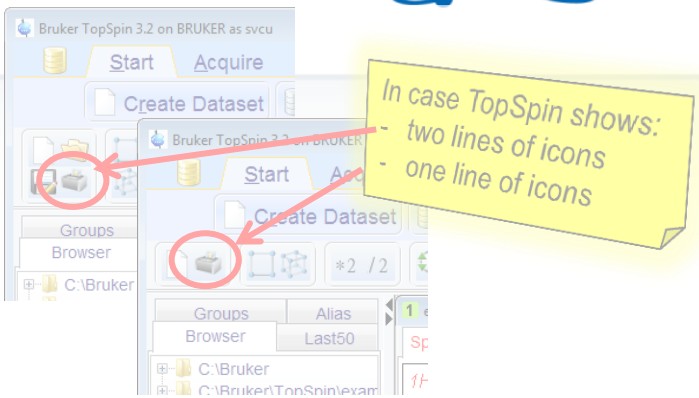
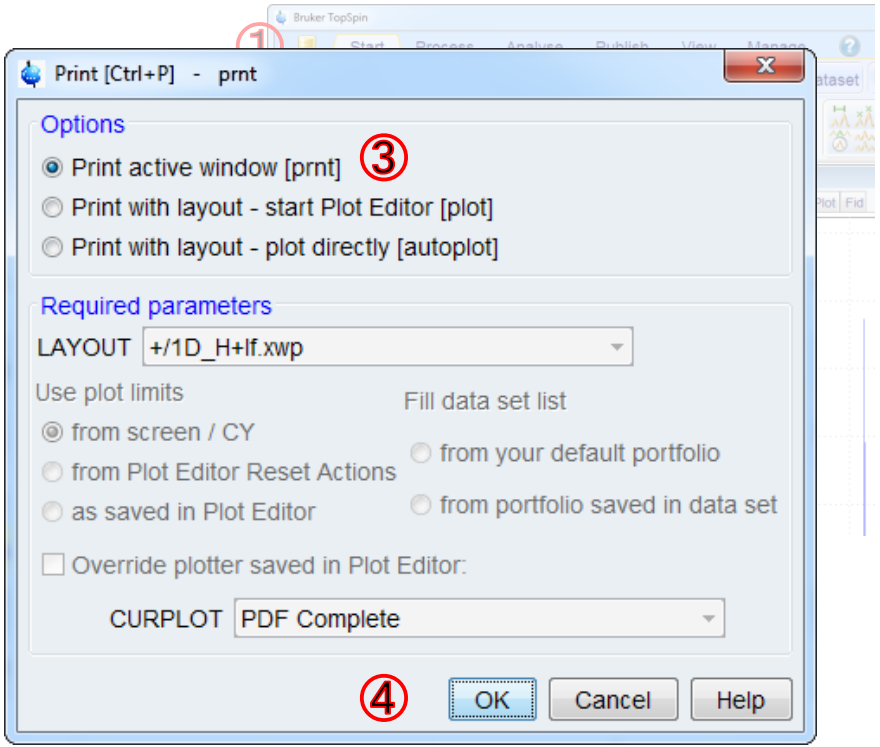


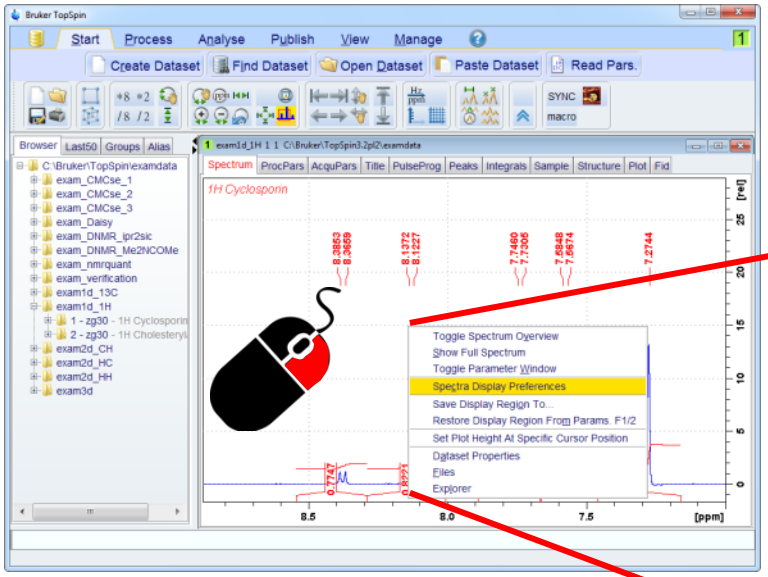


All four possibilities open the same window that offers all TopSpin print options.

Selecting the first option ③ and click **OK** ④ will execute the **prnt** command

I just want to easily print what I see in TopSpin – without anything else

The definition of what information is visible within TopSpin is available with a right mouse click inside the spectrum area
→ click **Spectra Display Preferences**



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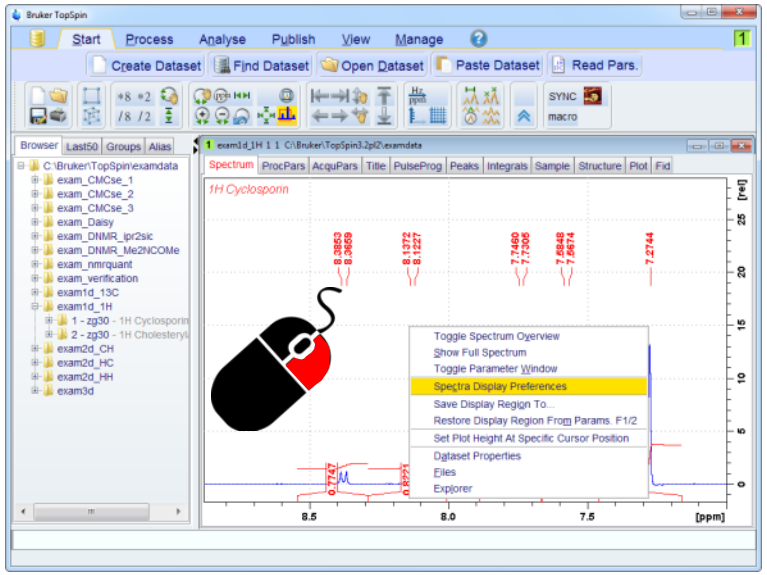
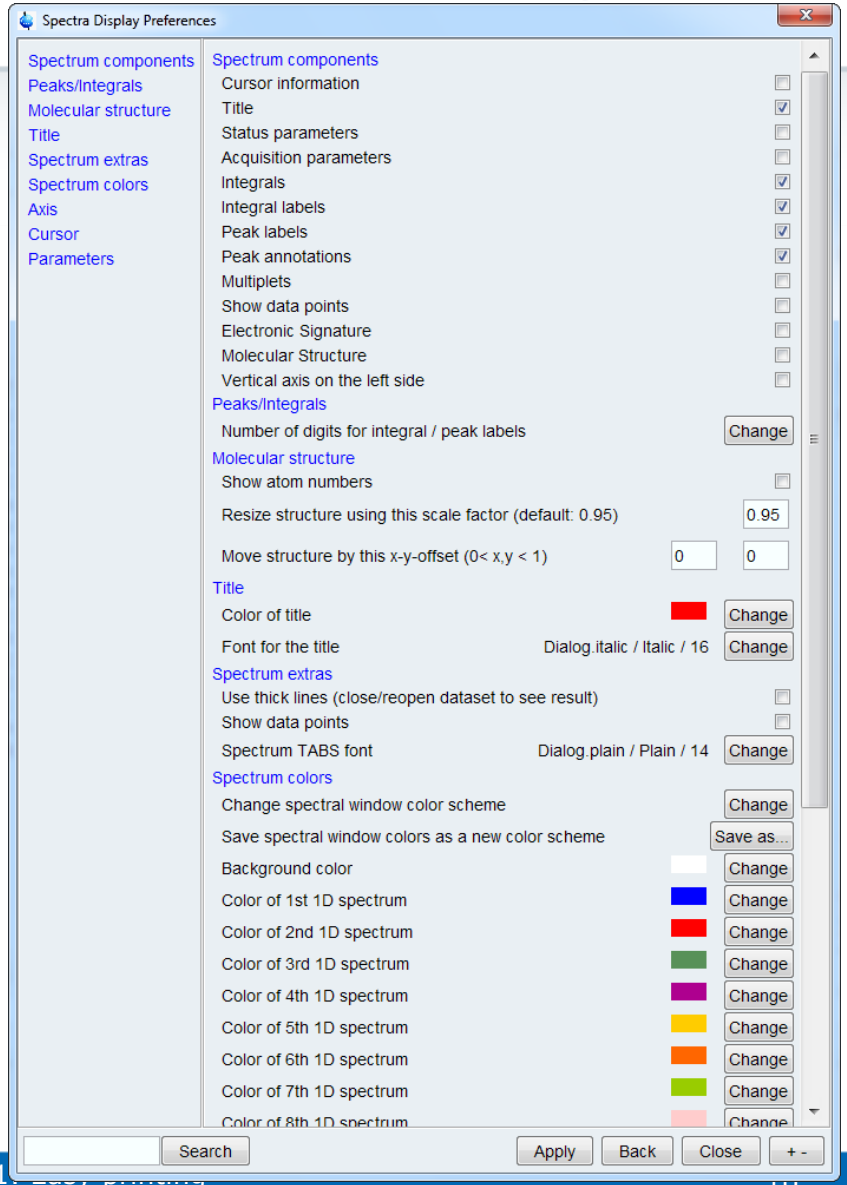
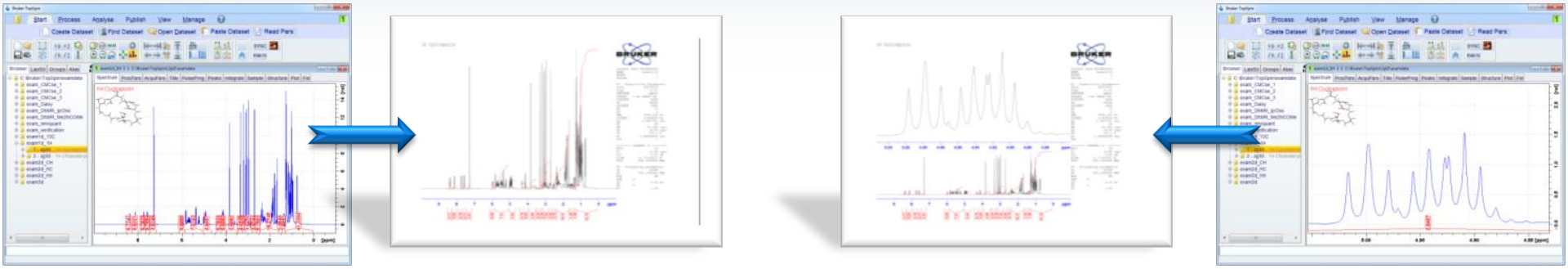




I just want to easily print what I see in TopSpin – with predefined layouts

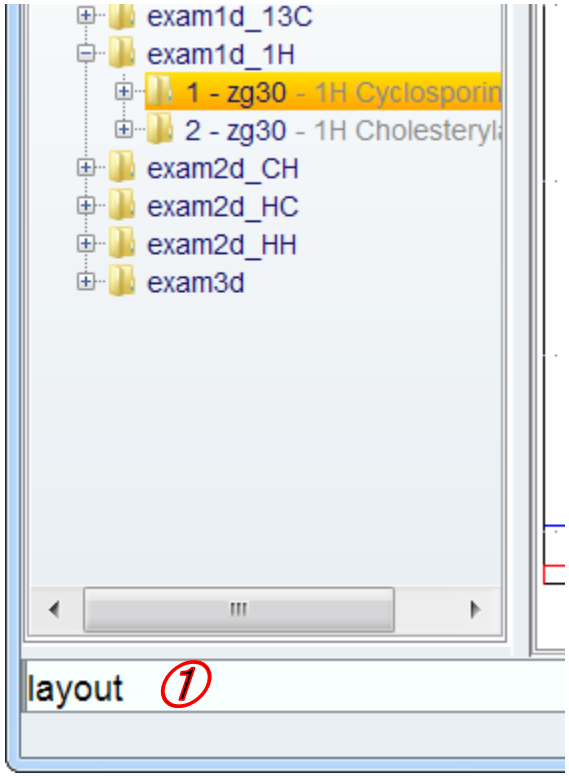


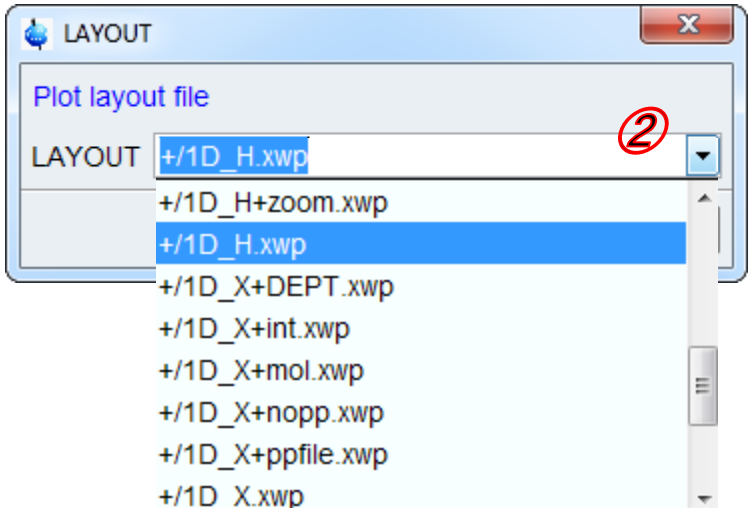
select one of the default layouts
and use the command:
autoplot

I just want to easily print what I see in TopSpin – with predefined layouts

To select a layout you can execute
either the command: **layout** ①
(or find the parameter in the processing parameter list)
and select one from the pull down list ②

More than 20 predefined layouts are delivered with TopSpin





1D_BB.xwp
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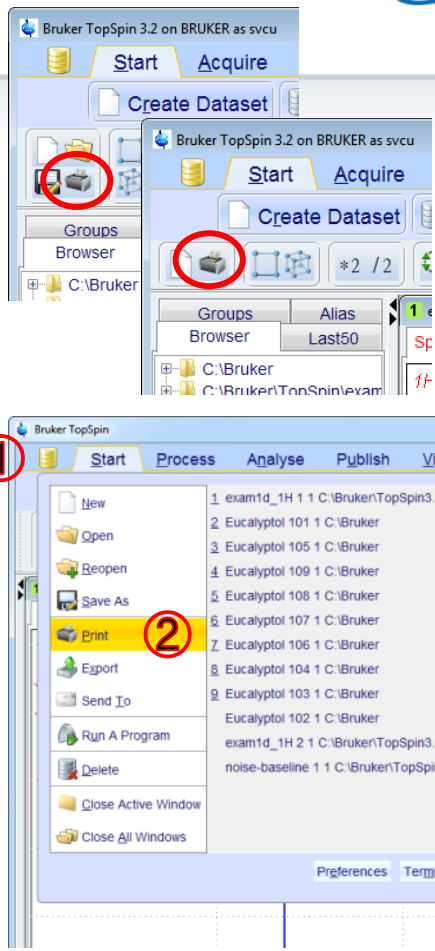
1D_H+lf.xwp
1D_H+mol.xwp
1D_H+noint+ppp.xwp
1D_H+pp.xwp
1D_H+pp+info.xwp
1D_H+pp+lf.xwp
1D_H+zoom.xwp
1D_noediff.xwp
1D_X.xwp
1D_X+DEPT.xwp
1D_X+int.xwp
1D_X+mol.xwp
1D_X+nopp.xwp
1D_X+ppfile.xwp
1D+1D+1D.xwp
1D+1D+int.xwp
1D+1D+pp.xwp
2D_2pro.xwp
2D_hom.xwp
2D_inv.xwp
t1norm.xwp

I just want to easily print what I see in TopSpin – with predefined layouts

Instead of typing in the command **prnt** you can also:

- press **Ctrl-p**
- or enter the command **print**
- or click on the printer icon: 
- or click on the TopSpin disk icon ①
  and select **Print** ②



I just want to easily print what I see in TopSpin – wit predefined layouts

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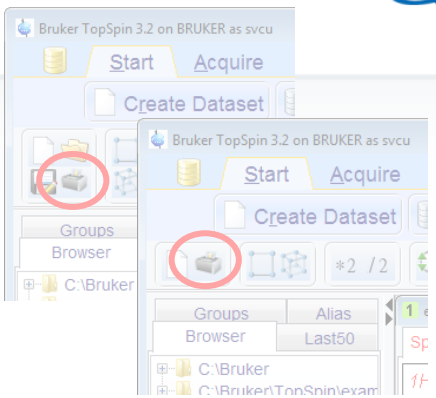
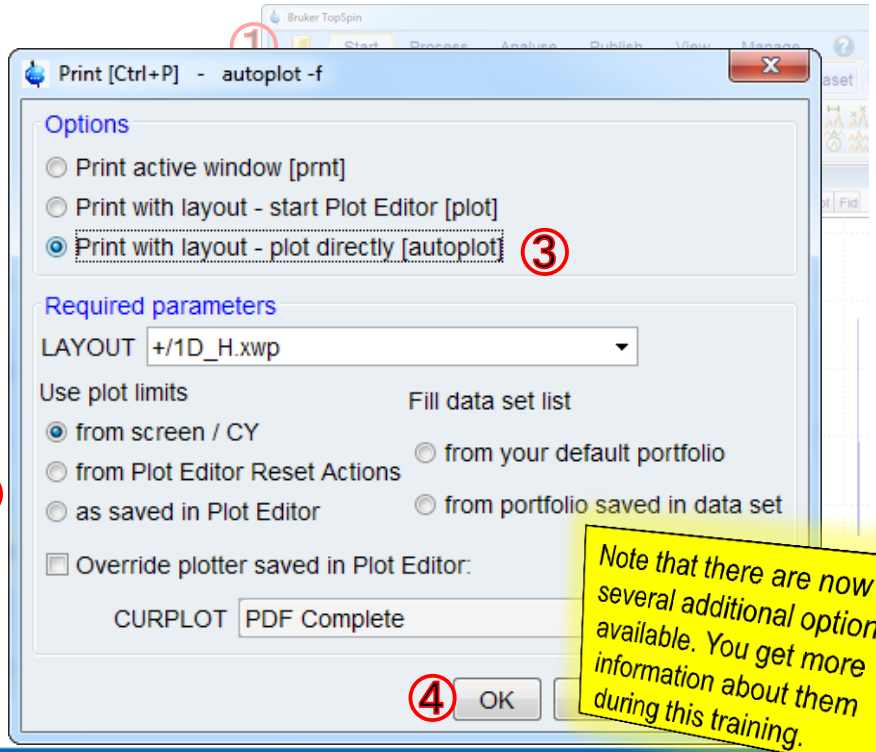




All four possibilities open the same window that offers all TopSpin print options.

Selecting the third option ③ and click **OK** ④ will execute the **autoplot** command

Different situations = different solutions
→ 1 tool

Situation 1

- I just want to easily print what I see in TopSpin
  - Fast print-out – without anything else
  - Fast print-out – with predefined layouts

Summary:

- To get printed what you see in TopSpin, use the command **prnt**

- To use a predefined layout, use the command **autoplot**
  Select a different layout with the command **layout**

Different situations = different solutions
→ 1 tool

Situation 1

- I just want to easily print what I see in TopSpin

Situation 2

- I want to easily print my own layout

Situation 3

- I would like to optimize my print-out for individual datasets

Situation 4

- I would like to get nice print-outs for all samples of my automation run

Different situations = different solutions → 1 tool

Situation 1

- I just want to easily print what I see in TopSpin

Situation 2

- I want to easily print my own layout
  - How to create my own layout
  - How to print my own layout

Situation 3

- I would like to optimize my print-out for individual datasets

Situation 4

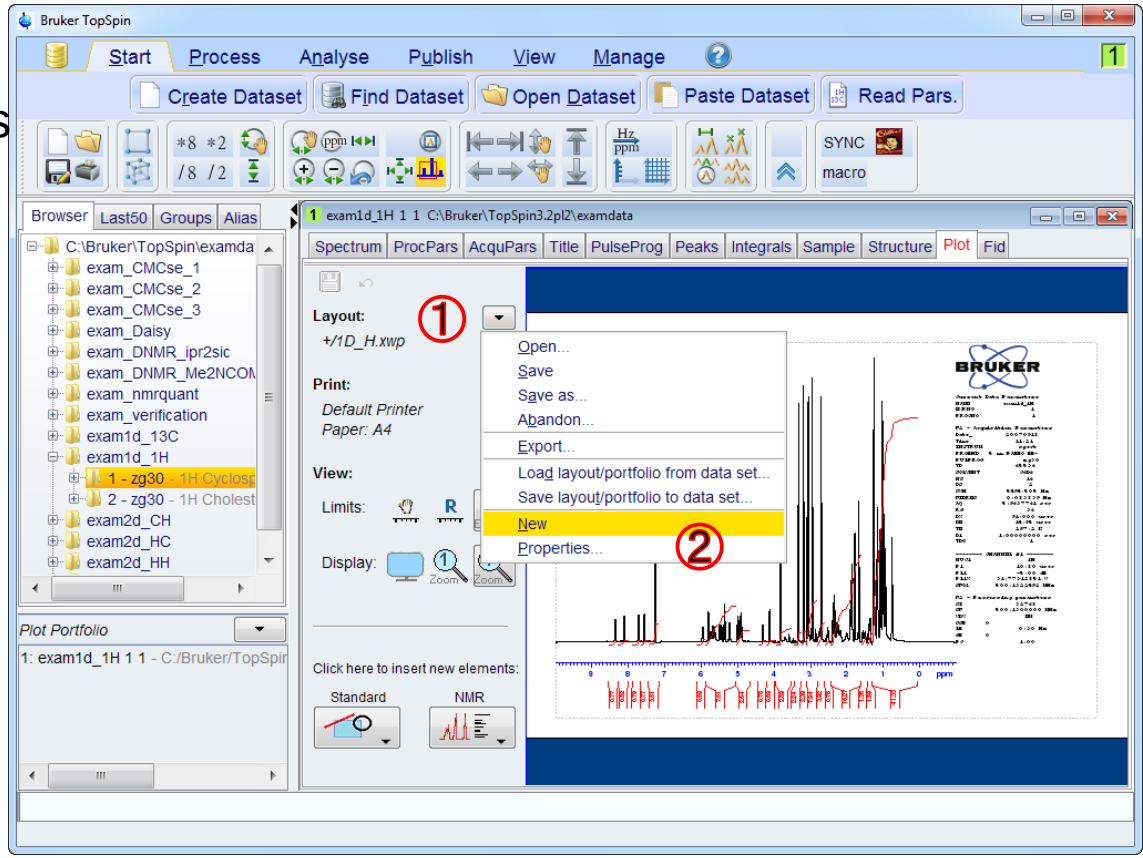
- I would like to get nice print-outs for all samples of my automation run

How to create my own layout - open an empty layout

You can take a predefined layout and modify it or you can start from scratch.
Let's have a look at the example to start from scratch (with a new, empty layout)

Opening the Plot tab always displays the predefined layout of the dataset.

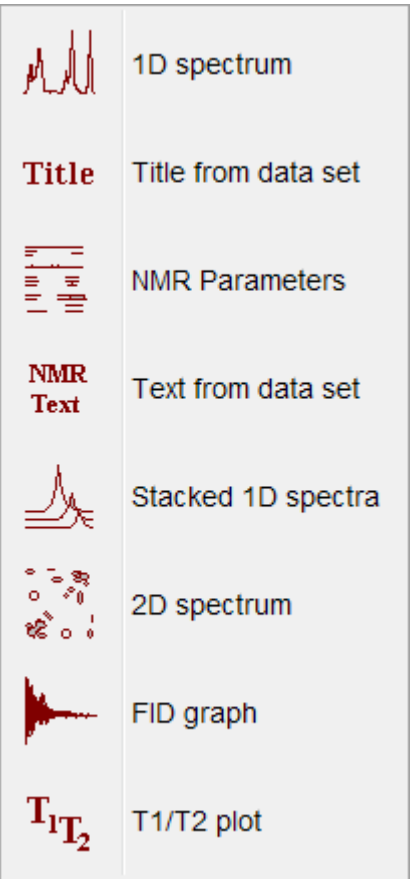
For a new layout click on the pull down menu right from **Layout** ① and select **New** ②

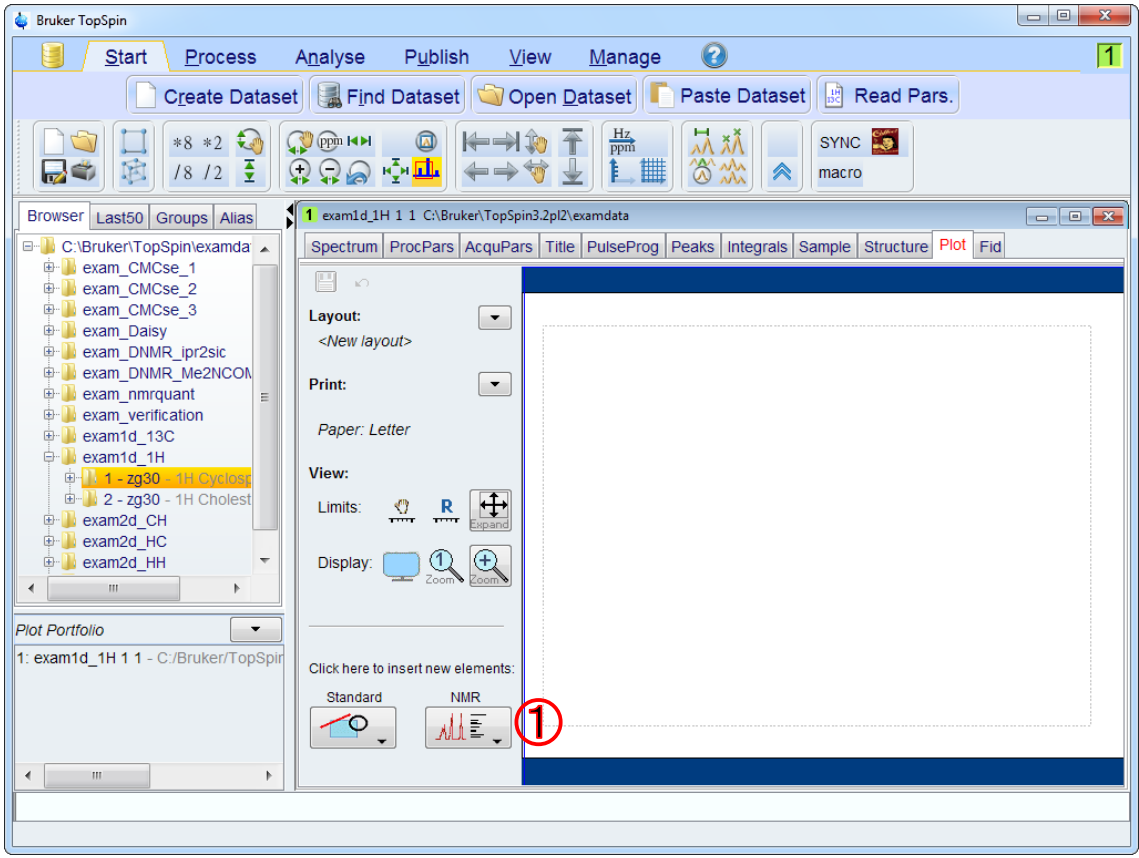


How to create my own layout - what do you want to add?

Open the pull down menu of **NMR** ①

→ you get a list of elements representing different NMR plot objects

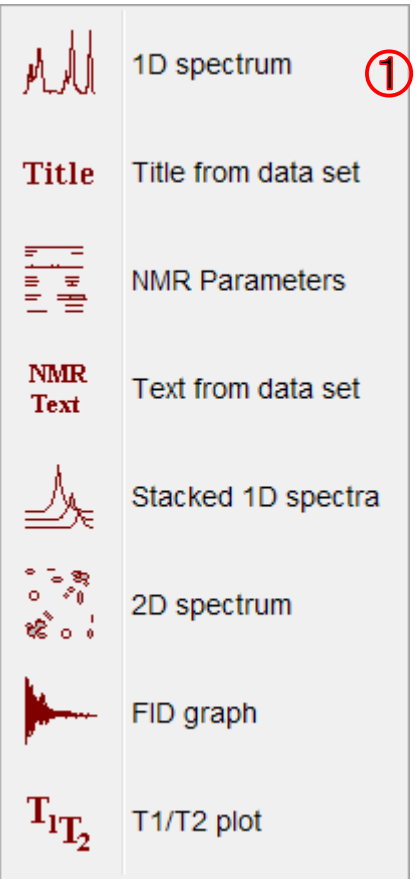




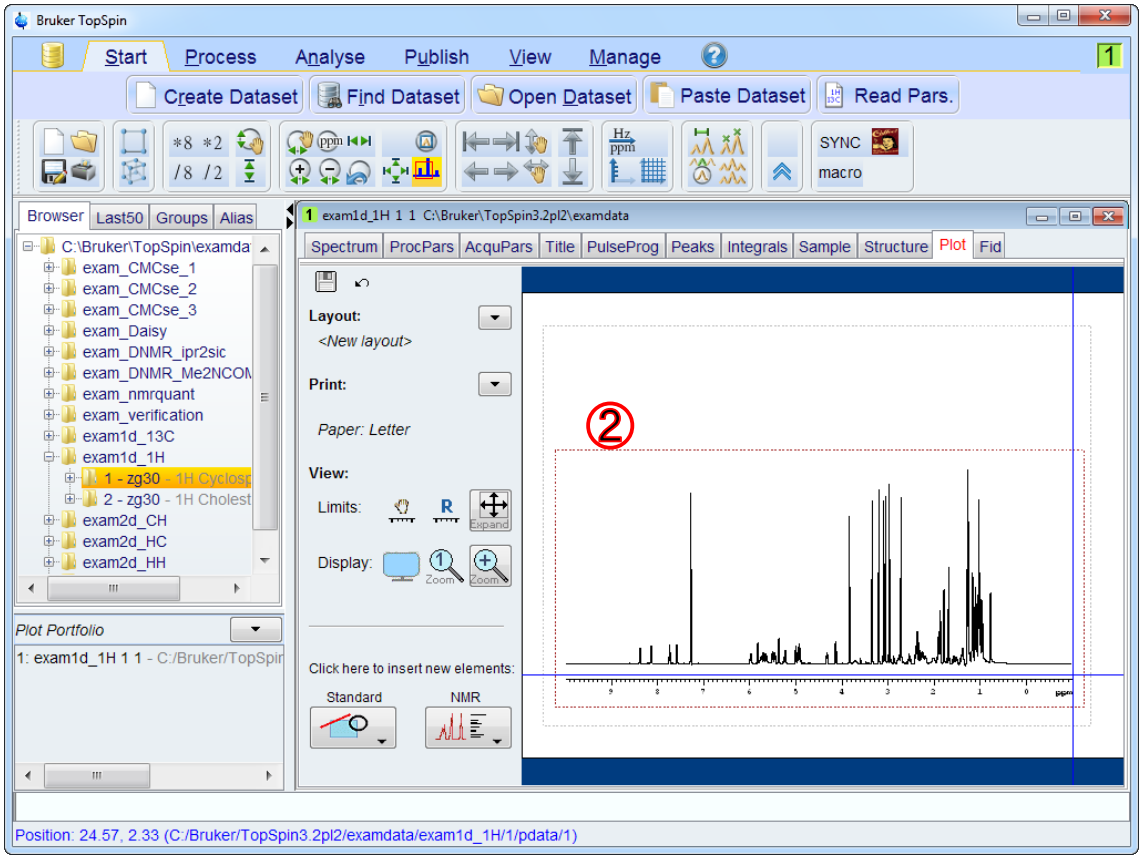
How to create my own layout - add a 1D spectrum

Select **1D spectrum** ①

→ with your mouse cursor you define position and size of your spectrum ②



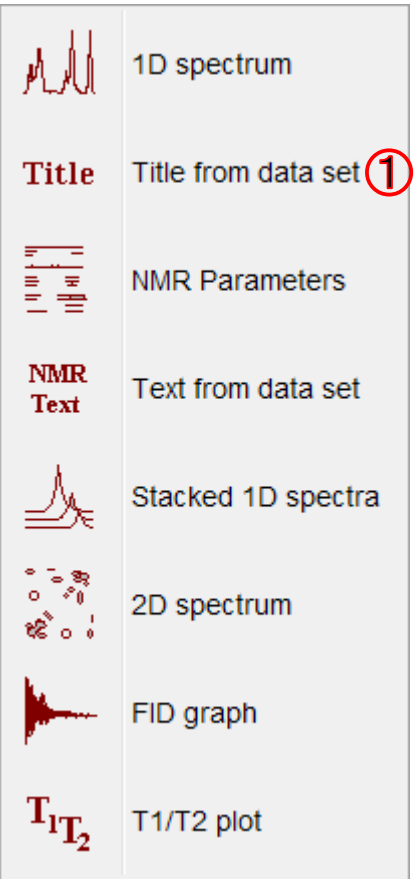
Click left mouse, keep it pressed and move the mouse to define spectrum size



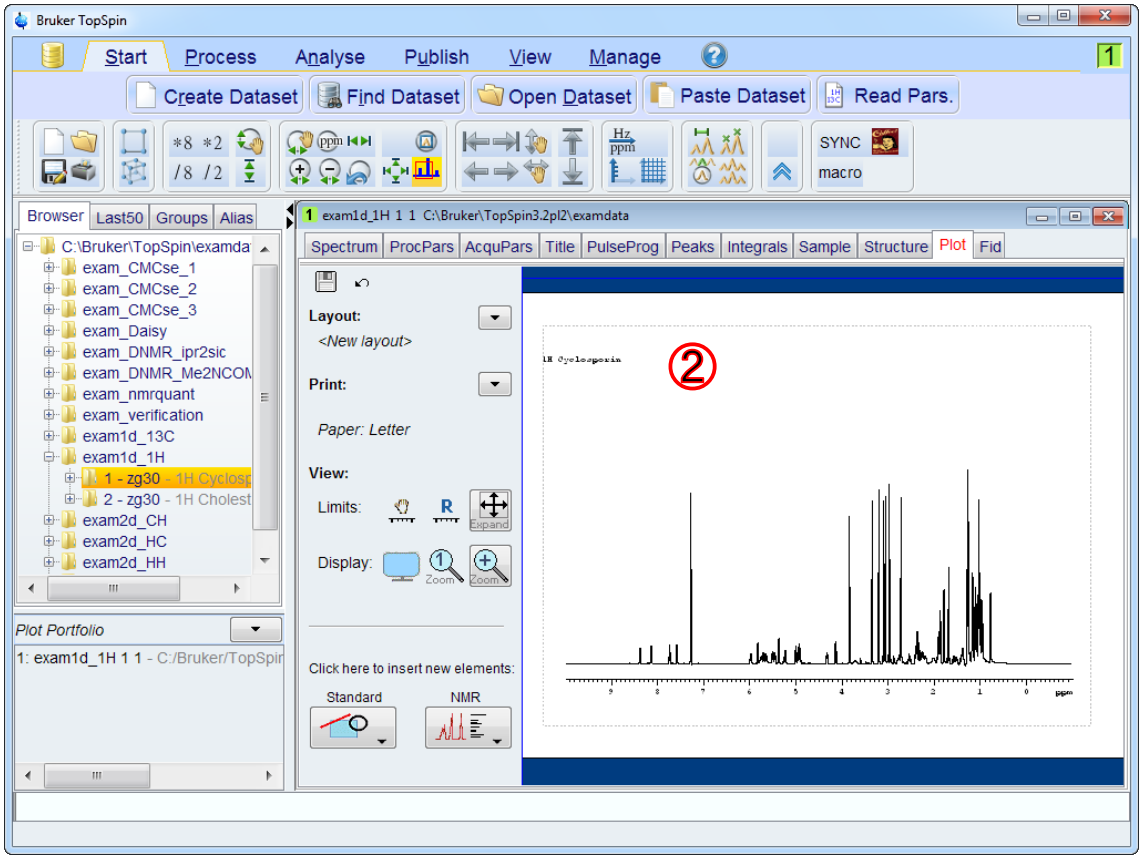
How to create my own layout - add the plot title

Select **Title** ①

→ with your mouse cursor you define position and size of your plot title ②

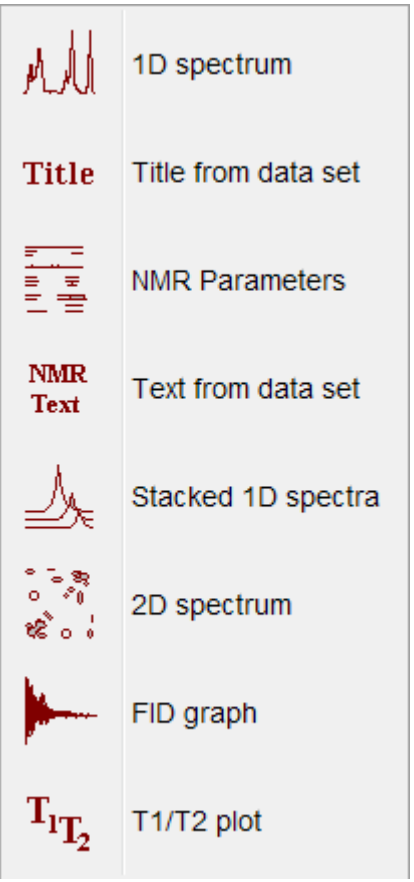


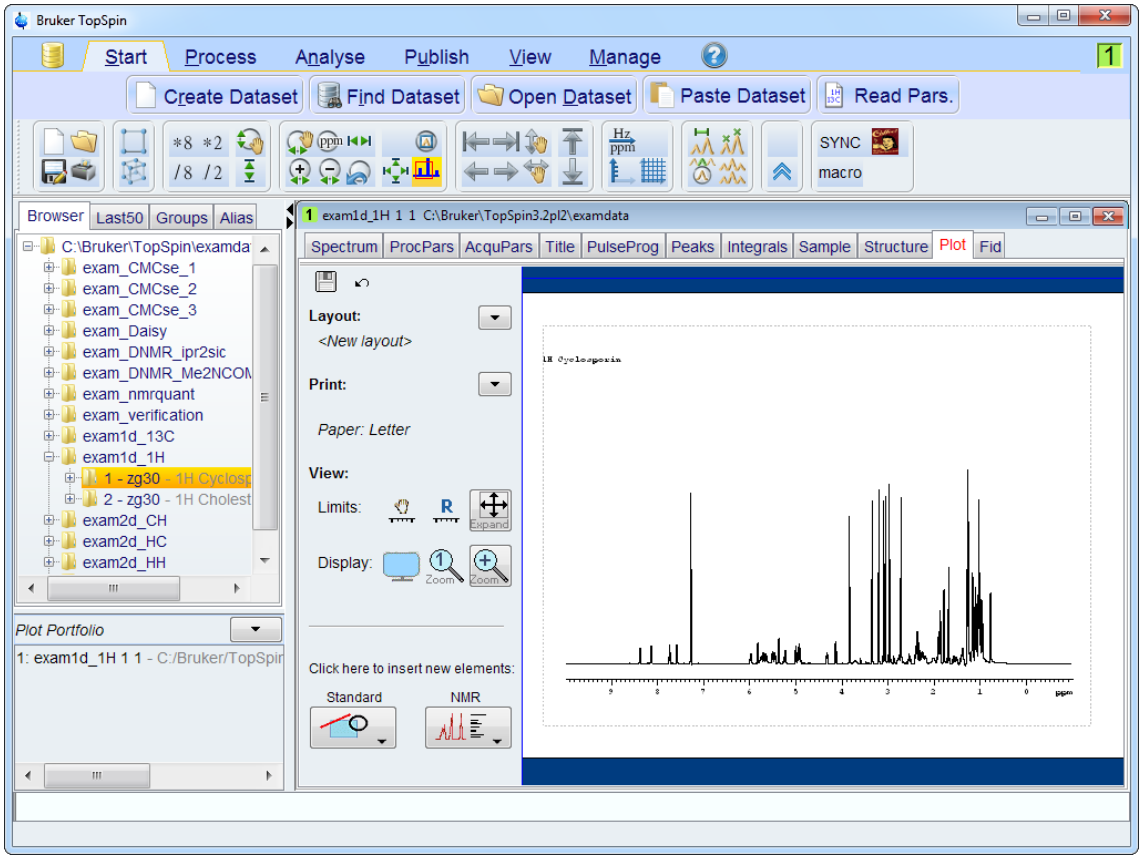
Click left mouse to put spectrum title in place



How to create my own layout - add other NMR elements

All other elements of this list can be inserted accordingly

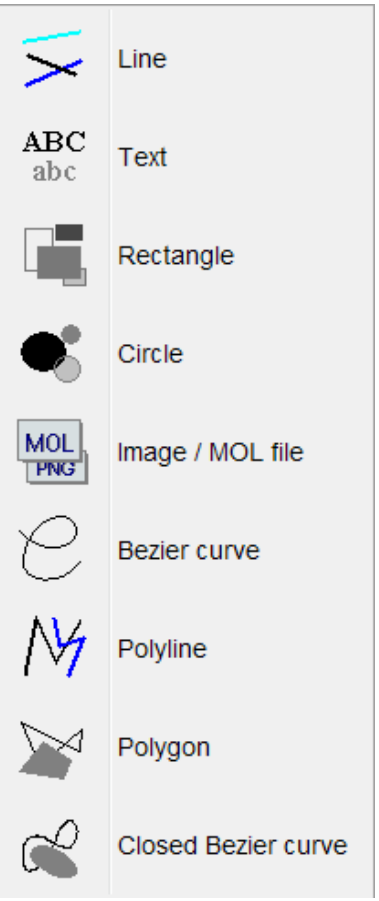


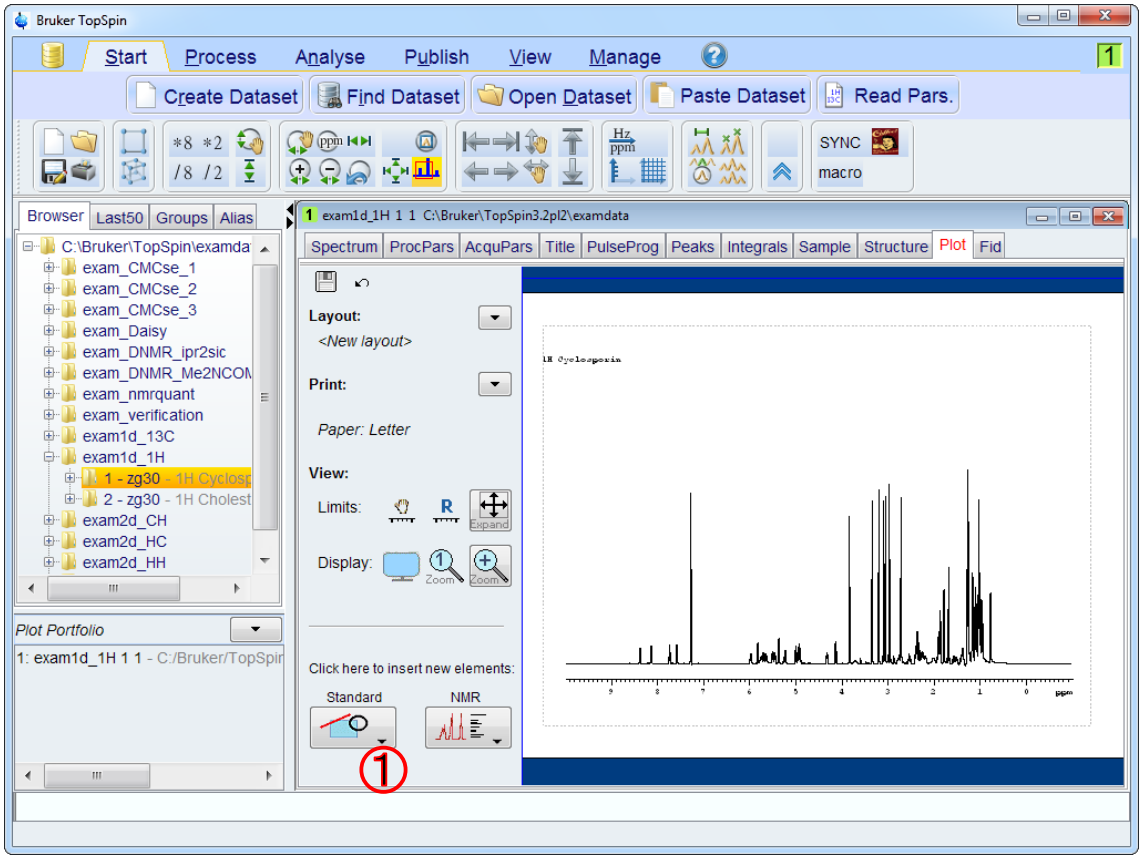


How to create my own layout
- what else do you want to add?

Open the pull down menu of **Standard** ①

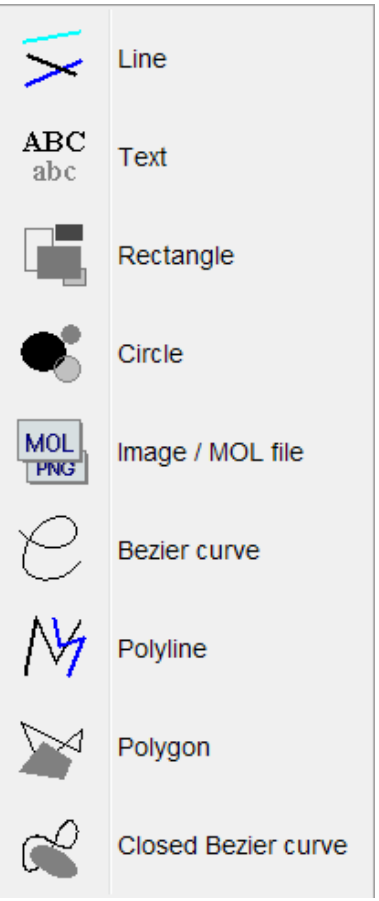
→ you get a list of elements representing different graphical objects

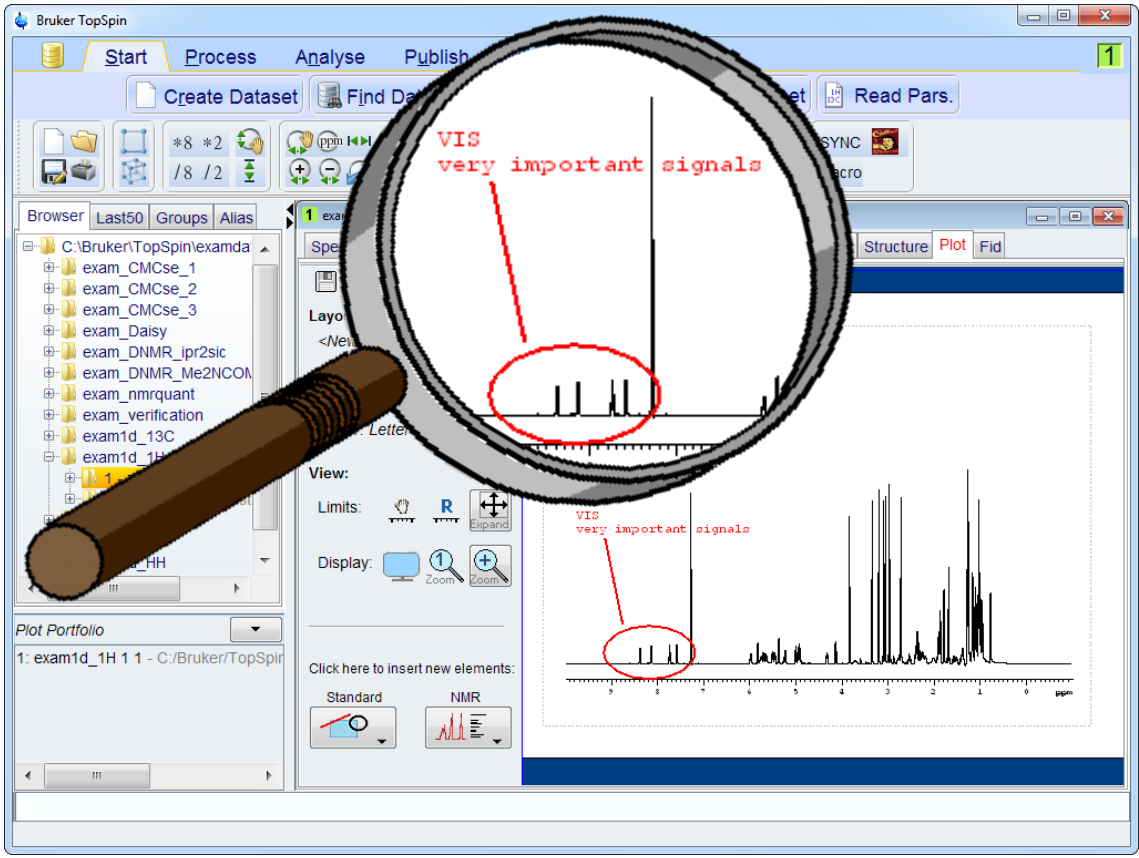




How to create my own layout
- highlighting important information

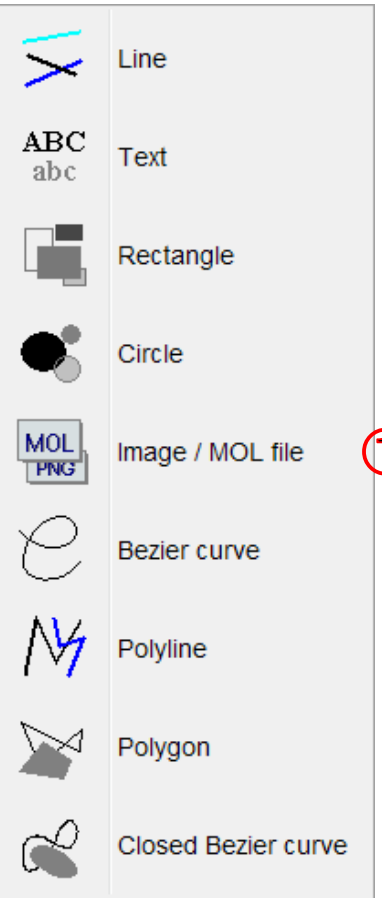
Using e.g. Circle, Line and Text



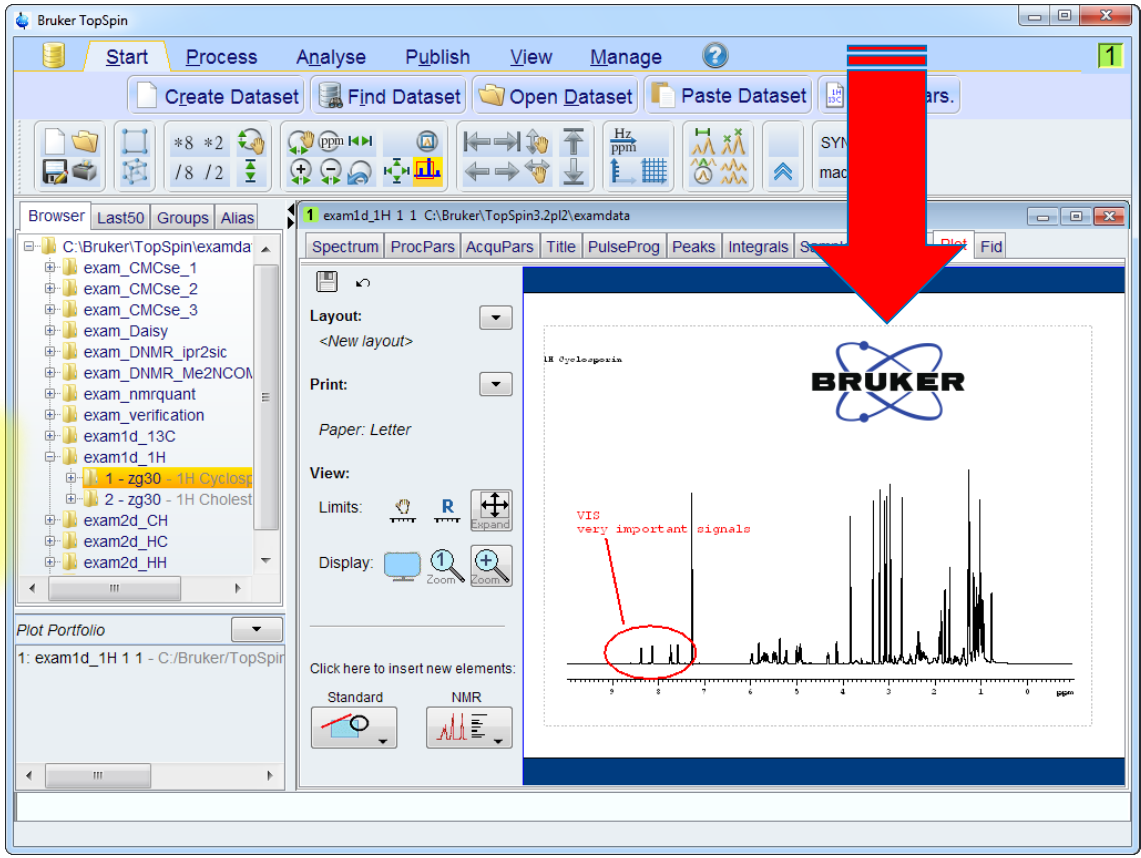


How to create my own layout - add graphics !

The most important tool in the list of Standard elements: add **Image/MOL file** ①
→ define size & position, then browse to the file on disk that should be displayed

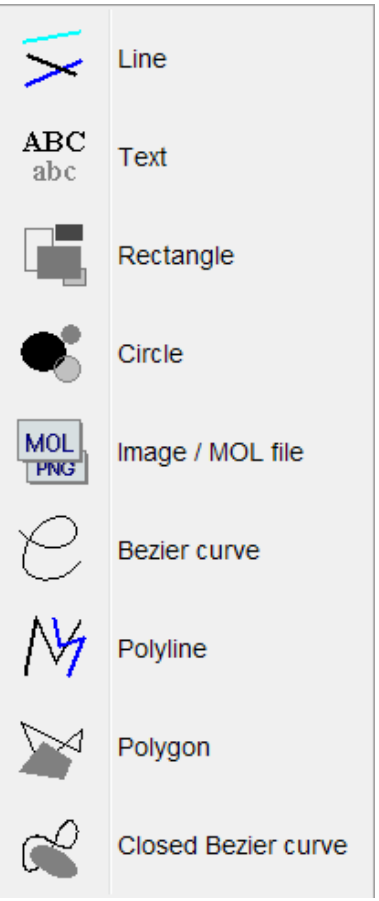


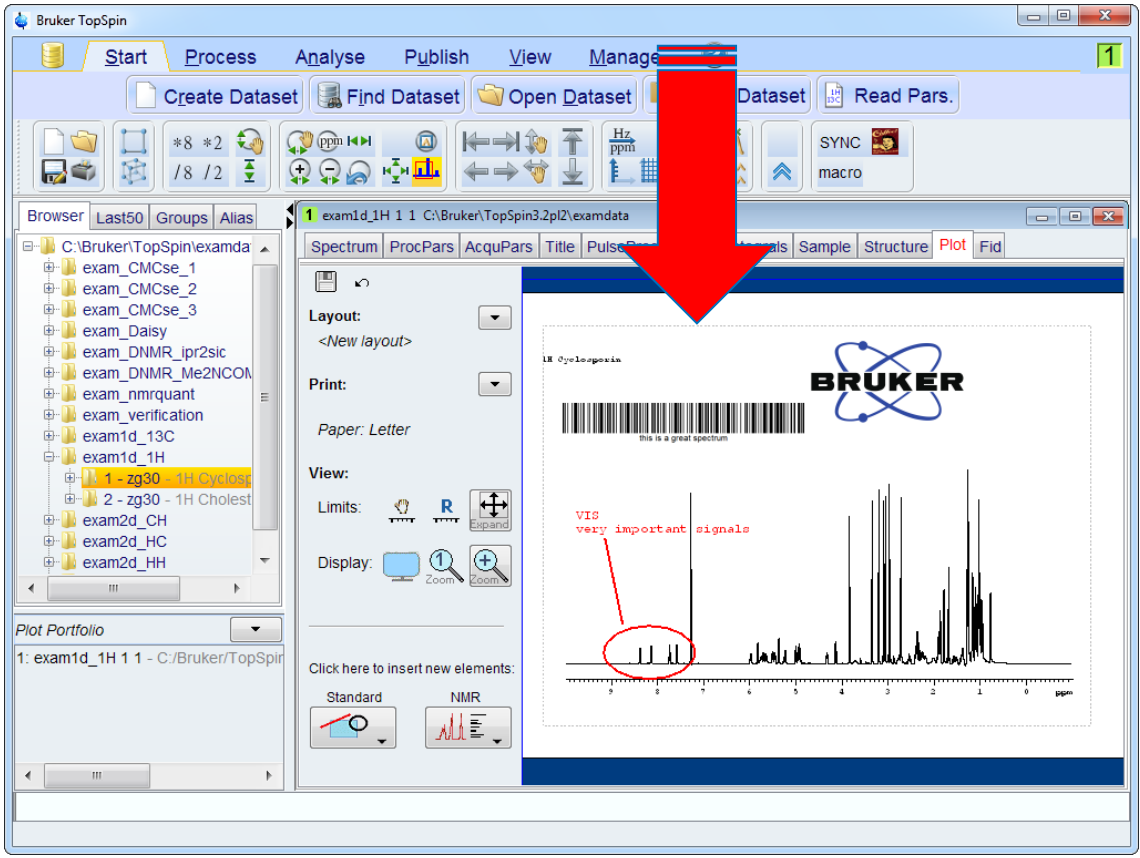
① The Bruker logo is available here: <TopSpin>/plot/bruker.png



How to create my own layout - add barcodes

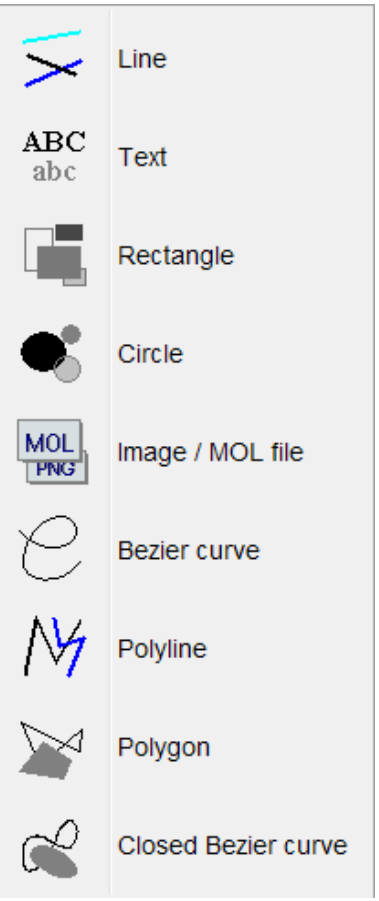
Barcodes are also graphical elements that can be displayed

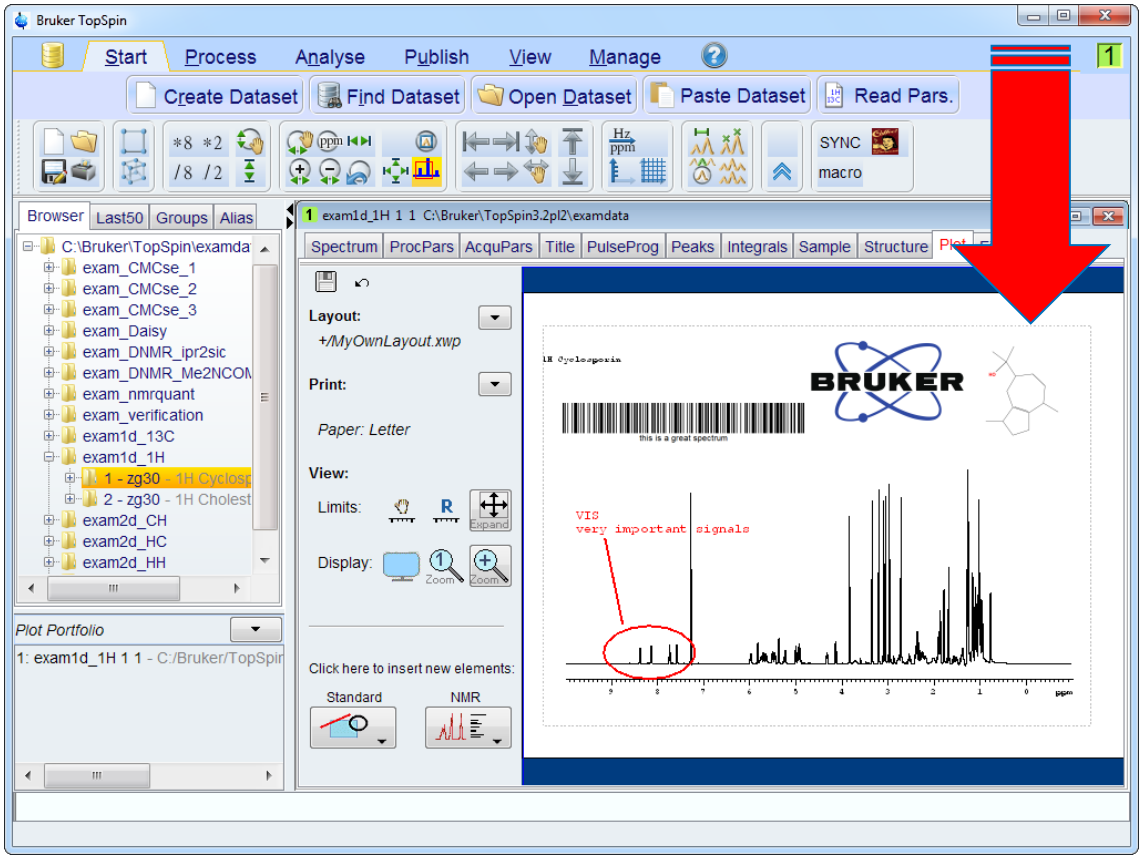




How to create my own layout
- add molecule structures (‘mol’ files)

Molecule structures can also be displayed

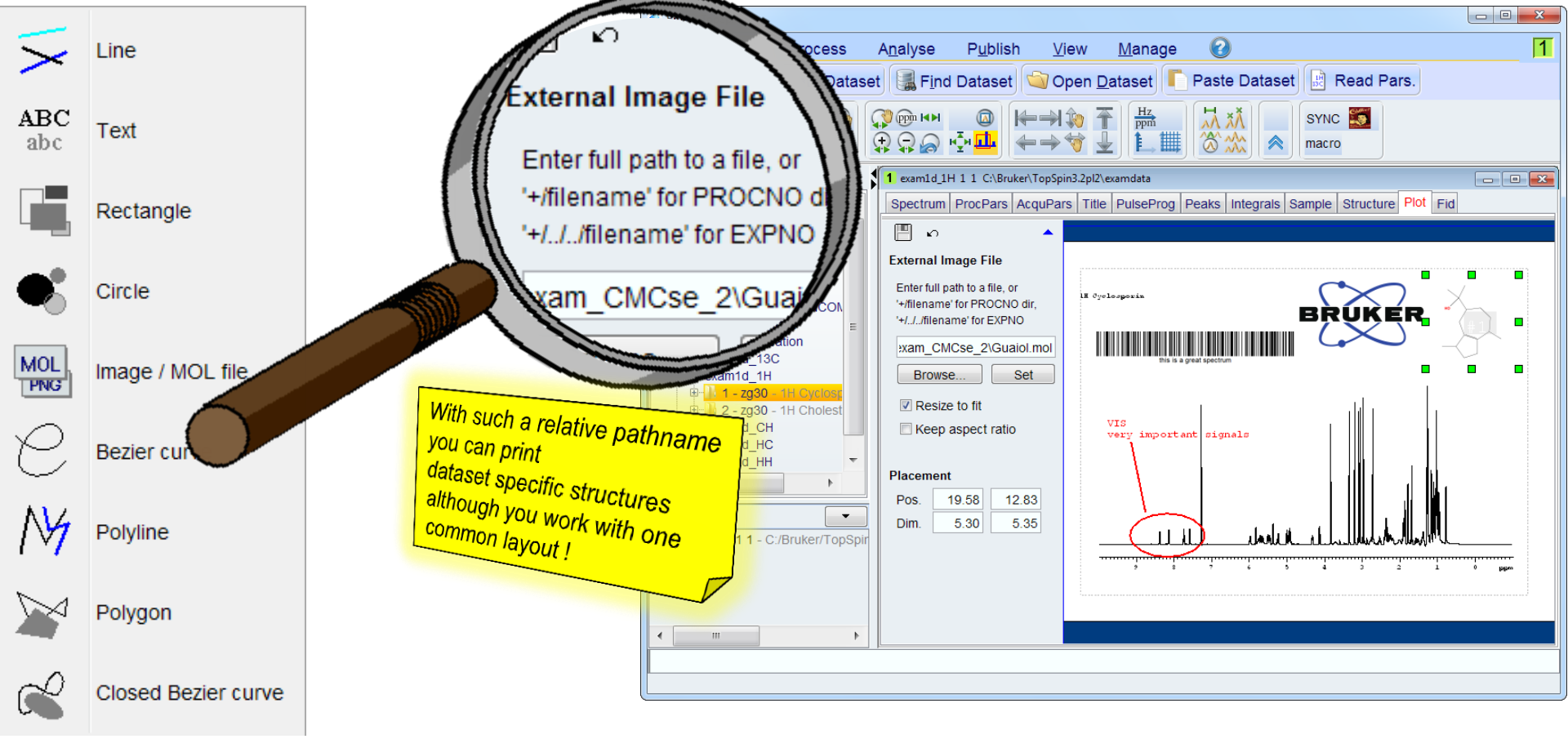




How to create my own layout
- take molecule structures from dataset

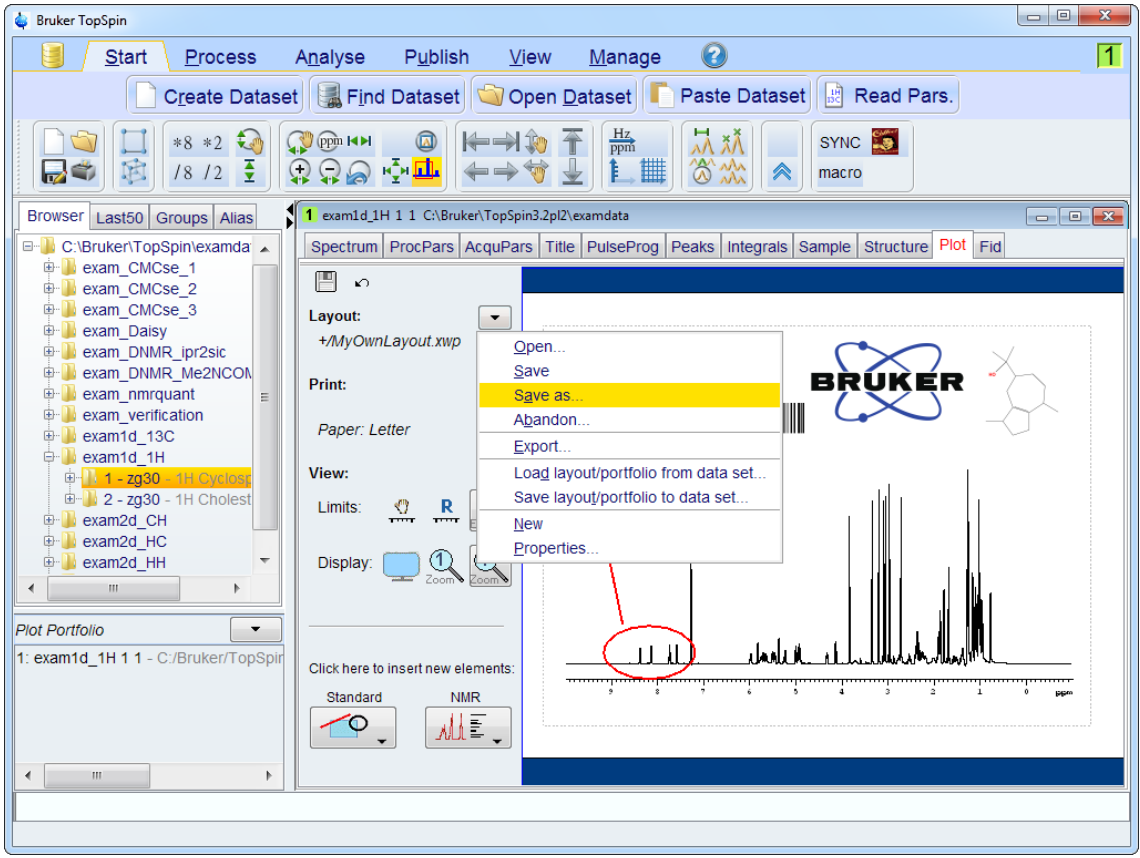
Define path to the molecule structure in a dataset specific way

→ The syntax is shown: '+/filename' for PROCNO, '+/../../filename' for EXPNO



How to create my own layout
- last step: save under a new name

Click on the pull down menu right from **Layout** and select **Save As**
→ Your layout is stored in the standard directory and can now be used for any dataset just like the Bruker layouts !



How to create my own layout
- last step: save under a new name

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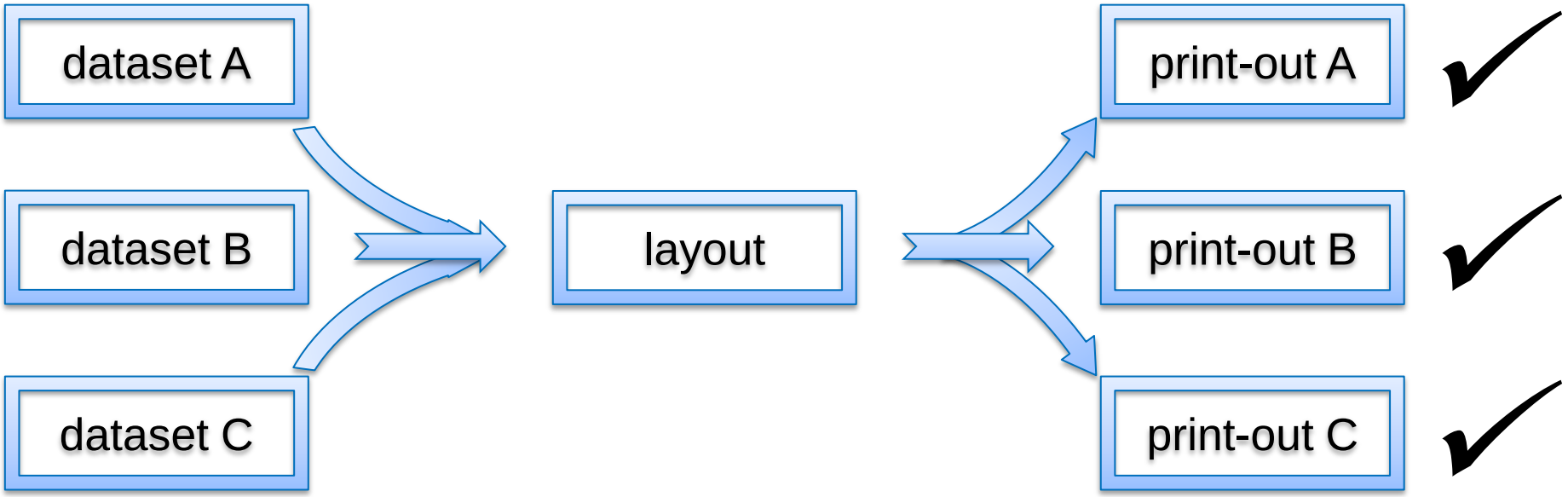
→ Your layout is stored in the standard directory and can now be used for any dataset just like the Bruker layouts !

This is the philosophy and procedure:



Different situations = different solutions
→ 1 tool

Situation 2

- I want to easily print my own layout

Summary:

- Setting up own layouts is easy and offers nice functionalities
- Own layouts can be used in the same way as Bruker layouts with the command:
  autoplot
  They appear in the standard list of all layouts and can be selected with the command:
  layout

Different situations = different solutions
→ 1 tool

Situation 1

- I just want to easily print what I see in TopSpin

Situation 2

- I want to easily print my own layout

Situation 3

- I would like to optimize my print-out for individual datasets

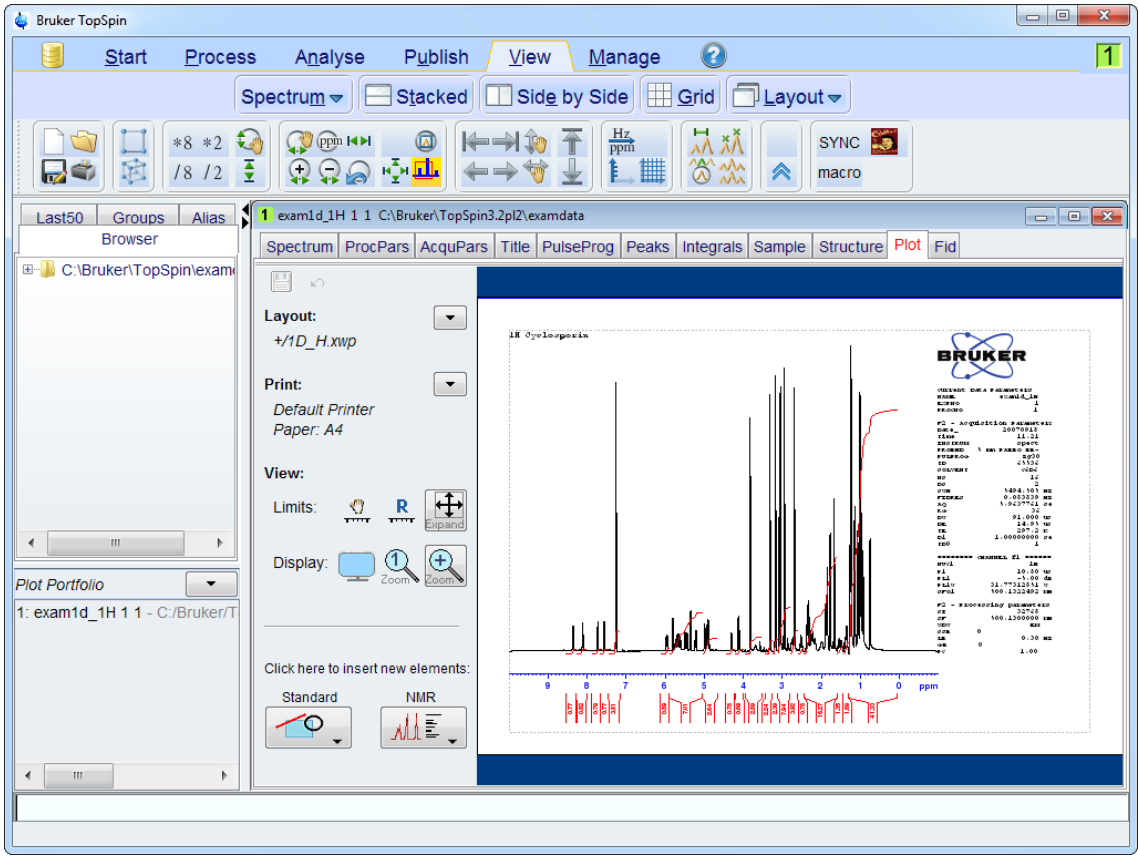
Situation 4

- I would like to get nice print-outs for all samples of my automation run

Interactive/dataset specific manipulations - these are the possibilities

Overview about interactive manipulations:

- spectrum area & information
- position & size
- colors & fonts
- alignment
- …



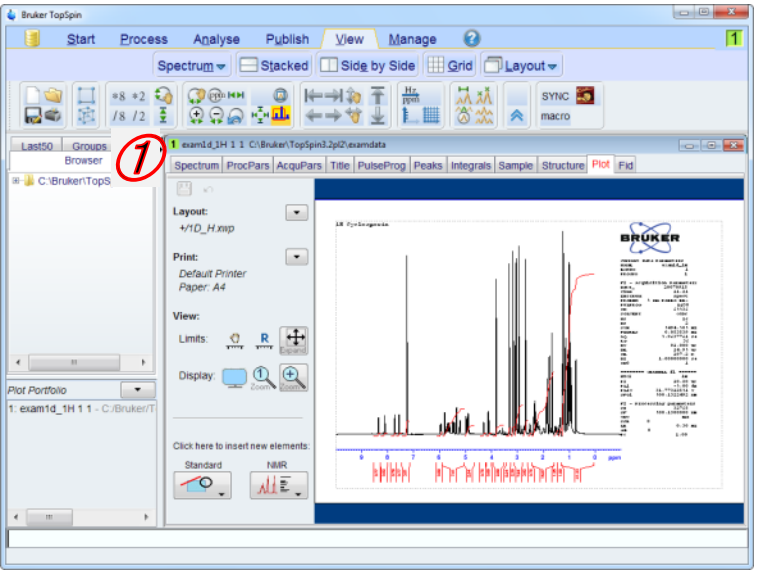
Note:
The most important settings are discussed in detail on the following slides.

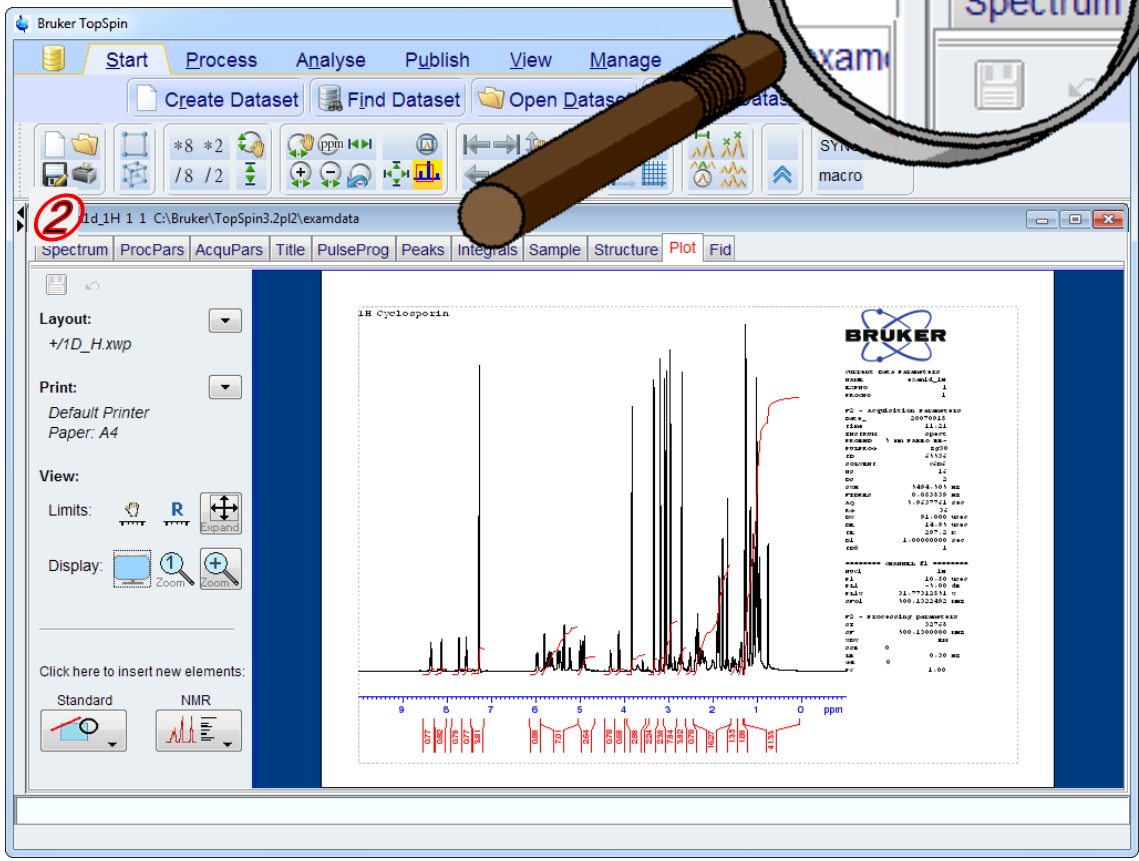
For all details please refer to the manual or just play a little bit with the program.

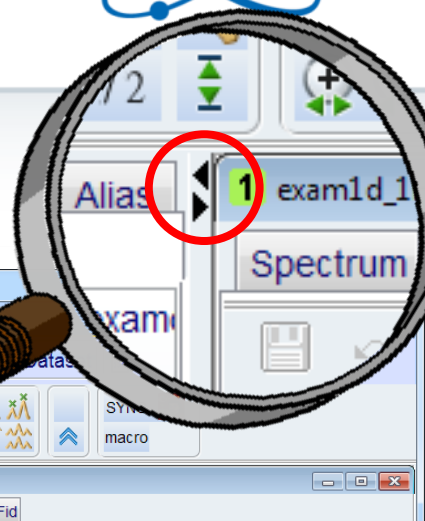
Interactive/dataset specific manipulations
- for your convenience: increase the size on screen

To see the plot layout with increased size, you can temporarily hide the left panels by clicking the arrow ‘left’ ①:

You can reopen the panel anytime by clicking the arrow ‘right’ ②



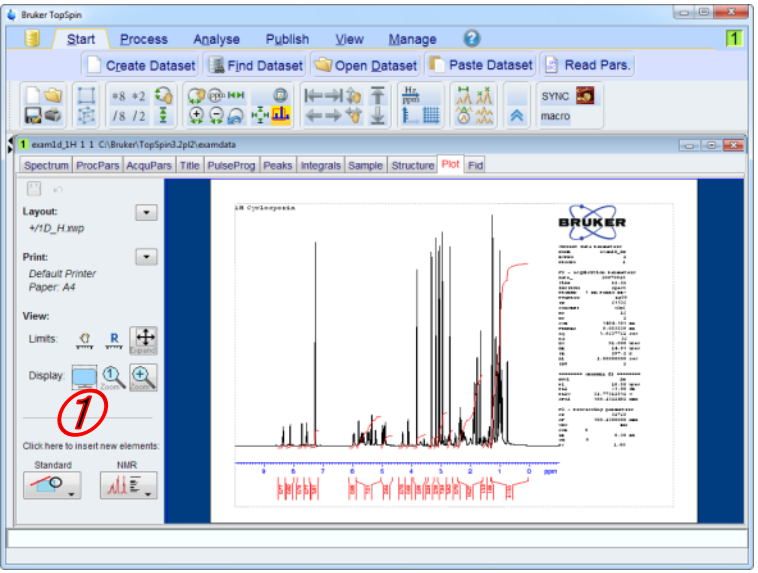


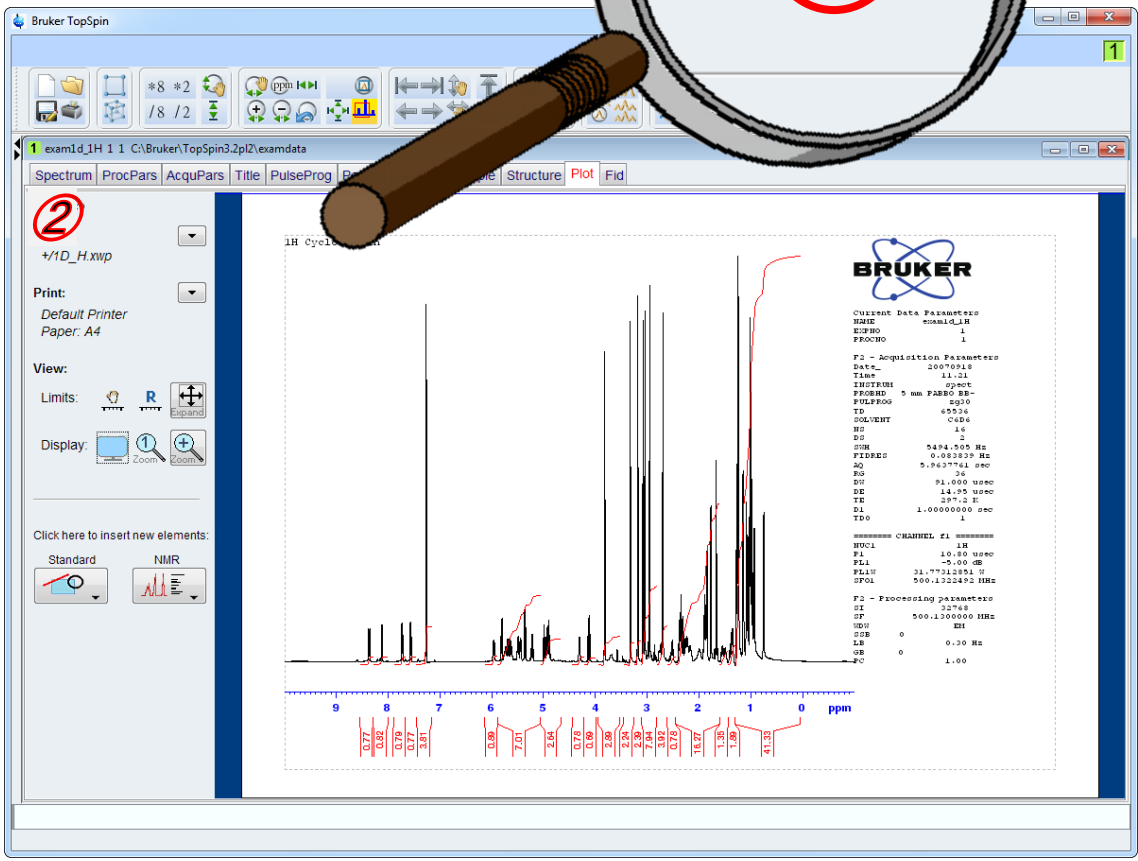


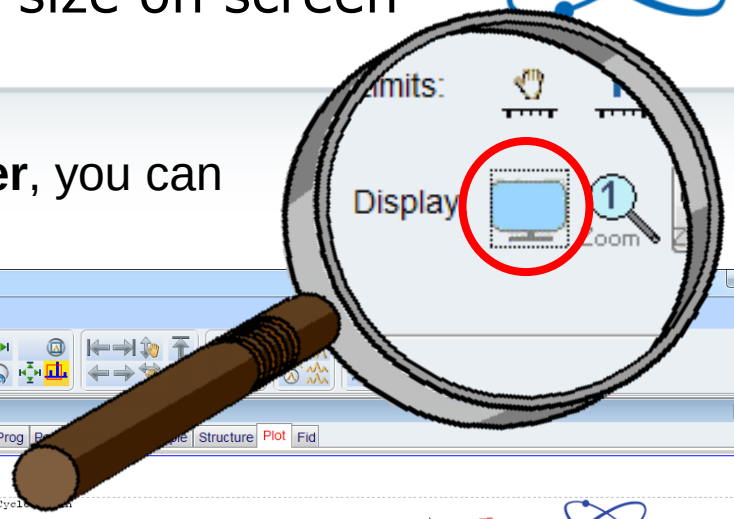
Interactive/dataset specific manipulations
- for your convenience: increase the size on screen

To increase the size of the plot layout **even further**, you can temporarily hide the left panels and menus ①:

You can get them back by switching to the Spectrum tab ②







Interactive/dataset specific manipulations - select an element

To change any setting, an element must be selected first

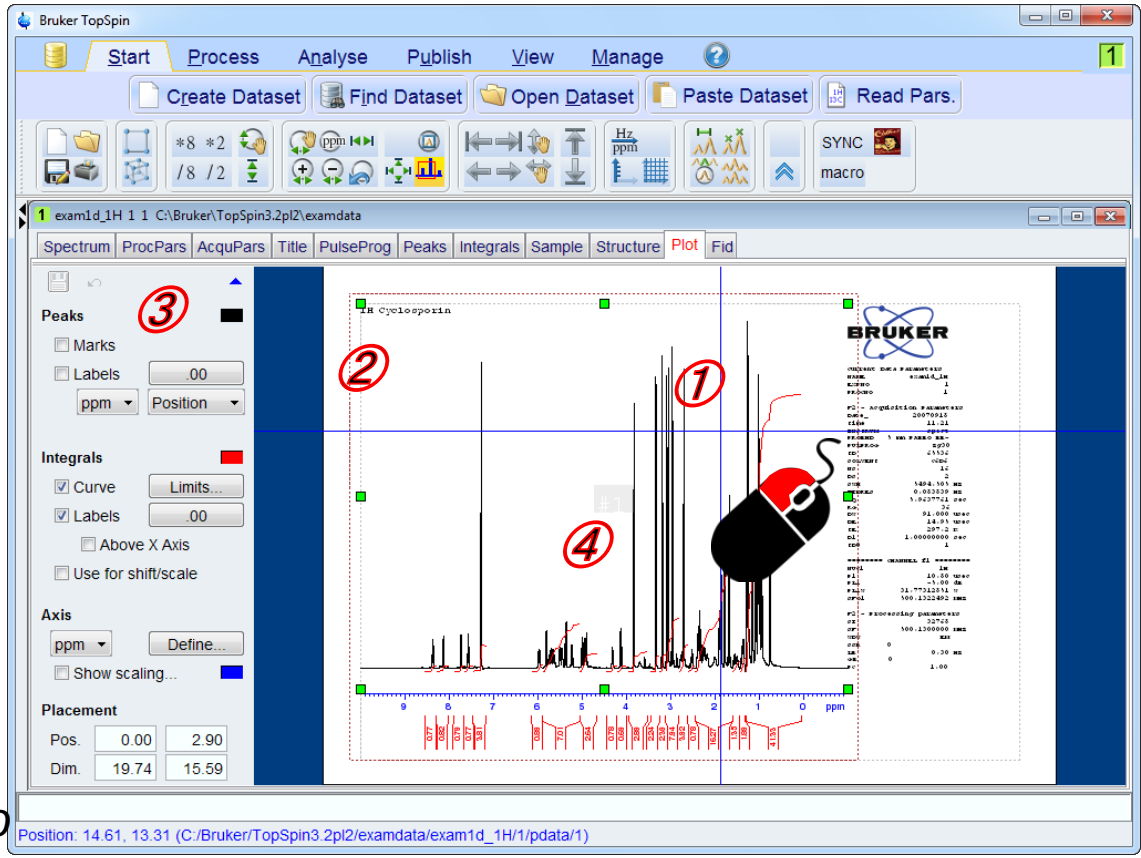
To select an element, click left anywhere on the element ①

→ *green boxes appear at the frame of the element ②*

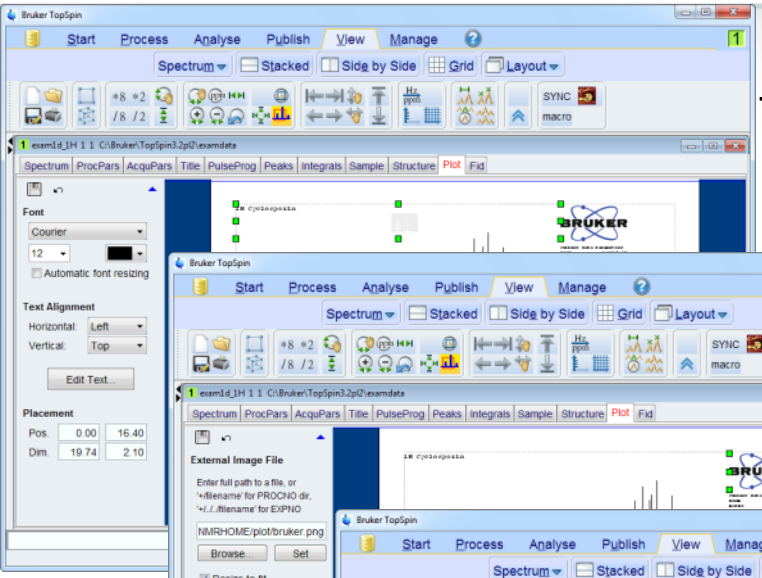
→ *left panel now offers manipulation possibilities ③*

→ *the element shows a transparent number ④*

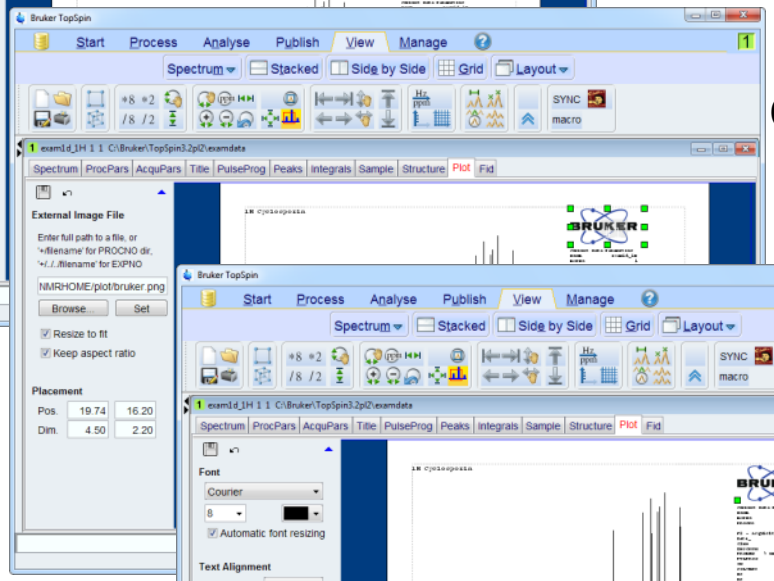
→ *identifier element / dataset number of position in portfolio*



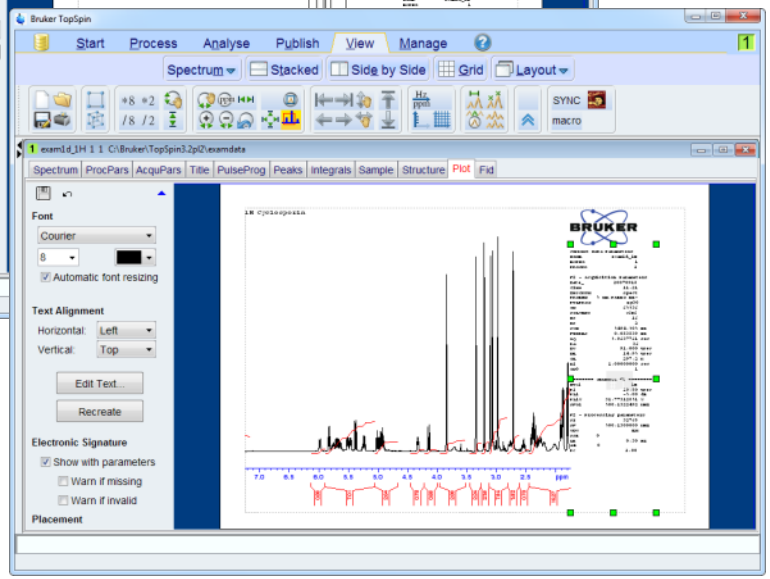
Interactive/dataset specific manipulations
- different configurations for different kind of elements



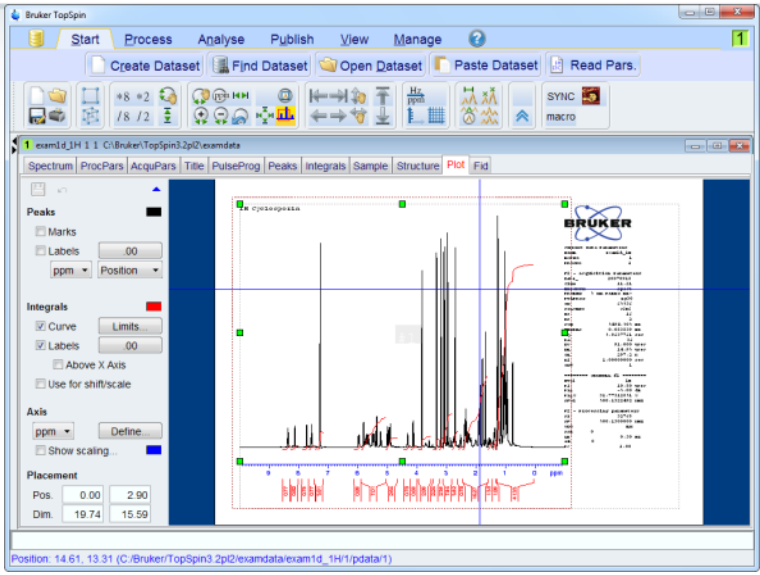
Title



Graphics



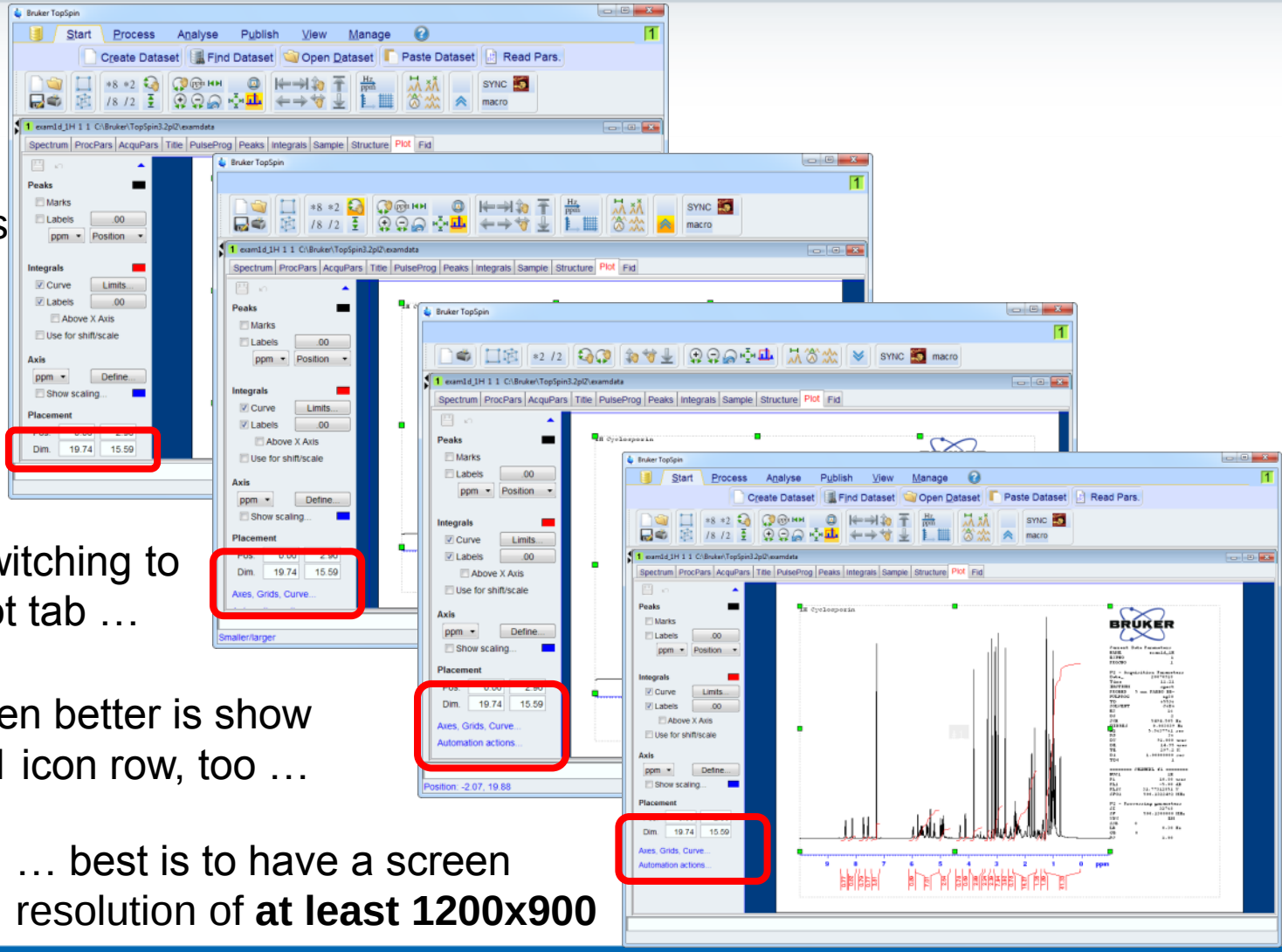
Parameter



1D spectrum

Interactive/dataset specific manipulations - minimum screen resolution required

A screen resolution of 1024x768 does not show all configuration settings …



… better is switching to full screen plot tab …

… even better is show only 1 icon row, too …

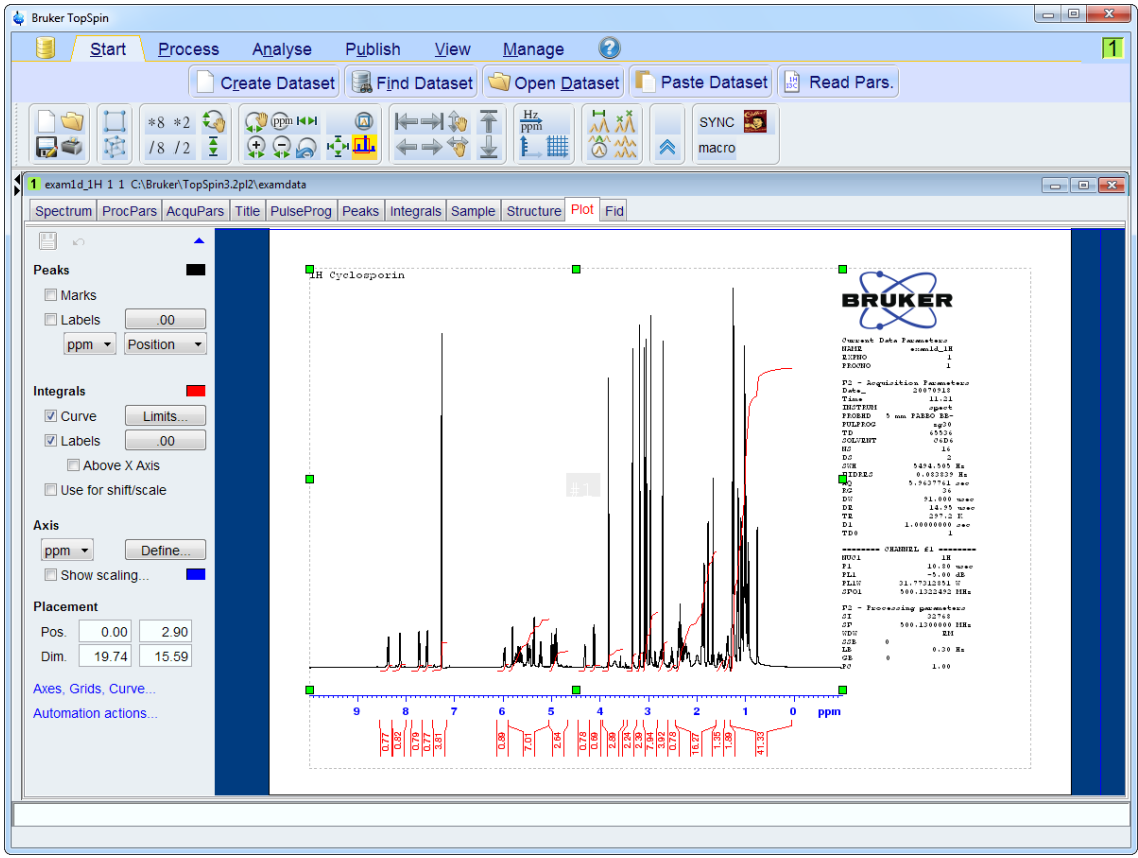
… best is to have a screen resolution of **at least 1200x900**

Jump back to last slide

Interactive/dataset specific manipulations - configuration for 1D spectra

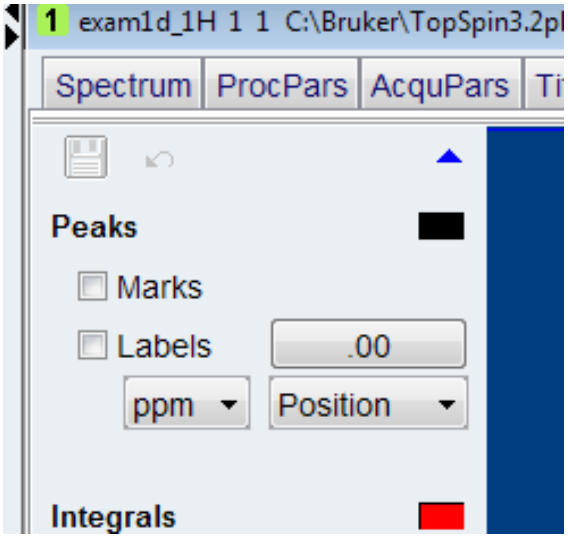
In 1D spectra elements, these configurations are available:

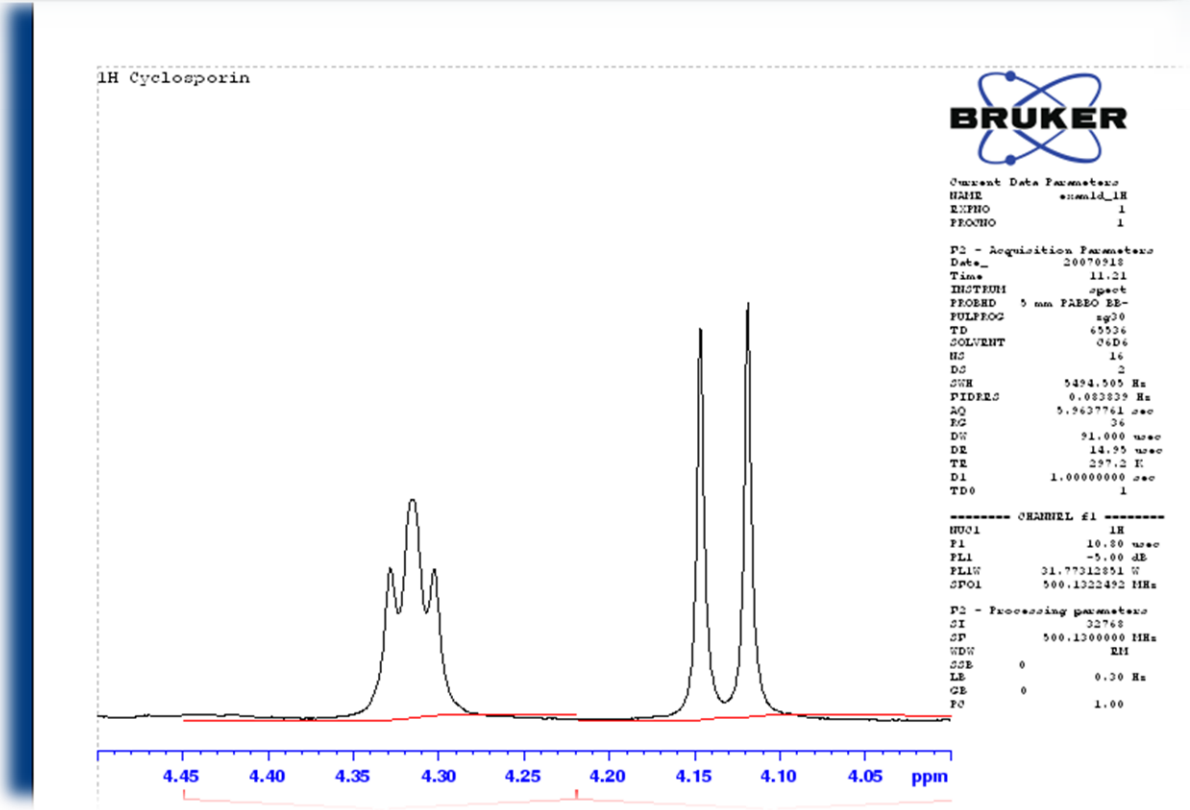
- peaks settings
- integrals settings
- axis settings
- size and position
- …



Interactive/dataset specific manipulations
- 1D spectra: peaks settings

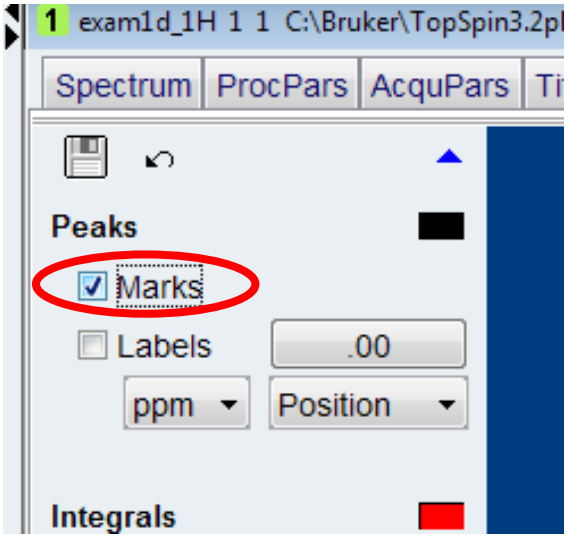
Peaks can be:
- not displayed

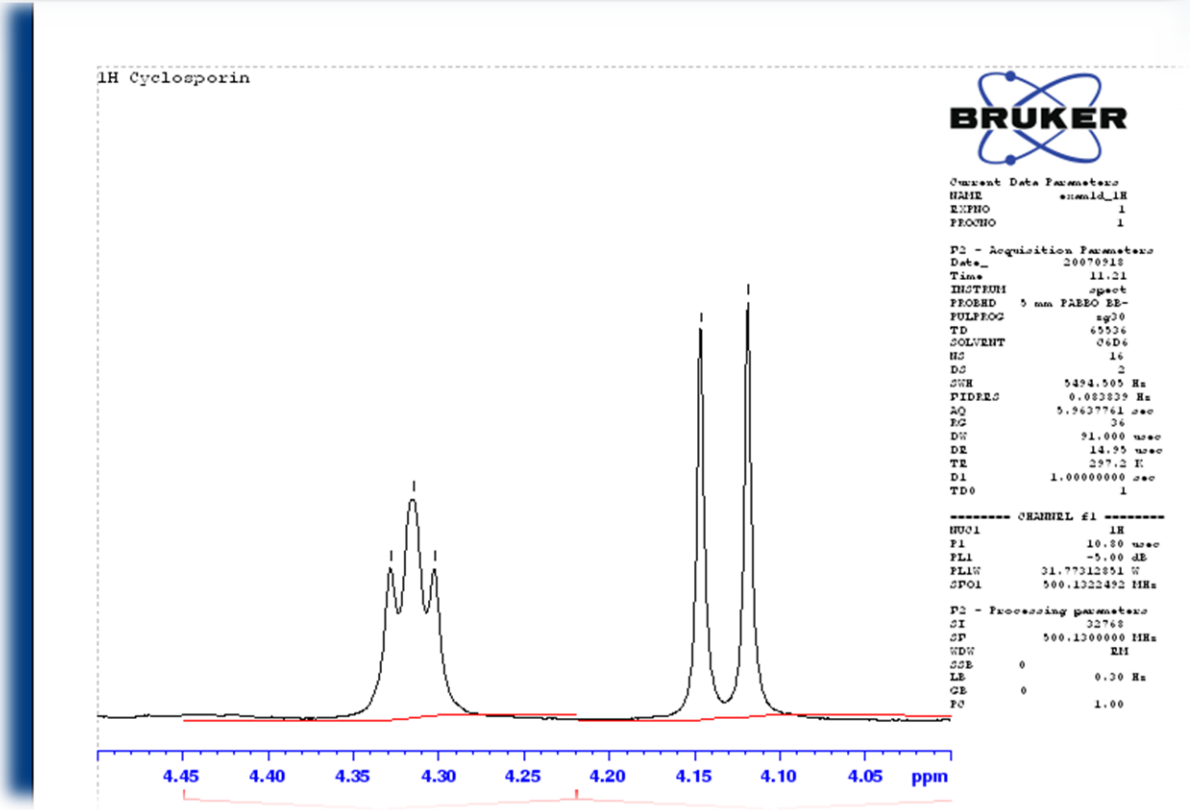




Interactive/dataset specific manipulations
- 1D spectra: peaks settings

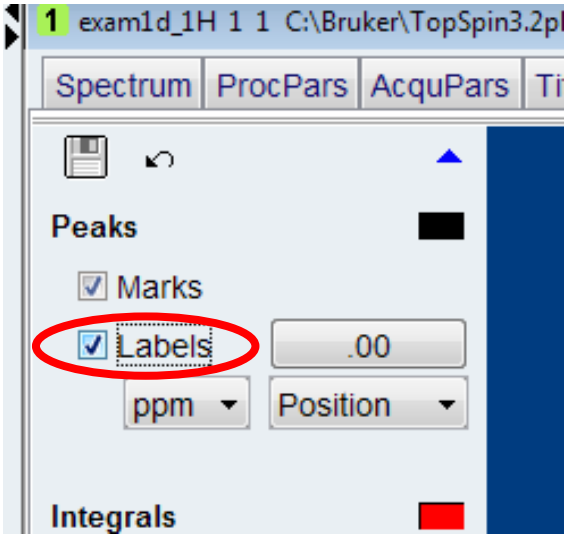
Peaks can be:
- not displayed
- displayed with marks

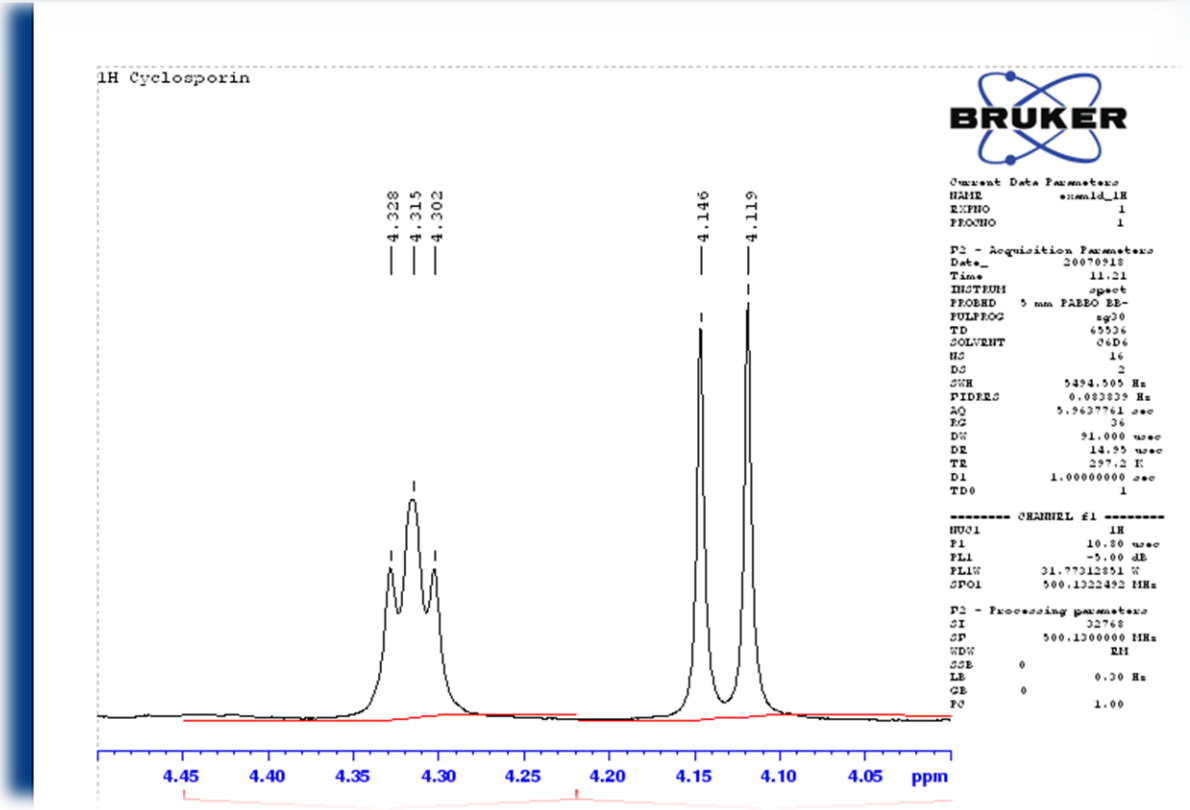




Interactive/dataset specific manipulations
- 1D spectra: peaks settings

Peaks can be:
- not displayed
- displayed with marks
- displayed with labels

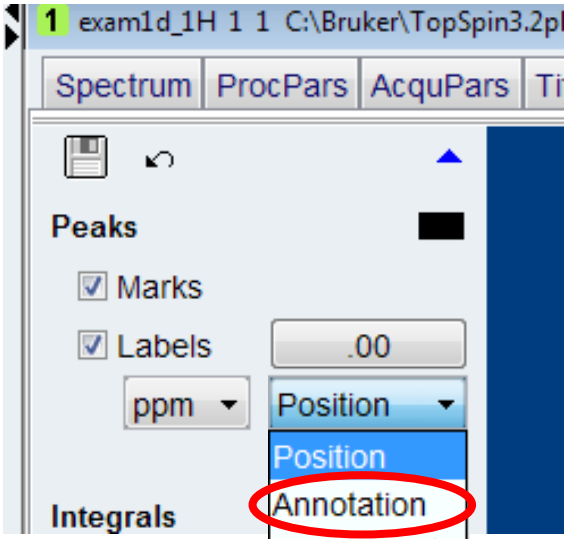


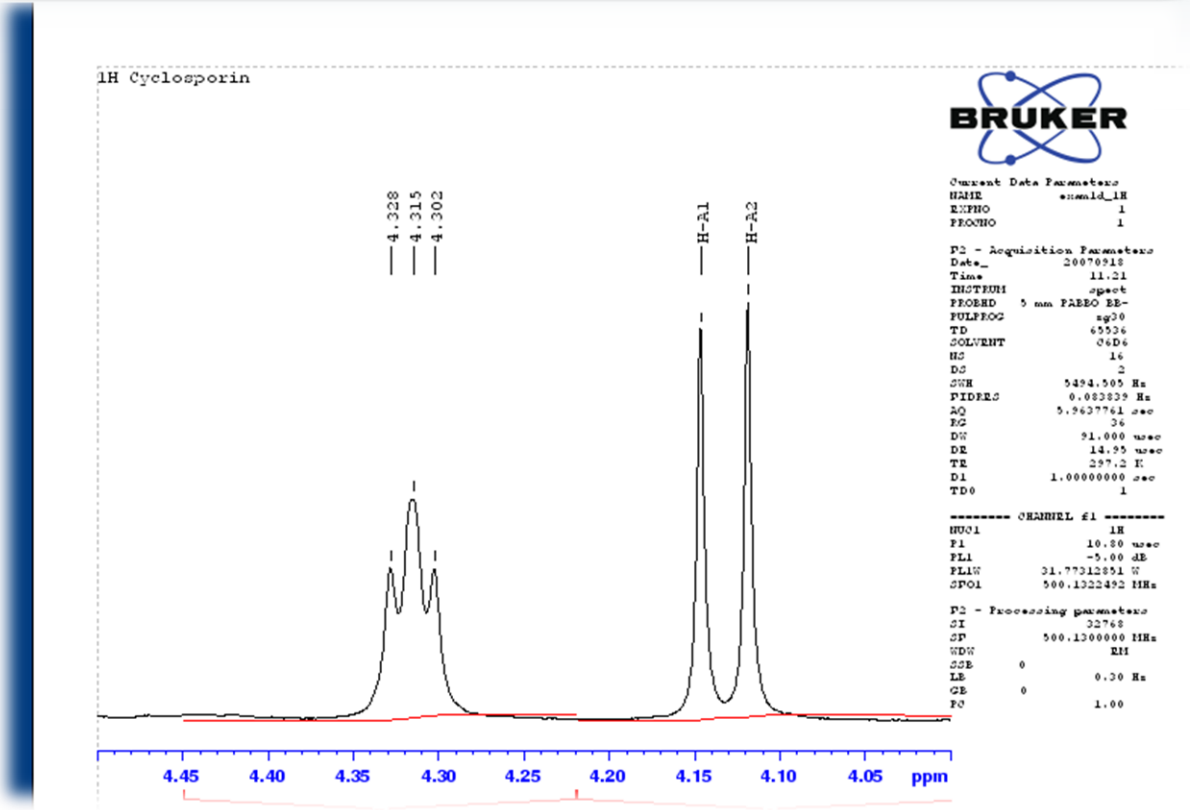


Interactive/dataset specific manipulations
- 1D spectra: peaks settings

Peaks can be:
- not displayed
- displayed with marks
- displayed with labels

They can show
- position or label or both

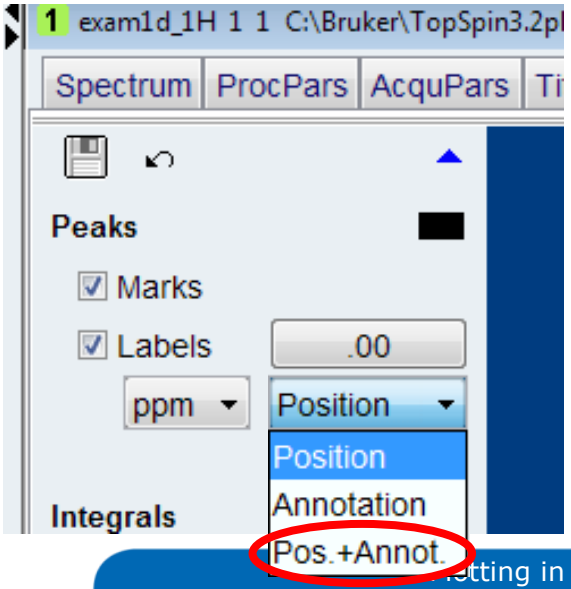


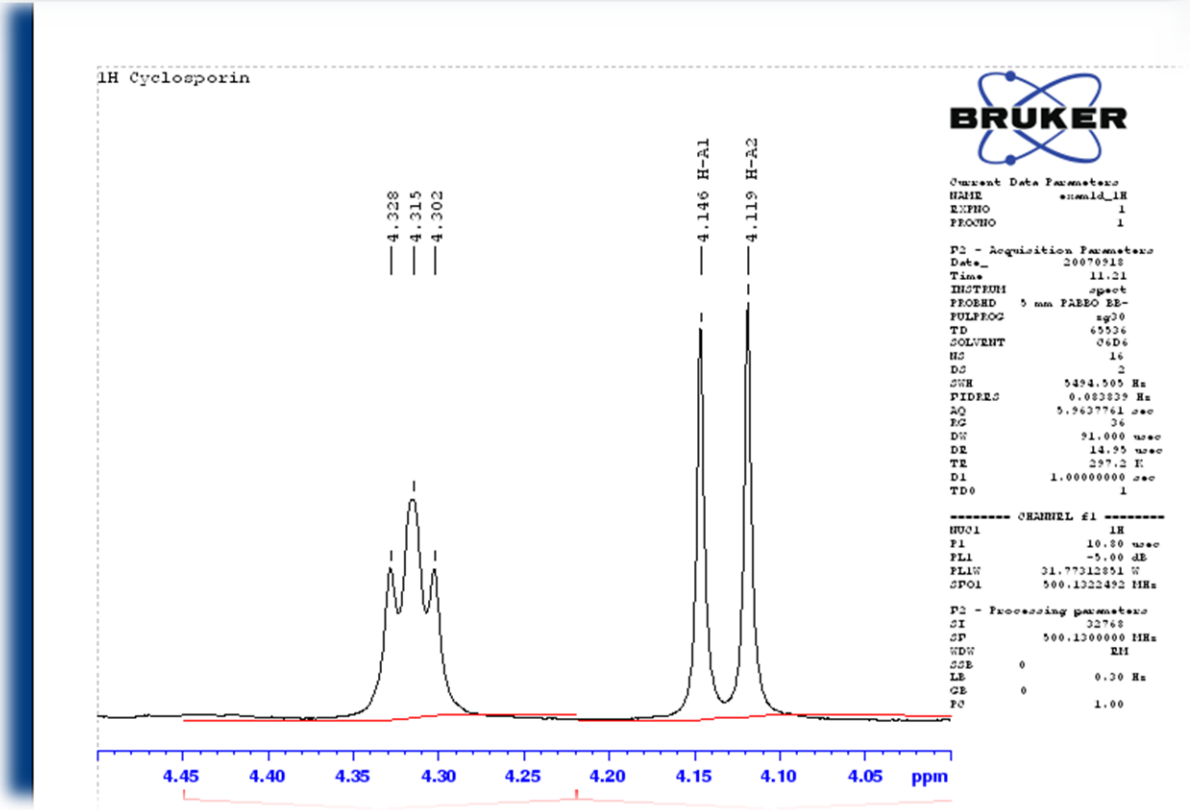


Interactive/dataset specific manipulations
- 1D spectra: peaks settings

Peaks can be:
- not displayed
- displayed with marks
- displayed with labels

They can show
- position or label or both

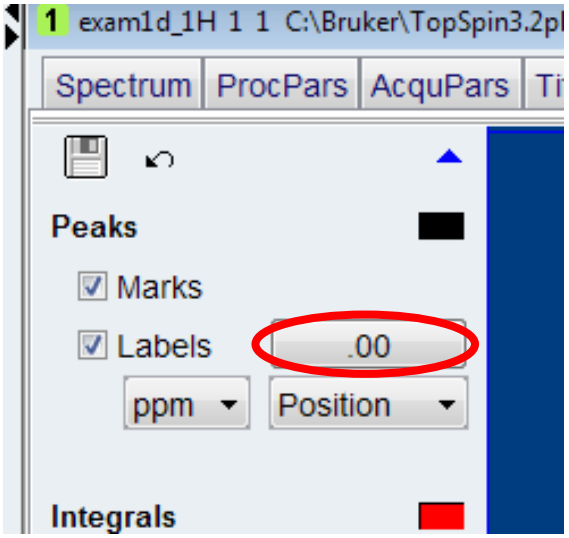


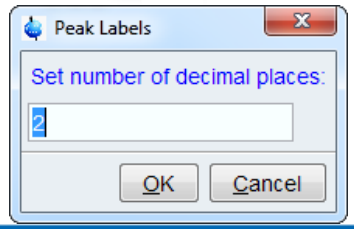


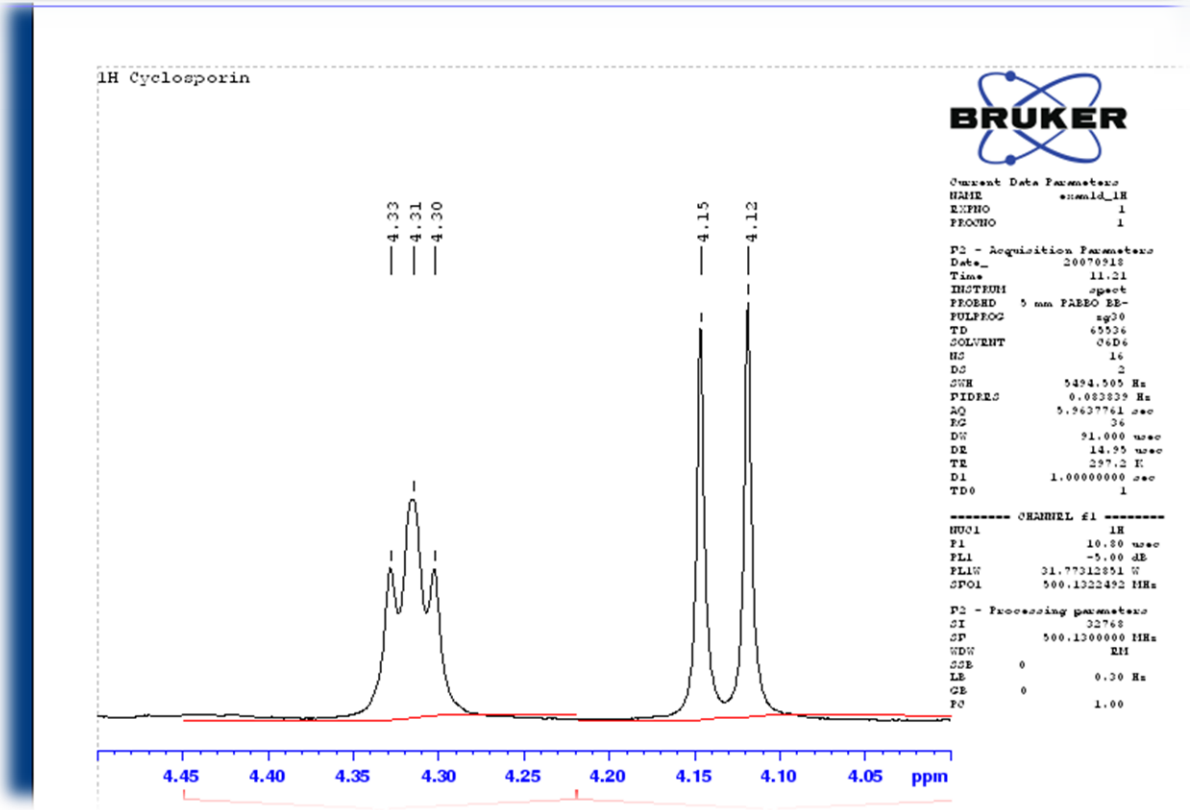
Interactive/dataset specific manipulations
- 1D spectra: peaks settings

Peaks can be:
- not displayed
- displayed with marks
- displayed with labels

They can show
- position or label or both
- user defined number of digits



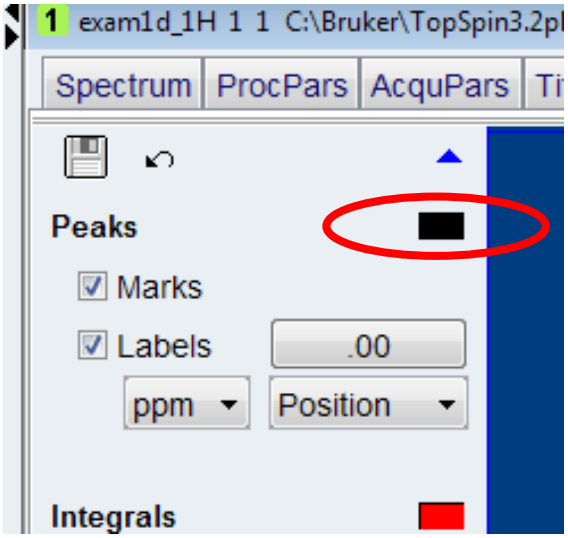


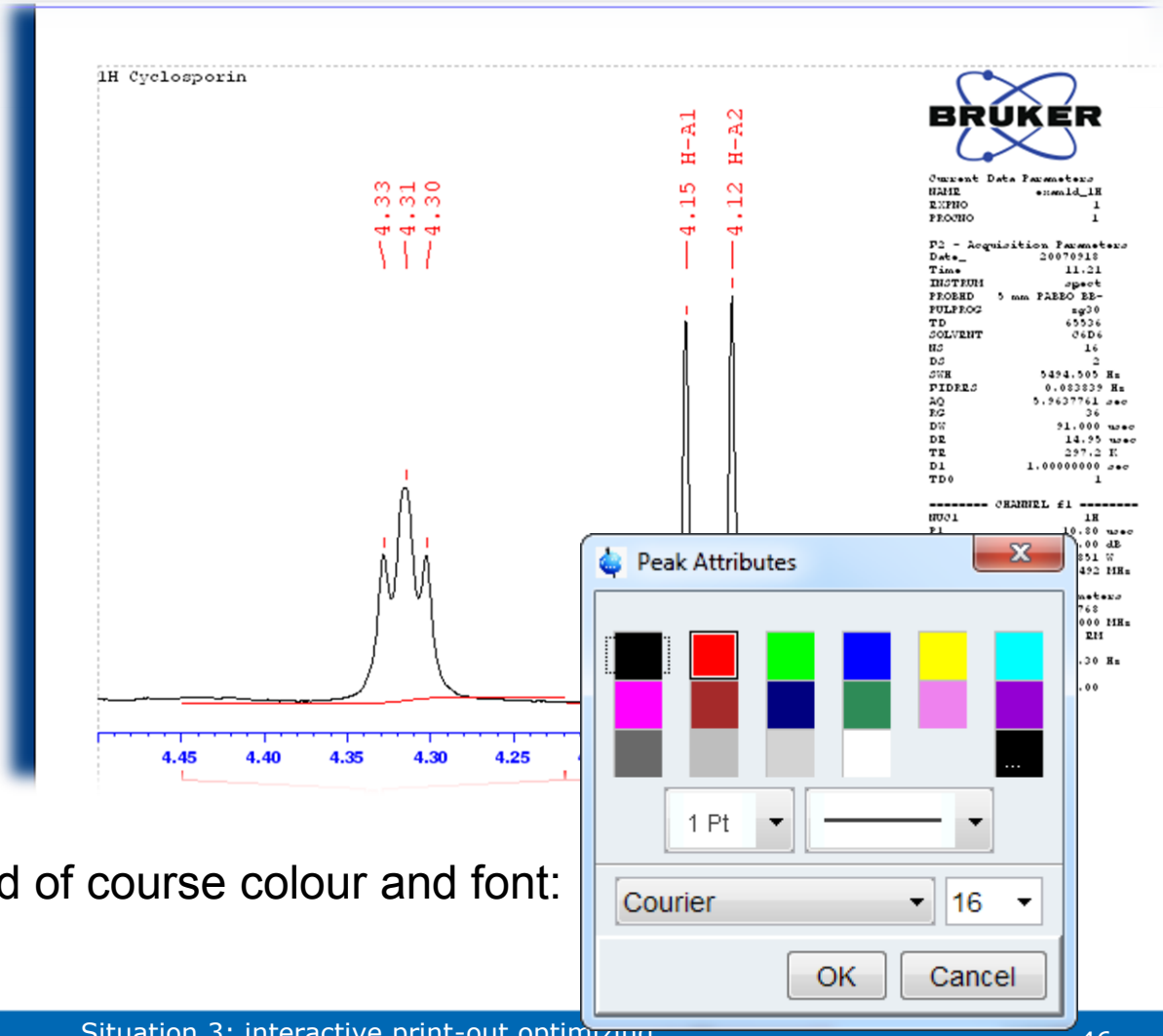


Interactive/dataset specific manipulations
- 1D spectra: peaks settings

Peaks can be:
- not displayed
- displayed with marks
- displayed with labels

They can show
- position or label or both
- user defined number of digits

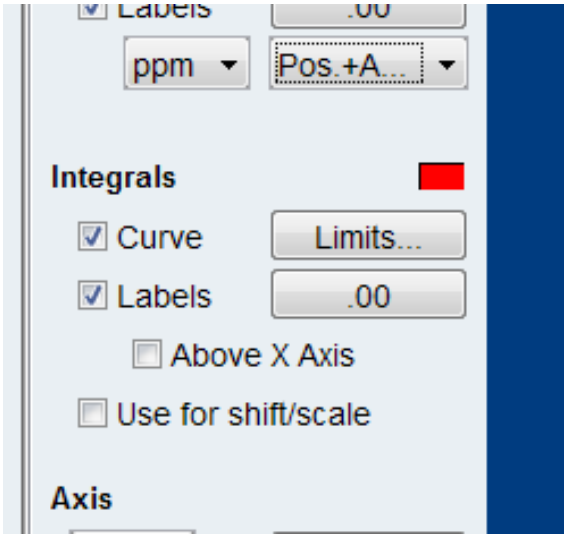


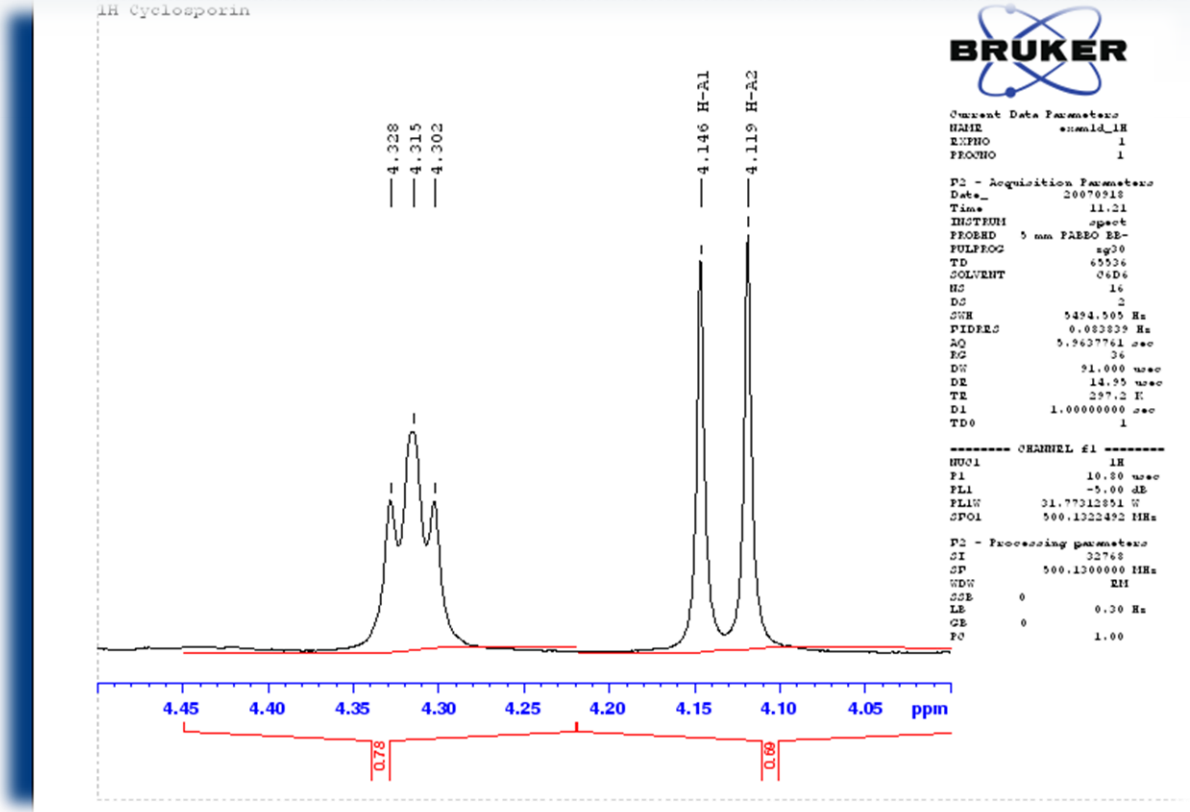


… and of course colour and font:

Interactive/dataset specific manipulations
- 1D spectra: special integral settings

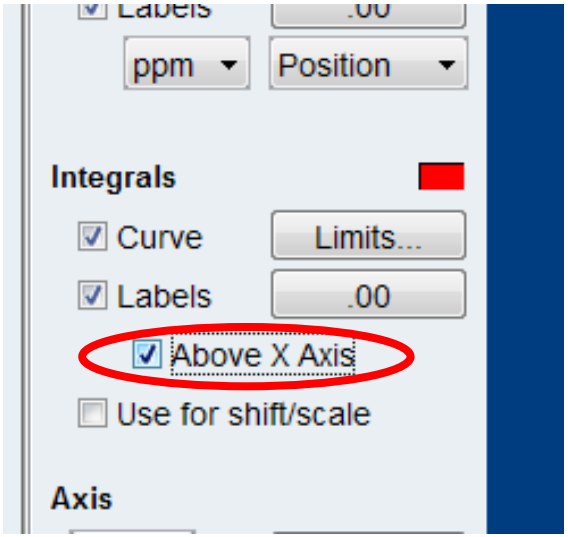
Integrals can be in addition:
- displayed below axis

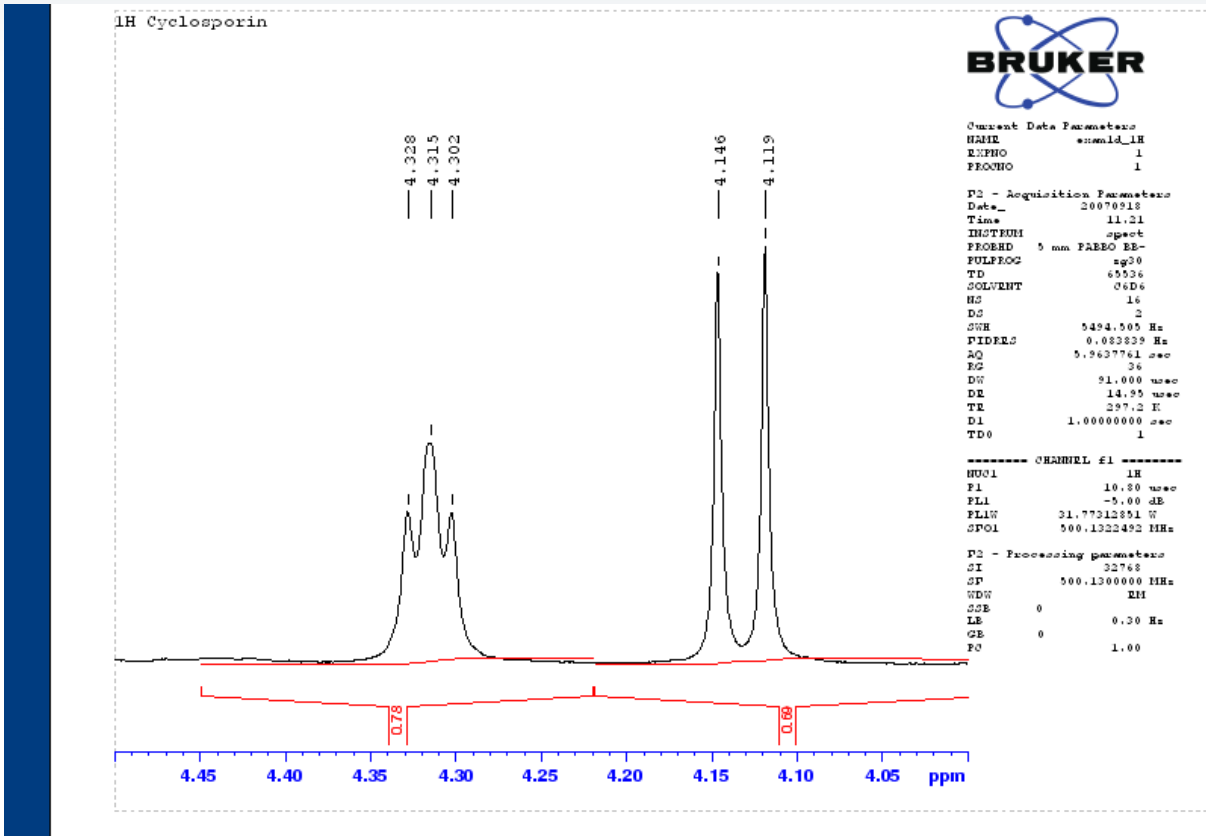




Interactive/dataset specific manipulations
- 1D spectra: special integral settings

Integrals can be in addition:
- displayed below axis
- displayed above axis

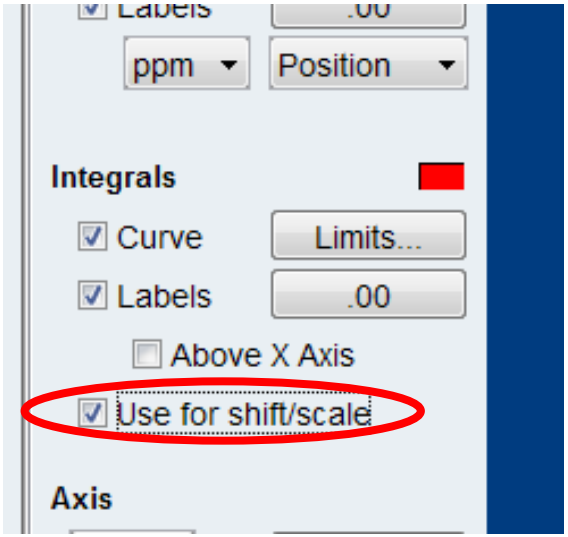


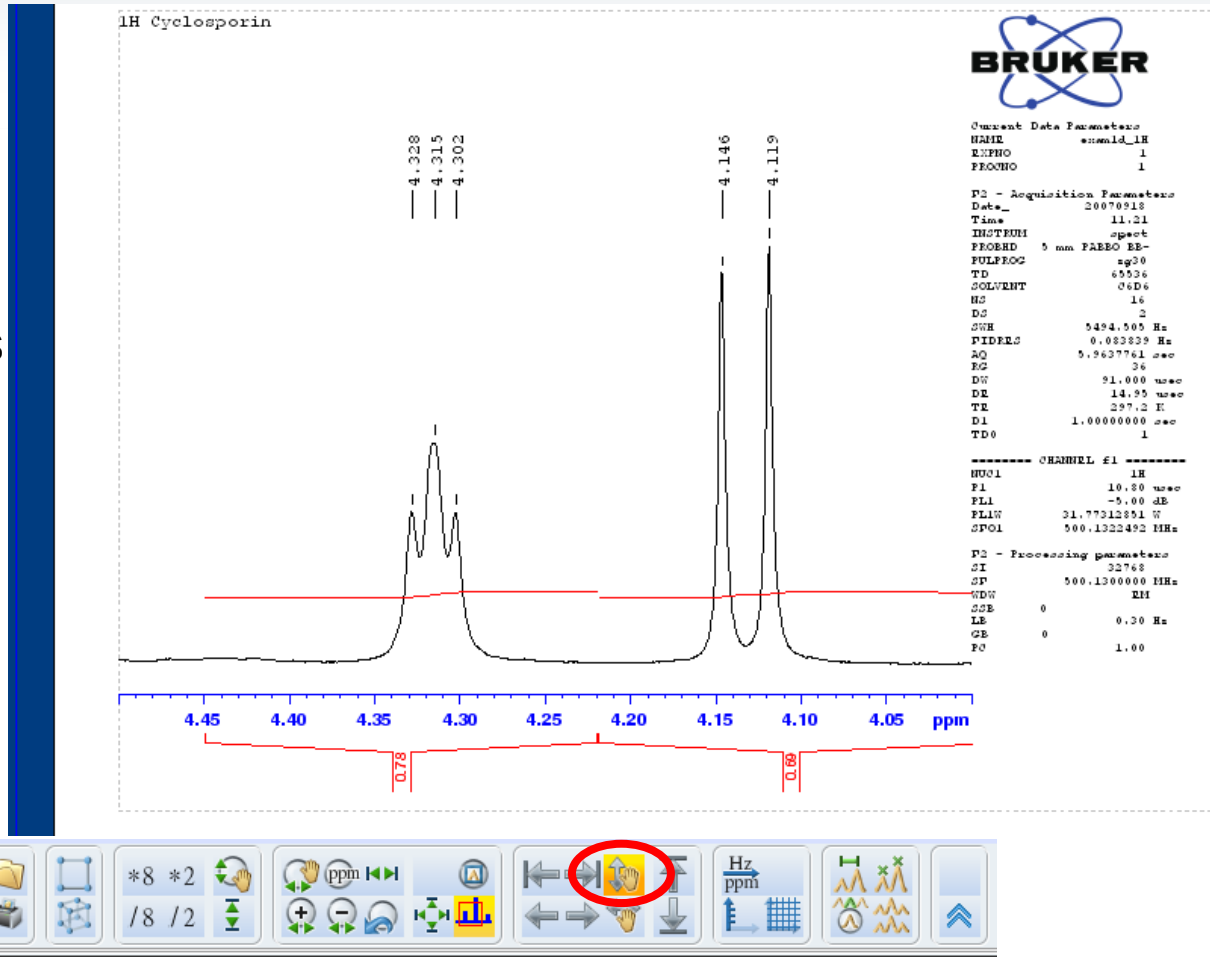


Interactive/dataset specific manipulations
- 1D spectra: special integral settings

Integrals can be in addition:
- displayed below axis
- displayed above axis

They can be used
- for scaling / shifting functions instead of the spectrum, e.g.

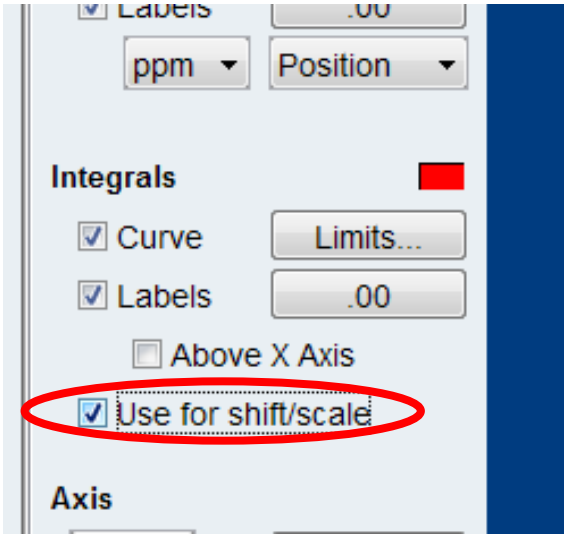


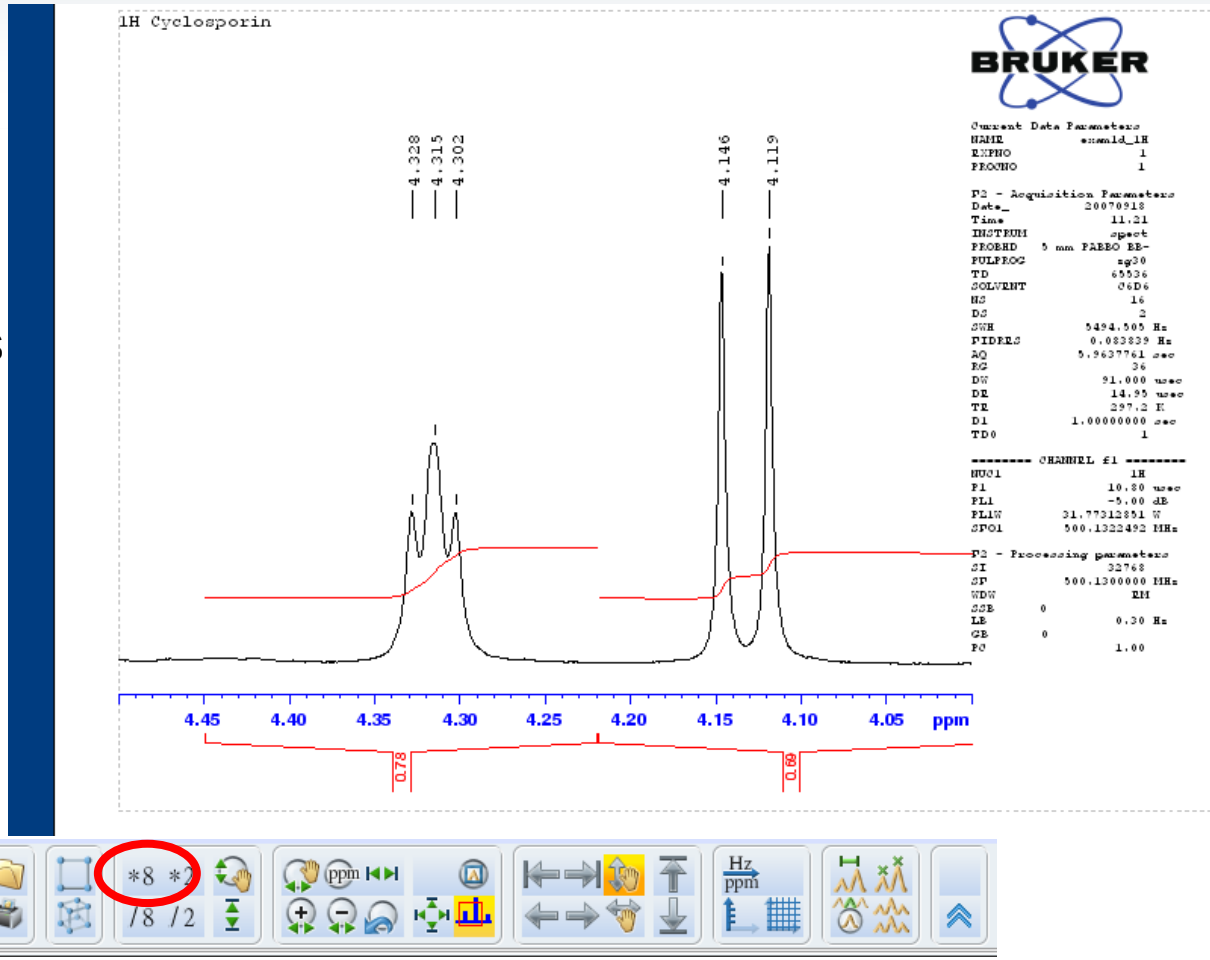


Interactive/dataset specific manipulations
- 1D spectra: special integral settings

Integrals can be in addition:
- displayed below axis
- displayed above axis

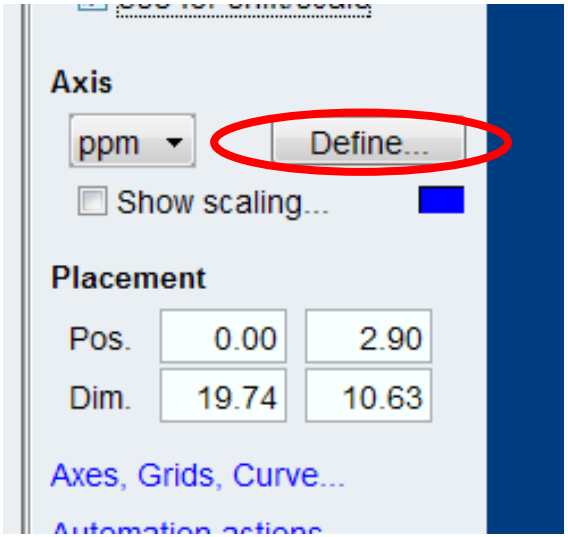
They can be used
- for scaling / shifting functions instead of the spectrum

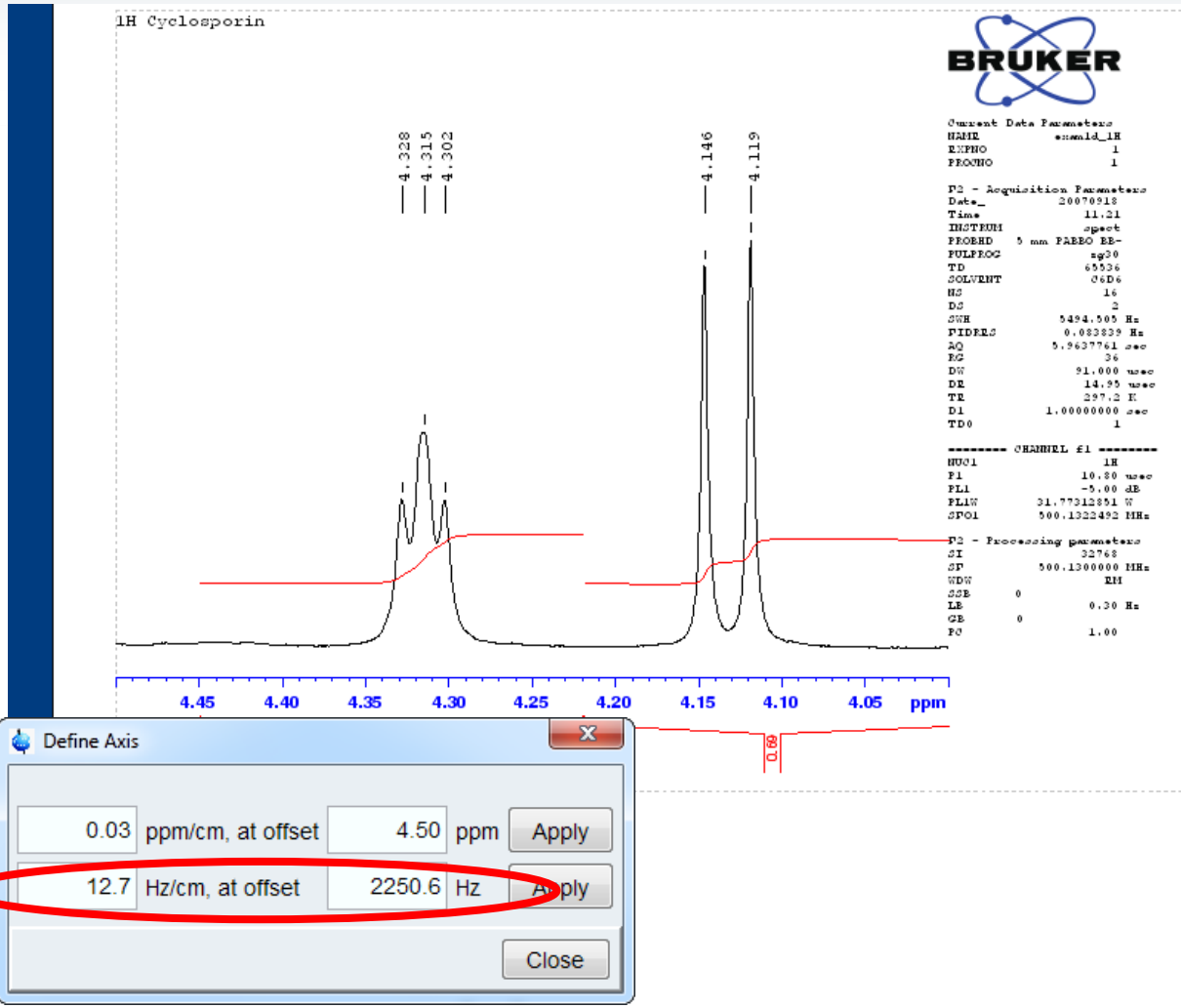




Interactive/dataset specific manipulations
- 1D spectra: special axis settings

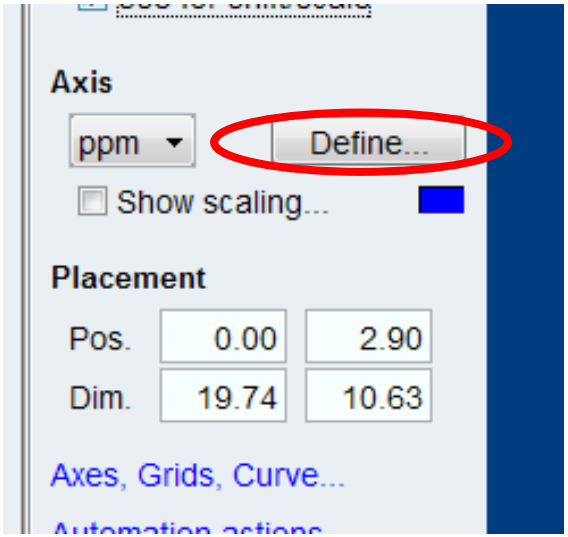
Axis can be in addition:
- numerically configured

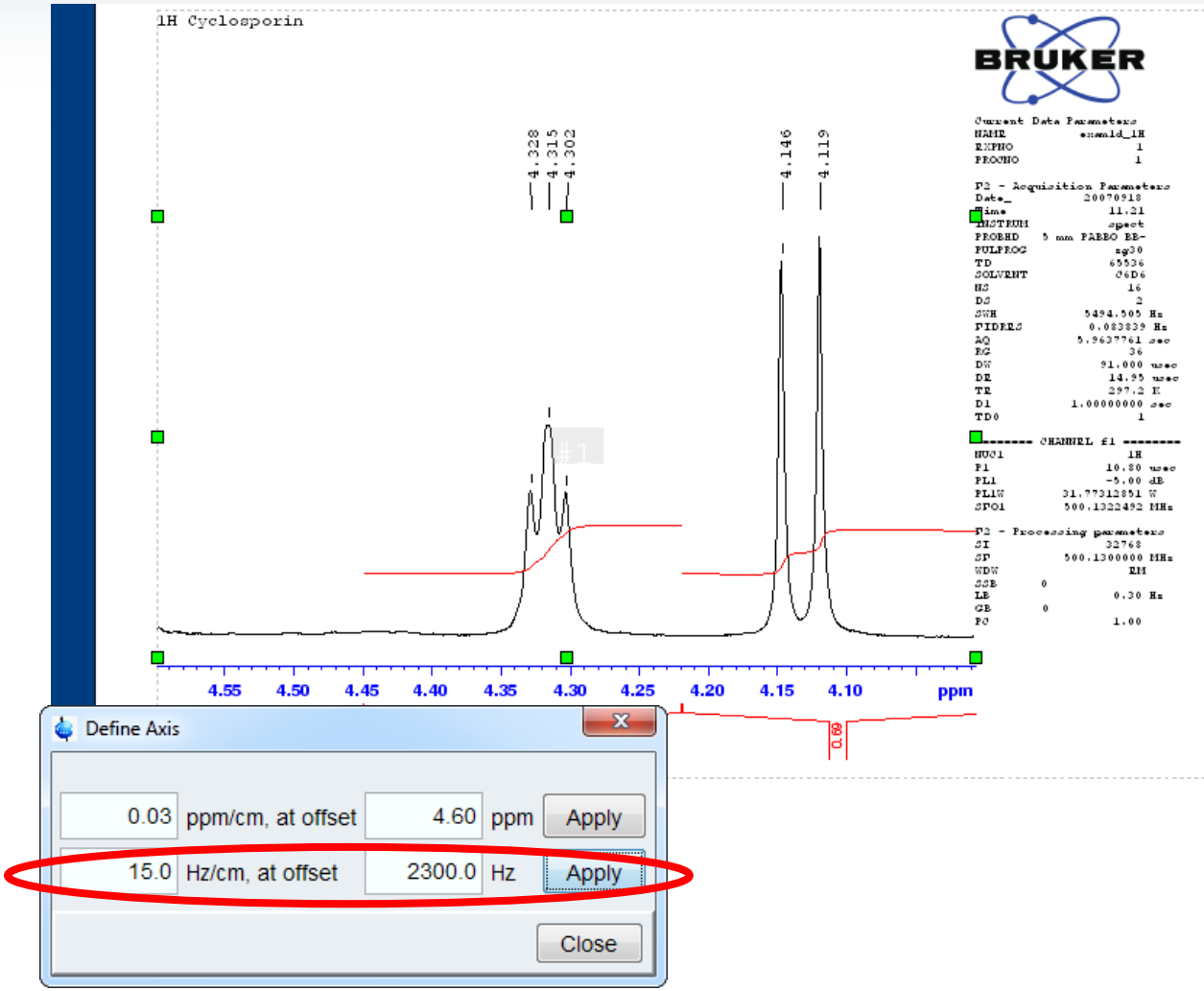




Interactive/dataset specific manipulations
- 1D spectra: special axis settings

Axis can be in addition:
- numerically configured

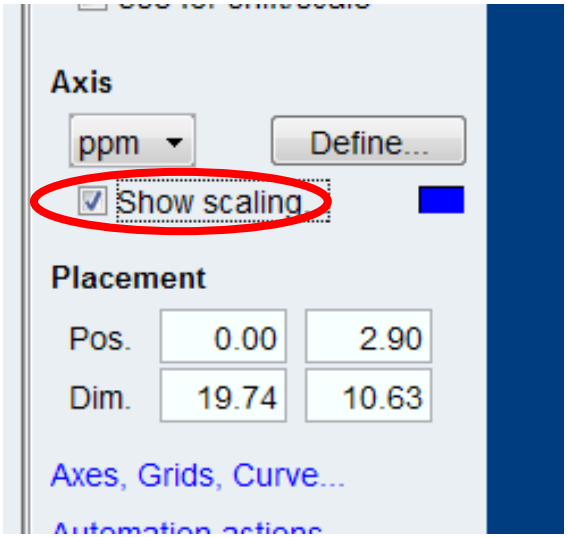


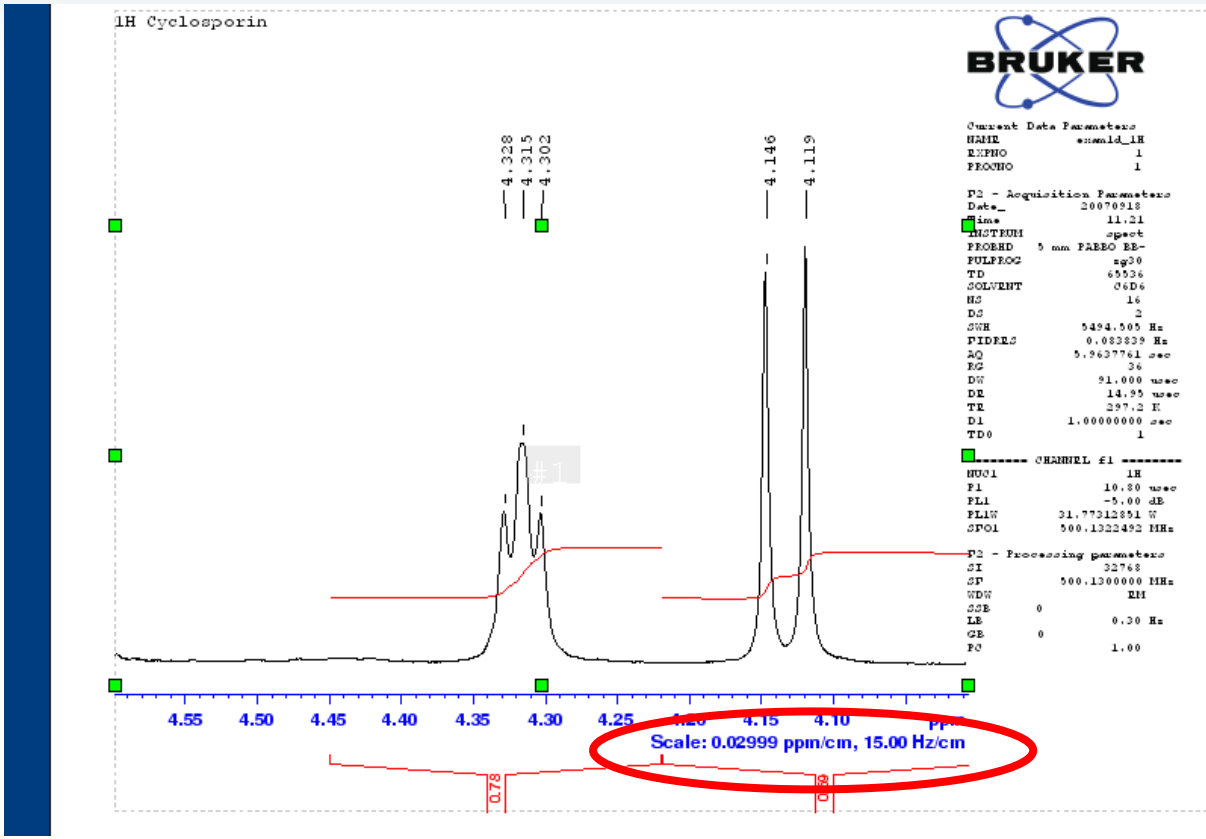


Interactive/dataset specific manipulations
- 1D spectra: special axis settings

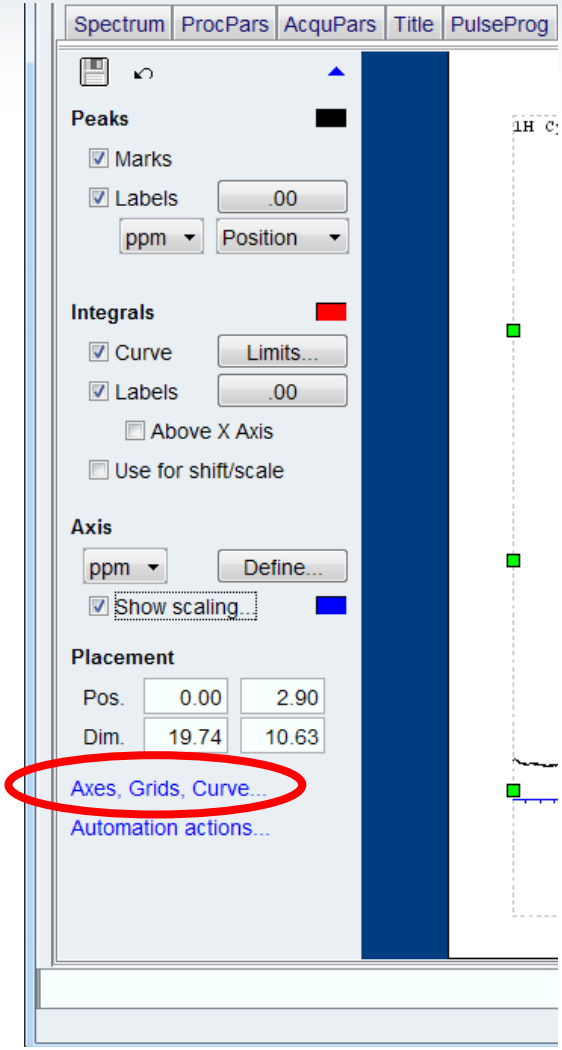
Axis can be in addition:
- numerically configured

Scaling information can be displayed



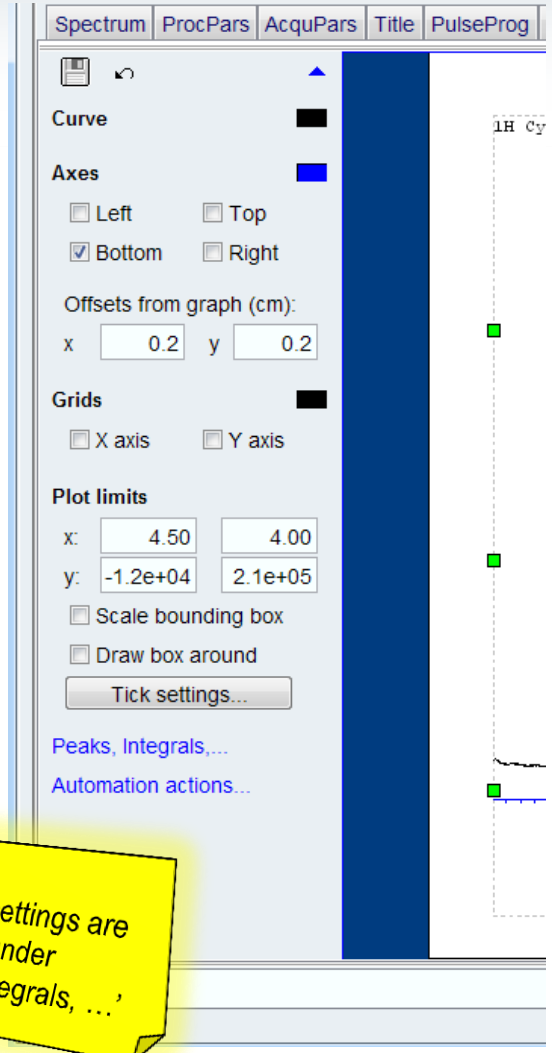


Interactive/dataset specific manipulations
- 1D spectra: more settings



More settings are available under:
'**Axes, Grids, Curve …**'
e.g.:

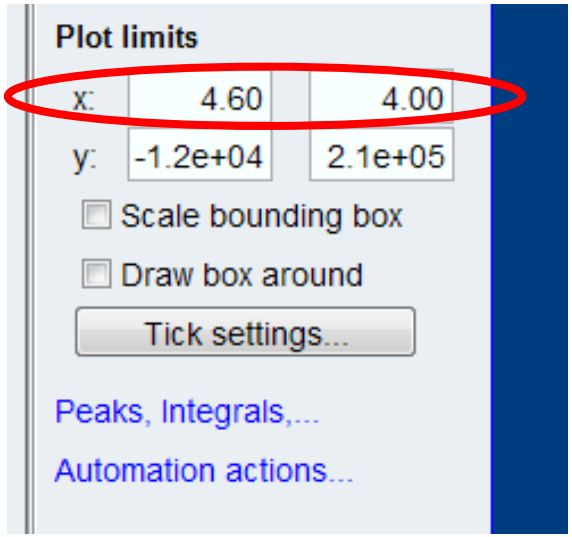
- Plot limits
- Tick settings

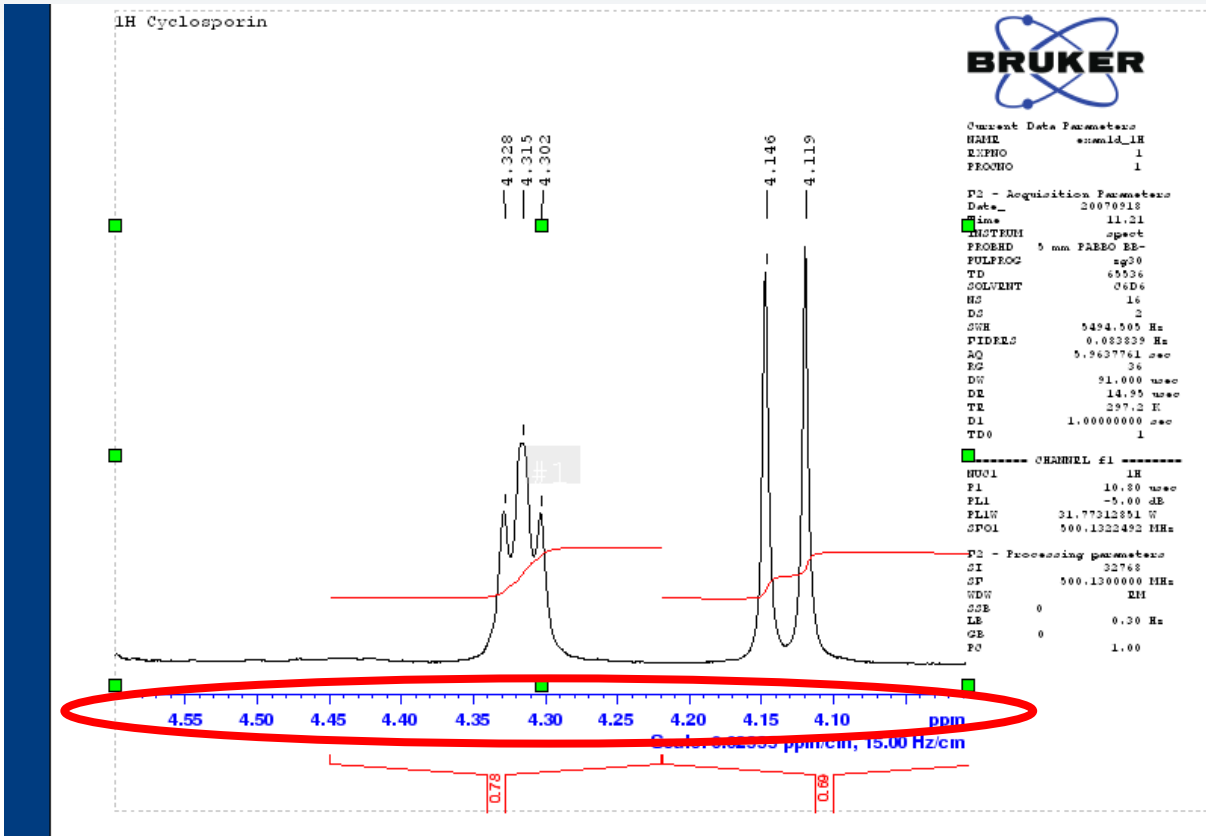


Note:
Previous settings are available under 'Peaks, Integrals, …'

Interactive/dataset specific manipulations
- 1D spectra: Plot limits

Plot limits:
- can be entered numerically*

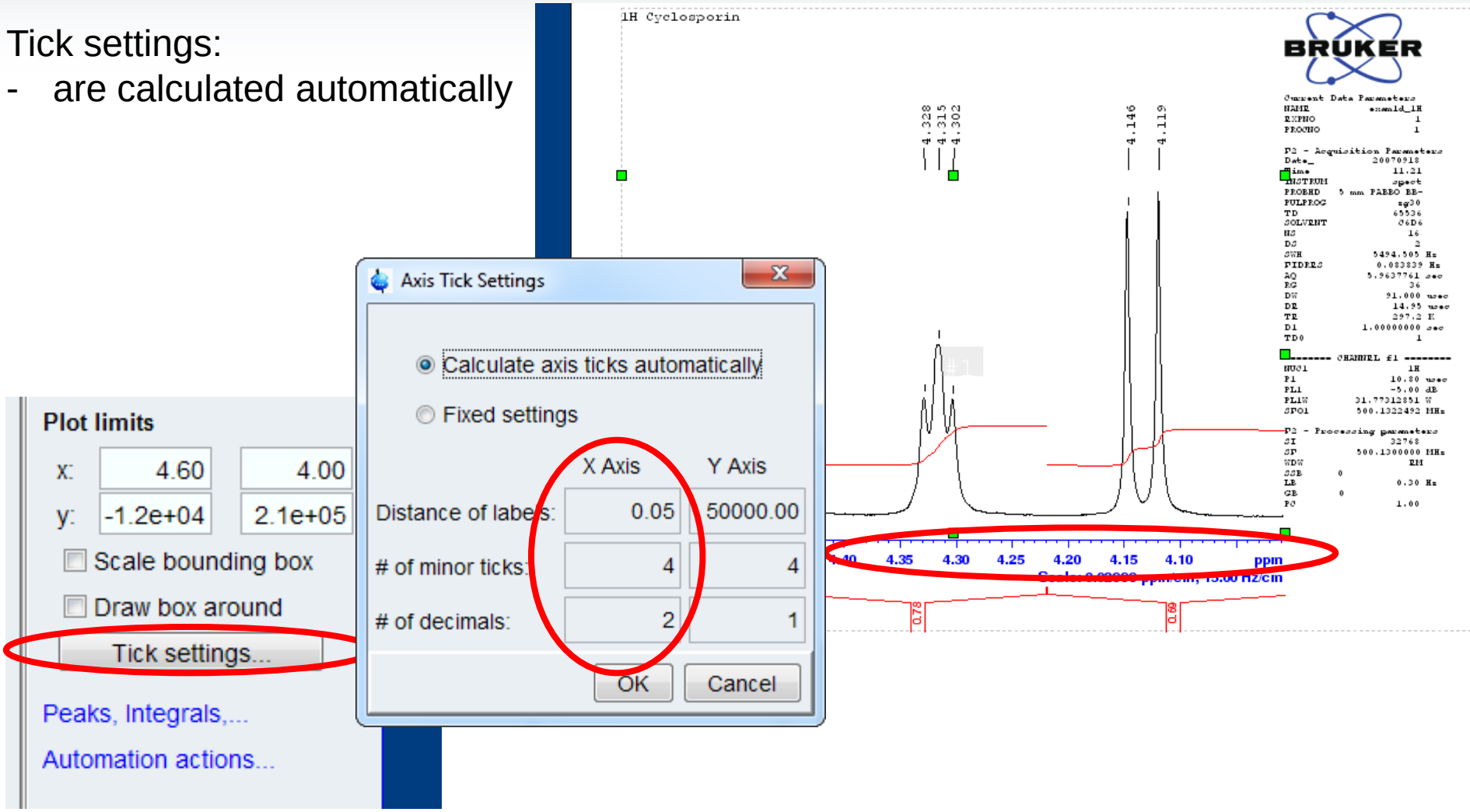




* the TopSpin icon ppm has the same functionality. Therefore, it is disabled in the plot tab, use this function to set exact values.

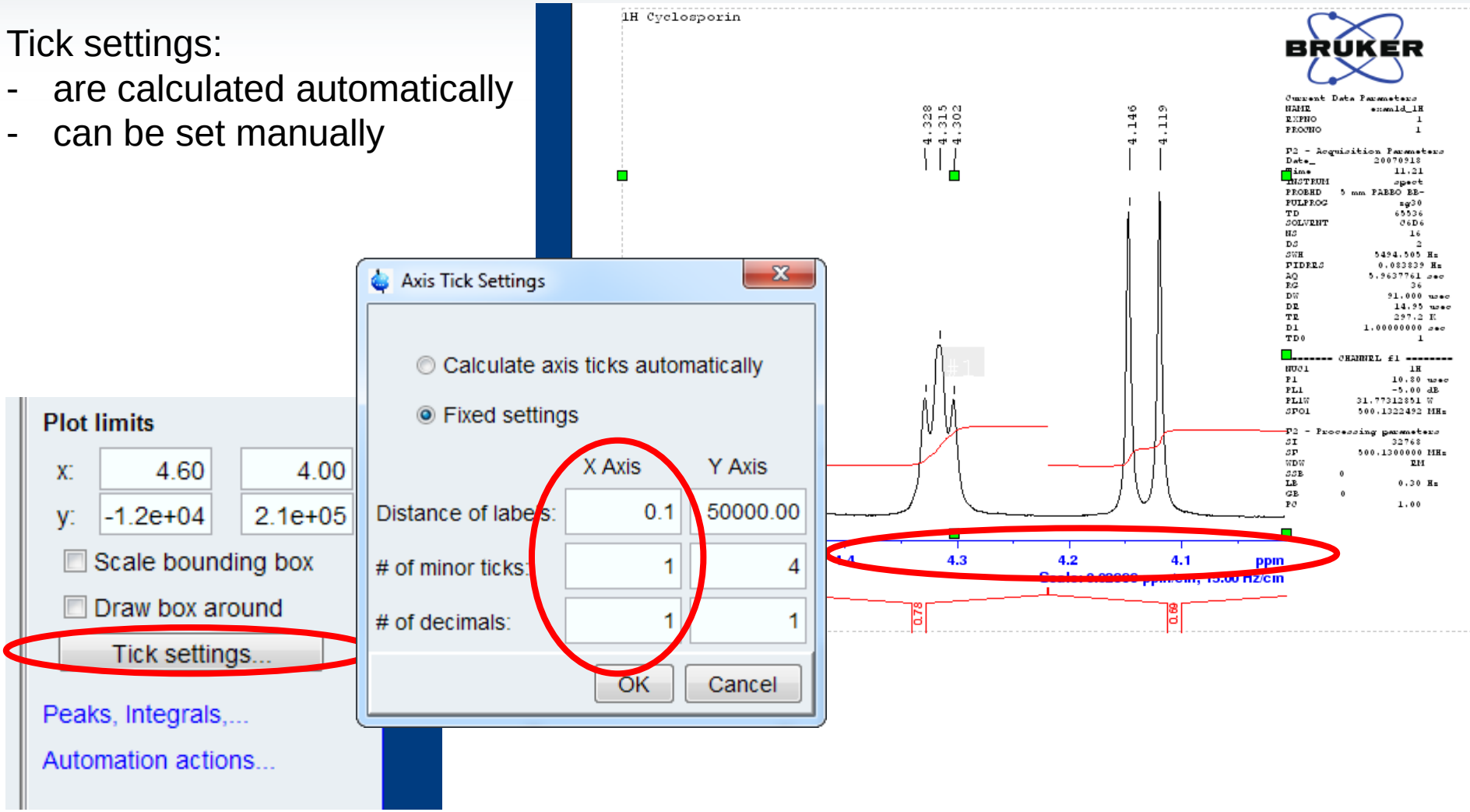
Interactive/dataset specific manipulations
- 1D spectra: special tick settings

Tick settings:
- are calculated automatically

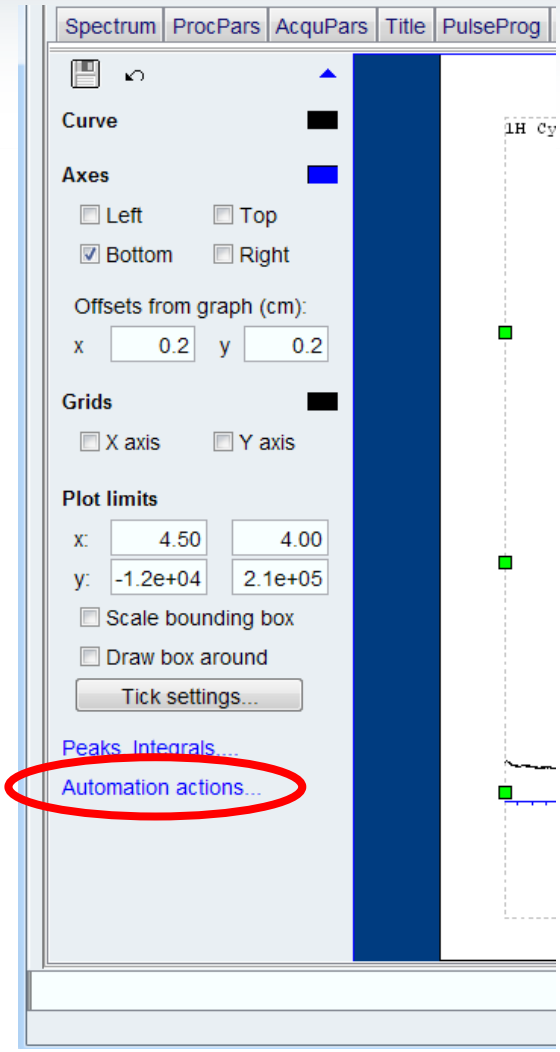


Interactive/dataset specific manipulations
- 1D spectra: special tick settings

Tick settings:
- are calculated automatically
- can be set manually

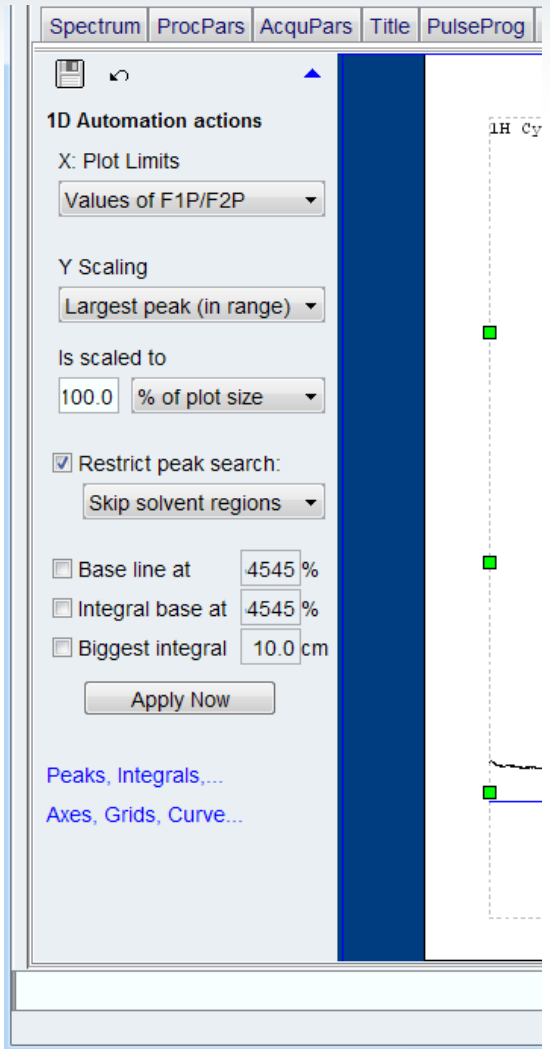


Interactive/dataset specific manipulations - 1D spectra: Automation actions



More settings are available under:
Automation actions …

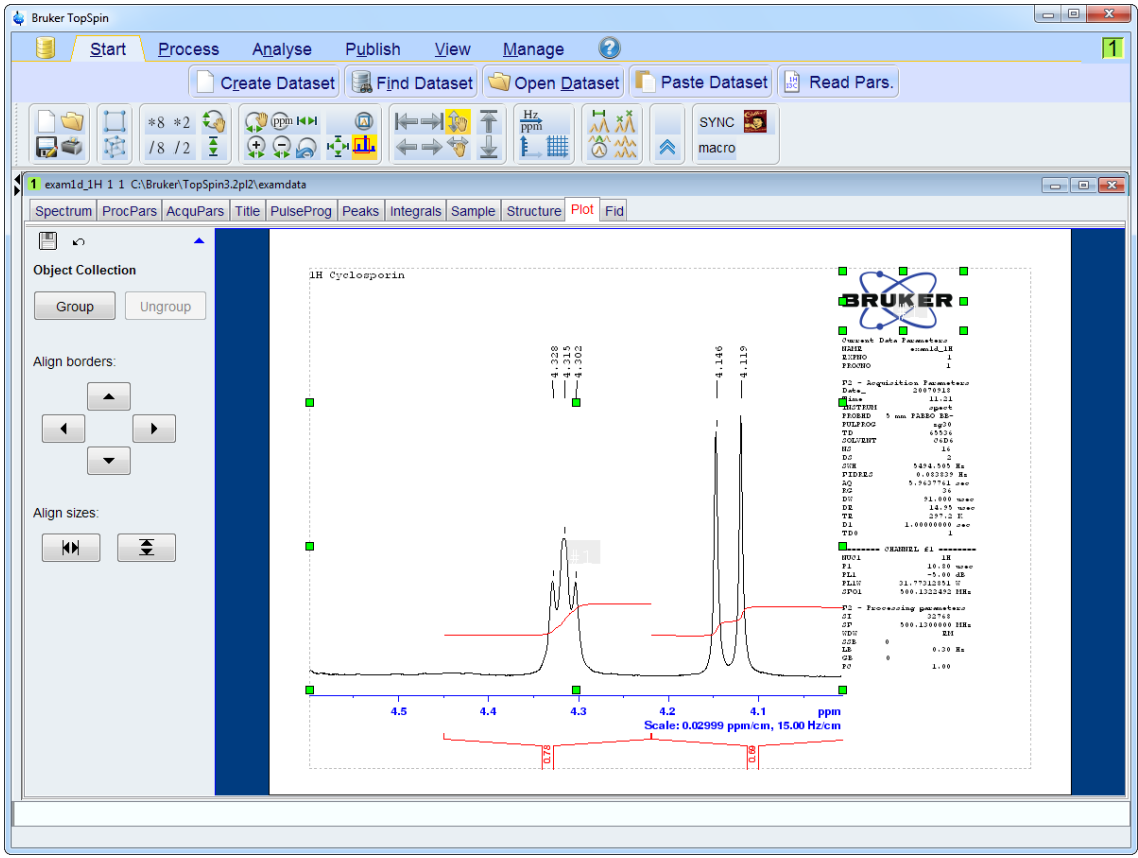
But these are discussed in the next chapter, Situation 4



Interactive/dataset specific manipulations - more than one element

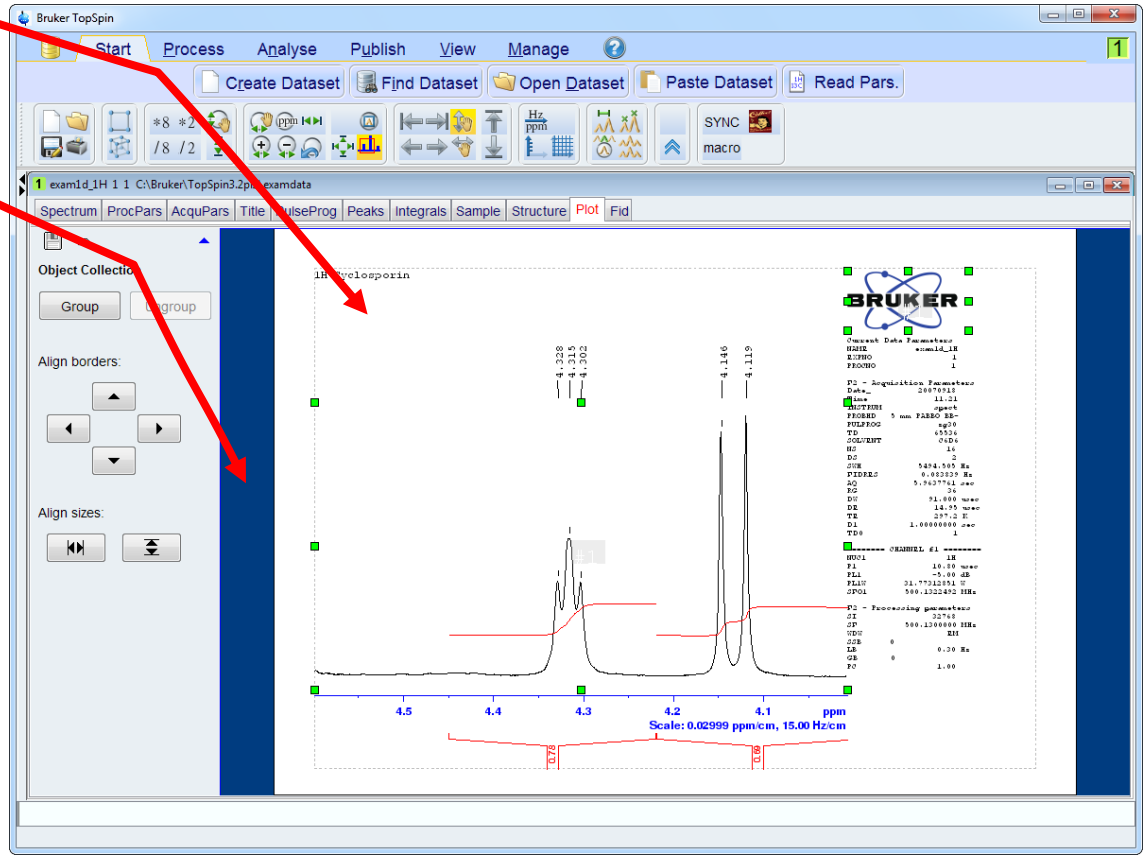
As soon as more than one element is selected (use **Ctrl** or **Shift**-key to select several elements): the following options appear:

- group (ungroup)
- align borders
- align sizes



Interactive/dataset specific manipulations - deselect an element

To deselect one or several elements just click in another area of the layout which does not contain an element.
Clicking in the blue area outside the layout would also work.



Different situations = different solutions
→ 1 tool

Summary:

Plot tab offers various possibilities to modify a print-out of an individual dataset.
NMR and drawing elements, fonts, colours, digits, alignment etc.

Situation 3

- I would like to optimize my print-out for individual datasets

Different situations = different solutions
→ 1 tool

Situation 1

- I just want to easily print what I see in TopSpin

Situation 2

- I want to easily print my own layout

Situation 3

- I would like to optimize my print-out for individual datasets

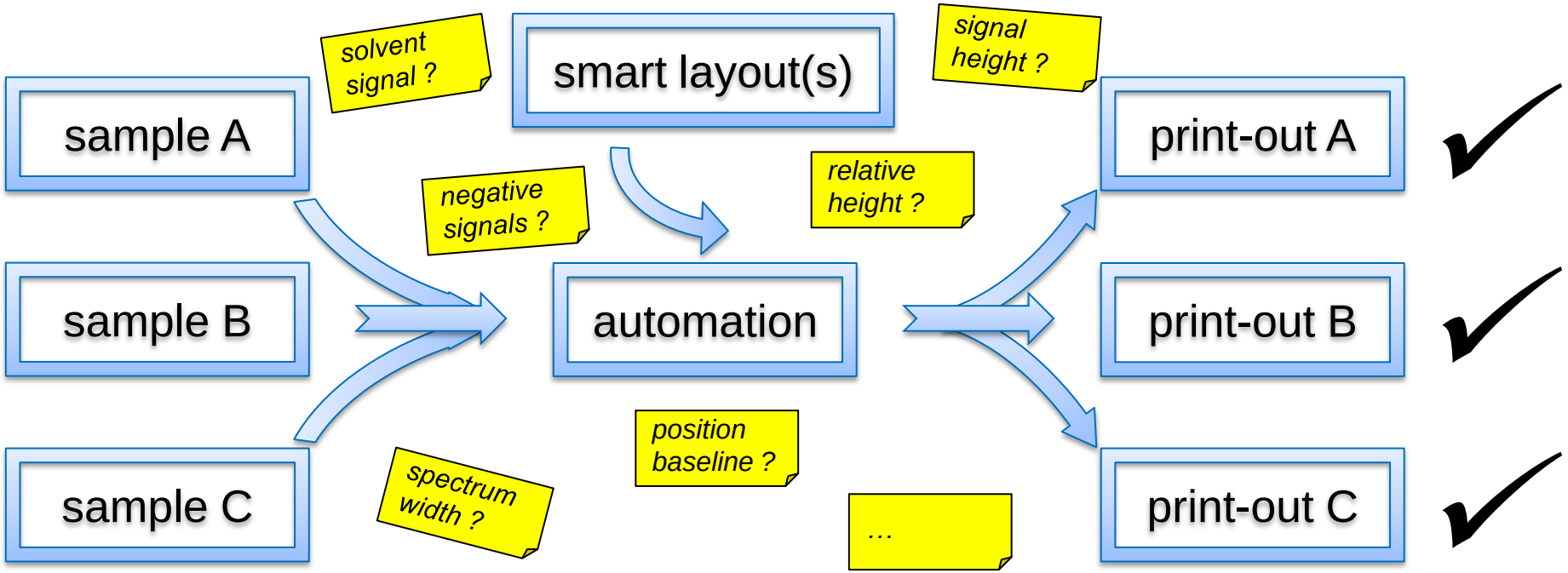
Situation 4

- I would like to get nice print-outs for all samples of my automation run

Situation 4:
nice print-outs for all samples in automation

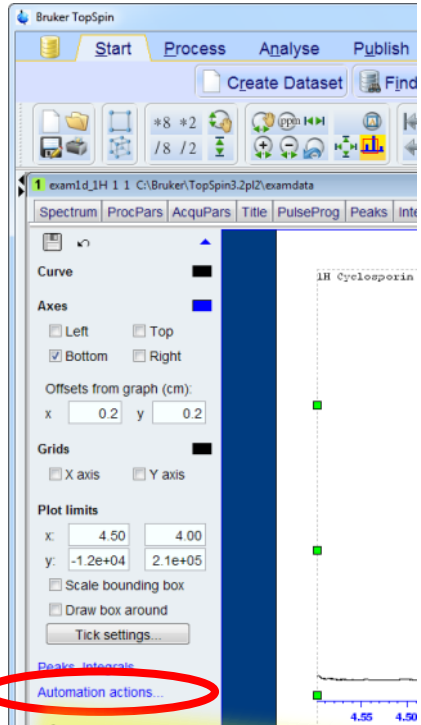
Getting the print-outs for all samples in automation in the best way requires:

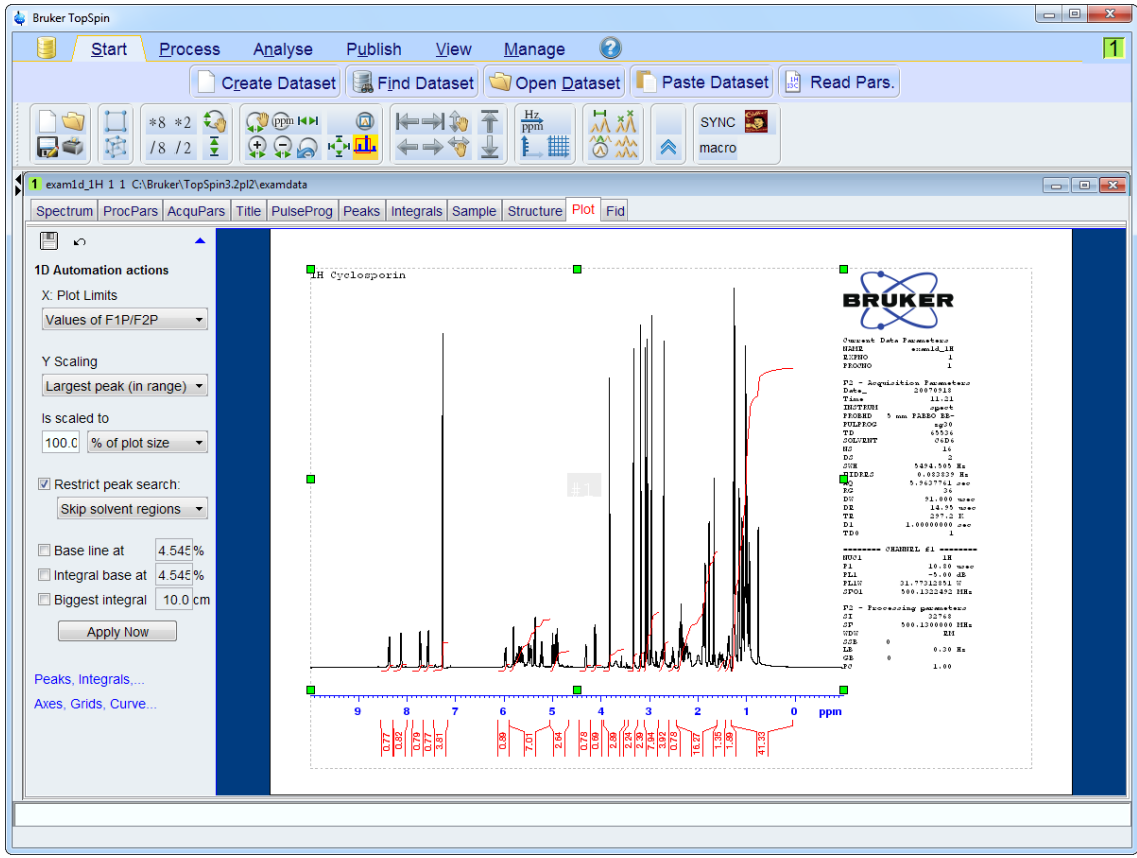
- smart features of the plot functionality
- user configurable according to your/all needs



Nice print-outs for all samples in automation - automation actions

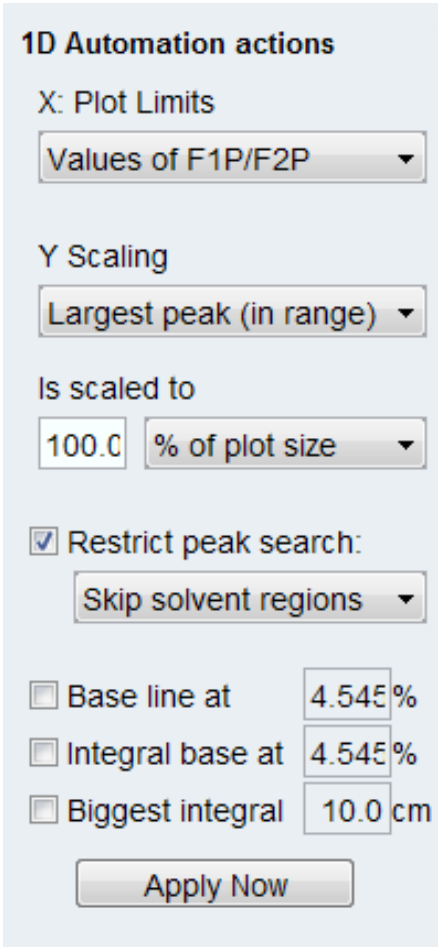
As soon as a spectrum element (1D or 2D) is selected, the left panel offers*:
Automation actions …





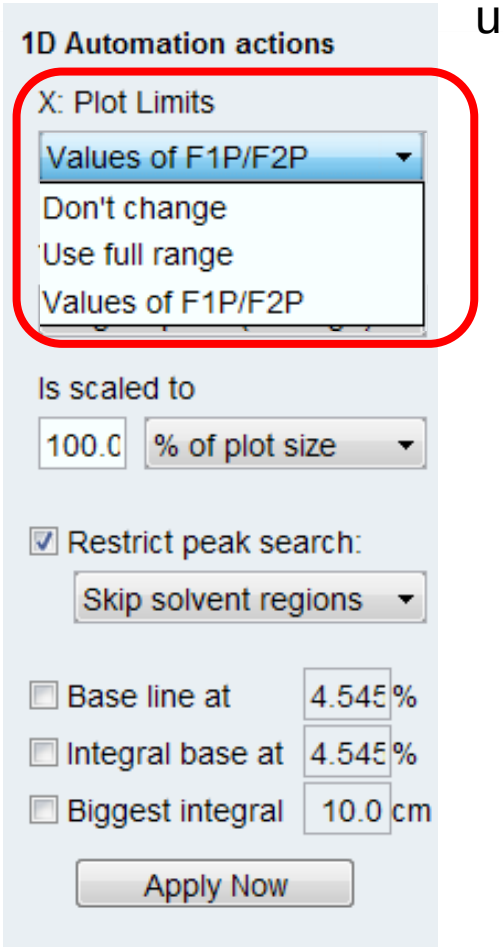
Automation actions

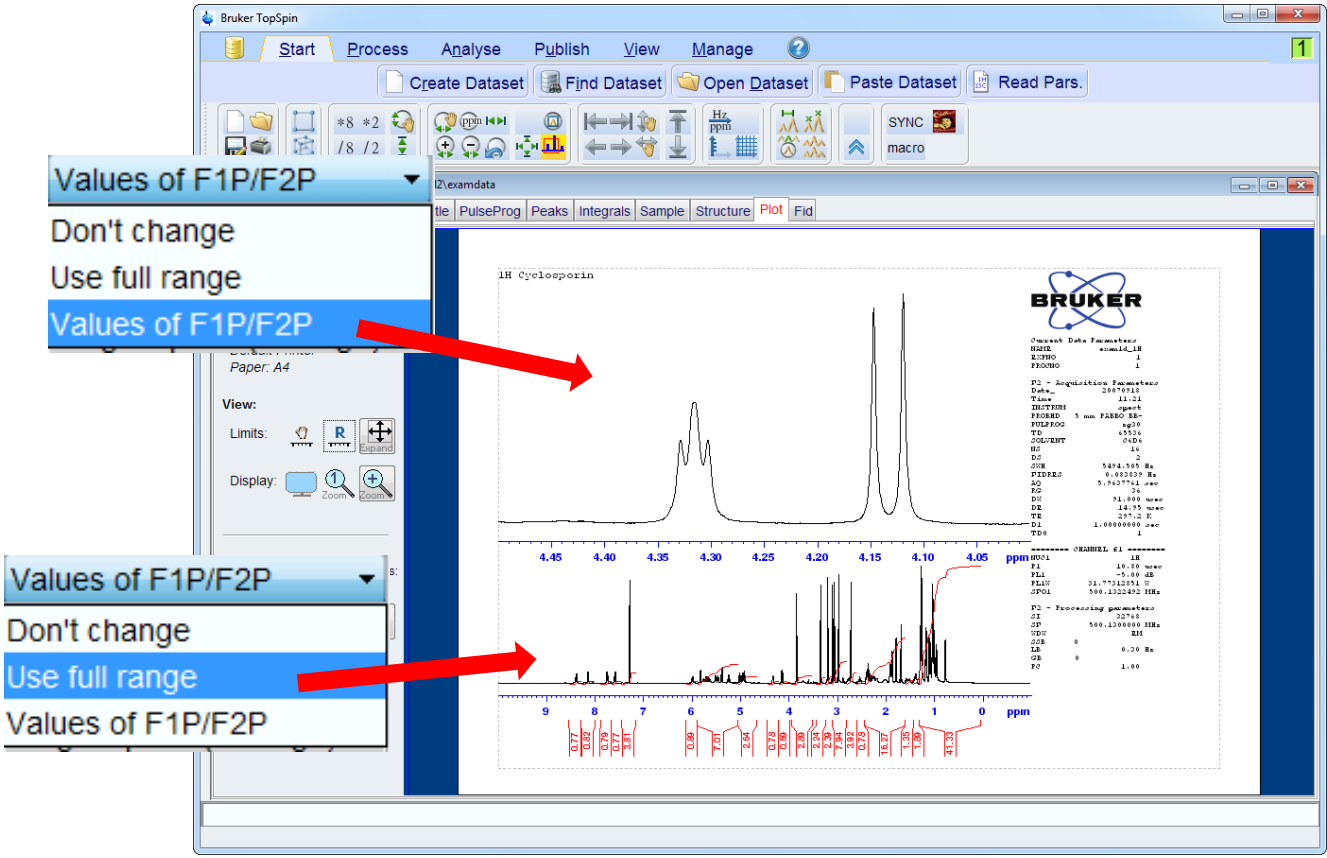
The next slides inform about the Automation actions including examples



Automation actions:
X-axis: Plot limits

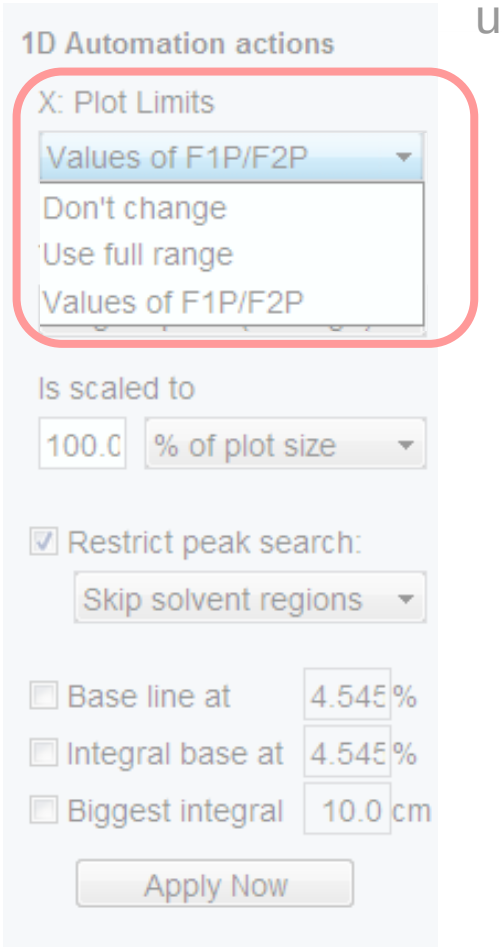
Layout **1D_H+zoom** shows the same spectrum twice: the bottom one is set up with **Use full range**, the top one uses **Values of F1P/F2P**

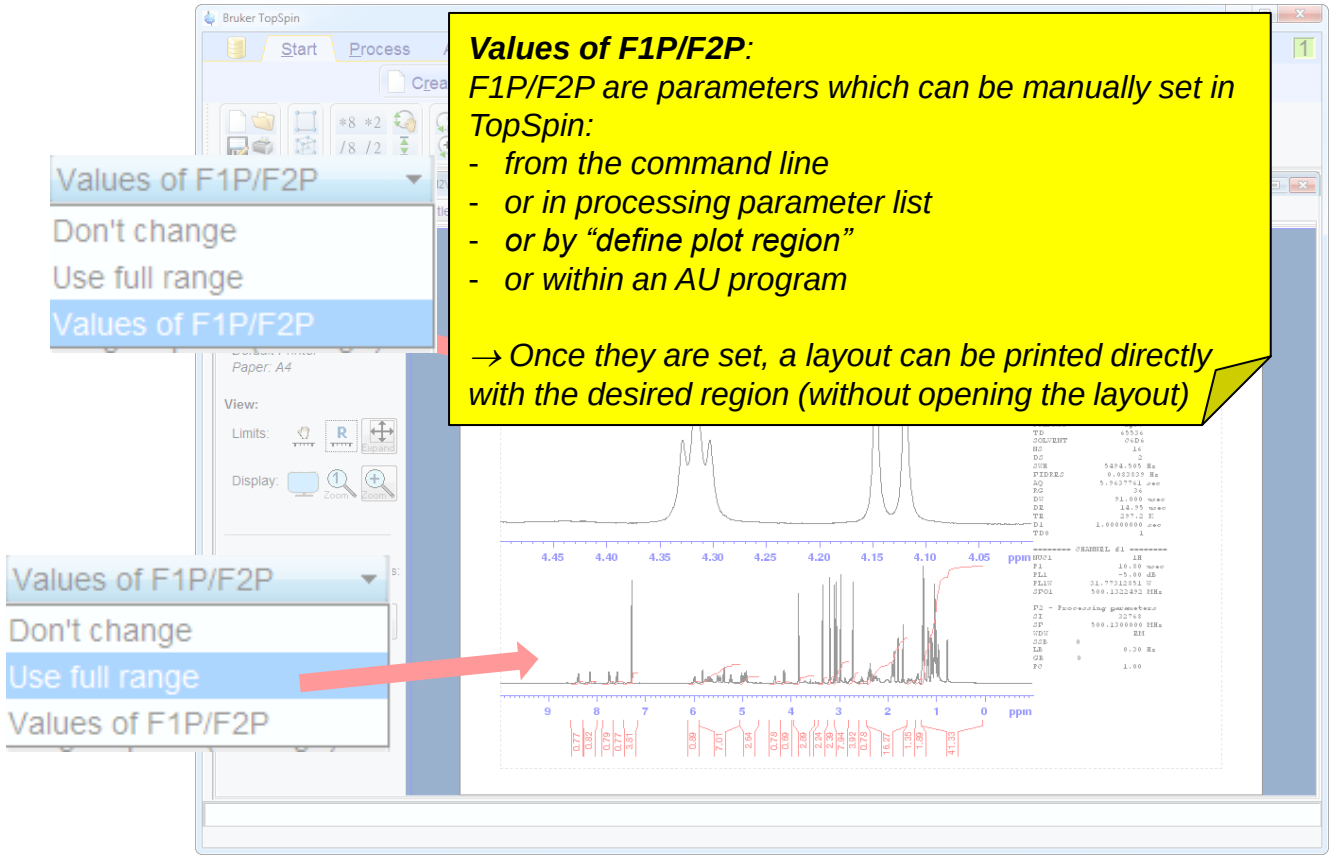




Automation actions:
X-axis: Plot limits

Layout **1D_H+zoom** shows the same spectrum twice: the bottom one is set up with **Use full range**, the top one uses **Values of F1P/F2P**





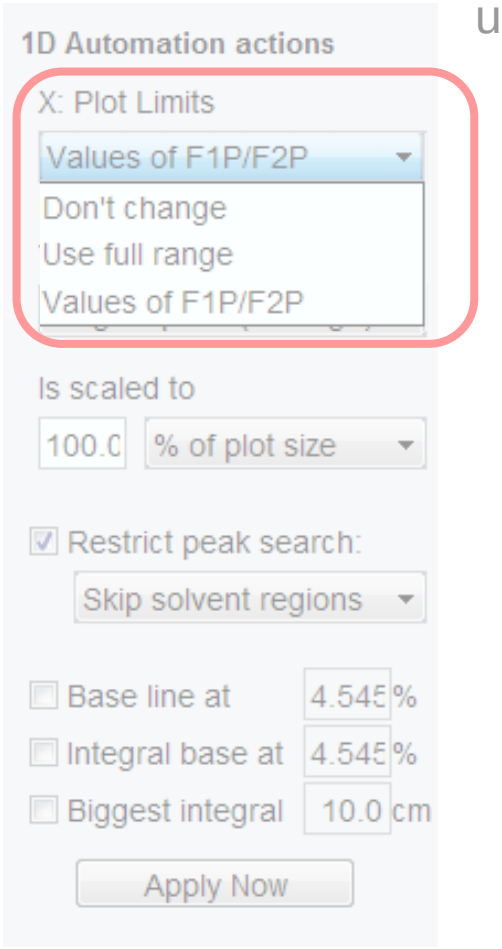
Values of F1P/F2P:
F1P/F2P are parameters which can be manually set in TopSpin:

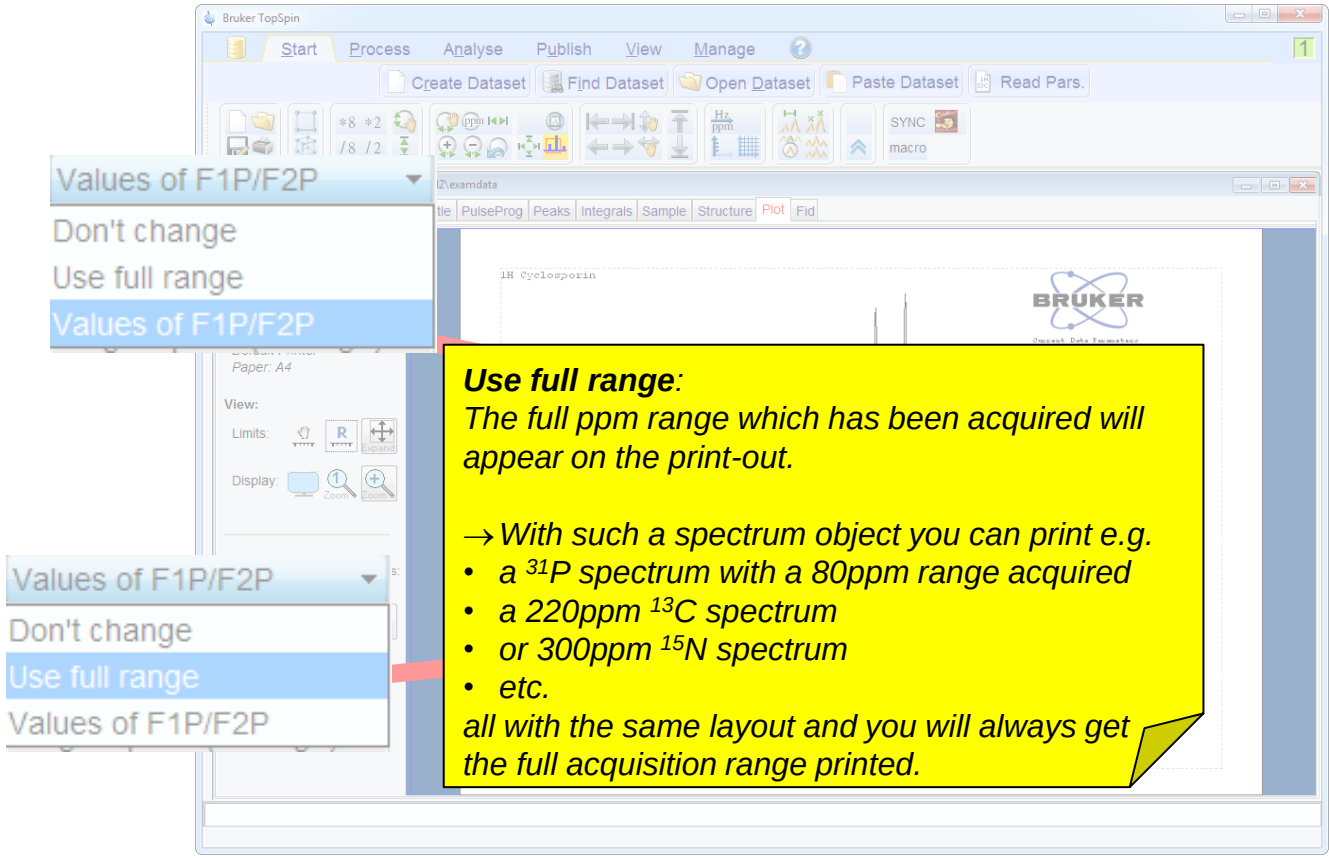
- *from the command line*
- *or in processing parameter list*
- *or by "define plot region"*
- *or within an AU program*

→ Once they are set, a layout can be printed directly with the desired region (without opening the layout)

Automation actions:
X-axis: Plot limits

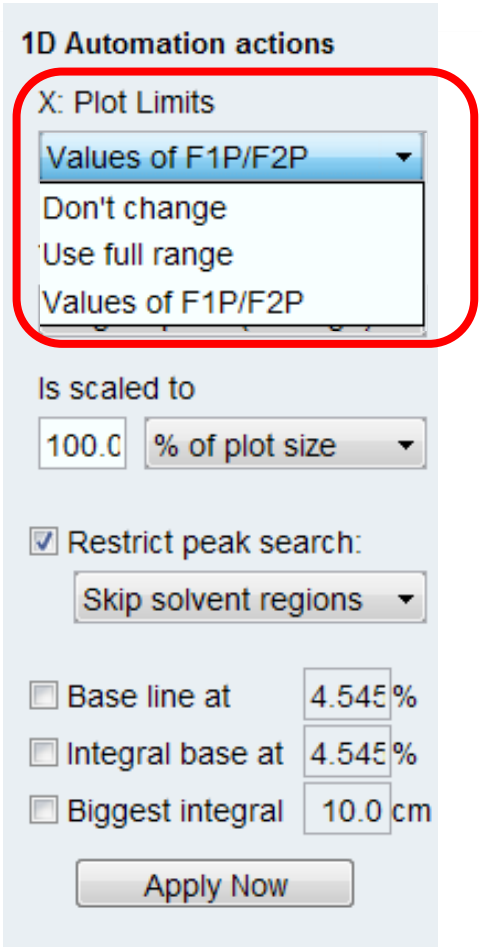
Layout **1D_H+zoom** shows the same spectrum twice: the bottom one is set up with **Use full range**, the top one uses **Values of F1P/F2P**

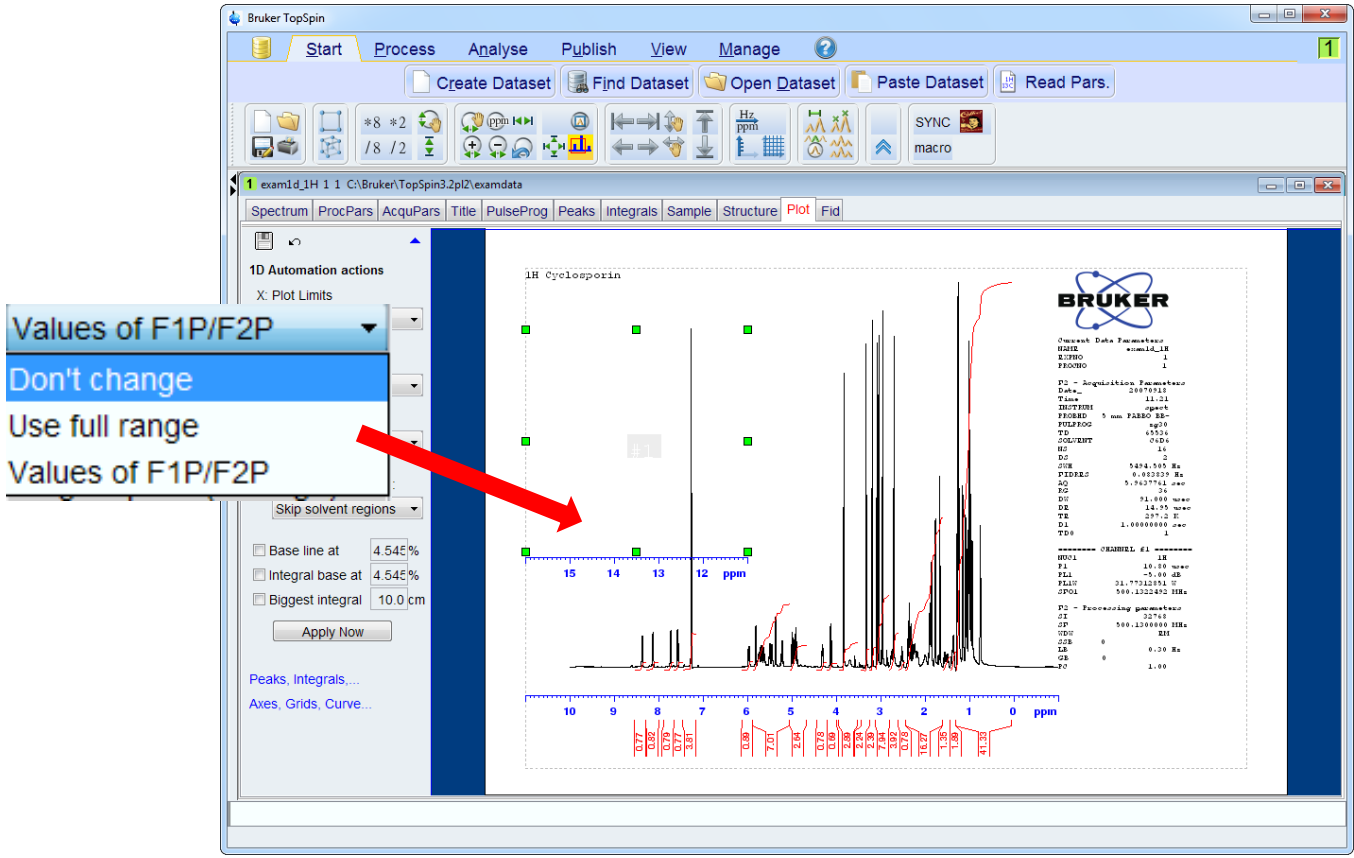




Automation actions:
X-axis: Plot limits

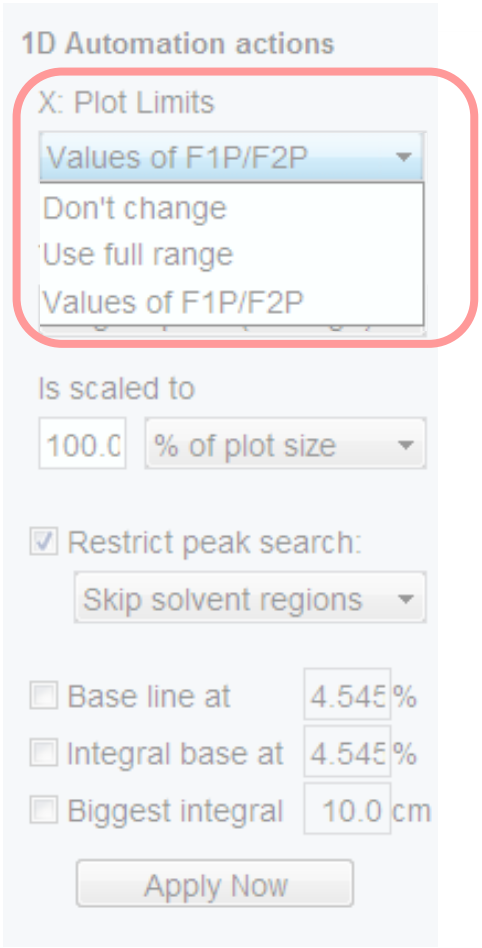
Layout **1D_H+If** uses the automation action for x-axis **Don't change**

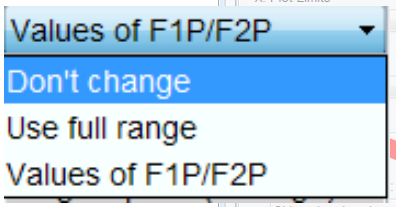


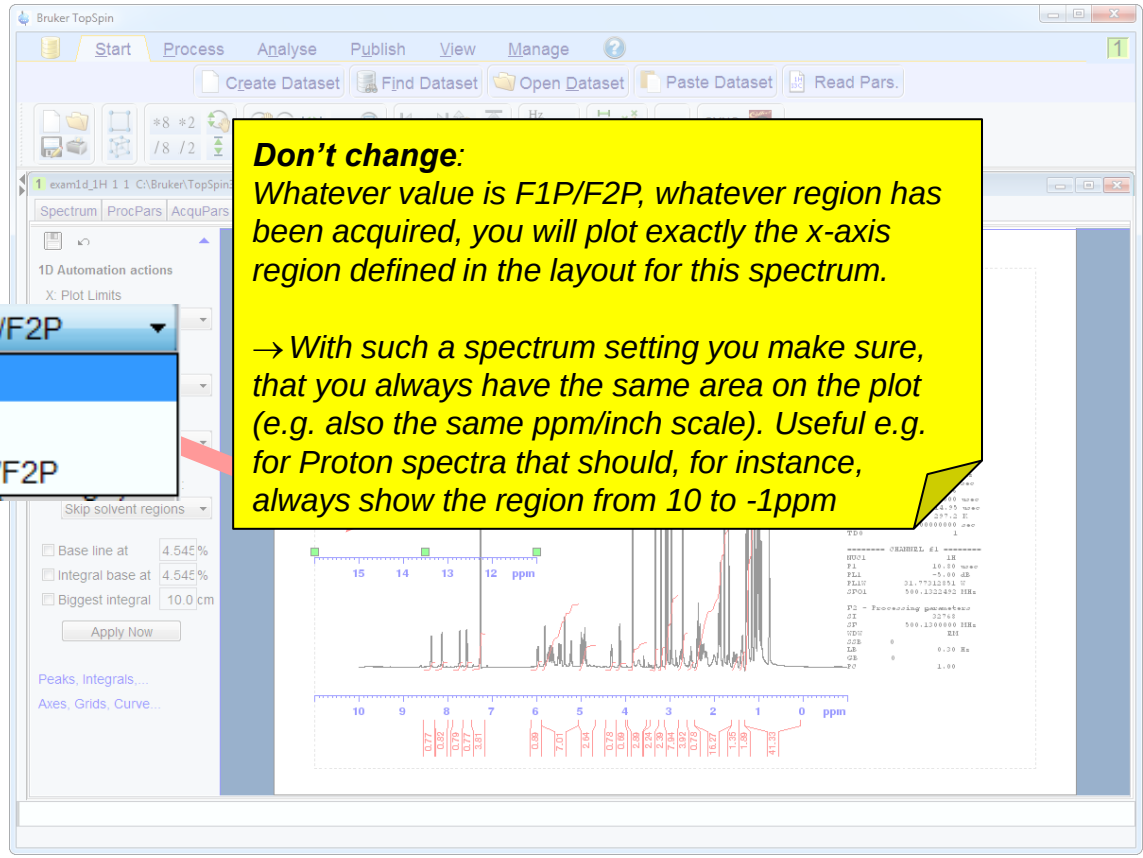


Automation actions:
X-axis: Plot limits

Layout **1D_H+lf** uses the automation action for x-axis **Don't change**





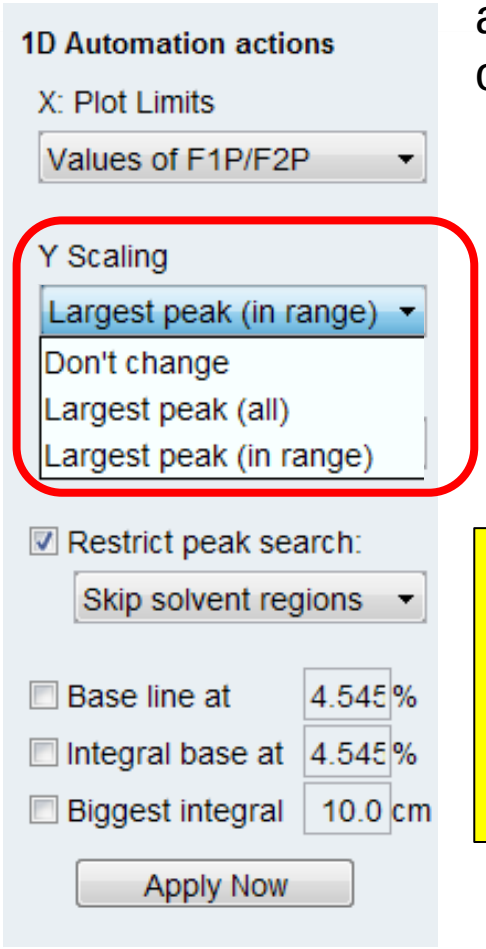


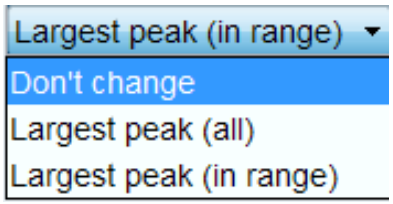
Don't change:
Whatever value is F1P/F2P, whatever region has been acquired, you will plot exactly the x-axis region defined in the layout for this spectrum.

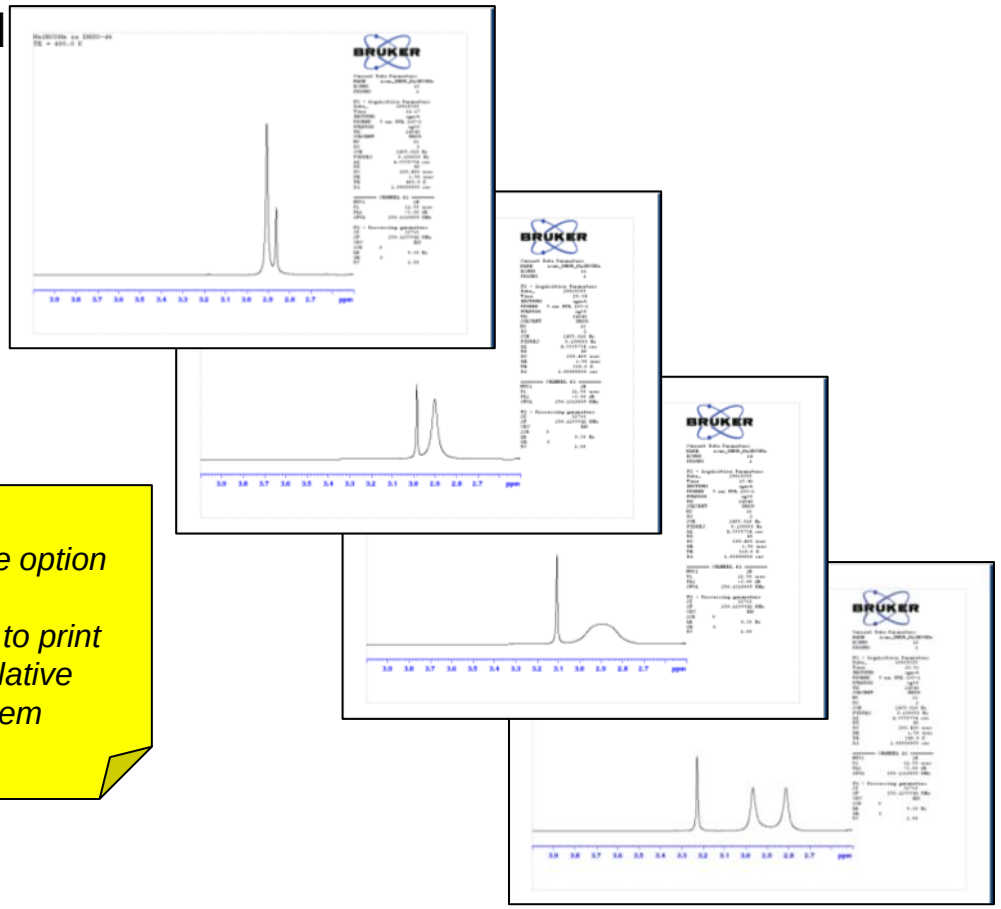
→ With such a spectrum setting you make sure, that you always have the same area on the plot (e.g. also the same ppm/inch scale). Useful e.g. for Proton spectra that should, for instance, always show the region from 10 to -1ppm

Automation actions: Y scaling relative to the intensity of a reference spectrum

Don't change: Y scaling should be used like it is stored within the layout (i.e. all datasets are printed with the intensity scale of the dataset the layout has originally be created





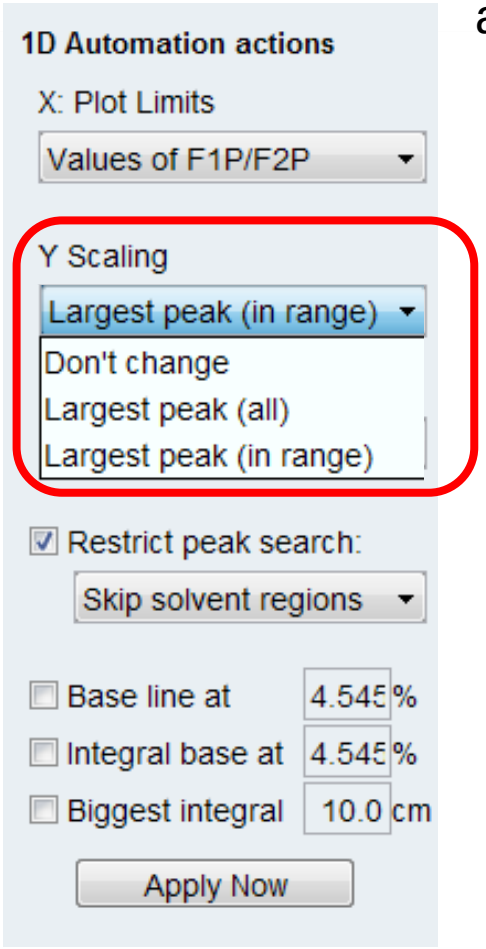


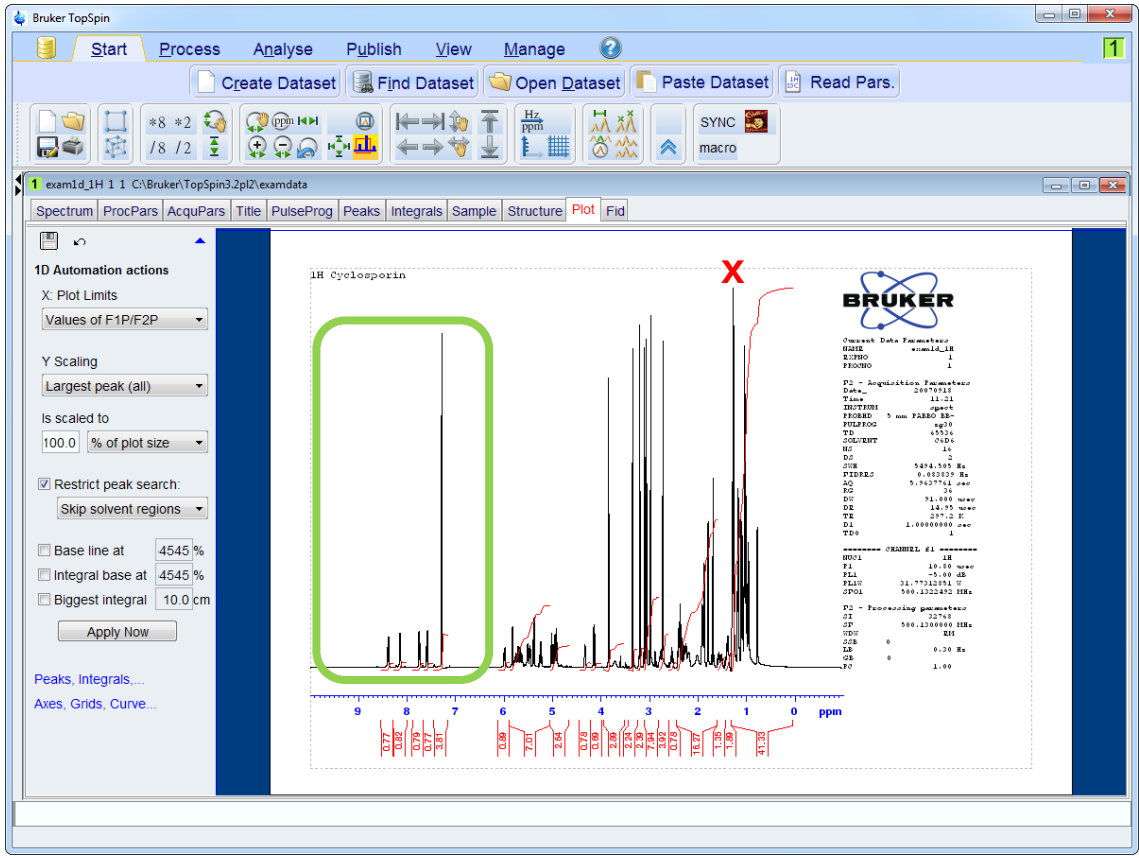
***Don't change**:*
This is a rarely used, but nice option

→ Can be useful if you want to print several datasets all with a relative height according to one of them (kinetics, tube reactions …)

Automation actions:
Y scaling: what is the biggest peak?

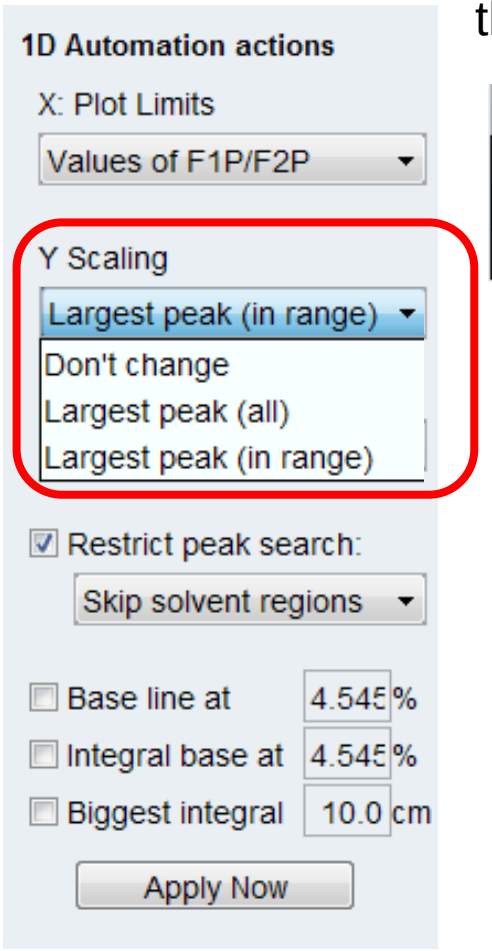
The area shown in the green box does not contain the biggest signal of the spectrum (**x**)
and the biggest signal in this area is the solvent signal

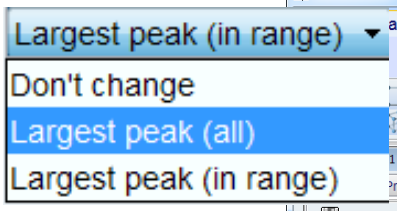


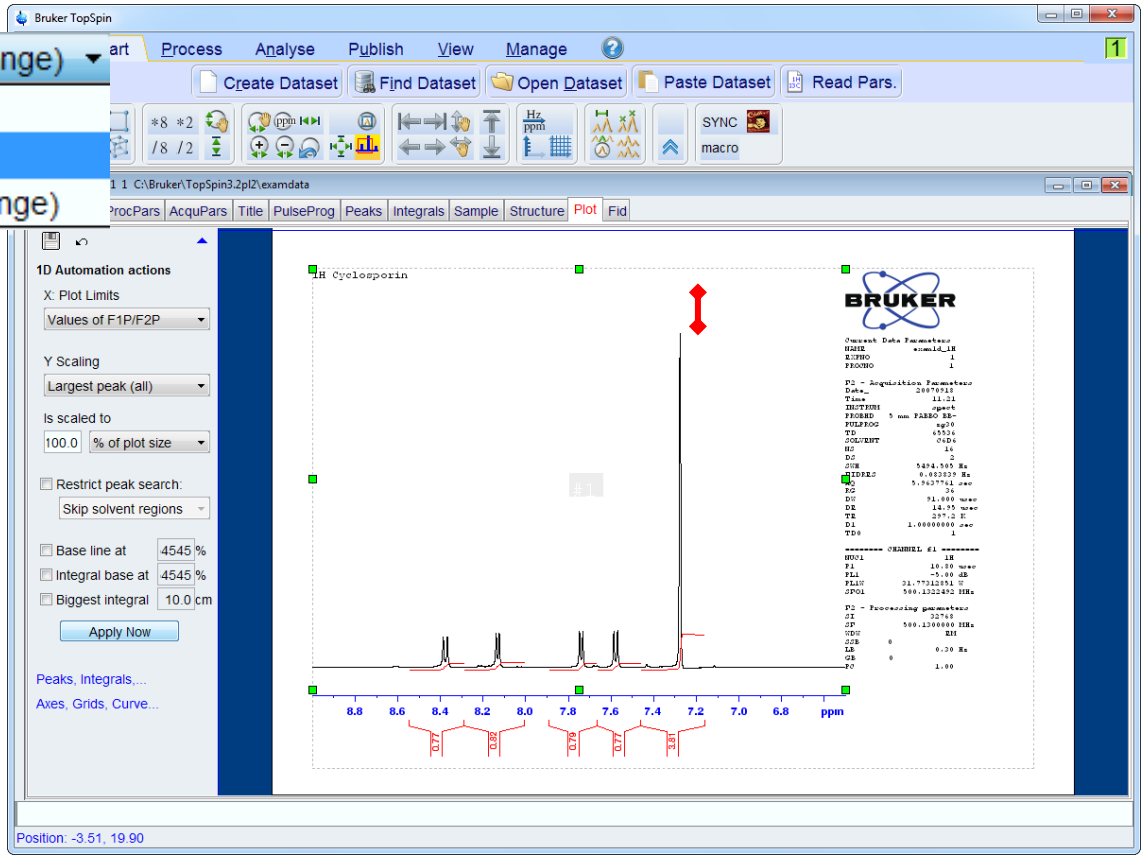


Automation actions:
Y scaling: what is the biggest peak?

Largest peak (all) scales the signals relative to the biggest signal in the spectrum:
therefore the visible peaks are not as big as possible (cf. red line)

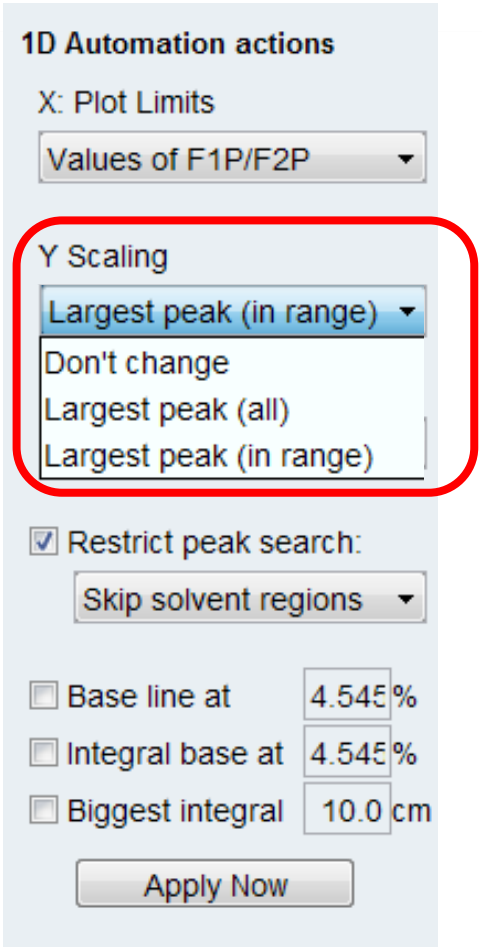


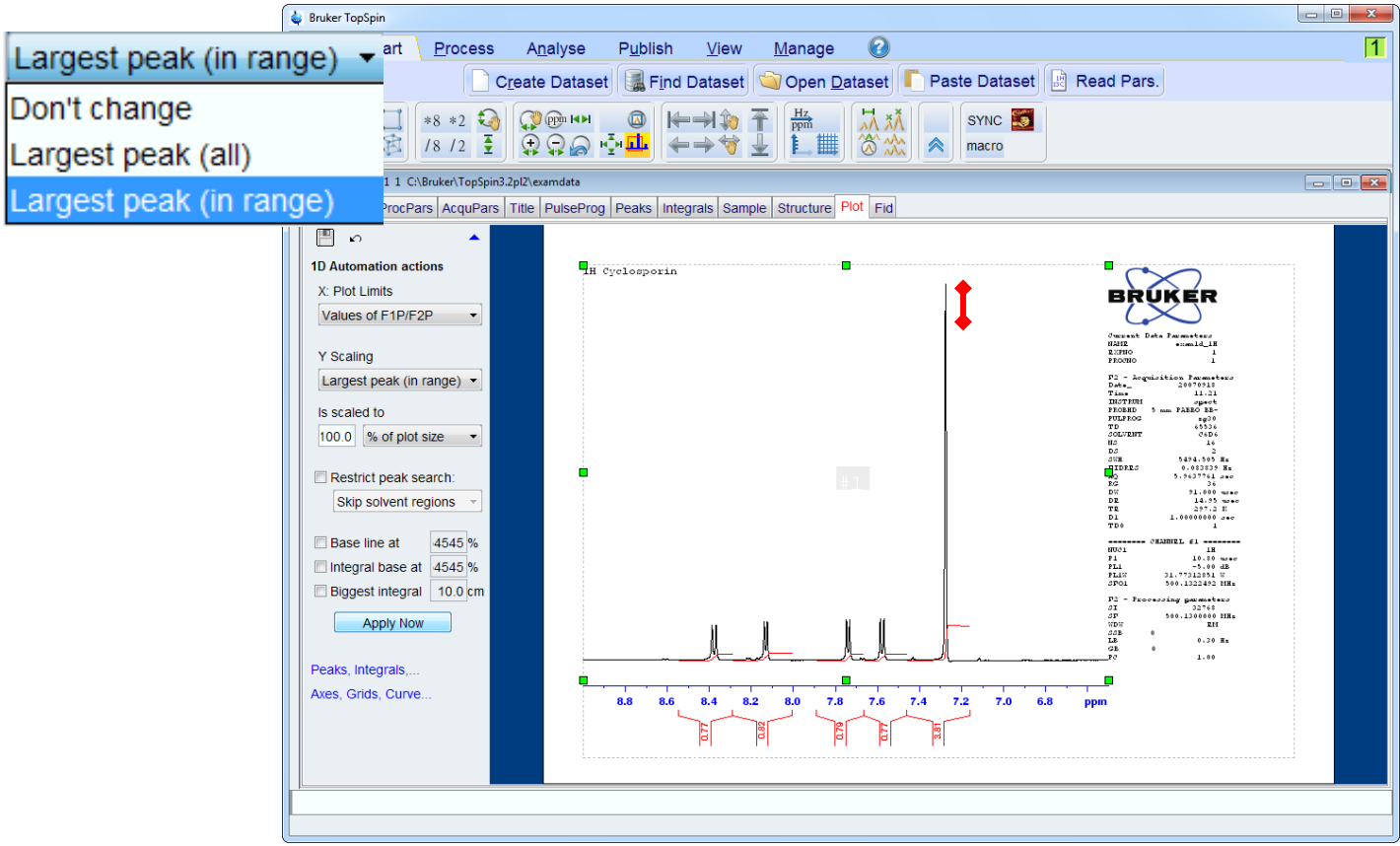




Automation actions:
Y scaling: what is the biggest peak?

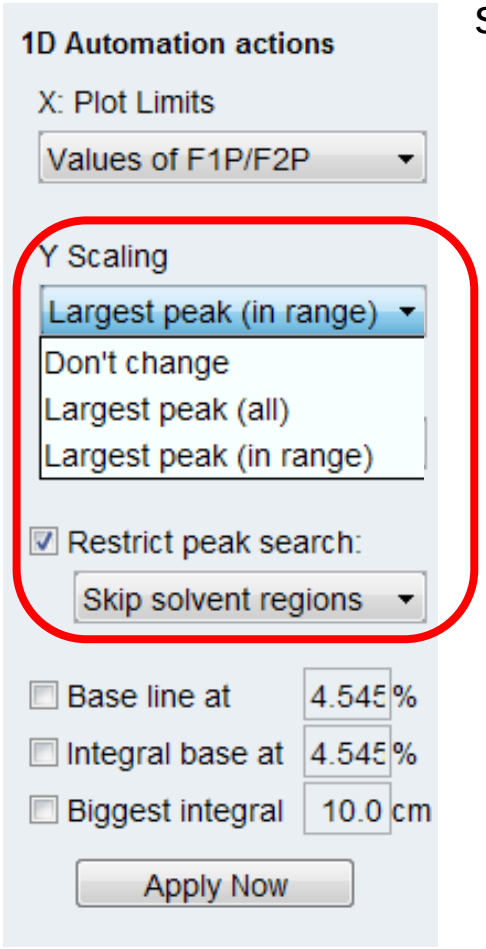
Largest peak (in range) instead scales the biggest visible signal as big as possible

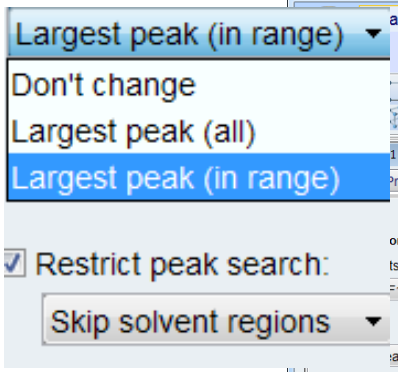


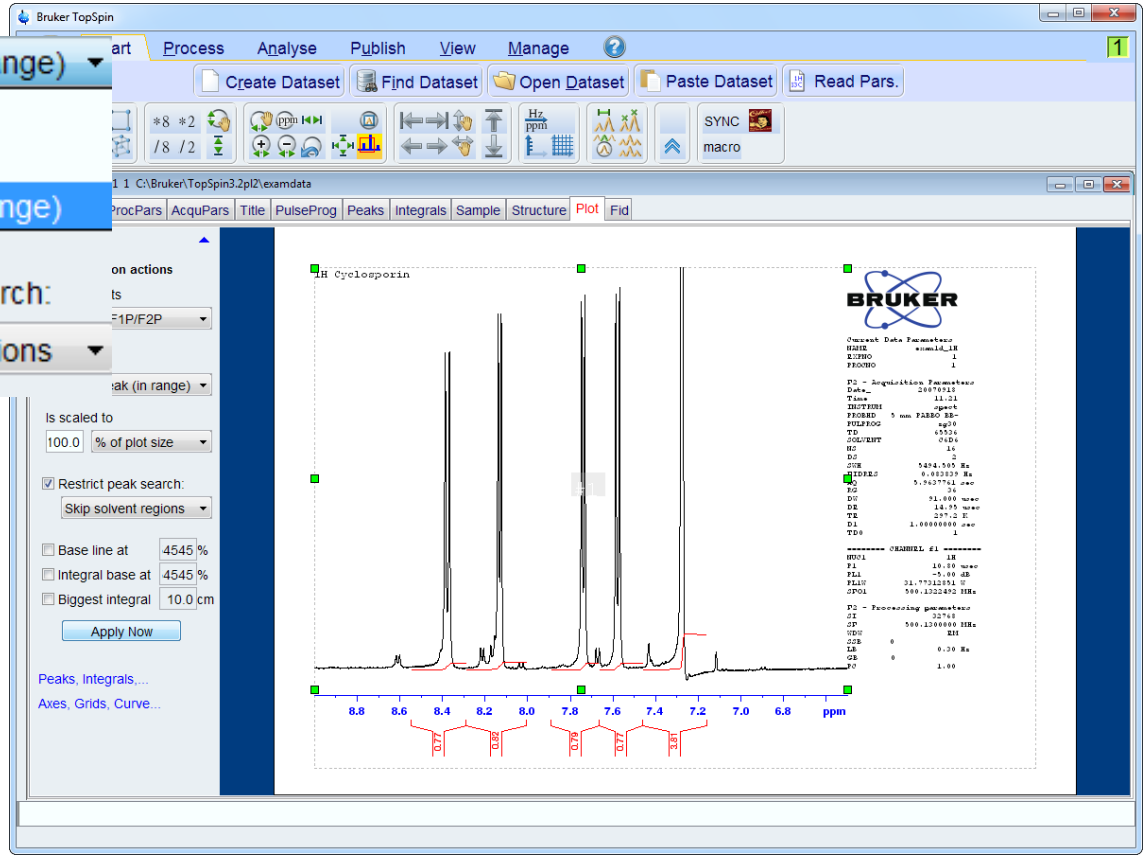


Automation actions:
Y scaling: what is the biggest peak?

Including **Skip Solvent regions** now ignores the biggest visible signal, because it is a solvent signal, and scales the small signals as big as possible

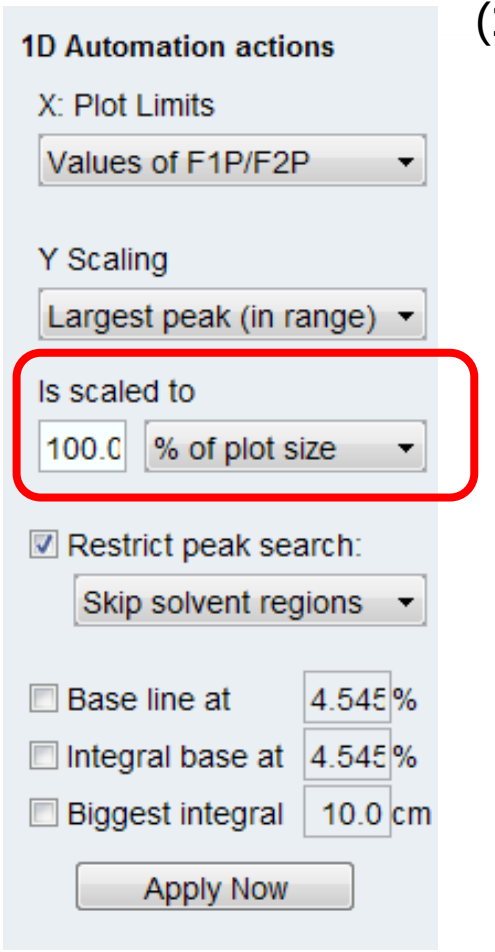


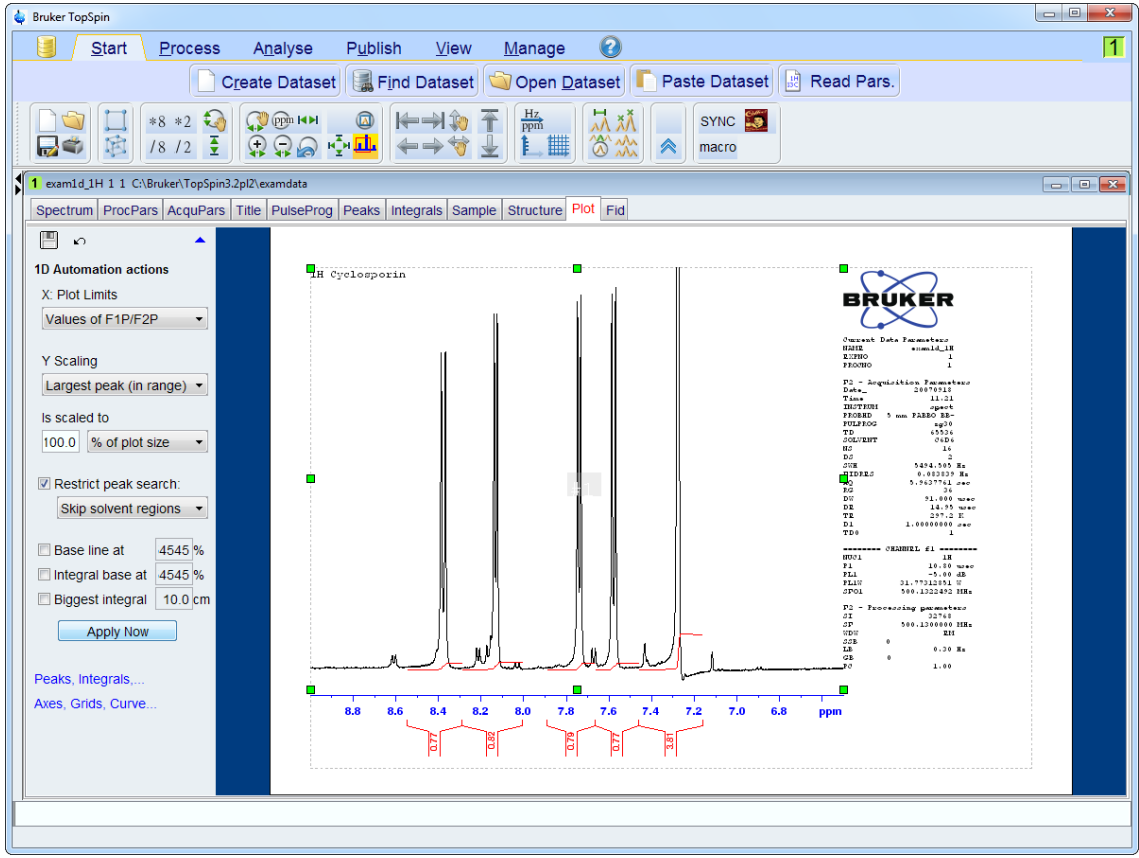




Automation actions:
Y scaling: what size is the biggest peak?

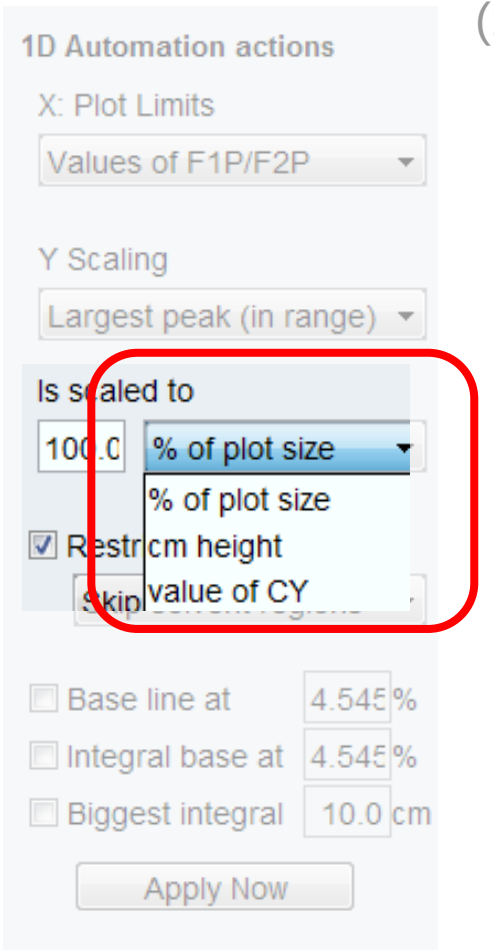
This setting defined the size of the biggest peak in the previous examples
(**100% of plot size** = as big as possible within the element size)

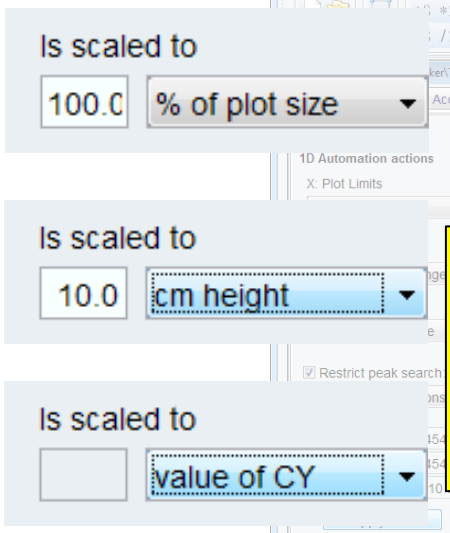


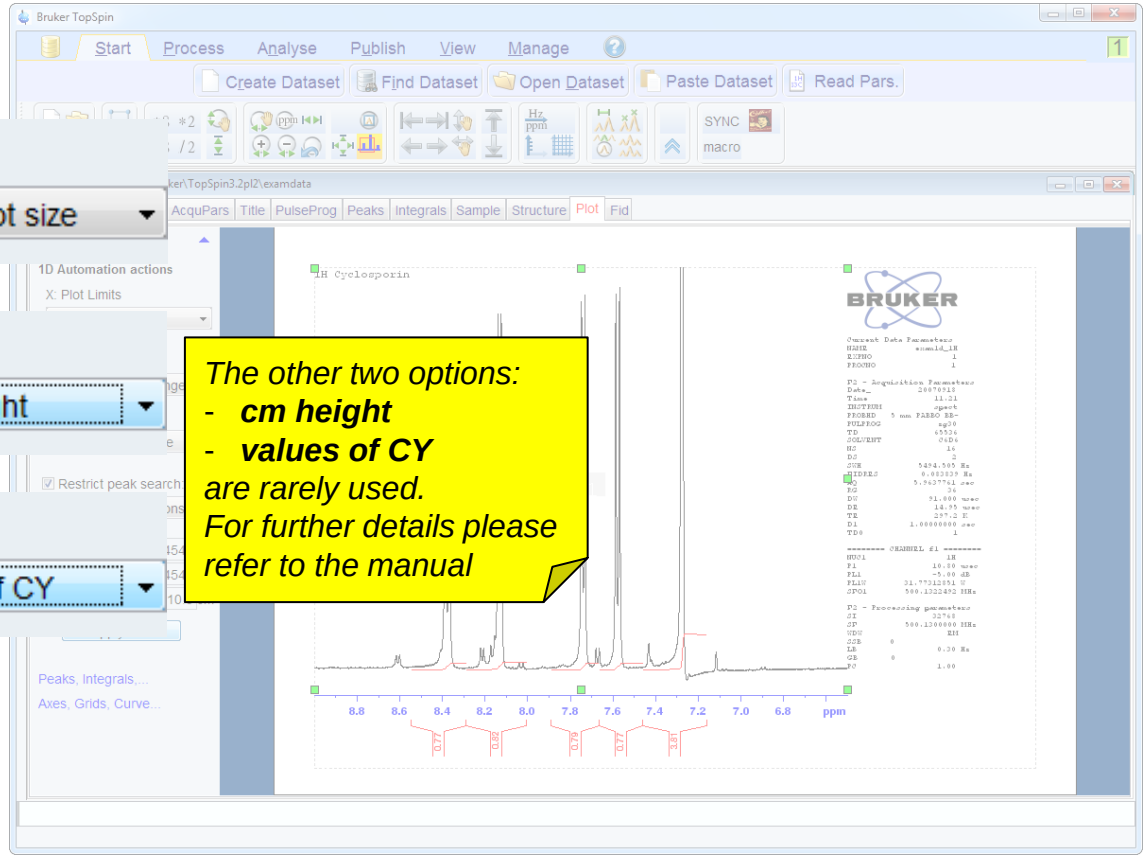


Automation actions:
Y scaling: what size is the biggest peak?

This setting defined the size of the biggest peak in the previous examples
(**100% of plot size** = as big as possible within the element size)





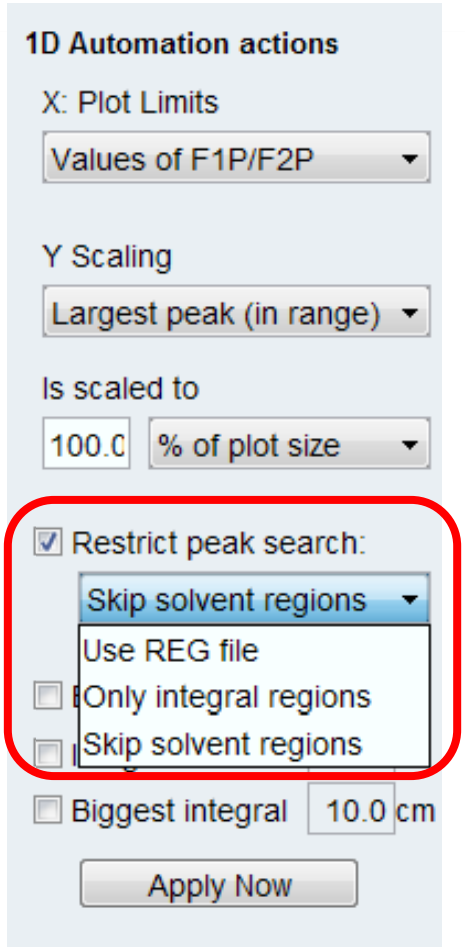


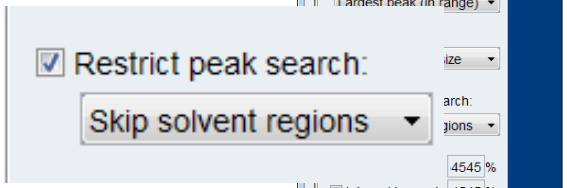
The other two options:
- ***cm height***
- ***values of CY***

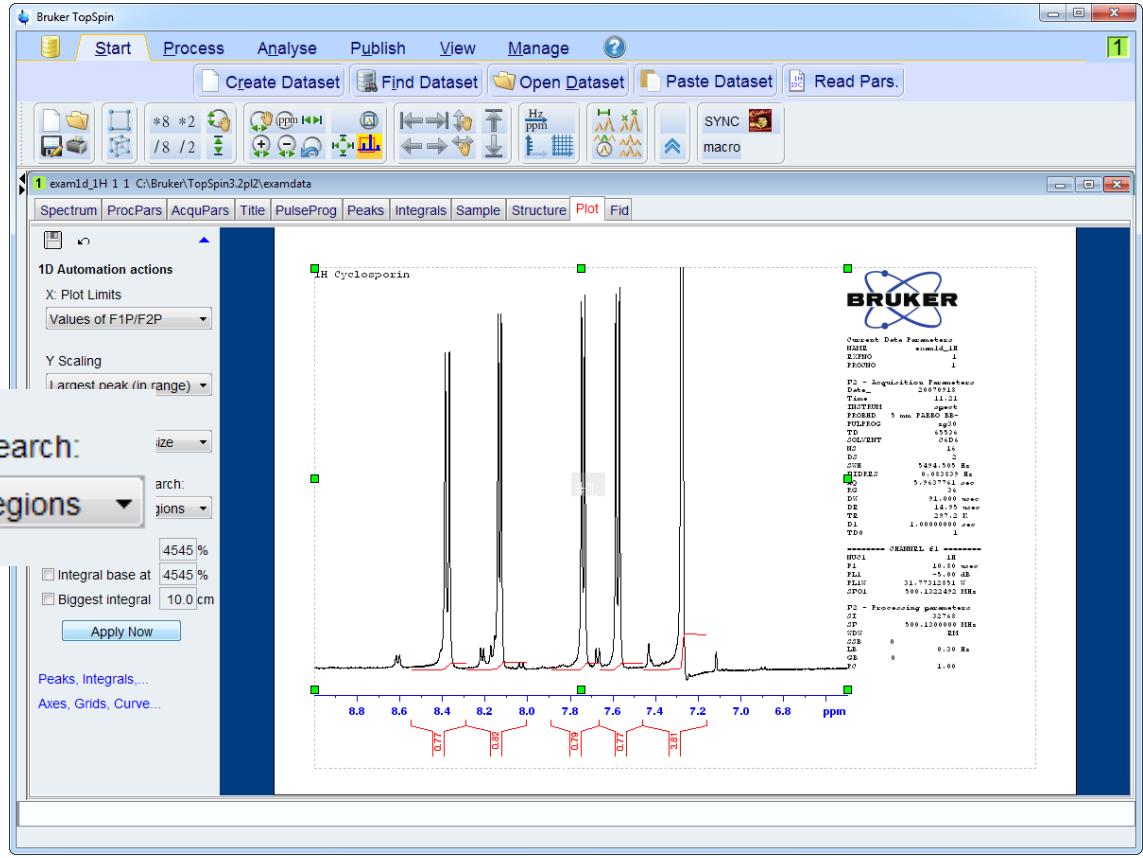
are rarely used.
For further details please refer to the manual

Automation actions:
Y scaling: which peaks are of (no) interest

Restrict peak search: the default **Skip solvent signal** has already been discussed

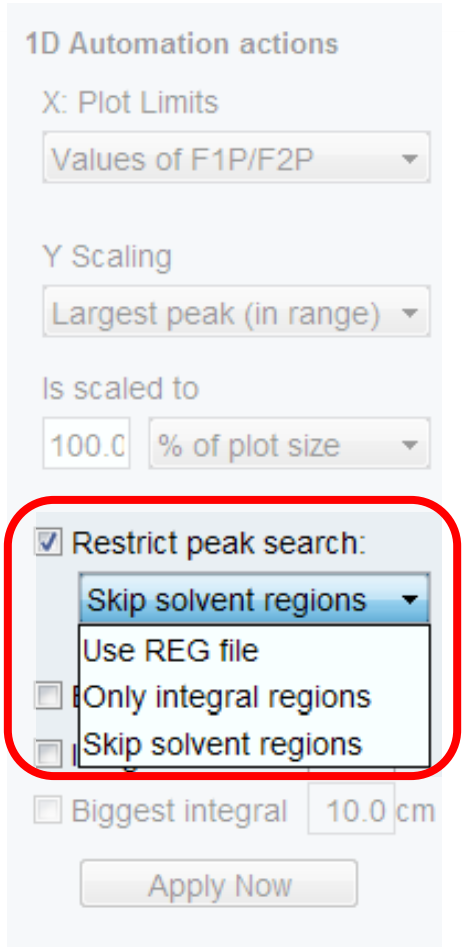


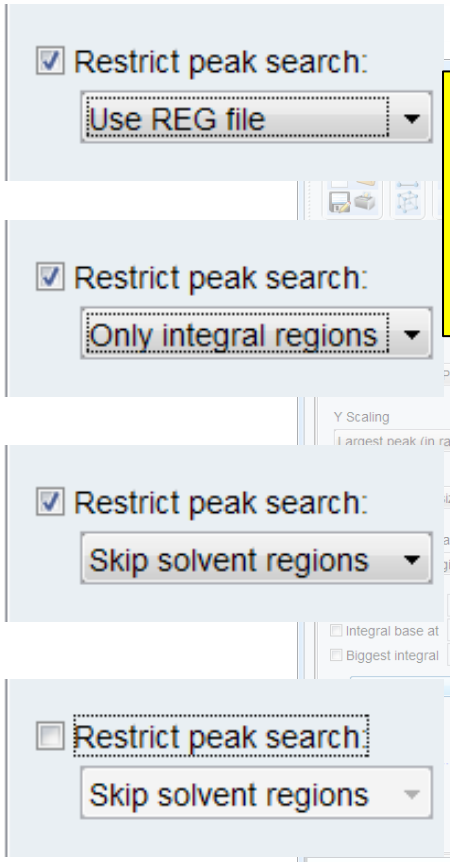




Automation actions:
Y scaling: which peaks are of (no) interest

Restrict peak search: the default **Skip solvent signal** has already been discussed





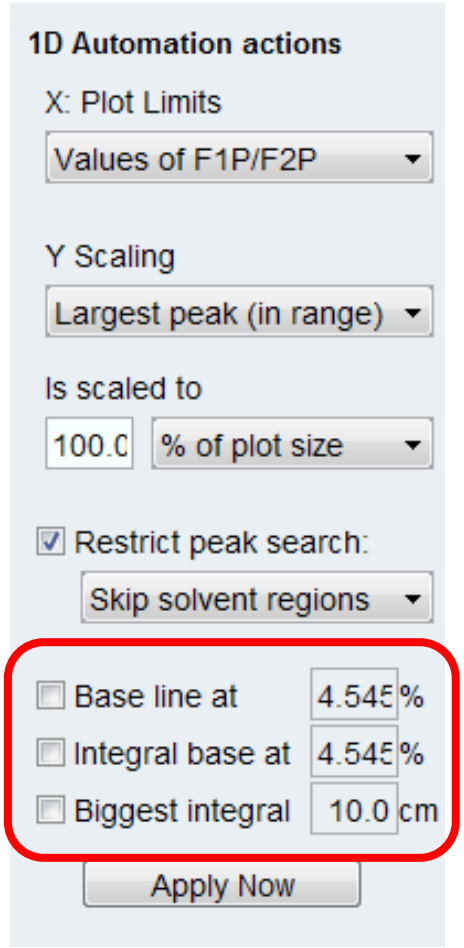
The other two options:
- ***Use REG file***
- ***Only integral regions***

are rarely used.
For further details please refer to the manual

*Uncheck **Restrict peak search** will consider all peaks for Y scaling*

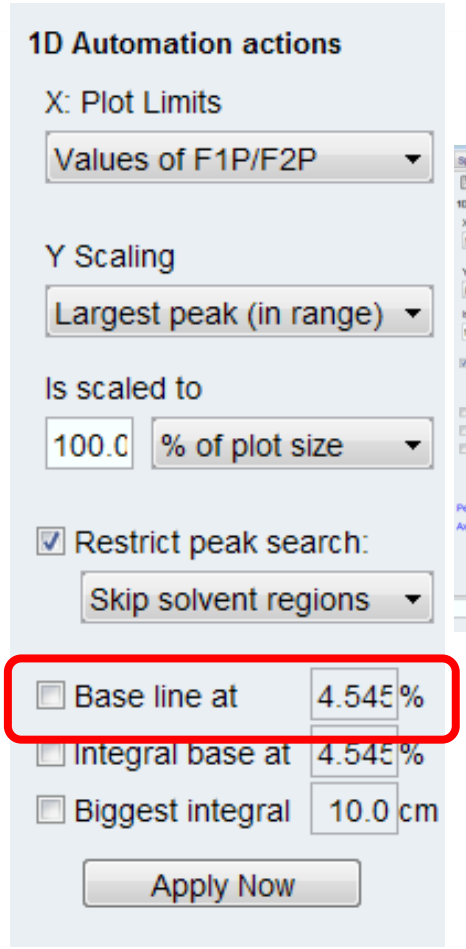
Automation actions:
further automation actions

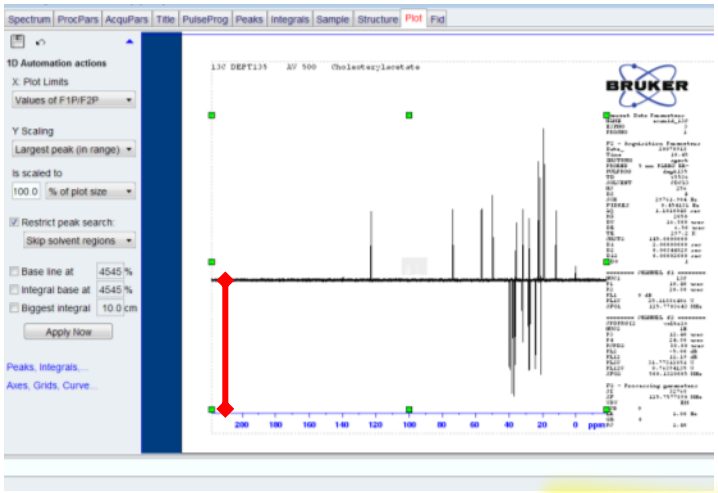
To complete the automation actions some settings for baseline and integrals are offered

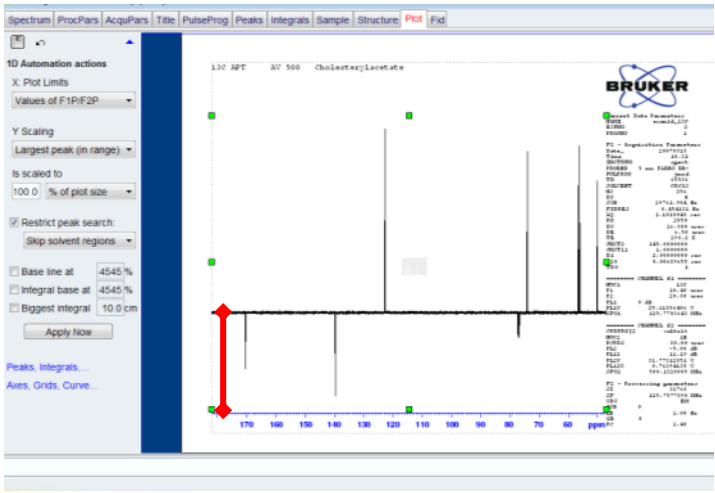


Automation actions:
further automation actions: Base line at x.xxx %

By default (**Base line at** unchecked) the base line of a spectrum is placed in such a way, that all positive AND all negative signals are visible (cf. red lines)





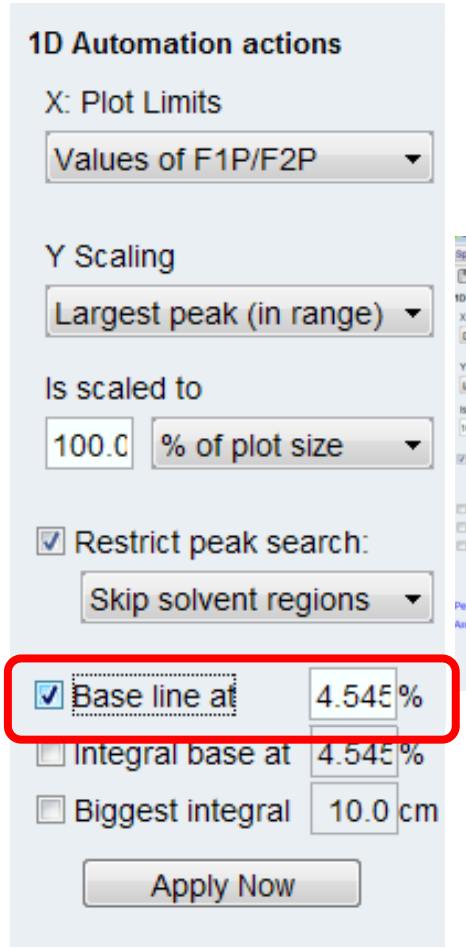


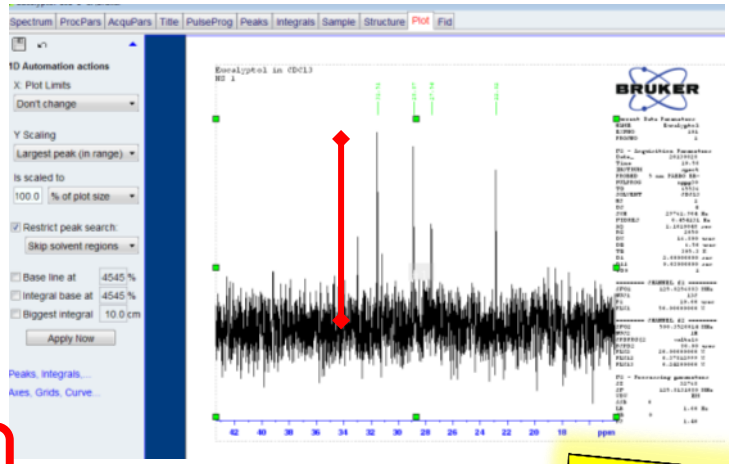
That's great e.g. for DEPT spectra.

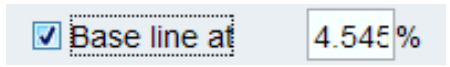
Base line is place automatically at the best position

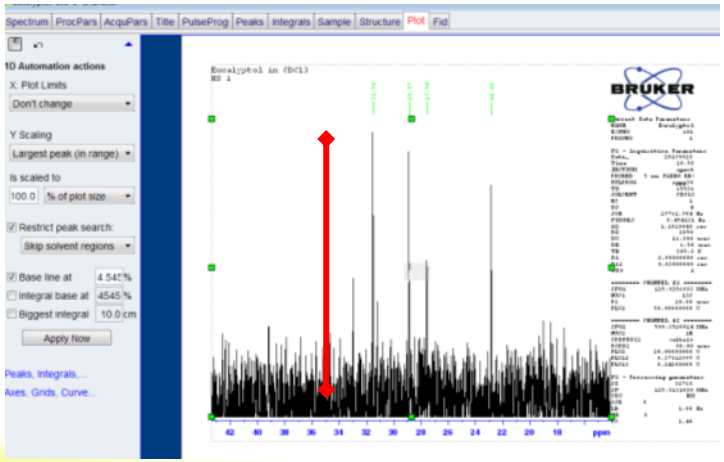
Automation actions:
further automation actions: Base line at x.xxx %

Checking **Base line at** keeps it fixed independent of negative signals. The default value 4.545% describes the standard position of a non moved base line.







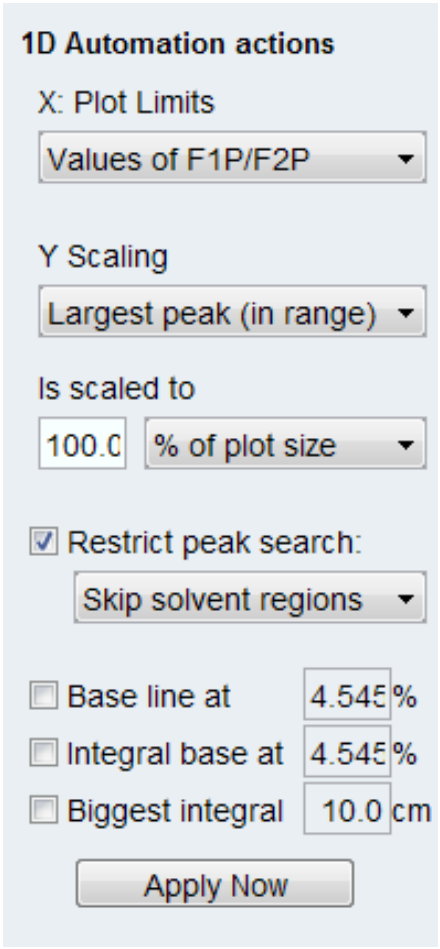


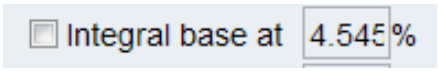
Keeping the base line fixed is useful for noisy spectra, e.g. from long term heteronuclei acquisitions, that have a fairly bad signal-to-noise ratio

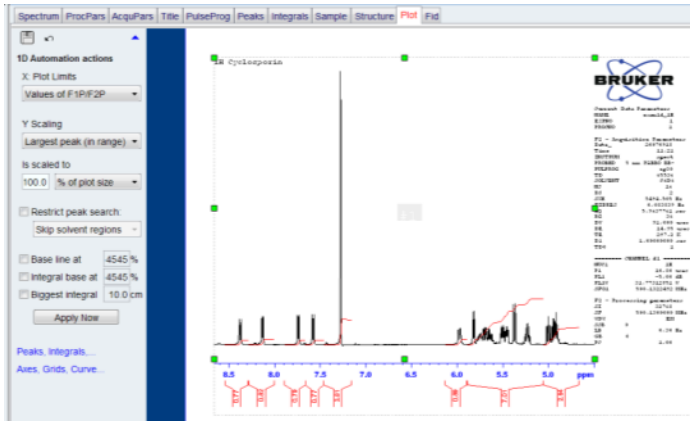
Automation actions:
further automation actions: Integrals base at x.xxx %

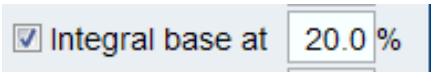
By default, drawing integrals starts at spectrum baseline, wherever baseline is placed.

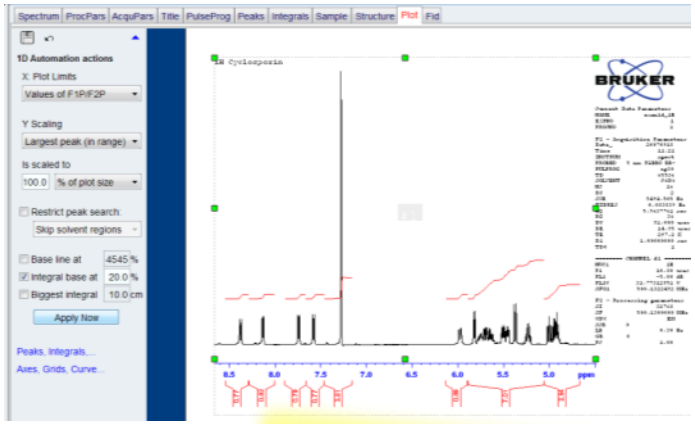
Integral base at allows you to change this.







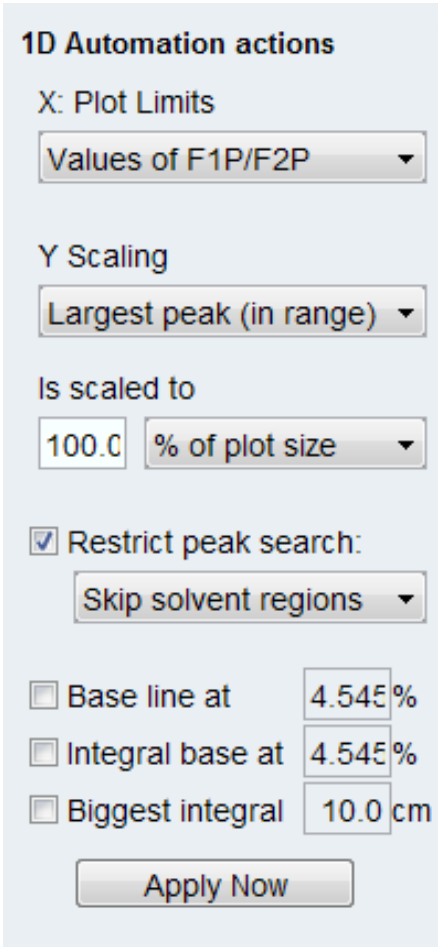


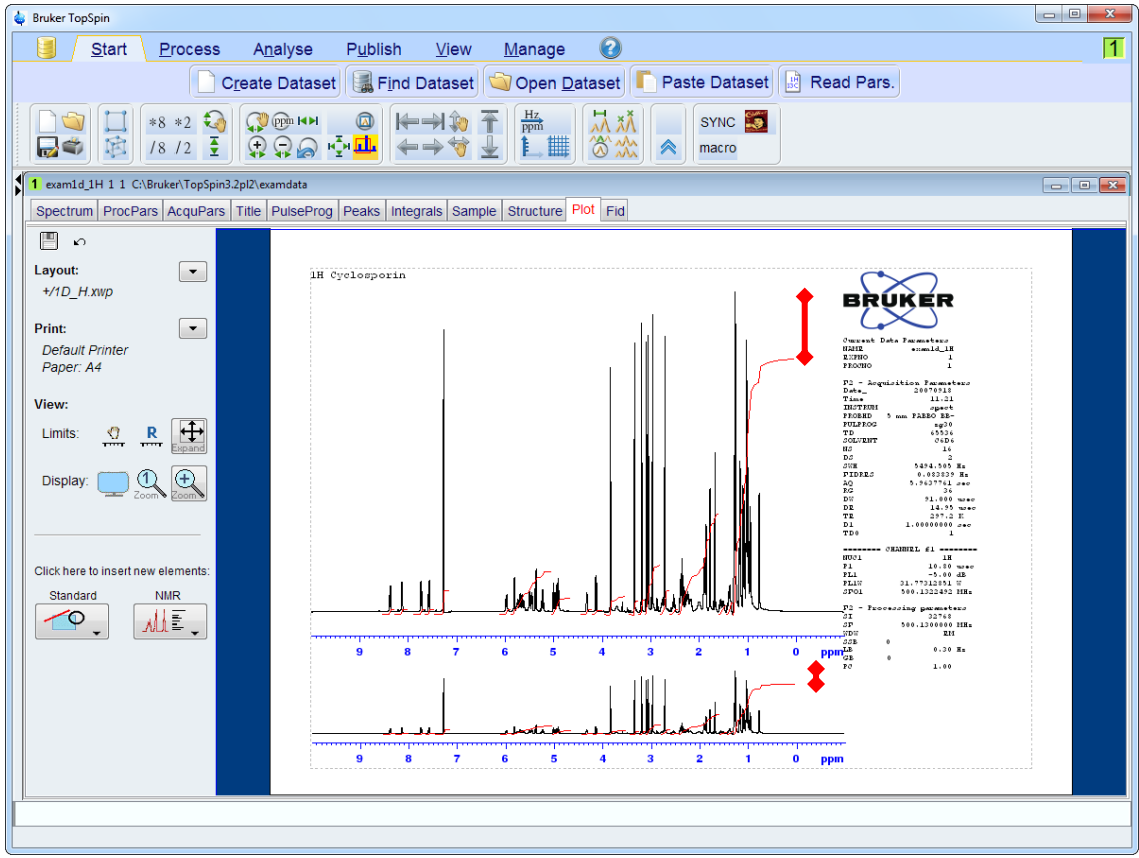


Moving integrals to a another position is useful if you want to measure printed integrals with a ruler, for instance.

Automation actions:
further automation actions: Biggest integral x.xx cm

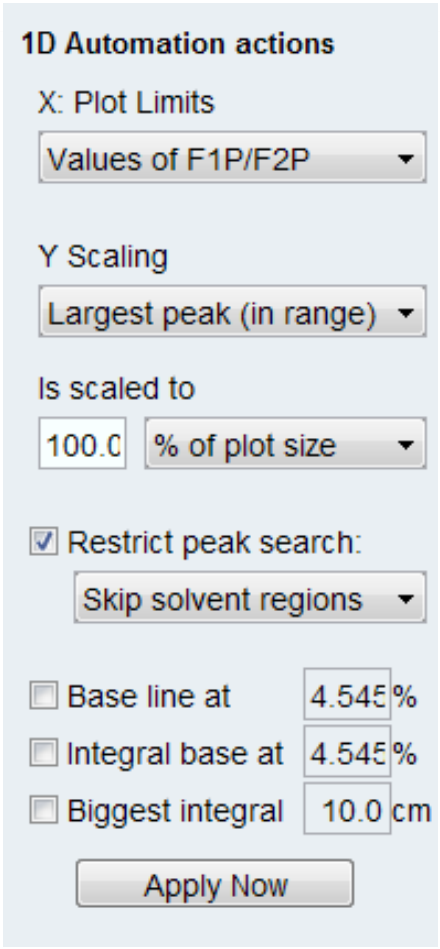
By default, the biggest integral is printed a little bit smaller than the biggest signal (cf. red lines).

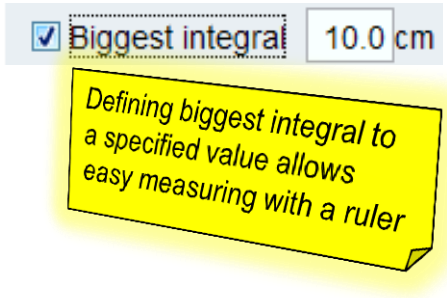




Automation actions:
further automation actions: Biggest integral x.xx cm

By default, the biggest integral is printed a little bit smaller than the biggest signal, but **Biggest integral** allows to define a fixed value.

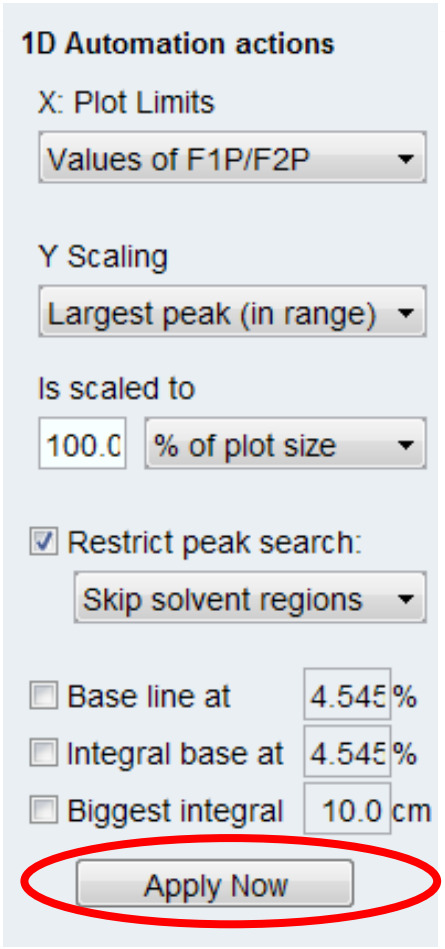




Automation actions: executing and testing

With the **Apply now** button you can execute the automation actions defined.

→ are the settings doing what you expected them to do?



Automation actions: executing and testing

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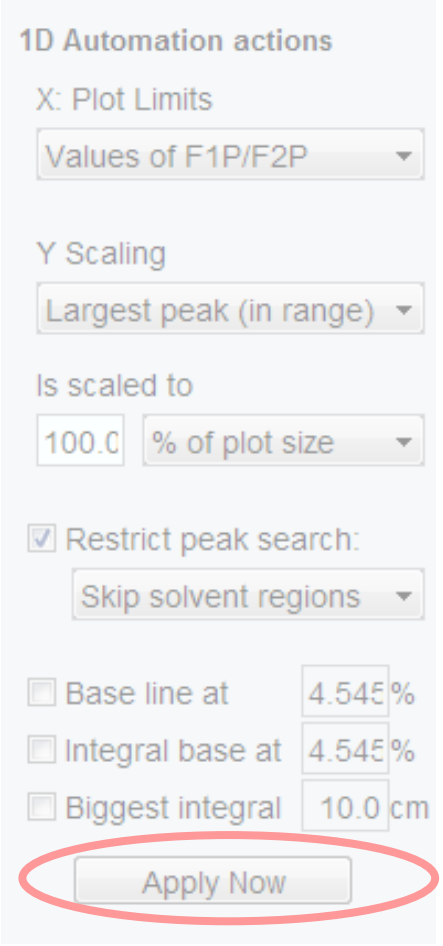
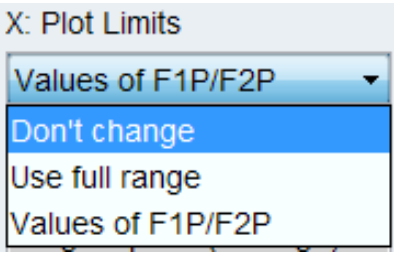


Note:
*The x-Axis setting **'Don't change'** is a bit tricky to test.*

If you have numerically defined a specific x-axis range in the layout and a different range becomes visible when you switch to the plot tab, then your spectrum is displayed in "current range" mode and not the one defined in the layout. Executing the x-axis automation action 'Don't change' will now overwrite the values in the layout with the limits read from the TopSpin spectrum display for this plot!

Tip:
Instead of clicking on the plot tab go there by executing the TopSpin command:
***plot –n** (no automation actions will be executed)*
***plot –r** (the automation actions are be executed and x-axis will show up in the area defined in the layout)*
Both ways will open the layout as defined without taking over the limits from the currently shown spectrum range.



Automation actions:
Only for automation?

Useful to know:

1. Automation (IconNMR) plots any layout according to all its automation actions*.

2. With the **Apply now** button in the **Automation actions** settings of an element you can test and execute the actions manually.

3. The TopSpin command:
   plot –r
   opens the plot tab and immediately executes all automation actions

4. The TopSpin command:
   plot –n
   opens the plot tab and ignores the limits set in the TopSpin spectrum display.

* IconNMR can also be configured to use user specific layouts instead of the Bruker predefined ones. More details are available in the training: 'Plotting in TopSpin – Advanced'

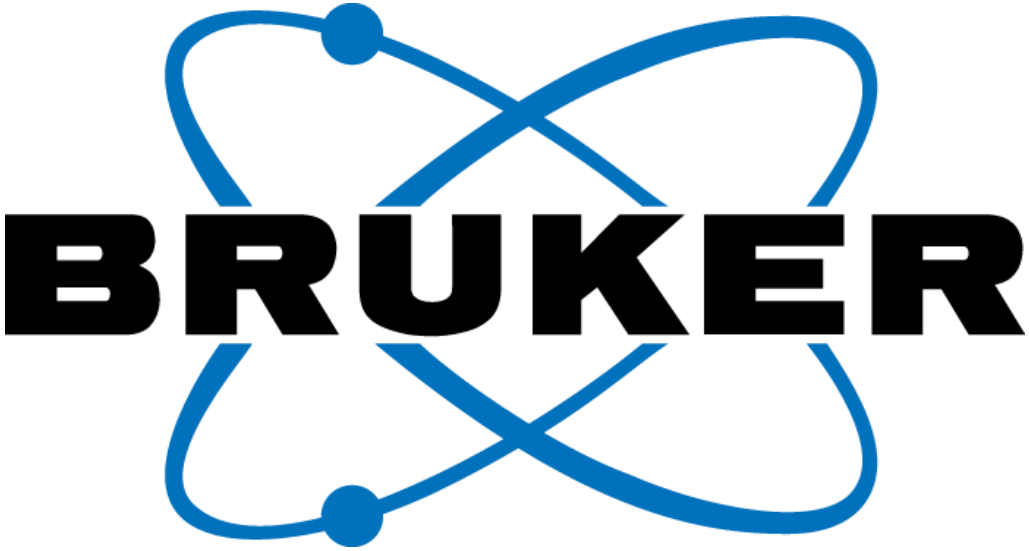
Different situations = different solutions
→ 1 tool

Summary:

Automation actions of each individual spectrum object can be precisely configured to get the desired print-out for any experiment measured in automation.
Should one layout not be enough to cover the needs of all automation experiments, then different layouts can be used.

Situation 4

- I want to get nice print-outs for all samples of my automation run



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