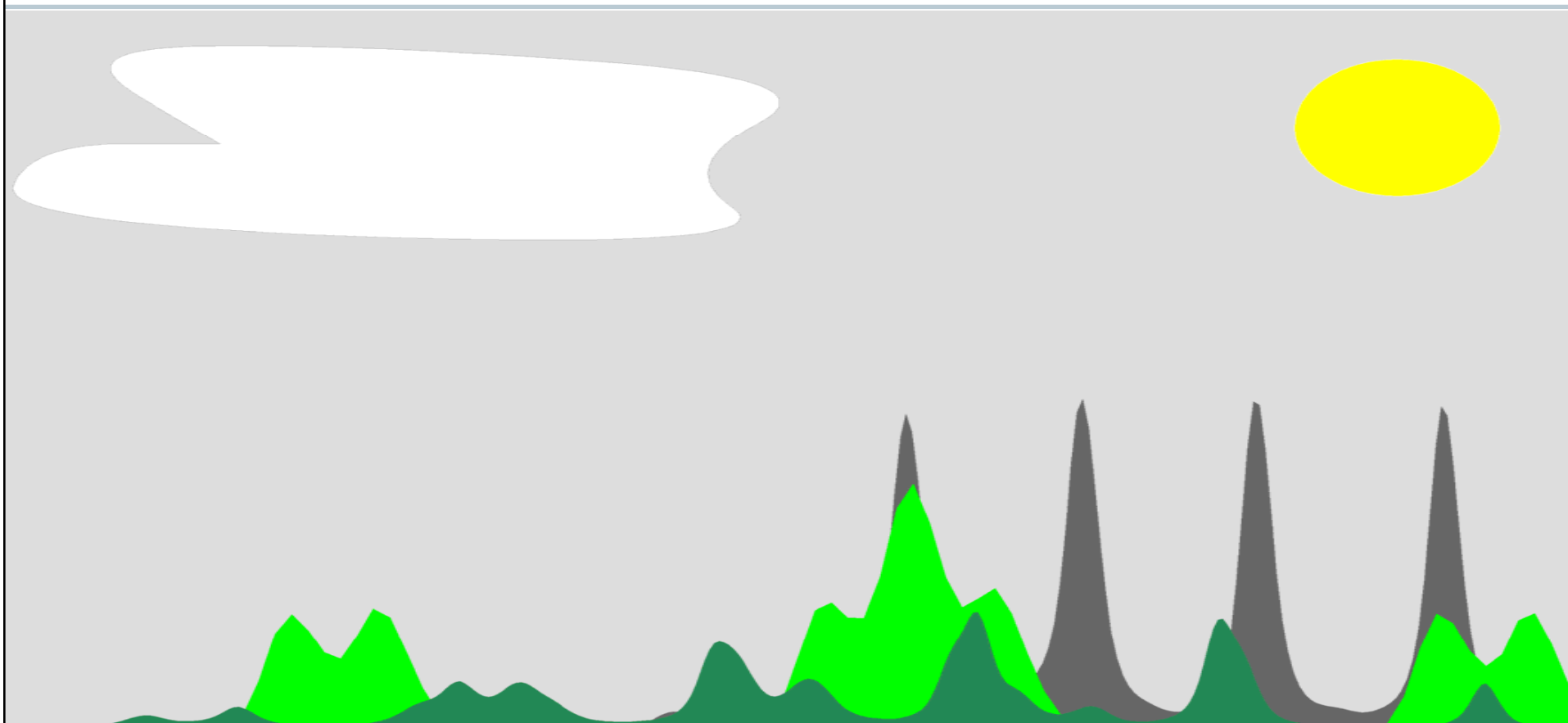


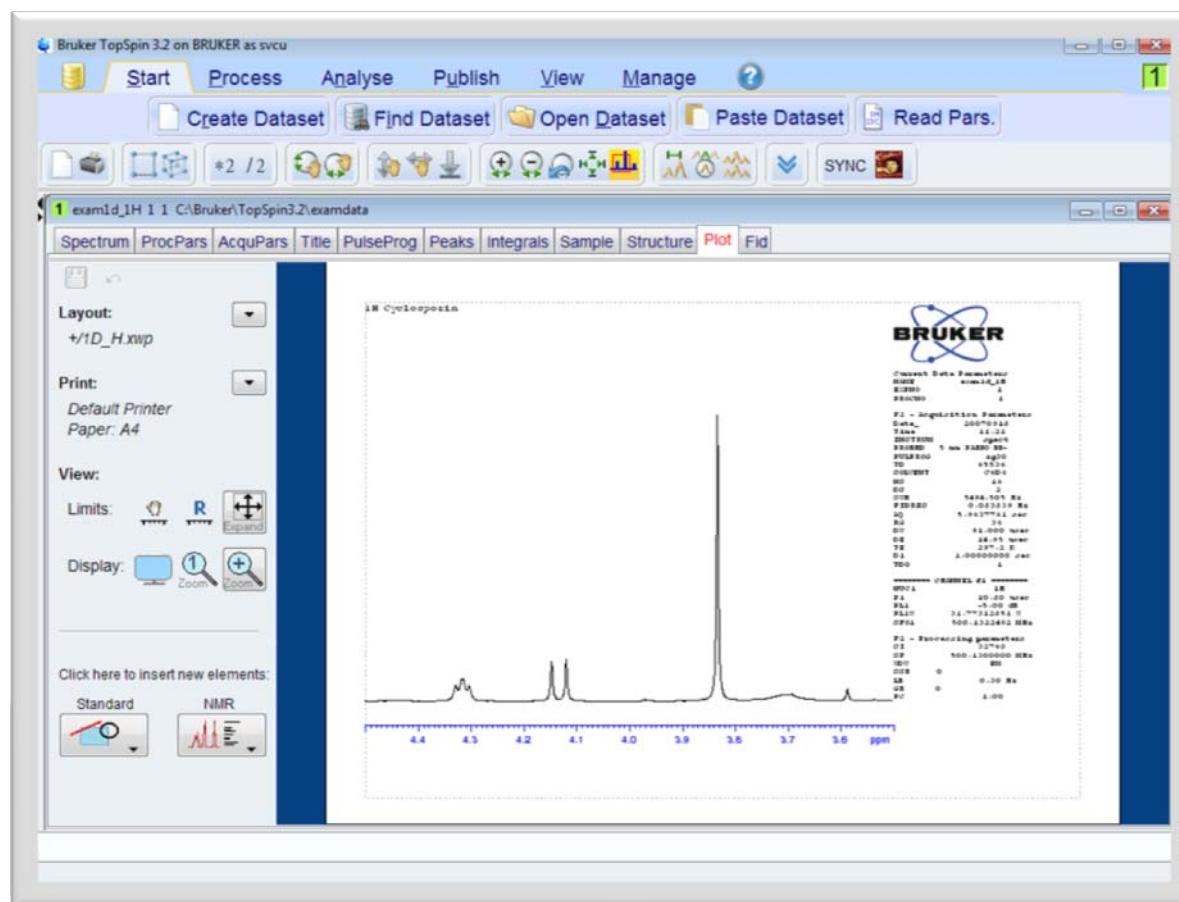
# Topspin plot editor



Clemens Anklin  
Bruker BioSpin Corp  
Avance-I course  
Billerica MA, June 10. – 13. 2013



# Plotting and creating output with Topspin 3.2



# The user interface



## Overview

The screenshot displays the Bruker TopSpin 3.2 software interface. The main window shows a 1D NMR spectrum of menthyltranilate-0712. The x-axis is labeled in ppm, ranging from 9.0 to 0.5. The spectrum shows several peaks, with a prominent one at approximately 1.0 ppm. The interface includes a menu bar (Start, Process, Analyse, Publish, View, Manage), a toolbar with various icons, a file browser on the left, and a status bar at the bottom right.

**Plot Portfolio**

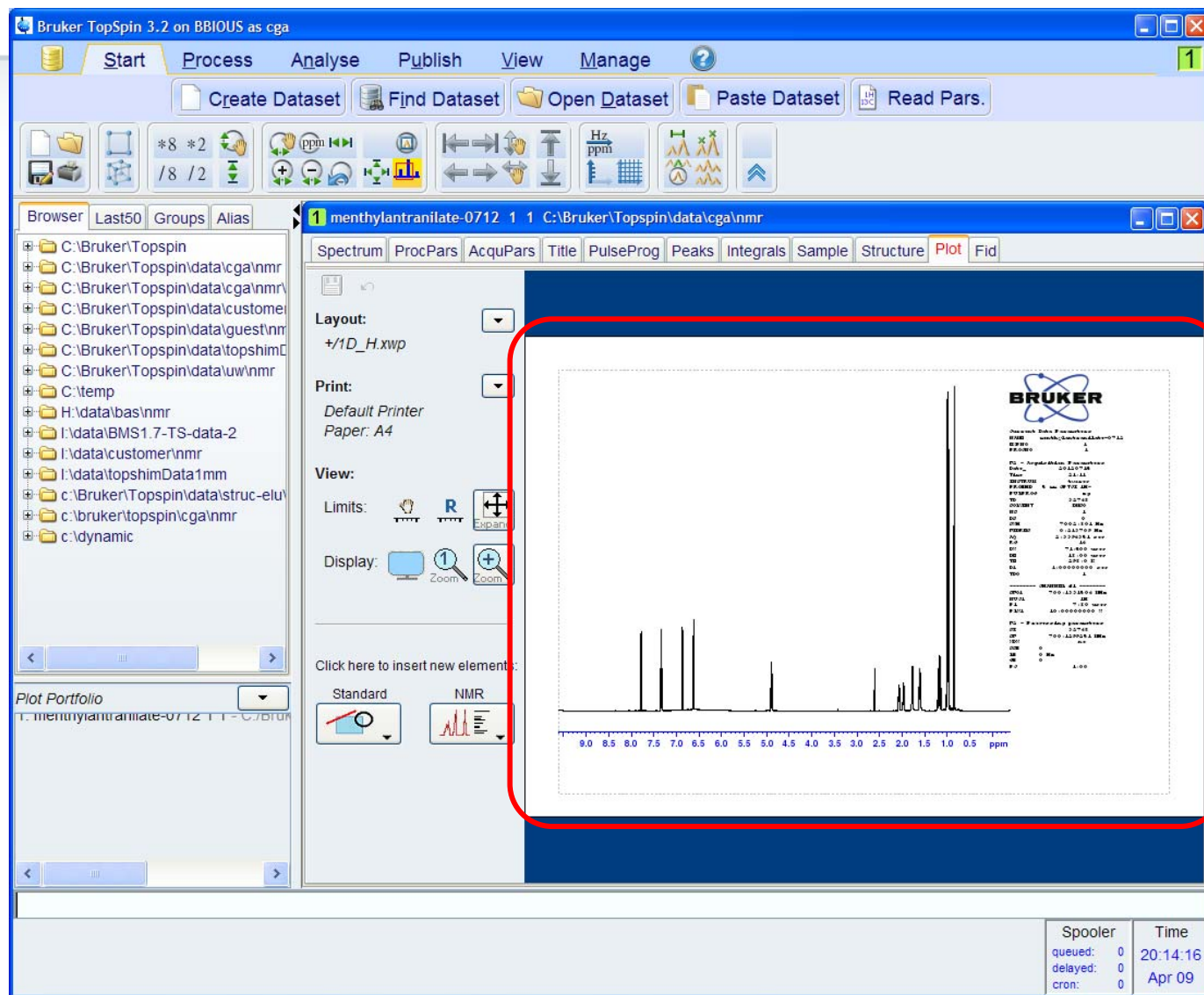
1. menthyltranilate-0712 1 1 - C:\Bruker\TopSpin\data\cga\nmr

Spooler	Time
queued: 0	20:14:16
delayed: 0	
cron: 0	Apr 09

# The user interface



Plot area



# The user interface



Plot functions

Layouts

Printers

View

Objects

The screenshot displays the Bruker TopSpin 3.2 software interface. The main window shows a spectrum plot with a Bruker logo and technical data on the right. A configuration panel is overlaid on the left side of the plot, containing the following sections:

- Layout:** A dropdown menu showing *+1D\_H.xwp*.
- Print:** A dropdown menu showing *Default Printer* and *Paper: A4*.
- View:** A section with icons for *Limits* (a lightbulb icon), *R* (a red 'R' icon), and *Expand* (a four-way arrow icon).
- Display:** A section with icons for *Zoom* (a magnifying glass icon) and *Zoom* (a magnifying glass with a plus sign icon).
- Click here to insert new elements:** A section with two buttons: *Standard* (a magnifying glass icon) and *NMR* (a spectrum plot icon).

The spectrum plot shows a series of peaks on a scale from 9.0 to 0.5 ppm. The configuration panel is highlighted with a red border.

Spooler	Time
queued: 0	20:14:16
delayed: 0	
cron: 0	Apr 09

# The new user interface



Data Browser

The screenshot displays the Bruker TopSpin 3.2 software interface. The main window is titled "Bruker TopSpin 3.2 on BBIOS as cga". The menu bar includes "Start", "Process", "Analyse", "Publish", "View", and "Manage". Below the menu bar are several toolbars with icons for file operations and data processing. The "Data Browser" window is highlighted with a red box and shows a tree view of the file system. The tree view includes folders such as "C:\Bruker\Topspin", "C:\Bruker\Topspin\data\cga\nmr", "C:\Bruker\Topspin\data\customer", "C:\Bruker\Topspin\data\guest\nmr", "C:\Bruker\Topspin\data\topshim", "C:\Bruker\Topspin\data\uw\nmr", "C:\temp", "H:\data\bas\nmr", "I:\data\BMS1.7-TS-data-2", "I:\data\customer\nmr", "I:\data\topshimData1mm", "c:\Bruker\Topspin\data\struc-el", "c:\brukertopspin\cga\nmr", and "c:\dynamic". The main window also displays a spectrum plot for "menthylantranilate-0712 1 1" with a Bruker logo and technical parameters. The status bar at the bottom right shows "Spooler" and "Time" information.

Spooler	Time
queued: 0	20:14:16
delayed: 0	
cron: 0	Apr 09

# The user interface



Portfolio area

The screenshot displays the Bruker TopSpin 3.2 software interface. The main window shows a 1D NMR spectrum with a chemical shift axis from 9.0 to 0.5 ppm. The spectrum features several peaks, with a prominent one at approximately 1.0 ppm. The interface includes a menu bar (Start, Process, Analyse, Publish, View, Manage), a toolbar with various icons, and a browser pane on the left showing a file tree. A 'Plot Portfolio' area at the bottom left is highlighted with a red box, containing a dropdown menu and a list of plots. The status bar at the bottom right shows 'Spooler' and 'Time' information.

Spooler	Time
queued: 0	20:14:16
delayed: 0	
cron: 0	Apr 09

# The plot and view functions



Plot functions

Layouts

Printers

View

Objects

The screenshot displays the Bruker TopSpin 3.2 software interface. The main window shows a 1D NMR spectrum plot with a Bruker logo and technical parameters on the right. A configuration panel is overlaid on the left side of the plot, enclosed in a red box. This panel includes settings for Layout (\*/1D\_H.xwp), Print (Default Printer, Paper: A4), View (Limits, Display), and options to insert new elements (Standard, NMR). The interface also features a menu bar (Start, Process, Analyse, Publish, View, Manage) and a toolbar with various icons for file operations and data analysis.

Spooler	Time
queued: 0	20:14:16
delayed: 0	
cron: 0	Apr 09



# The plot and view functions



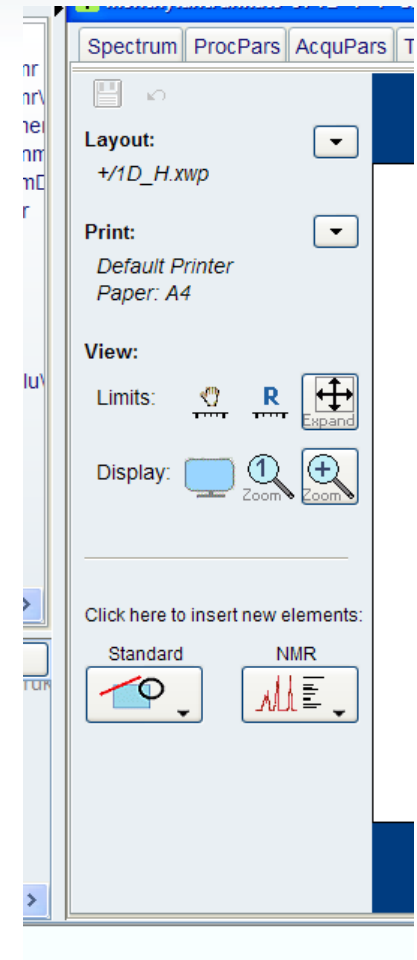
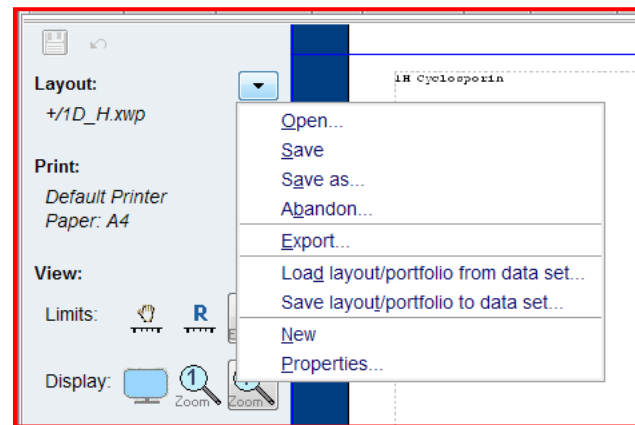
Plot functions

**Layouts**

Printers

View

Objects



# The plot and view functions



The layout is by default imported from the data set.

The screenshot displays the Bruker TopSpin 3.2 software interface. The main window is titled "menthylantranilate-0712 1 1 C:\Bruker\Topspin\data\cga\nmr". The interface is divided into several panels:

- Automation Panel:** This panel is highlighted with a red border and contains the following settings:
  - AUNMP: proc\_1d
  - PYNMP: proc.py
  - LAYOUT: +/1D\_H.xwp
  - CURPLOT: hp5000
- Miscellaneous Panel:** This panel is also highlighted with a red border and contains the following settings:
  - TI: [Empty]
  - DATMOD: proc
  - DC: 2
  - ALPHA: 0
  - GAMMA: 1
  - DFILT: [Empty]
  - SIGF1 [ppm]: 6.00000
  - SIGF2 [ppm]: 5.20000
  - NOISF1 [ppm]: 8.25834
  - NOISF2 [ppm]: 6.75833
  - SINO: 0
  - NSP: 1
  - NZP: 0

The interface also shows a file explorer at the bottom with a list of files including "8 - hsqcedtgpsp.3", "9 - hsqcedtgpsp.3", "10 - hsqcedtgpsp.3", "11 - hsqcedtgpsp.3", "12 - hsqcedtgpsp.3", "100 - zg - Menthyl Anthranilate", and "Me-rex-test".

# What is a layout



The layout contains information about locations, size properties of objects on your plot

It does NOT contain data.

It also contains information on what to do when data is loaded into the layout = automation actions or reset actions.

When a layout is applied to a dataset all of the above is applied and a view or printout is generated.

More later

# The plot and view functions



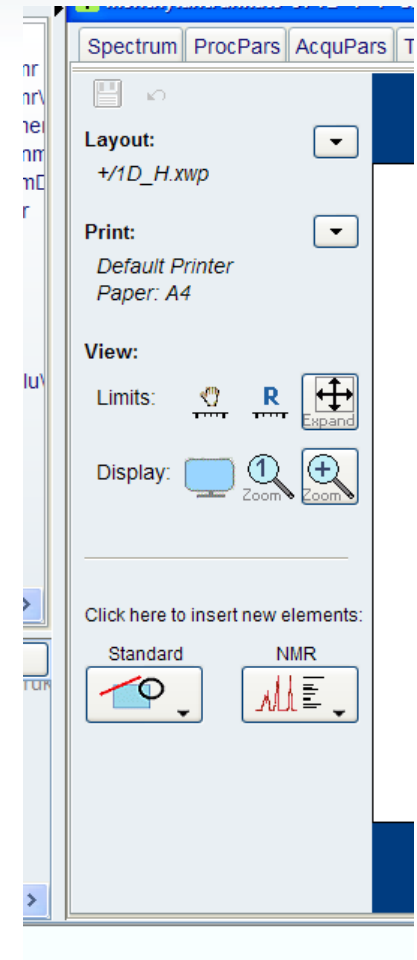
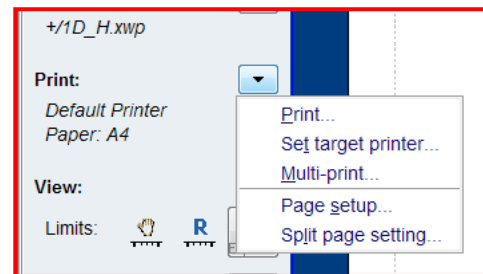
Plot functions

Layouts

**Printers**

View

Objects



# The plot and view functions



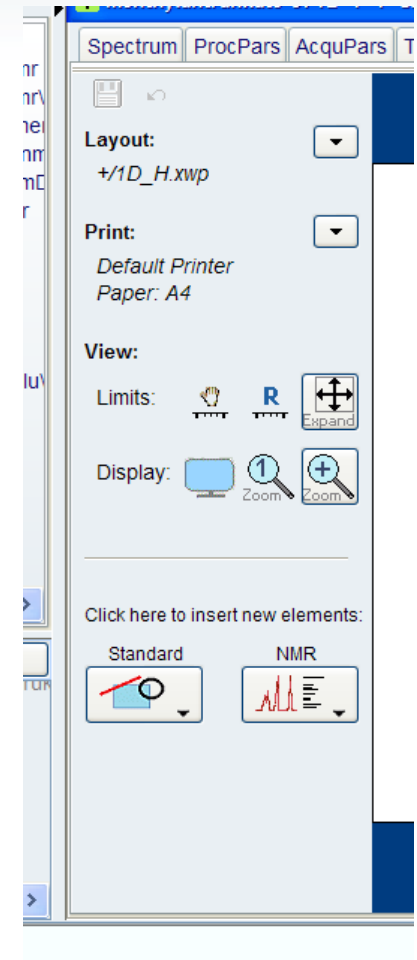
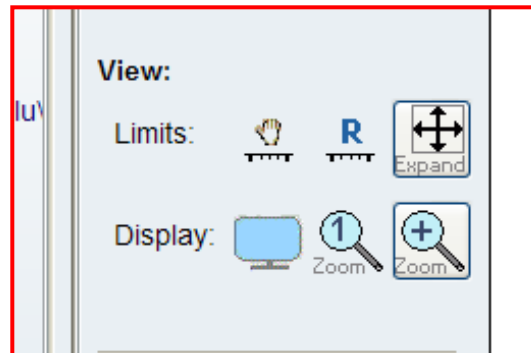
Plot functions

Layouts

Printers

**View**

Objects



# The view functions, more detail



View:

Limits:

Display:

Get more  
real estate



TopSpin 3.2.b.37 on BBIOS as cga

1 menthylantranilate-0712 1 1 C:\Bruker\Topspin\data\cga\nmr

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Plot Fid

Layout: +1D\_H.xwp

Print: Default Printer Paper: A4

View:

Limits:

Display:

Click here to insert new elements:

Standard NMR

Plot Portfolio

1: menthylantranilate-0712 1 1 - C:\Bruk

Position: -1.18, -2.32

Acquisition Parameters:

NAME	menthylantranilate-0712
EXPNO	1
F2 - Acquisition Parameters	
DATE_	20120714
TIME	13:11
PROBHD	1 mm QNP 5mm
PROBHD	51
CPDPRG2	zgpg30
TD	32743
DELTA	0
DECO	A
NUC1	13C
NUC2	1H
PROBHD	5 mm QNP 1H/13
AO	0.121700 mm
RO	2.1359213 mm
RF1	71.400 MHz
NUC1	13C
NUC2	1H
DE	200.0 MHz
TE	300.2 K
TD	1.00000000 gpc
RG	1

Processing Parameters:

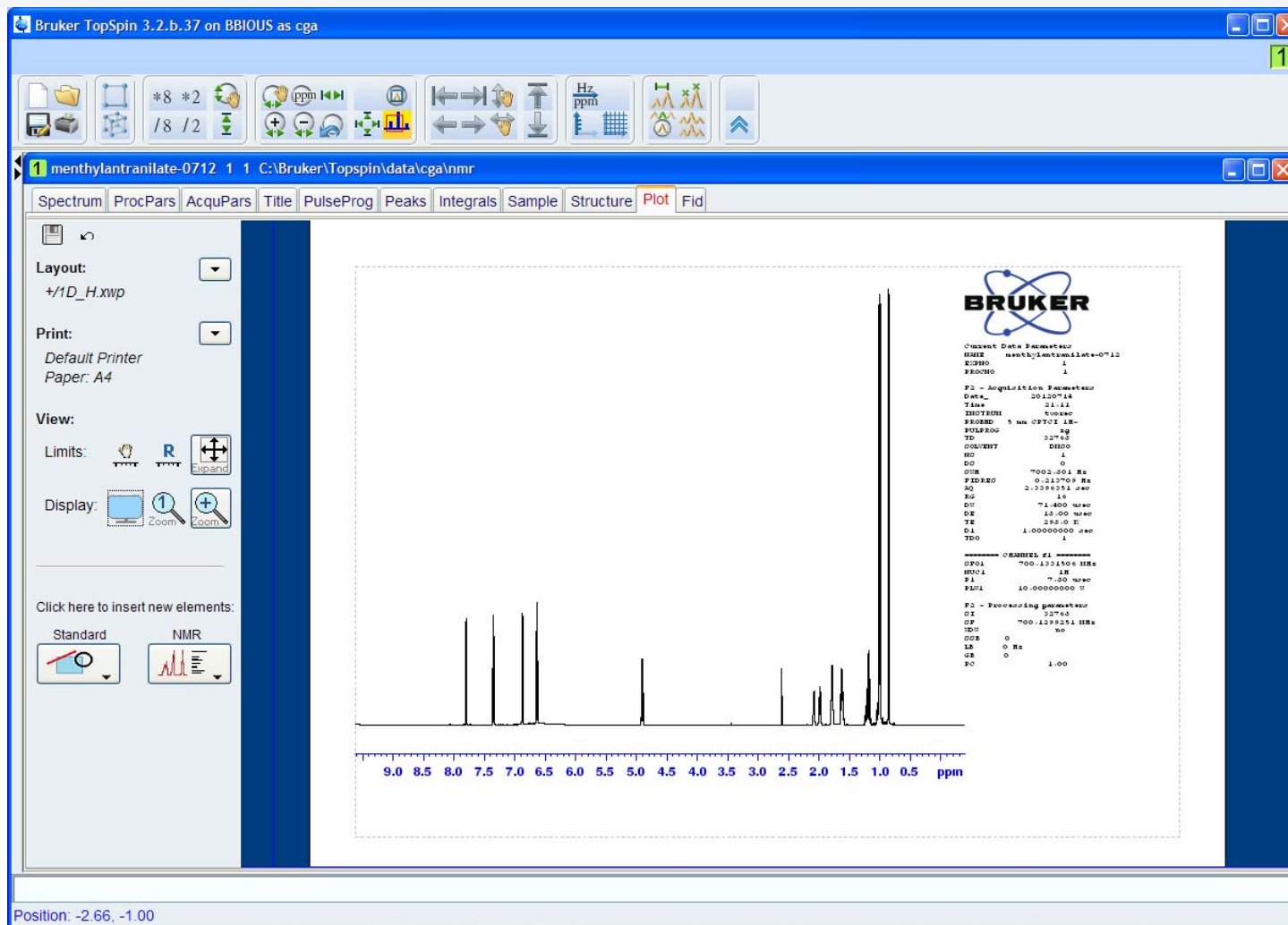
NAME	menthylantranilate-0712
EXPNO	1
F2 - Processing Parameters	
DATE_	20120714
TIME	13:11
PROBHD	1 mm QNP 5mm
PROBHD	51
CPDPRG2	zgpg30
TD	32743
DELTA	0
DECO	A
NUC1	13C
NUC2	1H
PROBHD	5 mm QNP 1H/13
AO	0.121700 mm
RO	2.1359213 mm
RF1	71.400 MHz
NUC1	13C
NUC2	1H
DE	200.0 MHz
TE	300.2 K
TD	1.00000000 gpc
RG	1

# The view functions, more detail

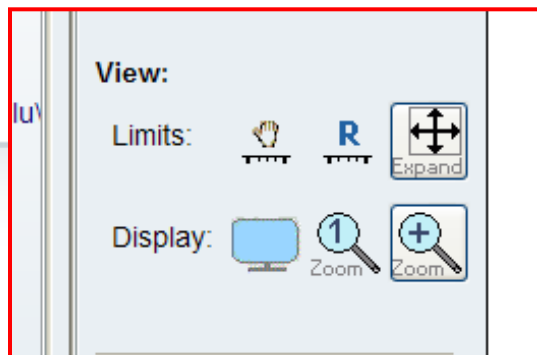


Get more  
real estate  
or optimize the  
window for  
plotting

**Ctrl d**  
to get back

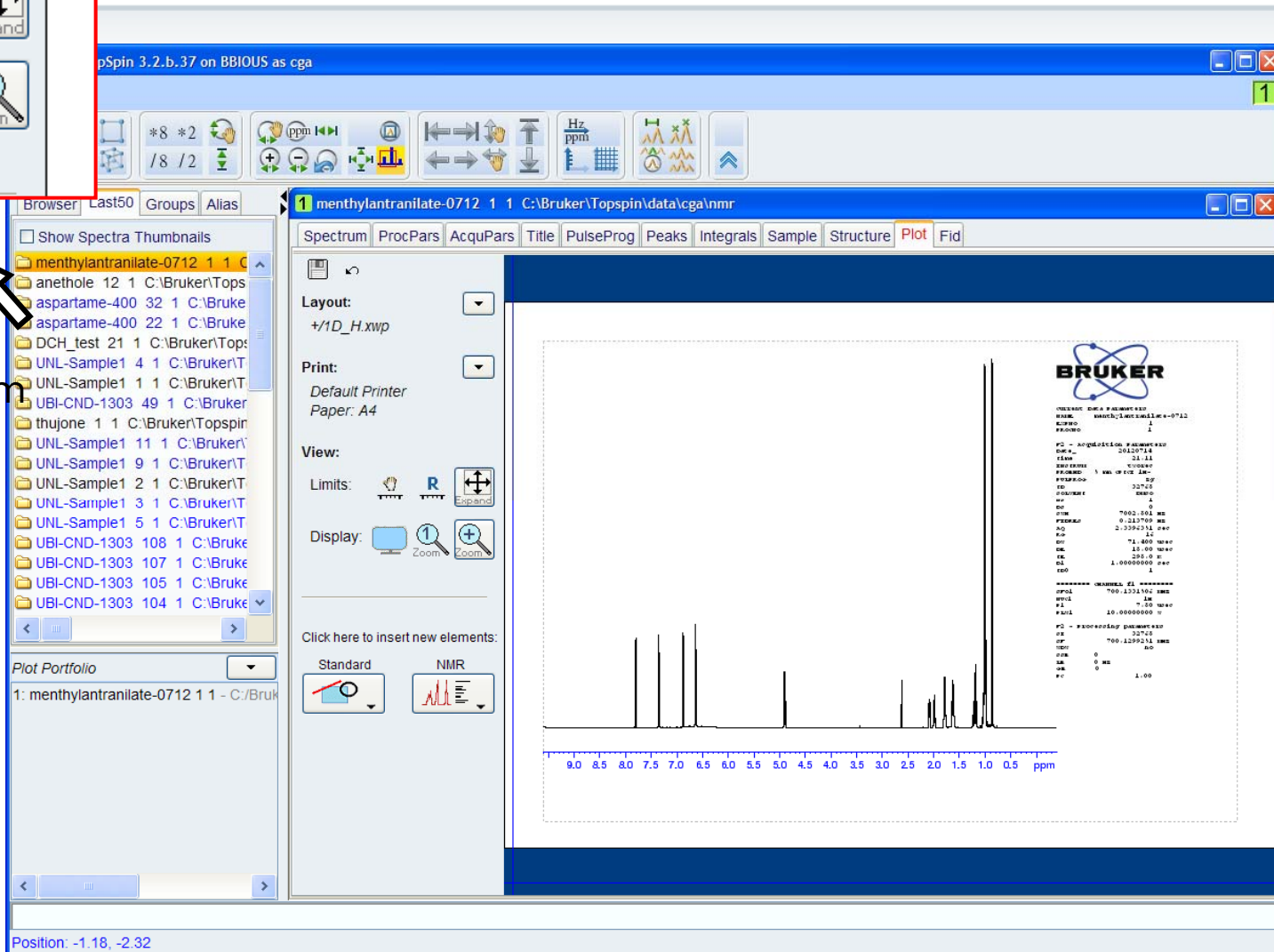


# The view functions, more detail



Zoom in  
no expansion  
of the spectrum  
just a closer  
look

Span a box  
and release



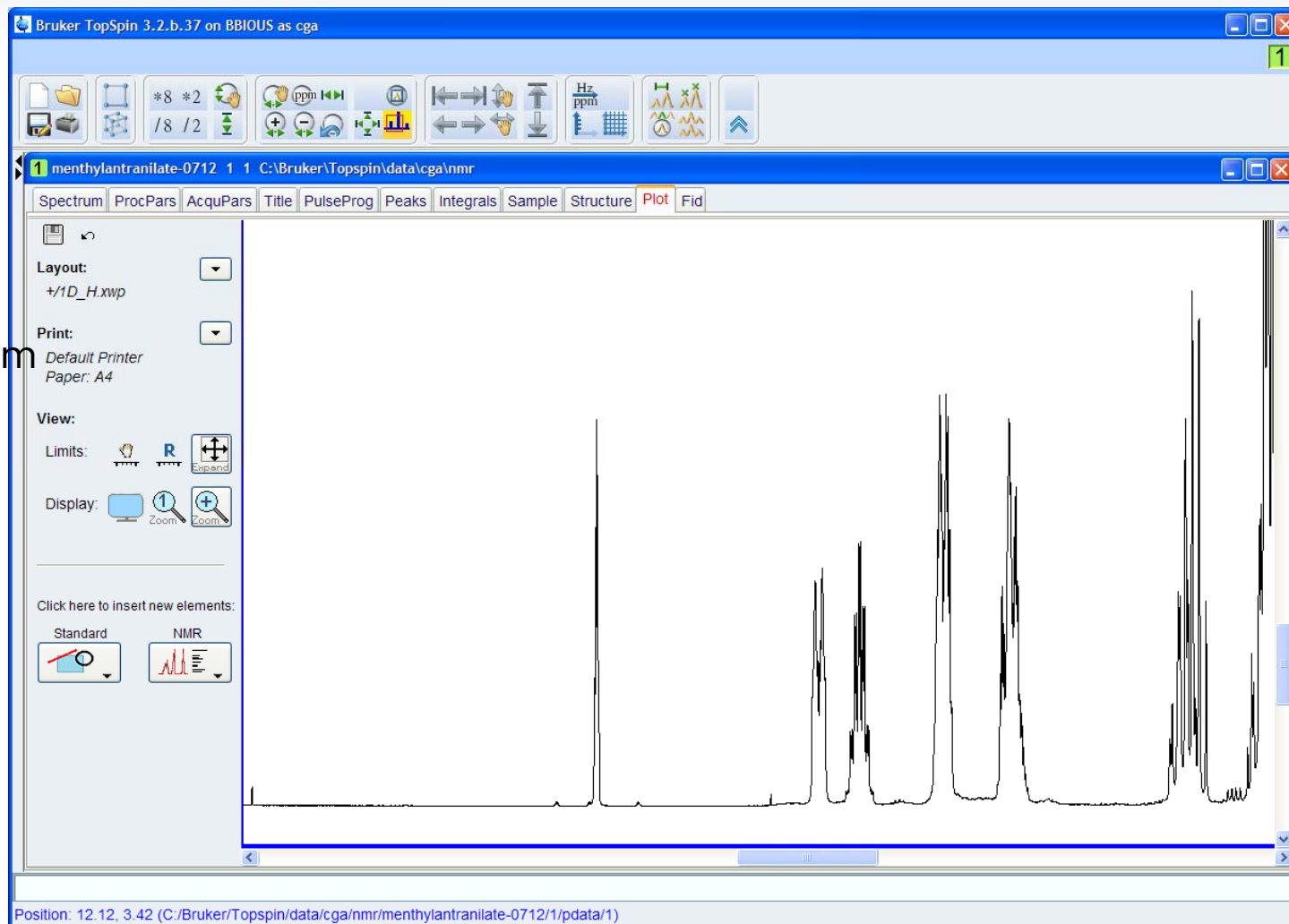


# The view functions, more detail

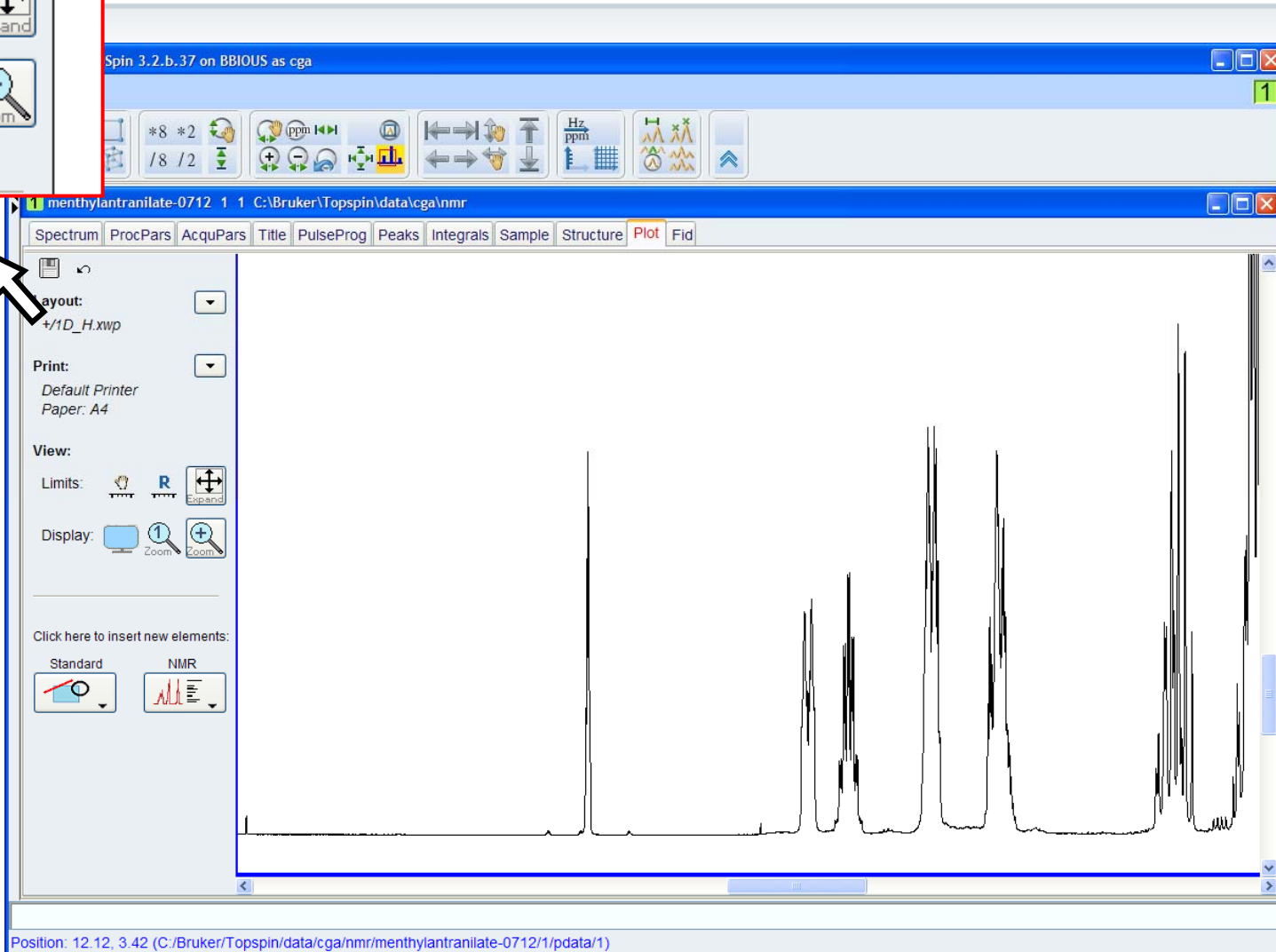
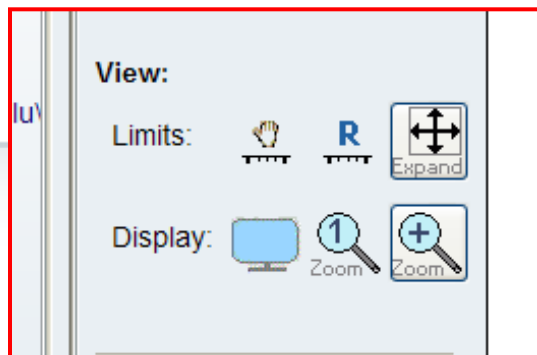


Zoom in  
no expansion  
of the spectrum  
just a closer  
look

Span a box  
and release



# The view functions, more detail



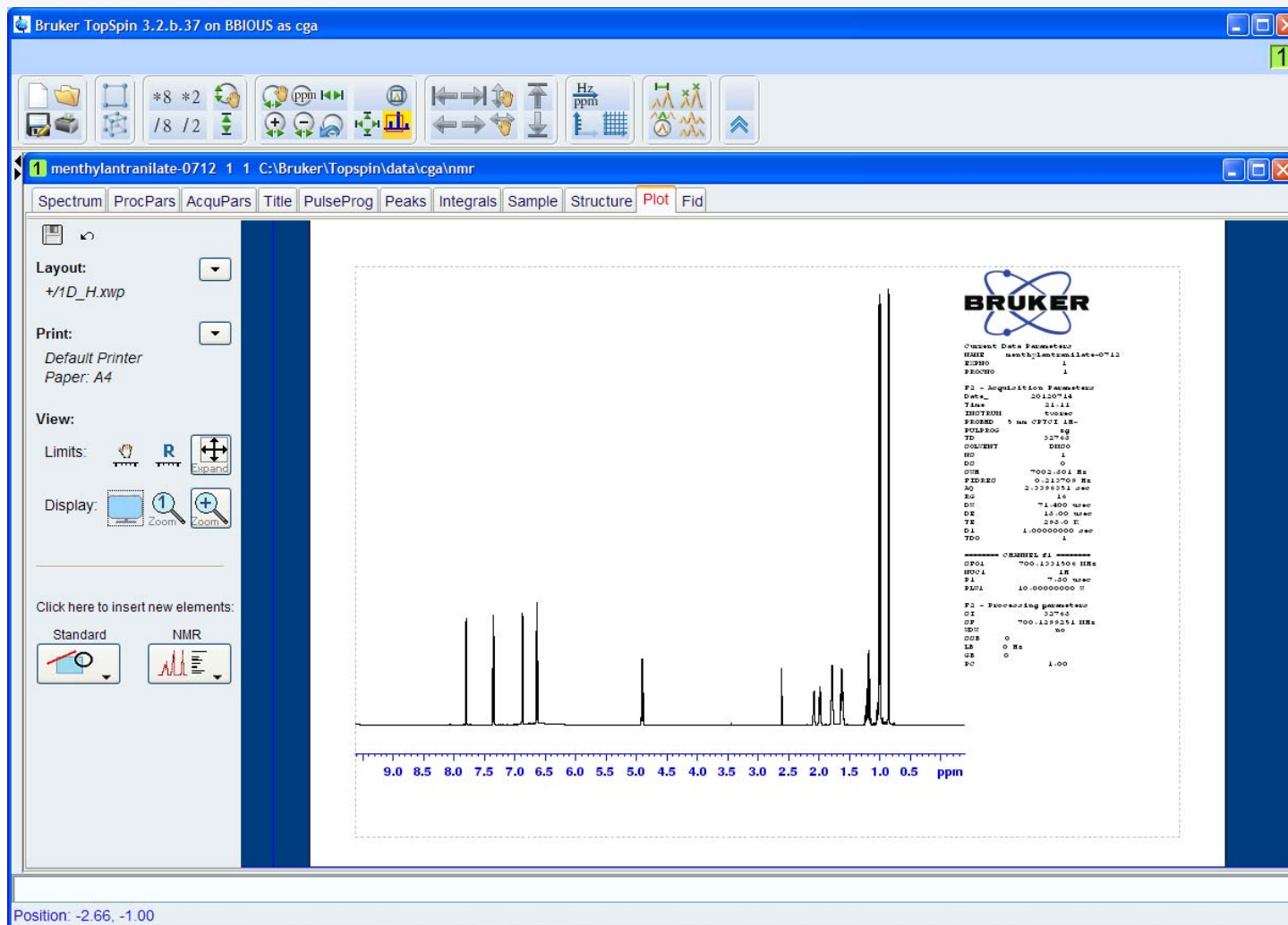
Zoom reset



# The view functions, more detail



Zoom reset



# The view functions, more detail



View:

Limits:

Display:

Spin 3.2.b.37 on BBIOS as cga

Expansions



menthyltranilate-0712 1 C:\Bruker\Topspin\data\cga\nmr

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Plot Fid

Layout:  +/1D\_H.xwp

Print:  Default Printer Paper: A4

View:

Limits:

Display:

Click here to insert new elements:

Standard  NMR

9.0 8.5 8.0 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 1.0 0.5 ppm

```
BRUKER
Current Data Parameters
NAME methyltranilate-0712
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100718
Time 21.11
INSTRUM spect
PROBHD 5 mm CPYQX 1H-
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1
DS 0
SWH 700.1301 MHz
FIDRES 0.212708 Hz
AQ 2.3398251 sec
RG 16
DT 71.800 usec
DE 13.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
----- CHANNEL f1 -----
CPD1 700.1271504 MHz
NUC1 1H
P1 7.00 usec
PL1 10.00000000 dB
F2 - Processing parameters
SI 32768
SF 700.1271504 MHz
AQ 2.3398251 sec
RG 16
DT 71.800 usec
DE 13.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
```

Position: -2.66, -1.00

# More on expansions



View:

Limits:

Display:

Spin 3.2.b.37 on BBI0US as cga

mentnylantranilate-0712 1 1 C:\Bruker\Topspin\data\cga\nmr

Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Plot Fid

Layout: +/1D\_H.xwp

Print: Default Printer Paper: A4

View:

Limits:

Display:

Click here to insert new elements:

Standard NMR

BRUKER

```
Current Data Parameters
NAME mentnylantranilate-0712
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120718
Time 21.11
INSTRUM spect
PROBHD 5 mm CPYQX 1H-
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1
DS 0
SWH 700.1301 MHz
FIDRES 0.212708 Hz
AQ 2.3398251 sec
RG 16
DT 71.800 usec
DE 13.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
CPD1 700.1321504 MHz
NUC1 1H
P1 7.20 usec
PL1 10.00000000 dB

F2 - Processing parameters
SI 32768
SF 700.1329251 MHz
AQ 2.3398251 sec
RG 16
DT 71.800 usec
DE 13.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
```

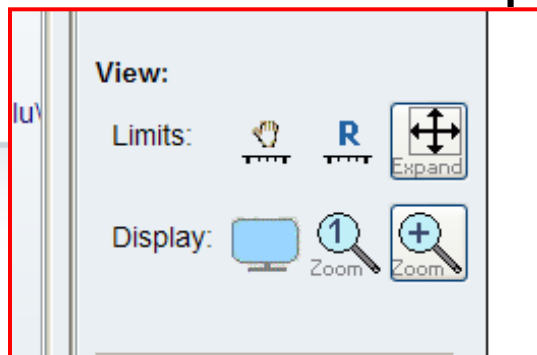
Shift – drag

Ctrl – drag

Alt - drag

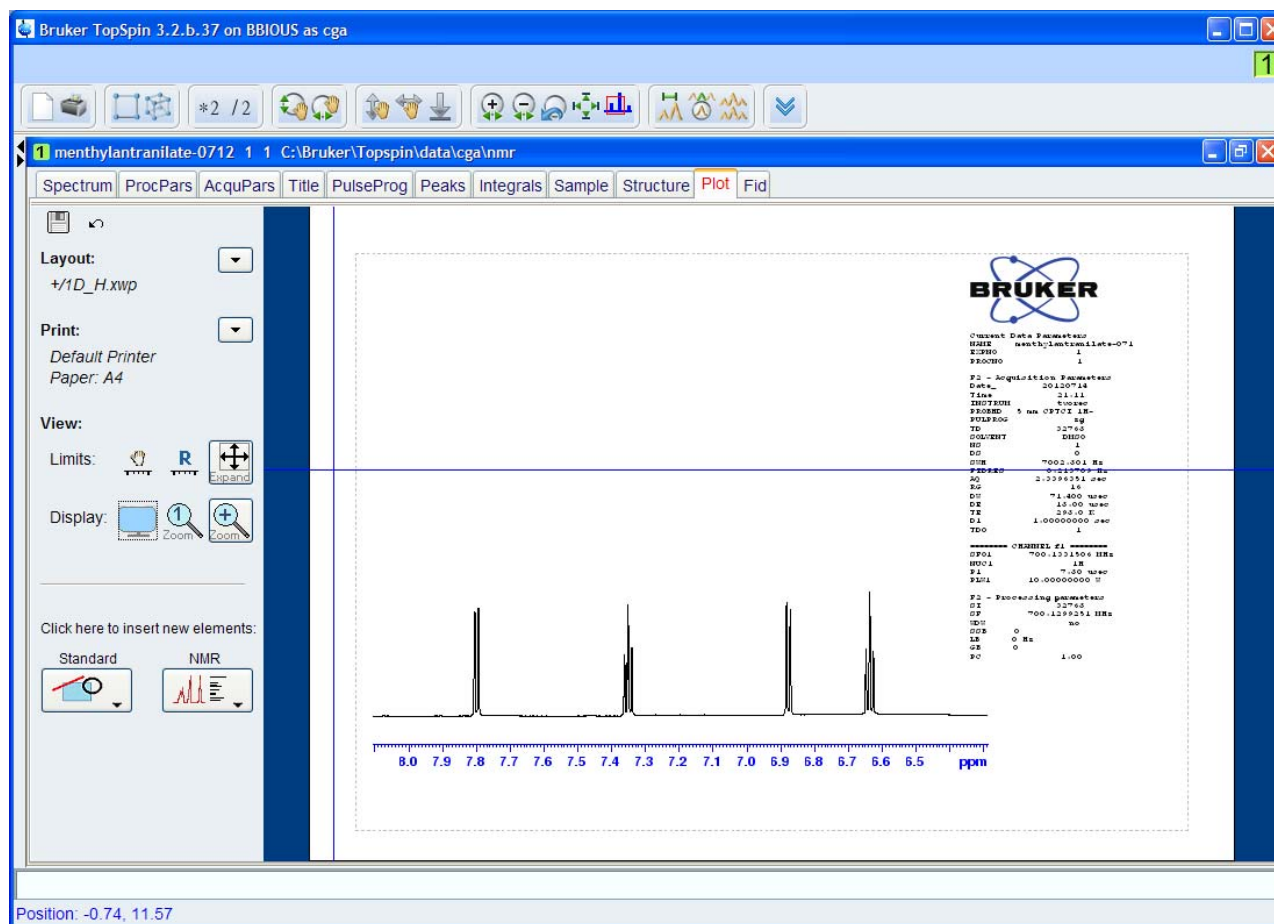
Position: -2.66, -1.00

# More on expansions

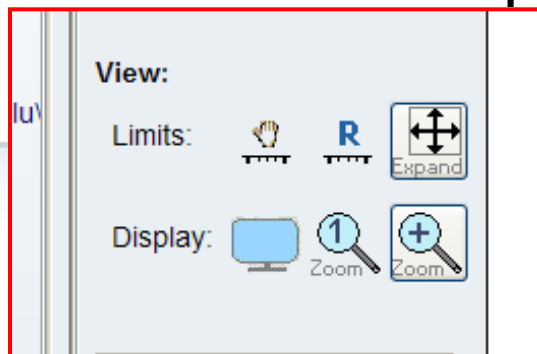


Shift – drag

Horizontal expansion only

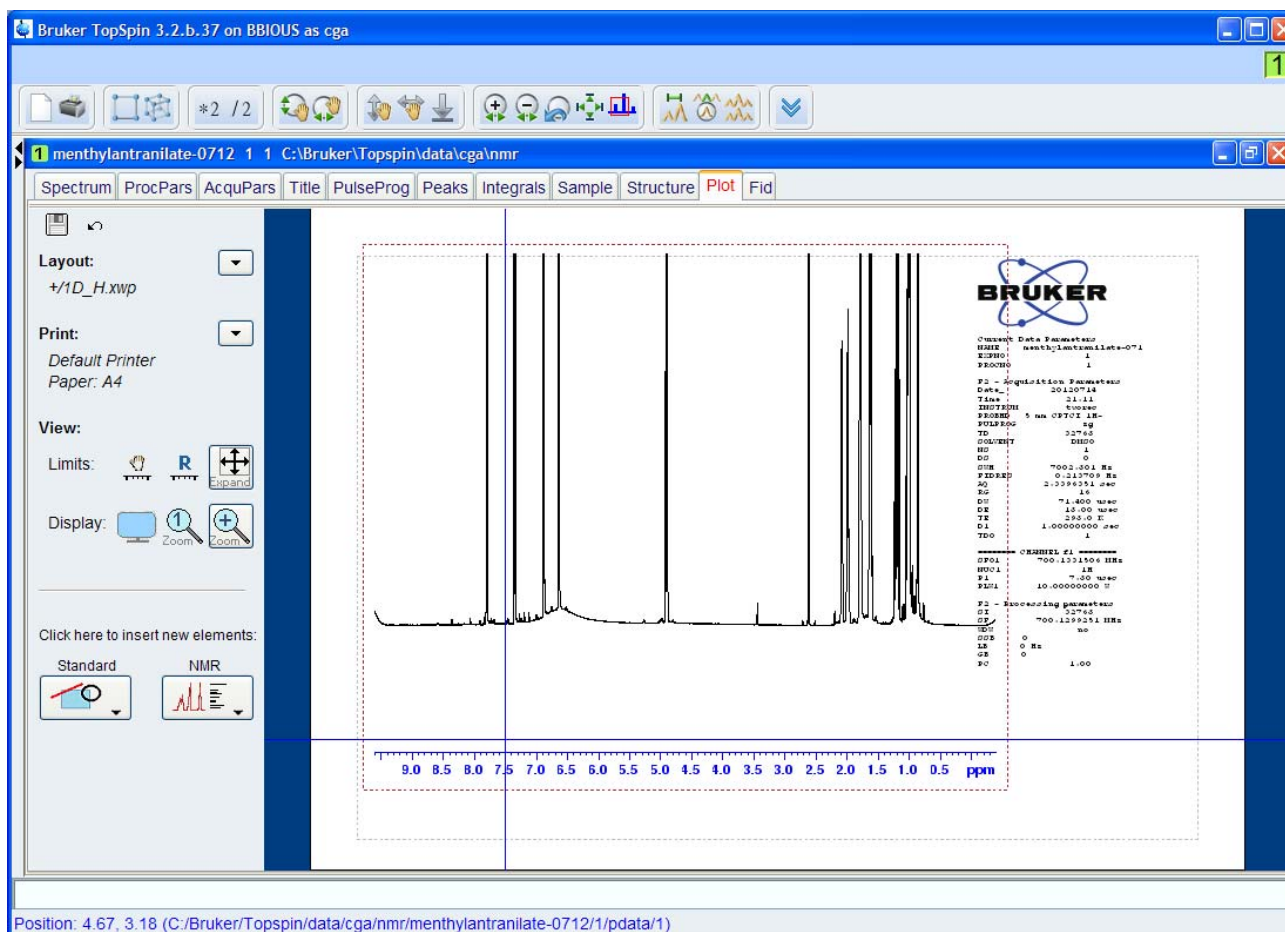


# More on expansions

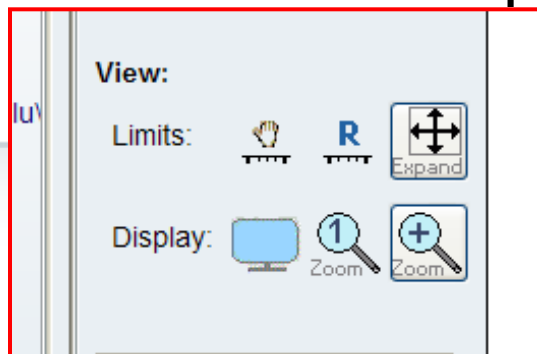


Ctrl – drag

Vertical expansion  
only

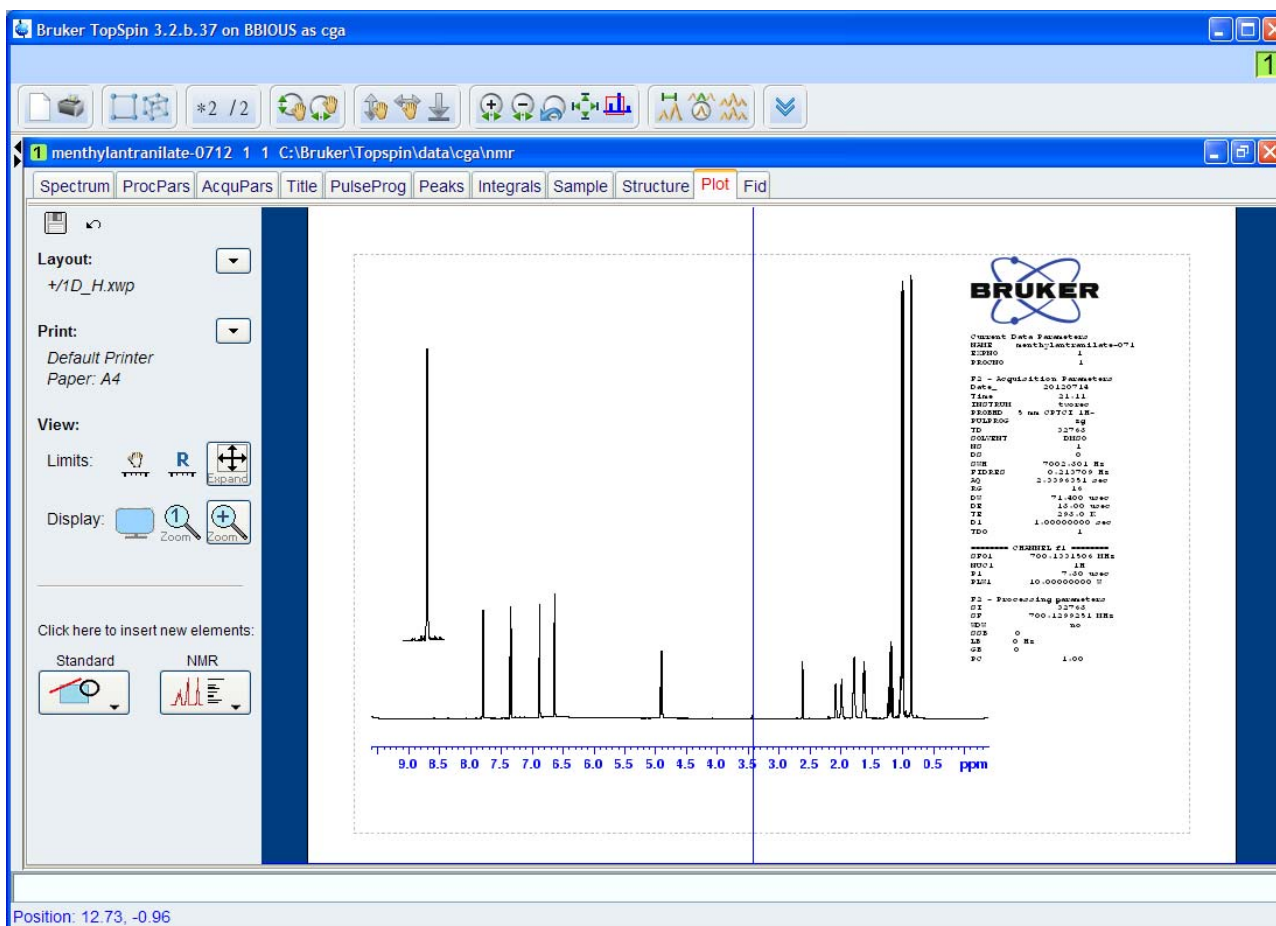


# More on expansions



Alt – drag

Creates new object  
with same horizontal  
scale and vert  
expansion





# The plot and view functions



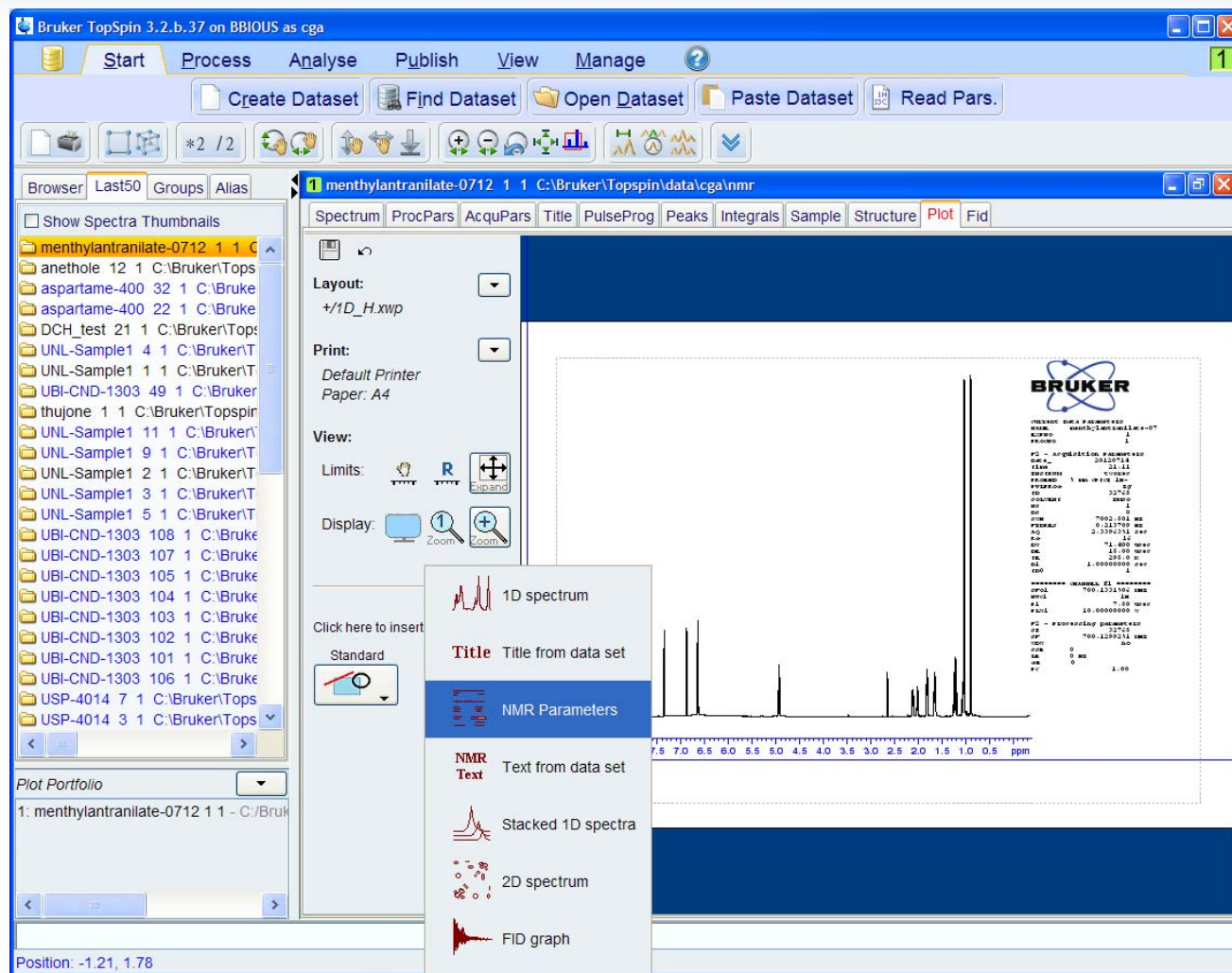
Plot functions

Layouts

Printers

View

Objects



# The plot and view functions



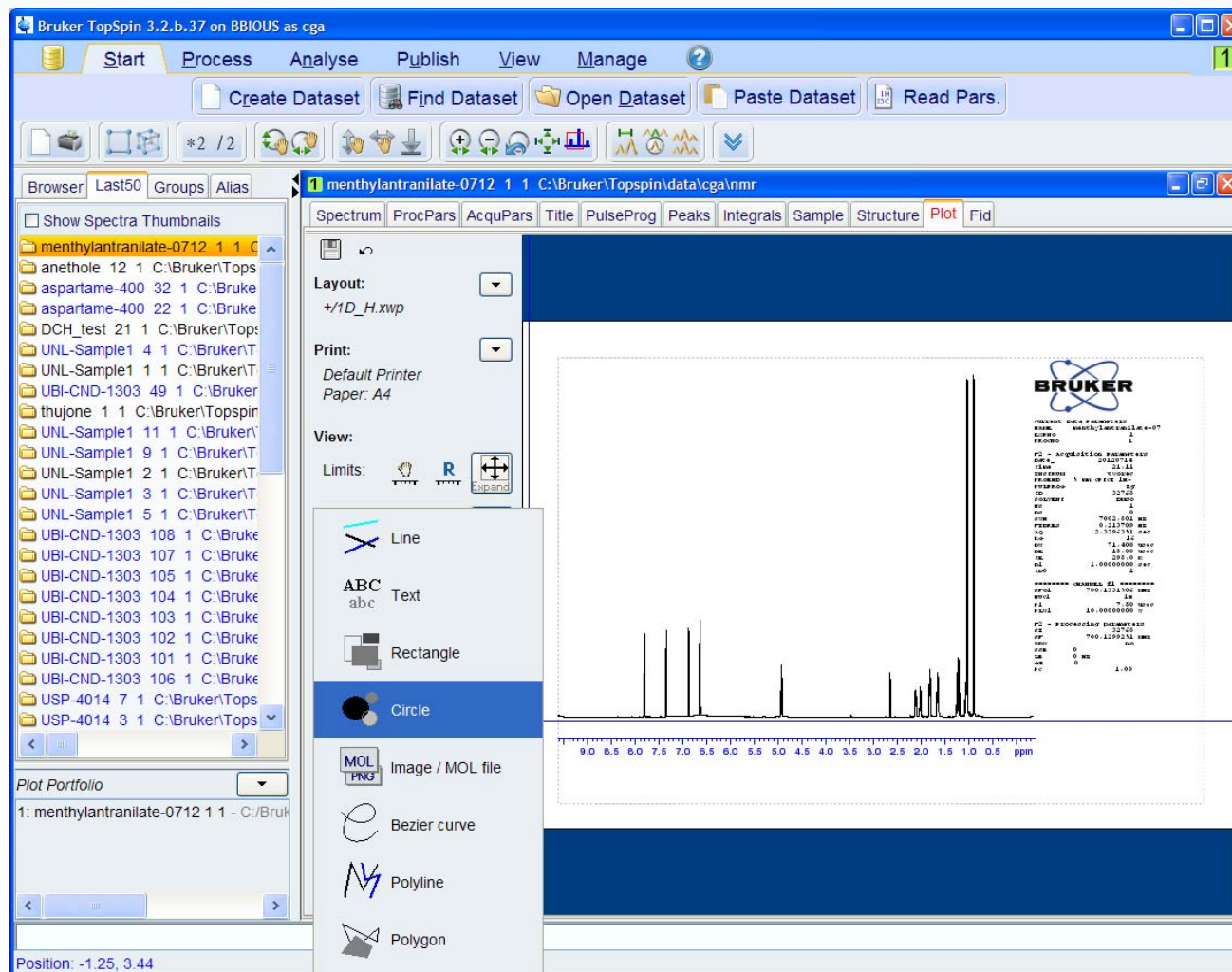
Plot functions

Layouts

Printers

View

Objects



# The plot and view functions



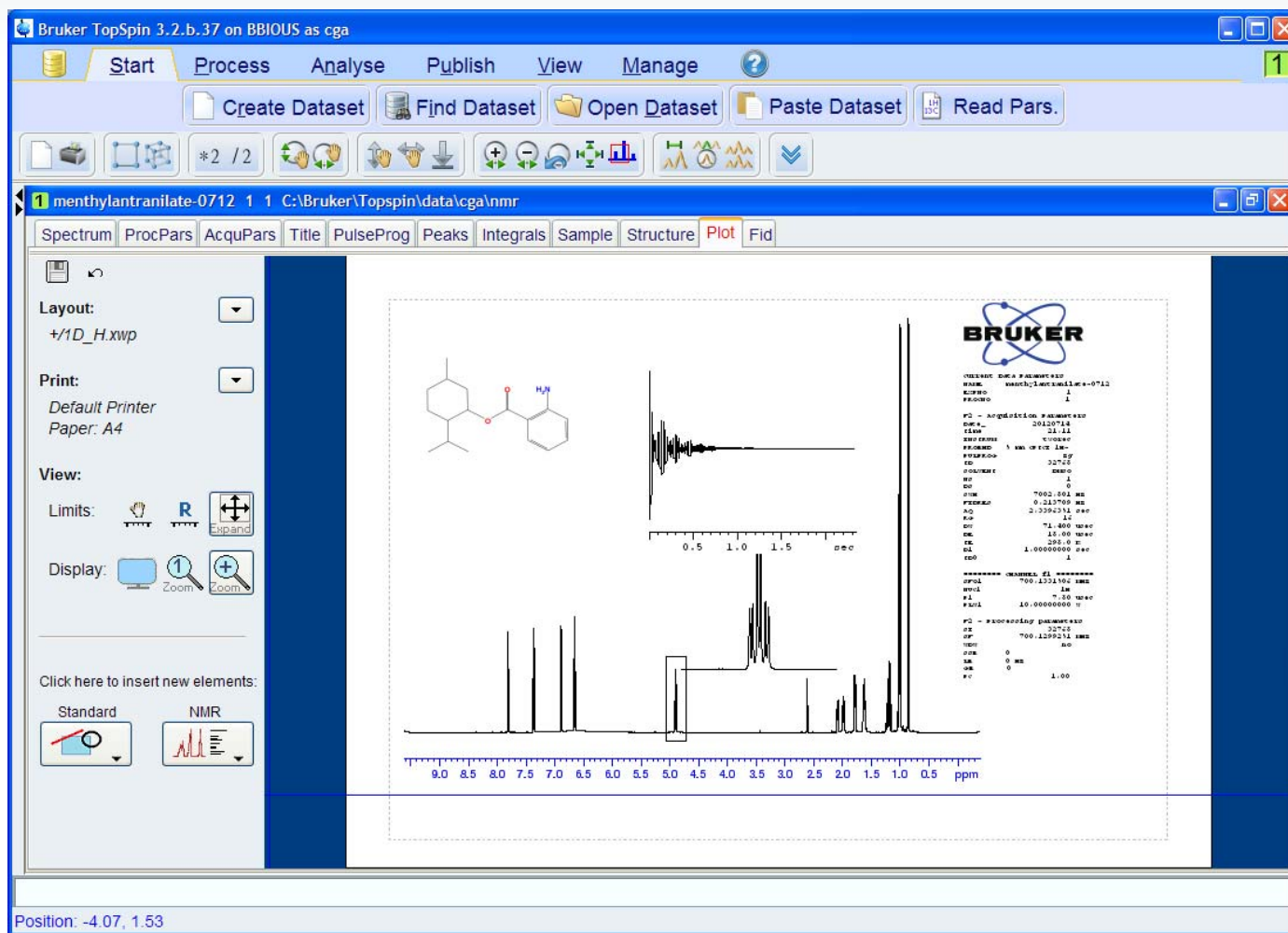
## Objects

Add more objects

The image shows two panels from a software interface. The left panel is a list of drawing objects, and the right panel is a list of plot types. In both panels, the 'Circle' and 'NMR Parameters' options are highlighted with a blue background.

Object / Plot Type	Description
Line	Line
Text	Text (ABC abc)
Rectangle	Rectangle
<b>Circle</b>	Circle
Image / MOL file	Image / MOL file (MOL PNG)
Bezier curve	Bezier curve
Polyline	Polyline
Polygon	Polygon
1D spectrum	1D spectrum
Title	Title from data set
<b>NMR Parameters</b>	NMR Parameters
NMR Text	Text from data set
Stacked 1D spectra	Stacked 1D spectra
2D spectrum	2D spectrum
FID graph	FID graph

# Applying all the tools so far



# Manipulating individual objects

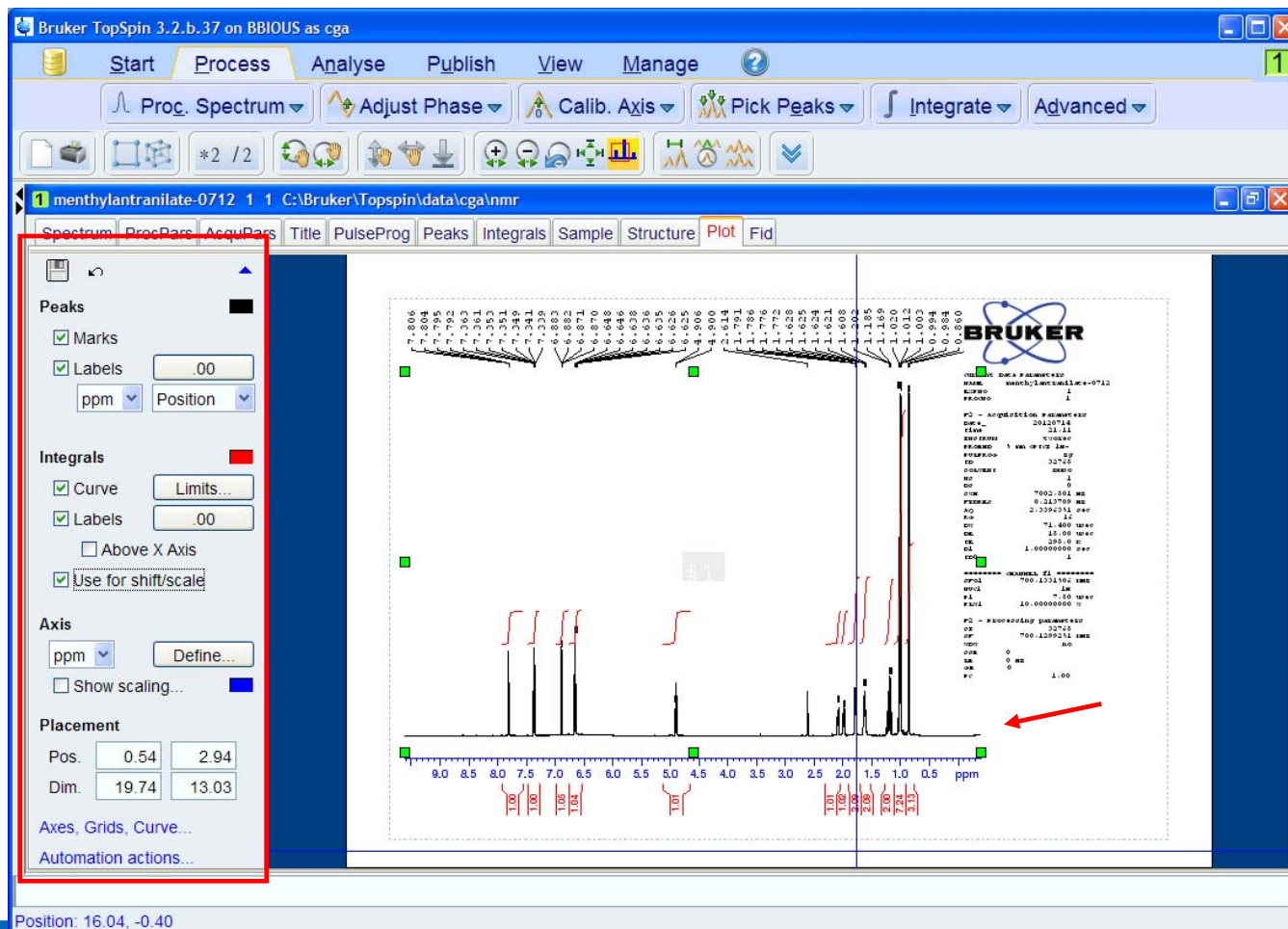


- How to change the properties of individual objects
  - Changing colors
  - Fonts
  - Line style and thickness
  - And more

# Manipulating individual objects



- Select the object (click on it)
- Green corners appear
- The menu on the left changes
- More options under links bottom



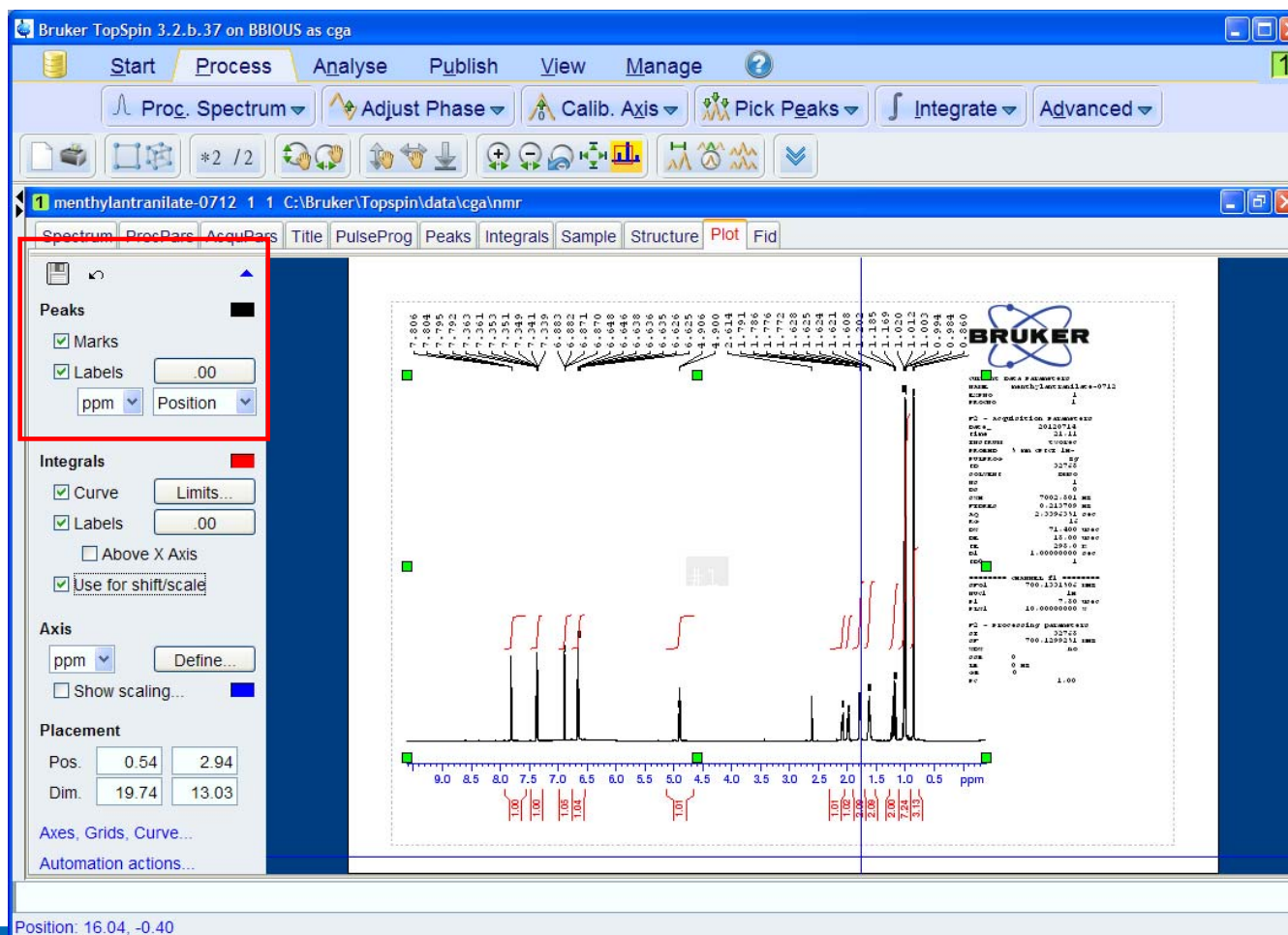
Position: 16.04, -0.40

# Manipulating individual objects



- Peaks

- Set the color of the marks and labels
- Choose marks on top of peaks
- Choose labels
- Set the number of decimal places

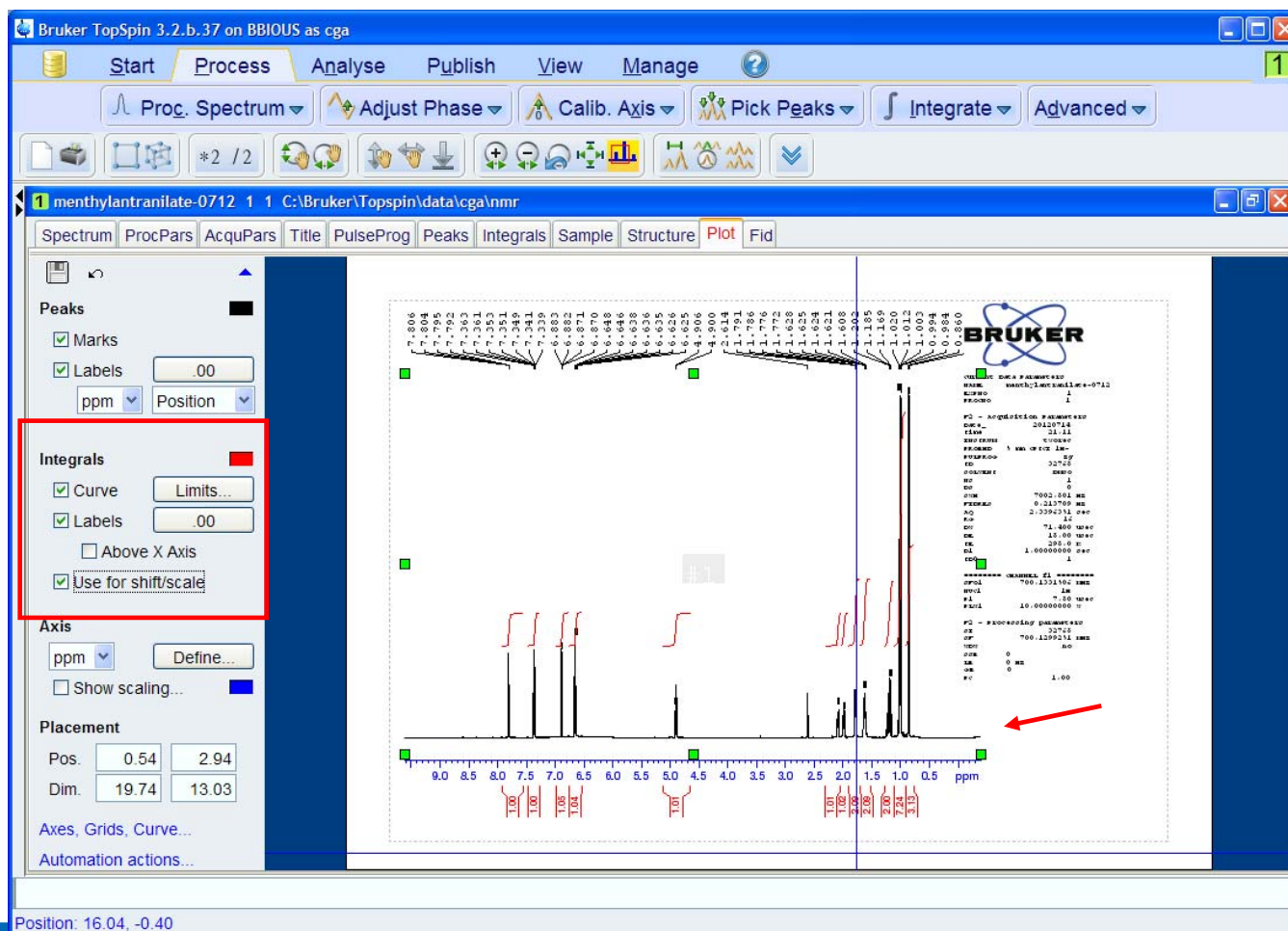


# Manipulating individual objects



- Integrals

- Set the color of the integral trails and labels
- Set the number of decimal places
- Choose the position of the labels. Below the axis or between axis and spectrum
- Check box to select interactive scaling functions



Position: 16.04, -0.40



# Manipulating individual objects



- Axis
- Choose ppm, Hz or points
- Define axis details

**Define Axis**

0.51 ppm/cm, at offset      9.50 ppm      Apply

354.8 Hz/cm, at offset      6652.0 Hz      Apply

Close

- Choose color
- Choose display of scaling info on plot

The screenshot shows the Bruker TopSpin 3.2.b.37 software interface. The main window displays an NMR spectrum with a chemical shift axis from 9.0 to 0.5 ppm. The spectrum shows several peaks, with integration values displayed below the baseline. The 'Define Axis' dialog box is open, showing the current axis settings: 0.51 ppm/cm, at offset (9.50 ppm) and 354.8 Hz/cm, at offset (6652.0 Hz). The 'Axis' dropdown menu is set to 'ppm'. The 'Show scaling...' checkbox is checked. The 'Placement' section shows 'Pos.' values of 0.54 and 2.94, and 'Dim.' values of 19.74 and 13.03. The 'Automation actions...' section is also visible.

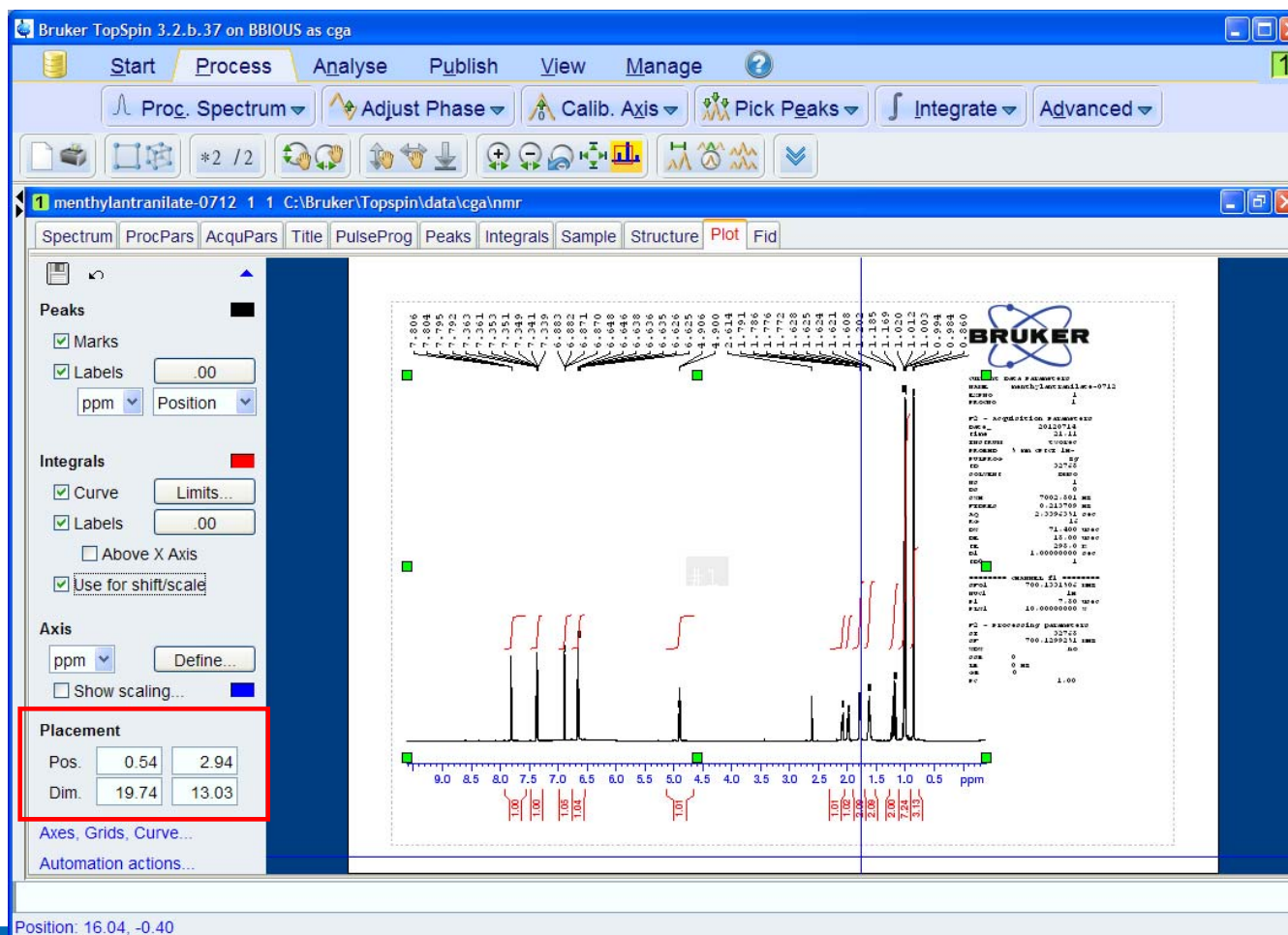
Position: 16.04, -0.40

# Manipulating individual objects



- Placement
- Pos: defines the lower left hand corner of the plot (the **green** corner)
  - See next page of options
- Dim: defines the size of the plot as shown by the green corners

Attention Spectrum scales vertically with the dimension

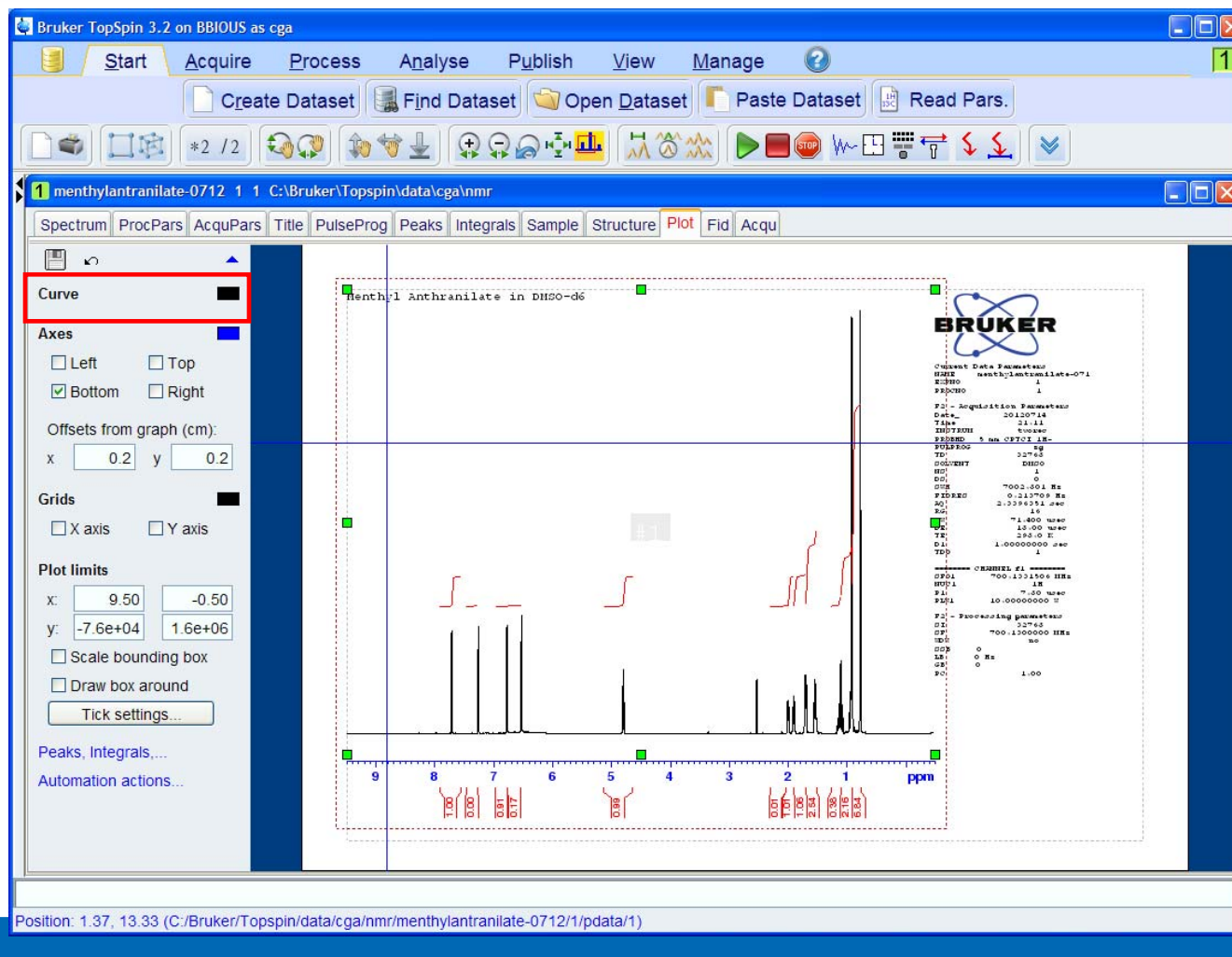
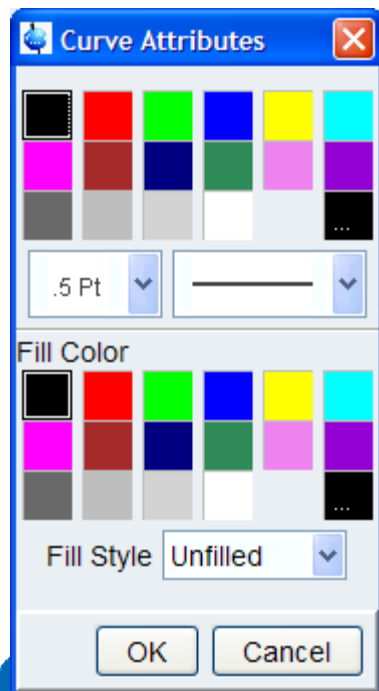


Position: 16.04, -0.40

# Manipulating individual objects



- Curve
- Defines the color and line thickness of the spectrum



That is how you do it.

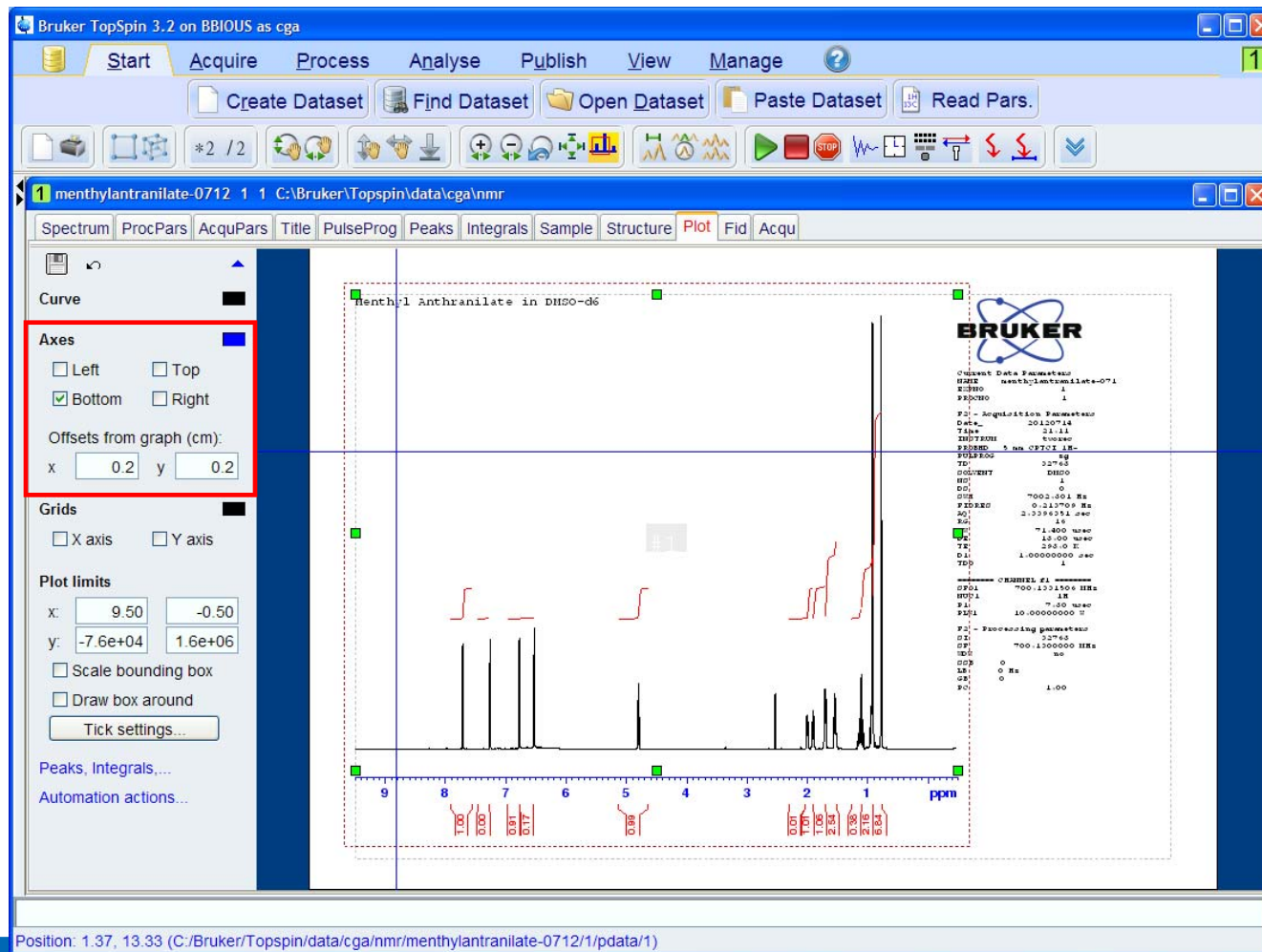


The screenshot displays the Bruker TopSpin 3.2 software interface. The main window shows an NMR spectrum of Menthyl Anthranilate in DMSO-d6. The x-axis is labeled in ppm, ranging from 1.13 to 1.05. The spectrum shows several peaks, with the most prominent ones between 1.05 and 1.13 ppm. A 'Curve Attributes' dialog box is open in the foreground, showing various settings for the selected curve. Red arrows point to specific settings: the 'Fill Color' (green), the 'Line Style' (3 Pt), and the 'Fill Style' (Solid). The dialog box also includes options for 'Top', 'Bottom', 'Left', and 'Right' alignment, and a 'Y axis' checkbox. The 'Curve Attributes' dialog box is titled 'Curve Attributes' and has a close button (X) in the top right corner. It contains a grid of color swatches, a line style dropdown set to '3 Pt', a 'Fill Color' section with another grid of color swatches, and a 'Fill Style' dropdown set to 'Solid'. There are 'OK' and 'Cancel' buttons at the bottom. The background software window shows a menu bar with 'Start', 'Acquire', 'Process', 'Analyse', 'Publish', 'View', and 'Manage'. Below the menu bar is a toolbar with icons for 'Create Dataset', 'Find Dataset', 'Open Dataset', 'Paste Dataset', and 'Read Pars.'. The main window title is 'menthylantranilate-0712 1 1 C:\Bruker\Topspin\data\cga\nmr'. The 'Plot' tab is active, showing the spectrum. On the right side of the plot, there is a 'BRUKER' logo and a list of 'Current Data Parameters' and 'Acquisition Parameters'. The 'Acquisition Parameters' list includes: Date\_ 20100718, Time 21:11, INSTRUM spect, P2PROG 5 nm OPTIC 1B, PULPROG zg, TD 32768, SOLVENT DMSO, NS 1, DS 0, DSR 7002.501 Hz, FIDRES 0.215709 Hz, SFO 213283.11 MHz, EQ 16, DE 71.400 usec, TE 15.00 usec, TR 2.95.0 s, D1 1.00000000 usec, TDO 1. The 'Processing Parameters' list includes: SFO1 700.1301506 MHz, INU1 1B, P1 7.10 usec, PL1 10.00000000 dB, SFO 700.1300000 MHz, CP 127.65, DP 700.1300000 MHz, INU 1B, DSR 0, LR 0 Hz, OR 0, PC 1.00. At the bottom of the software window, the text 'Position: 3.00, 19.89' is visible.

# Manipulating individual objects



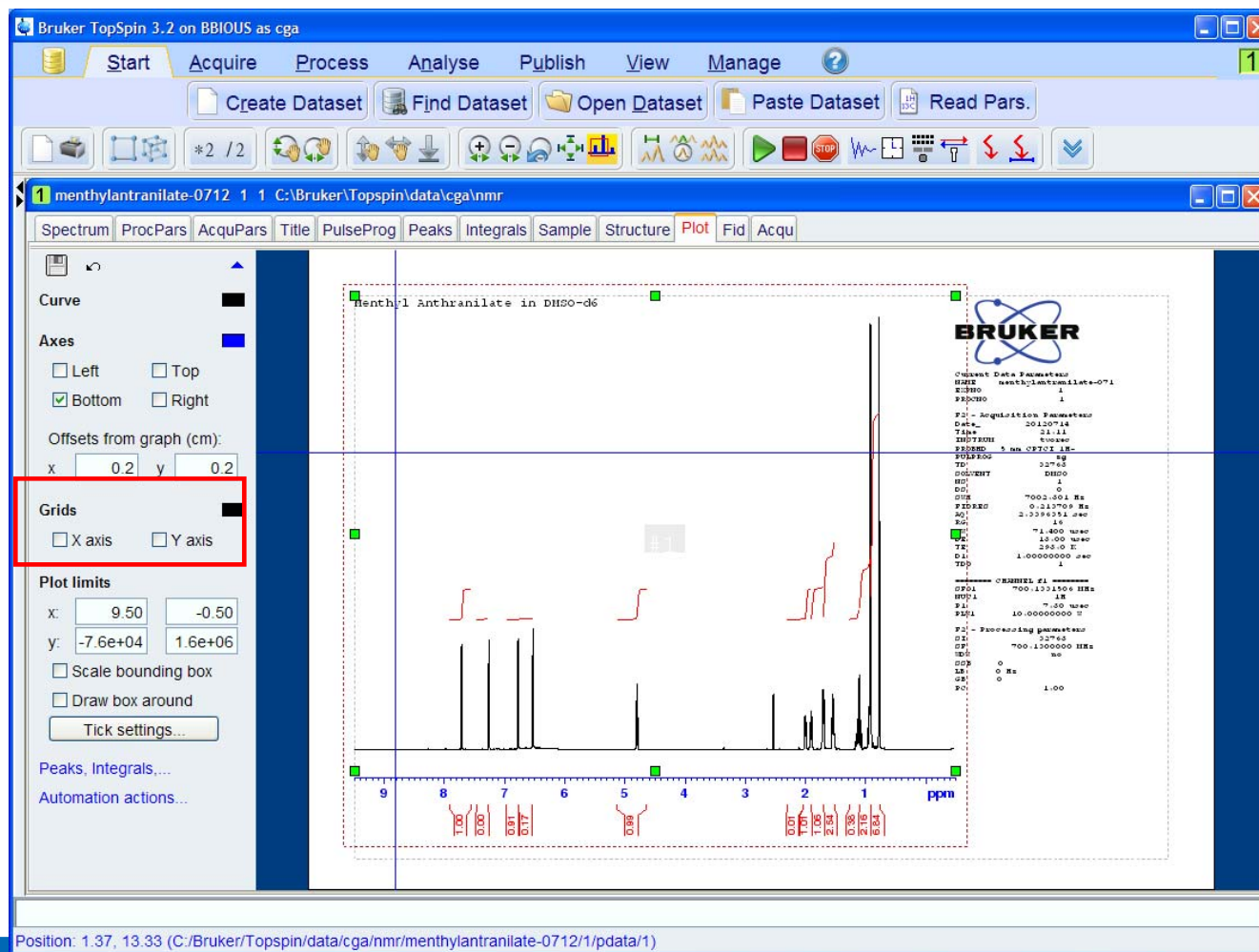
- Axes
- Choice of color, line style, font size and font for axis



# Manipulating individual objects



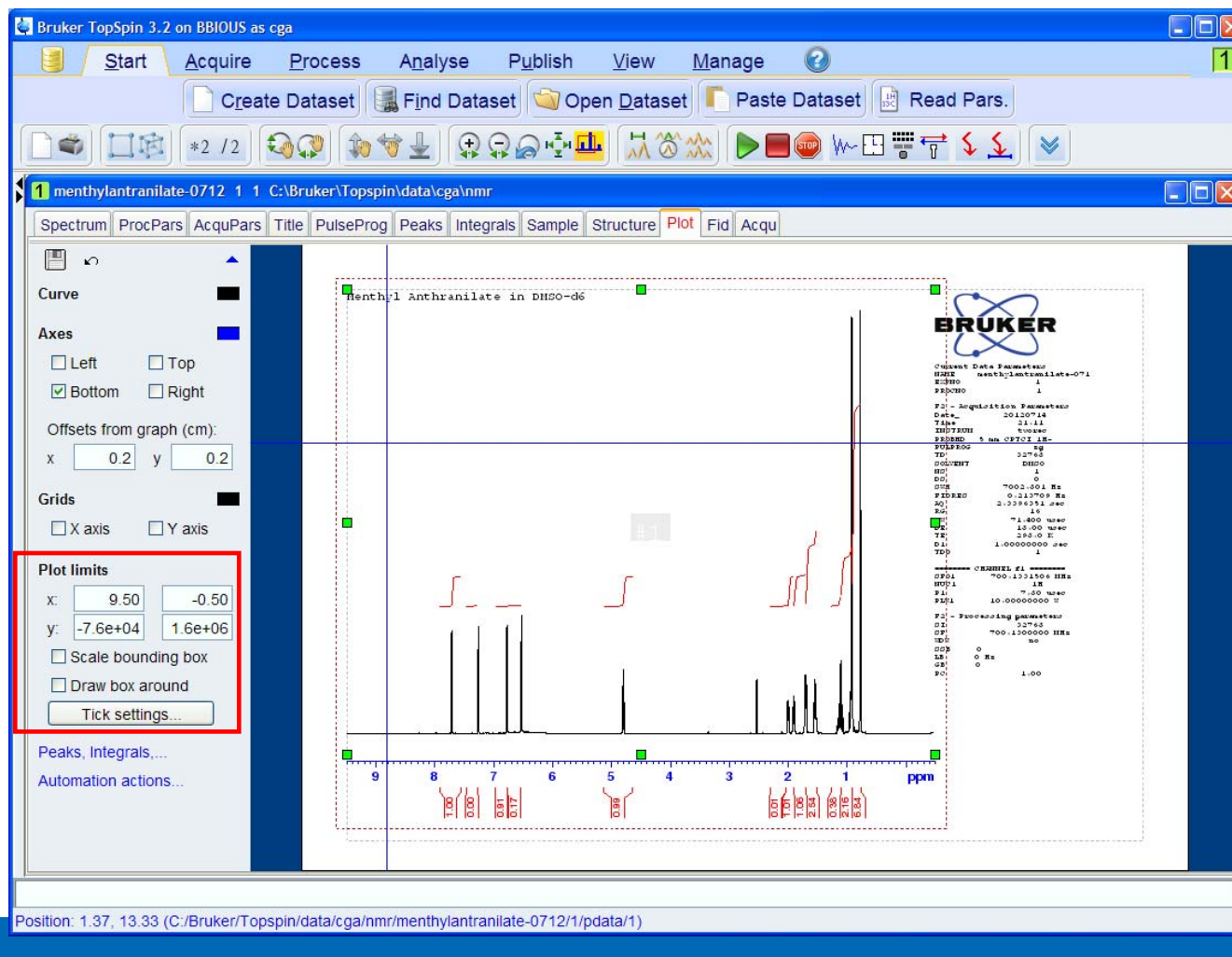
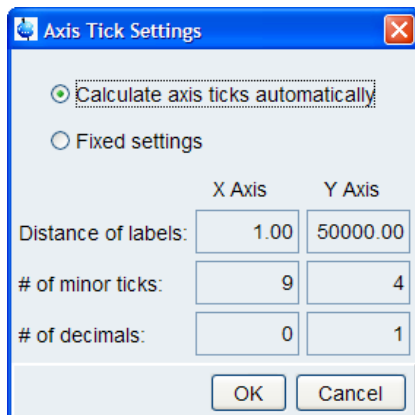
- Grid
- Choice of color, line style, for X and Y grid lines



# Manipulating individual objects



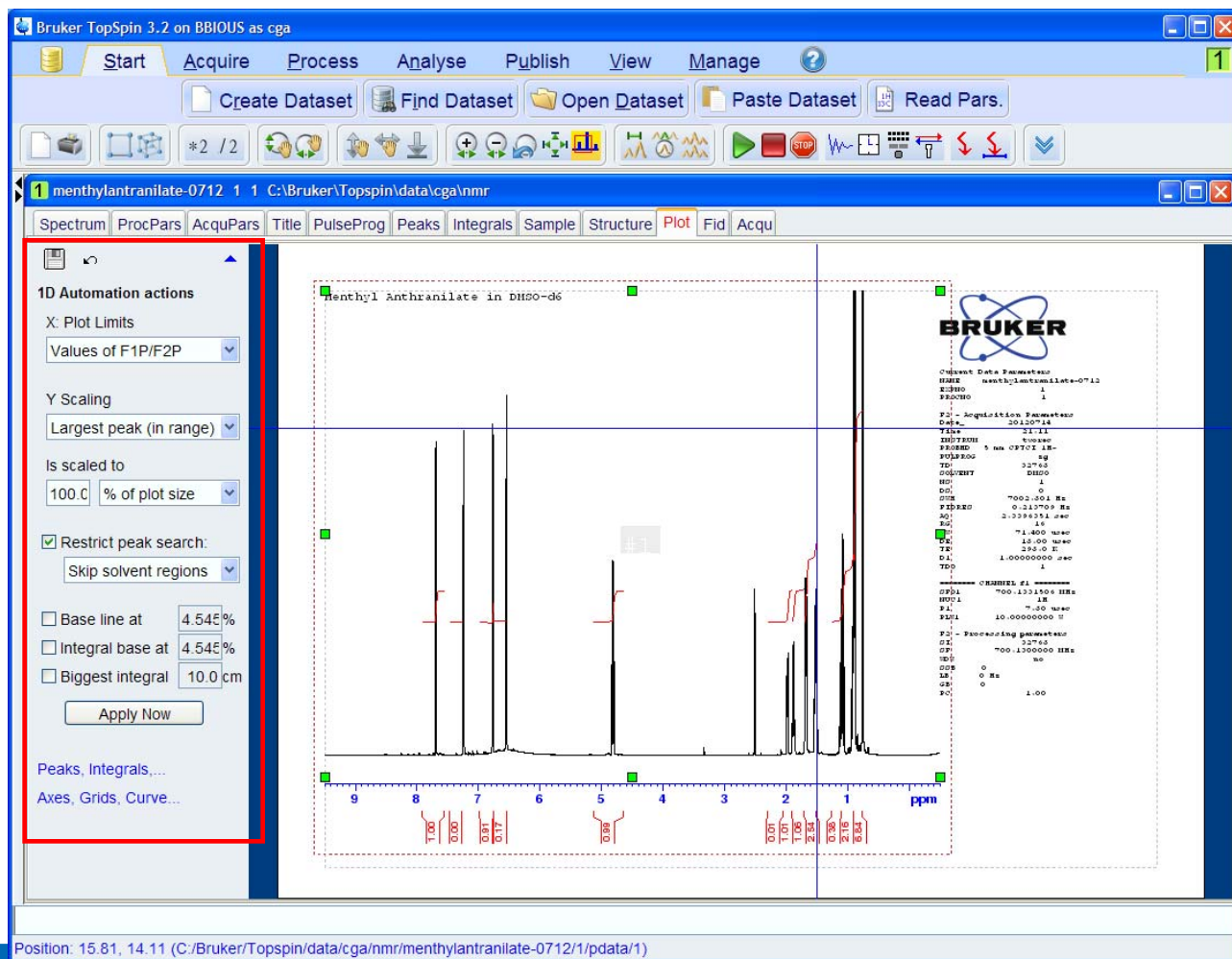
- Plot limits
- Choice of plot limits in the units define on the first page of options
- Scale bounding box
  - Include everything
  - Include spectrum only
- Tick mark settings



# Defining Automation actions



- Define what happens when you reset a spectrum, when you plot in automation or use autoplot
- Vertical and horizontal scaling
- Exclusions such as solvent or other peaks.
- Vertical arrangement of spectrum and integral

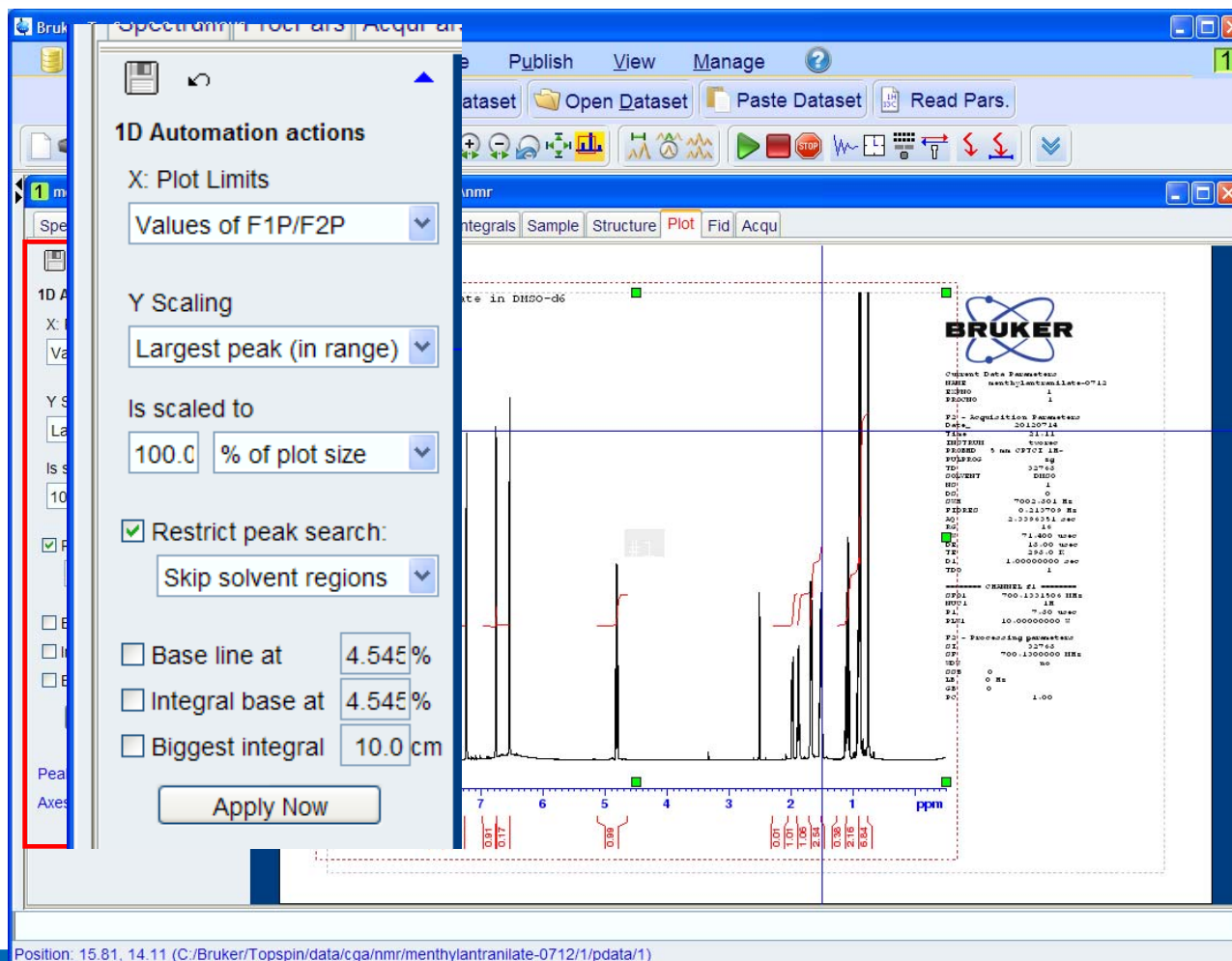




# Defining Automation actions



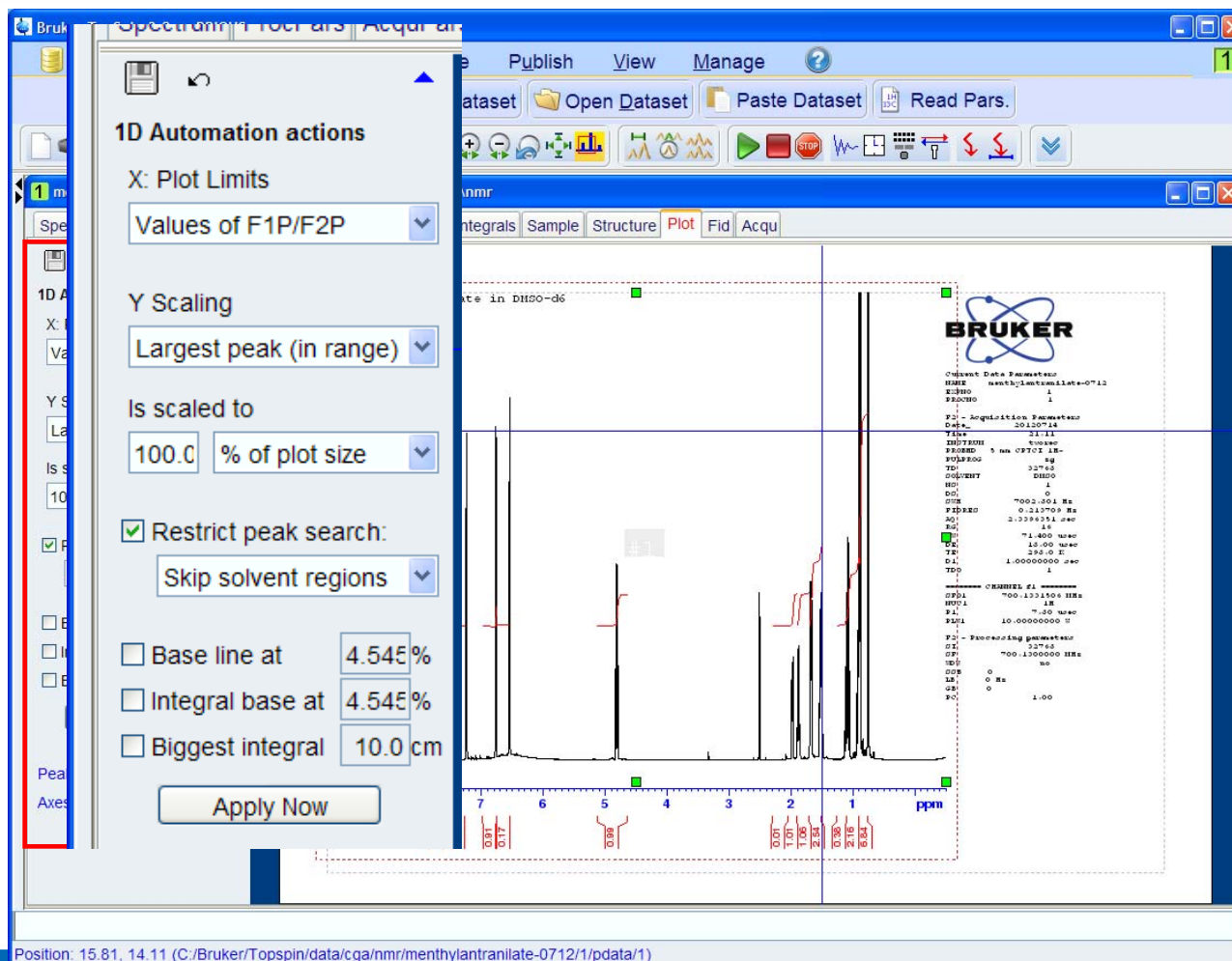
- **X plot Limits**
- Don't change
  - As is in spectrum tab
- Full Range
  - The whole spectrum
- Values of F1P/F2P



# Defining Automation actions



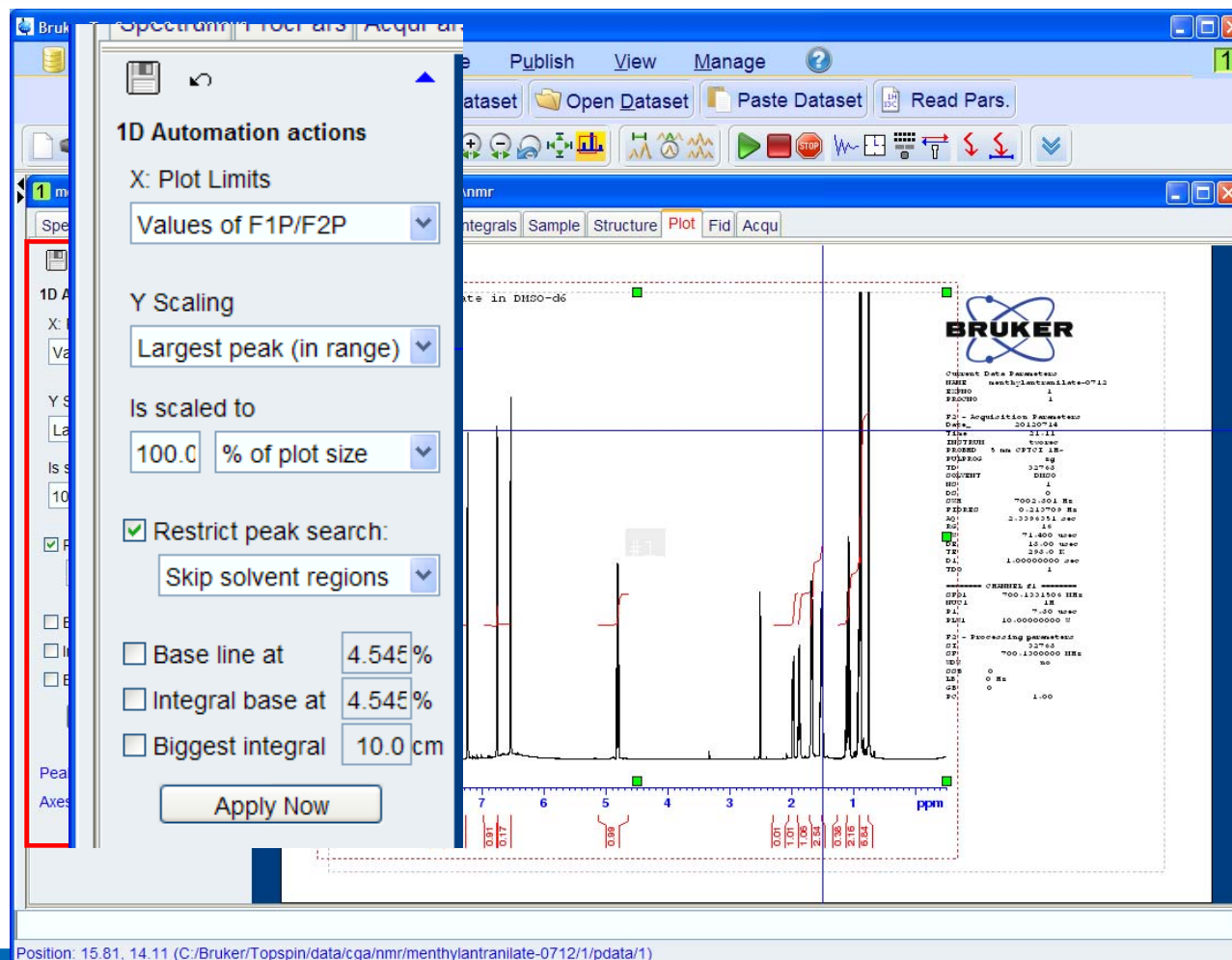
- **Y Scaling**
- Don't change
  - As is in spectrum tab
- Largest peak (all)
- Largest peak (in range)
- **Is scaled to**
- Percentage of Plot size
- Specific height in cm
- Value of CY



# Defining Automation actions



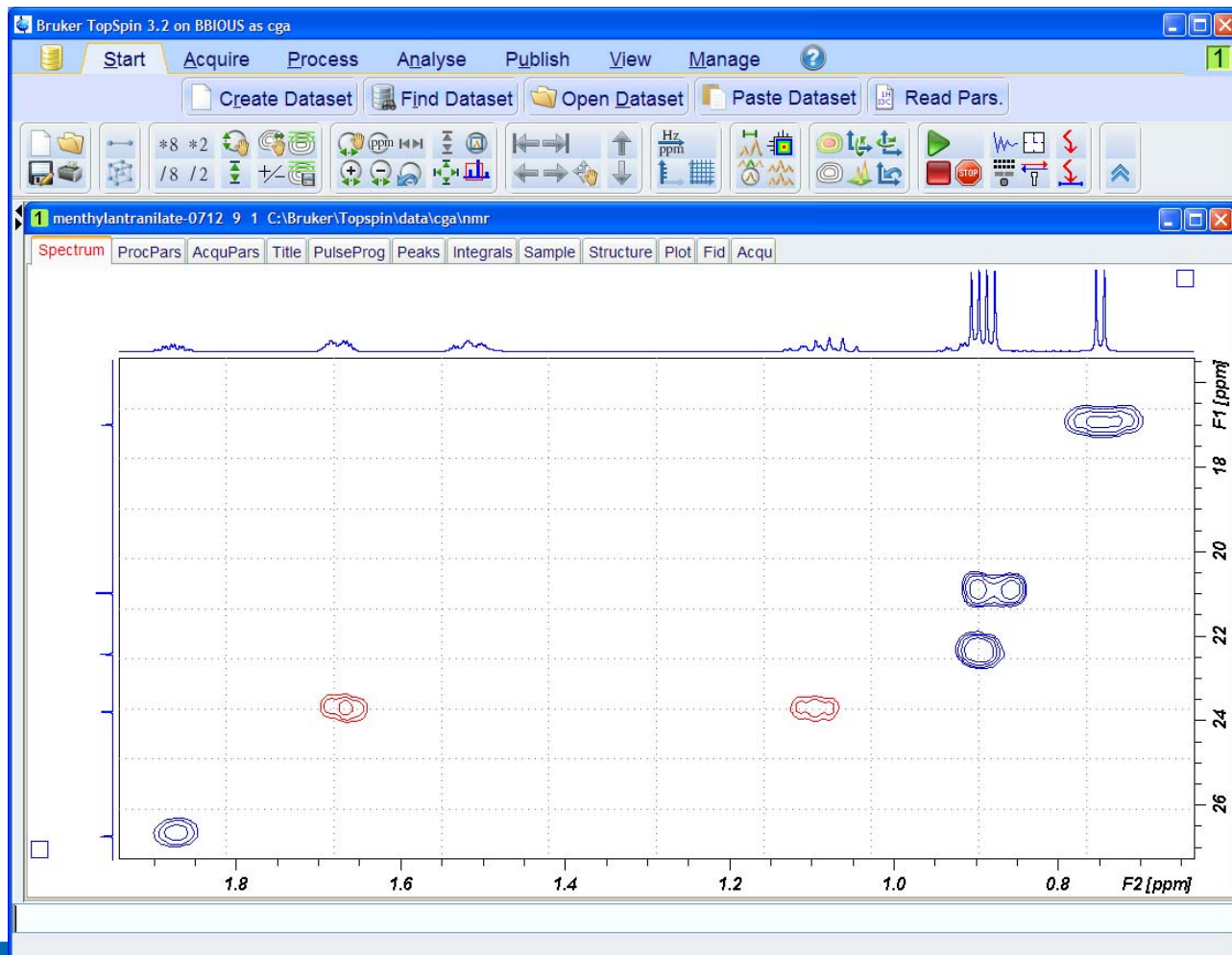
- **Restrict peak search**
- Use REG file
- Only integral regions
- Skip Solvent regions
- **Baseline settings**



Now some 2D



- Preparation
- Set projections  
1d spectra
- Set levels

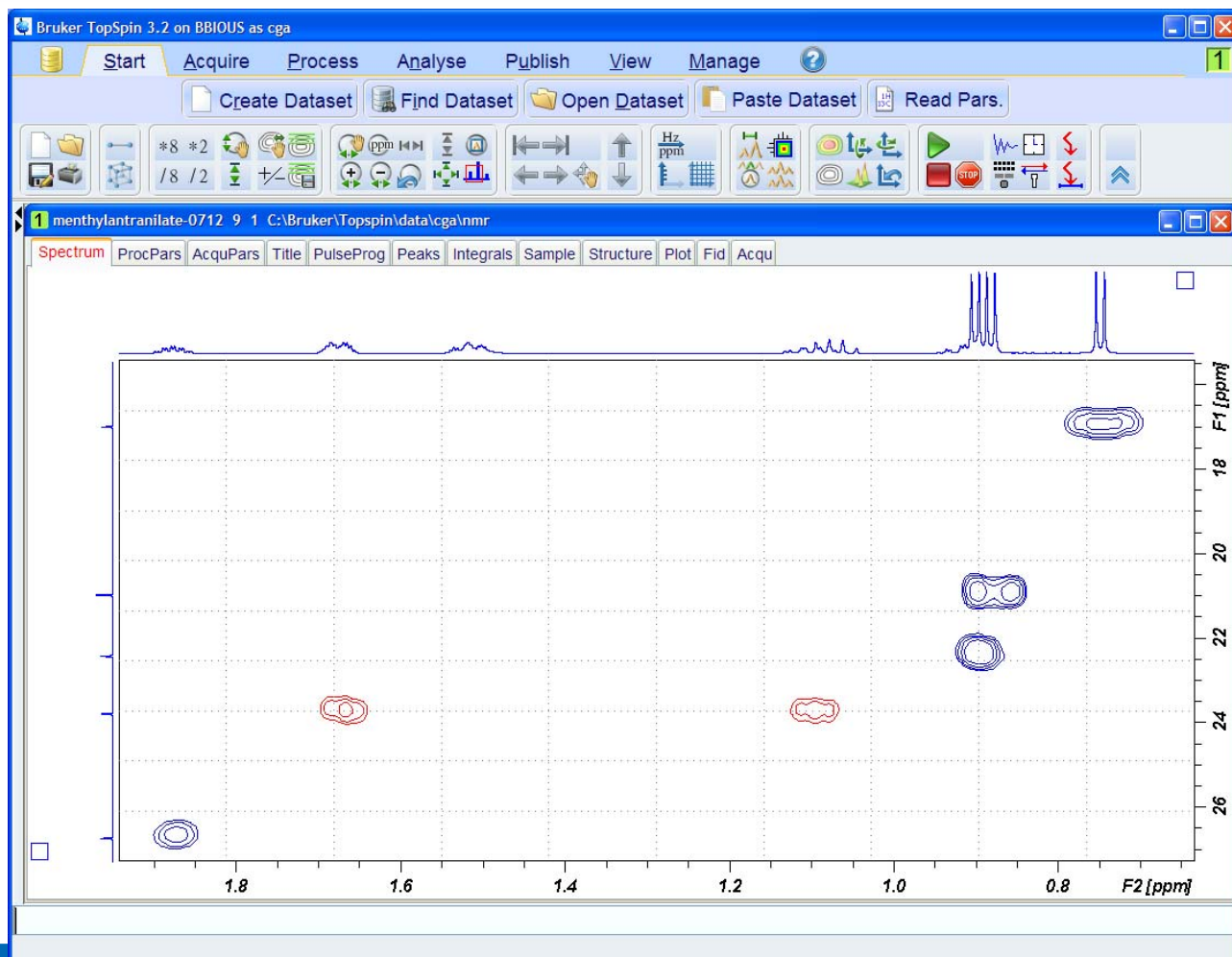


Now some 2D



Set levels

Default  
8 levels  
factor 1.8  
between  
levels



Now some 2D



Set levels

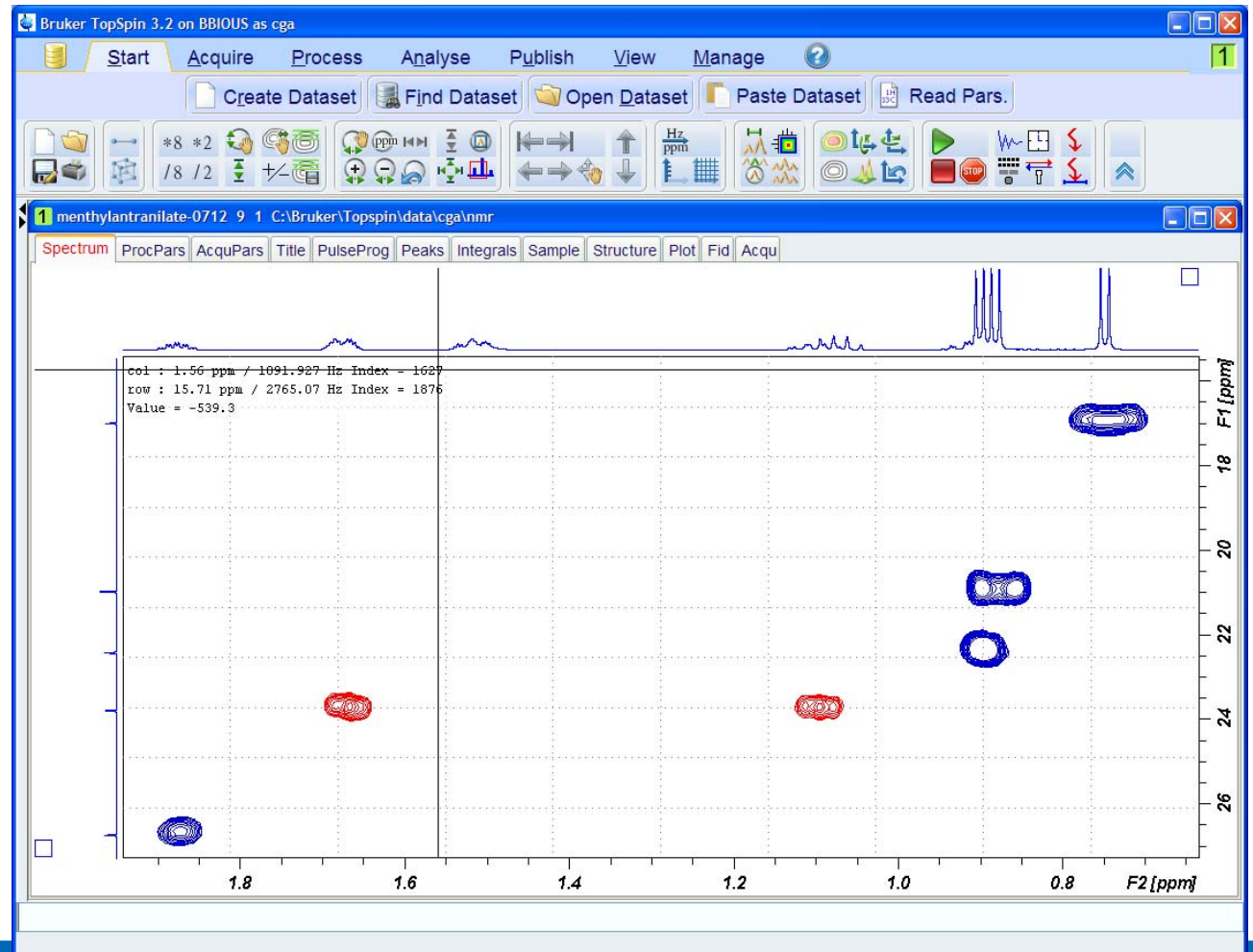
Better

32 levels

factor 1.2

between  
levels

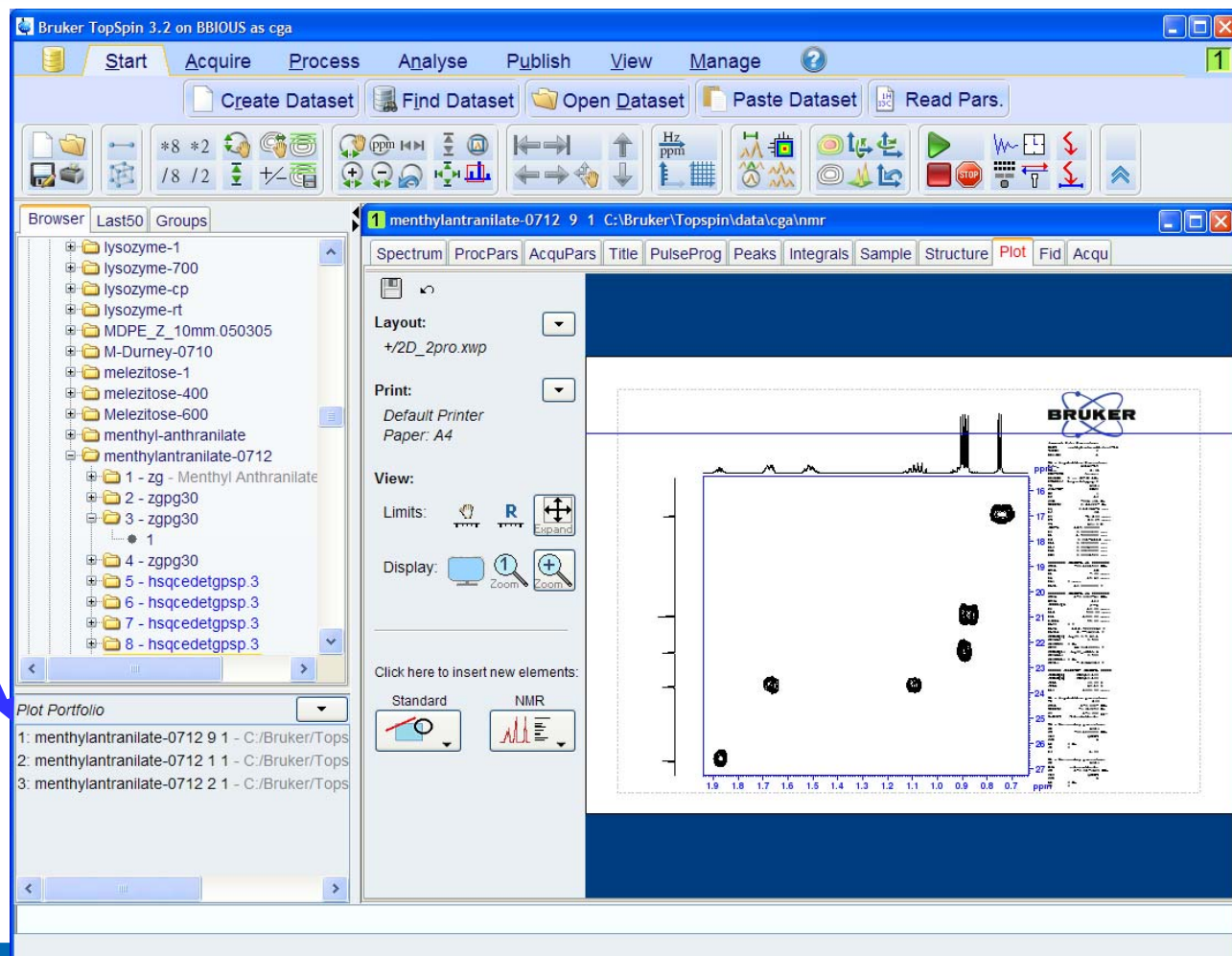
Now into the  
plot editor



# 2D Plot Editor



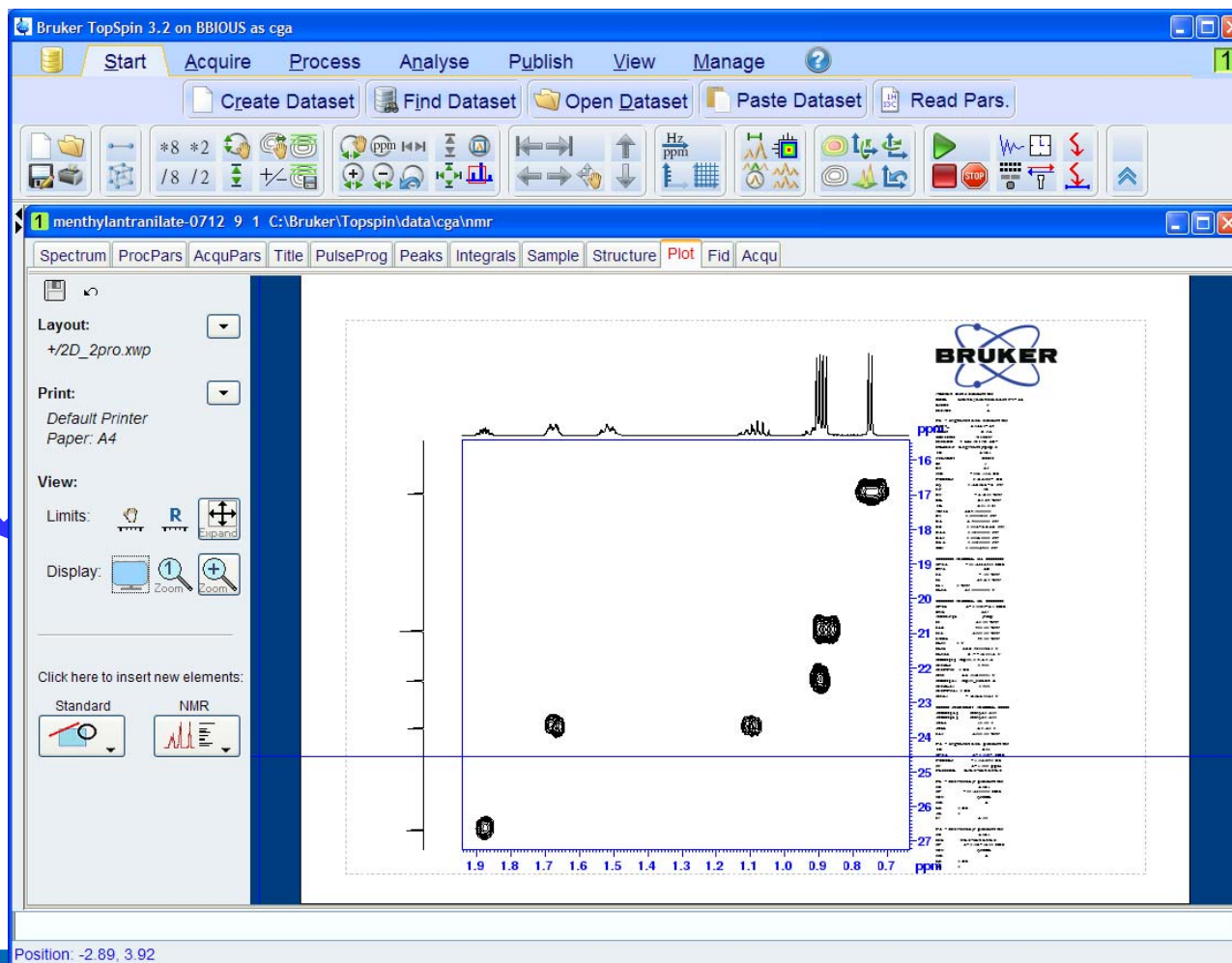
Portfolio window shows path of projections



# 2D Plot Editor



Basic options  
same as 1D



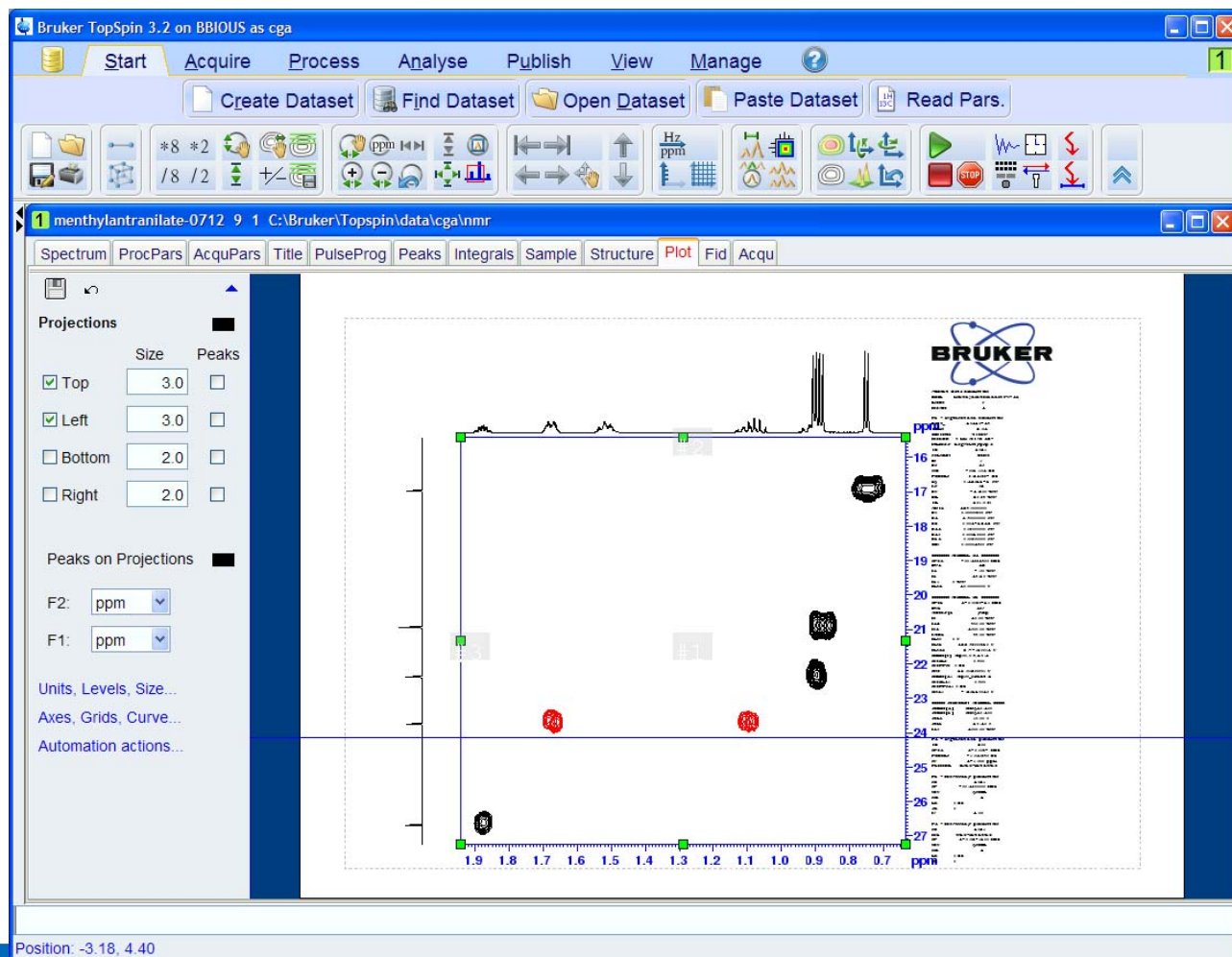


# 2D Plot Editor



## Projections

- Top, bottom, left and right
- Size of projections
- Peak display

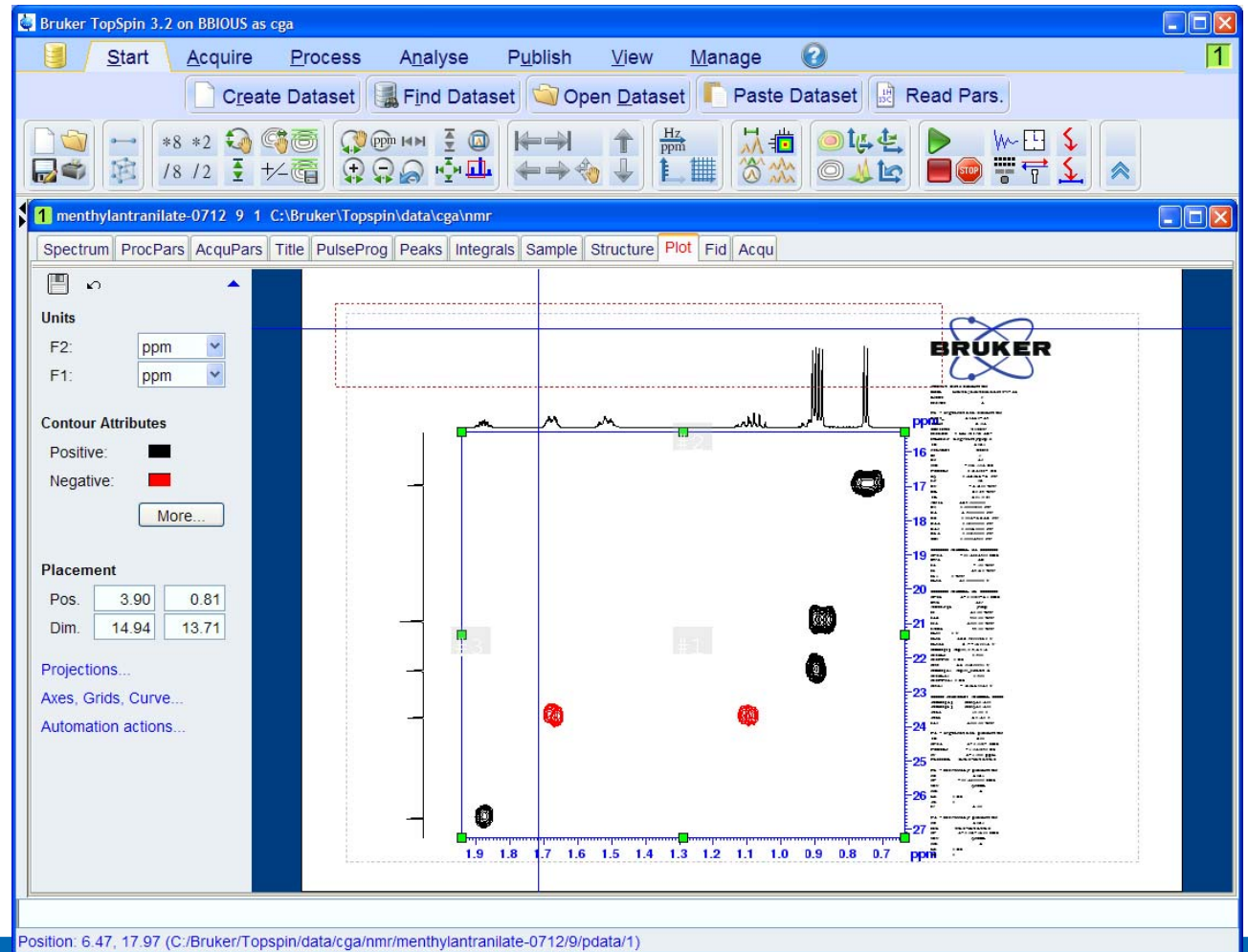


Position: -3.18, 4.40

# 2D Plot Editor



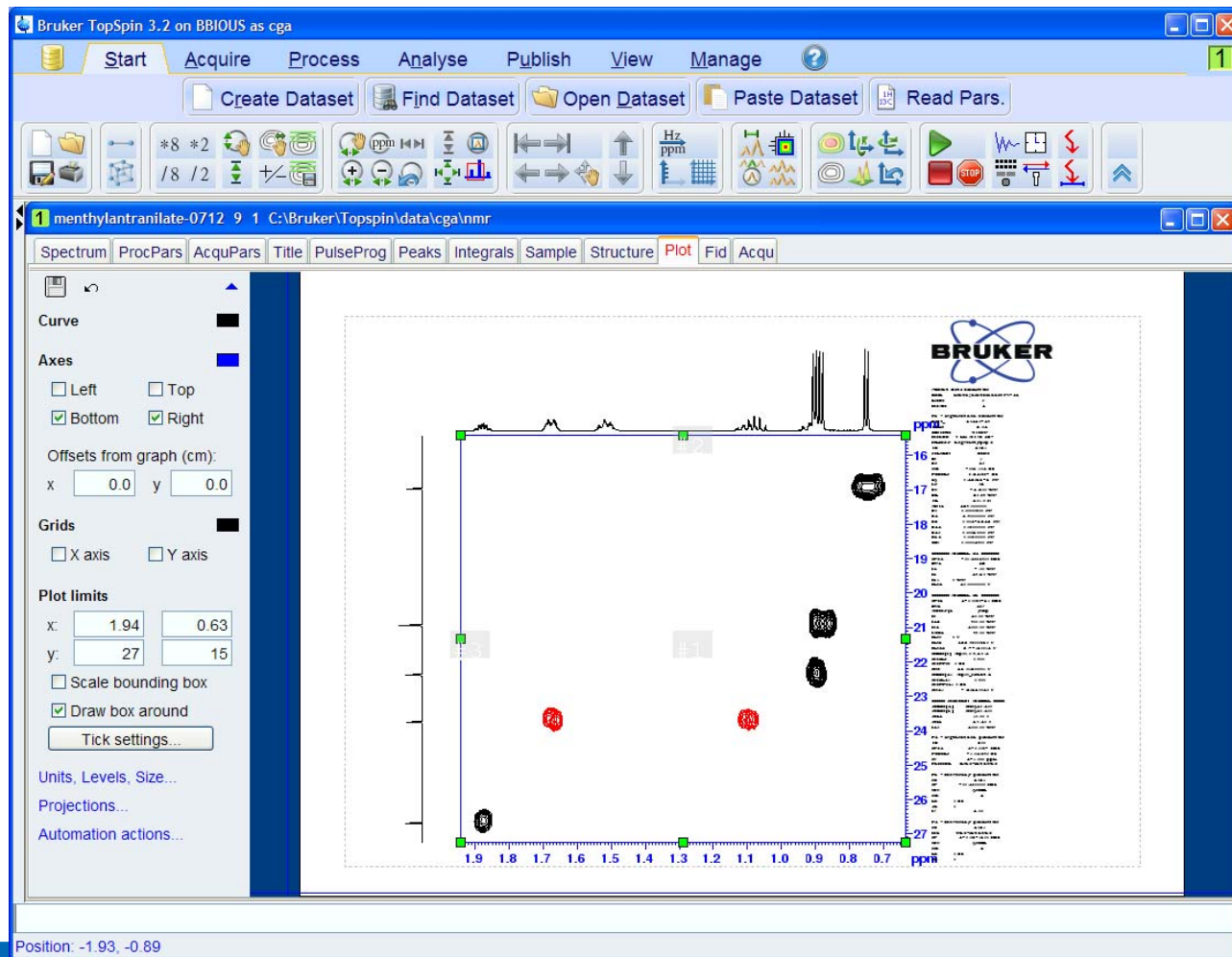
- **Units, Contours and placement**
- Contours
  - Choice of colors
- Placement
  - Location of spectrum



# 2D Plot Editor



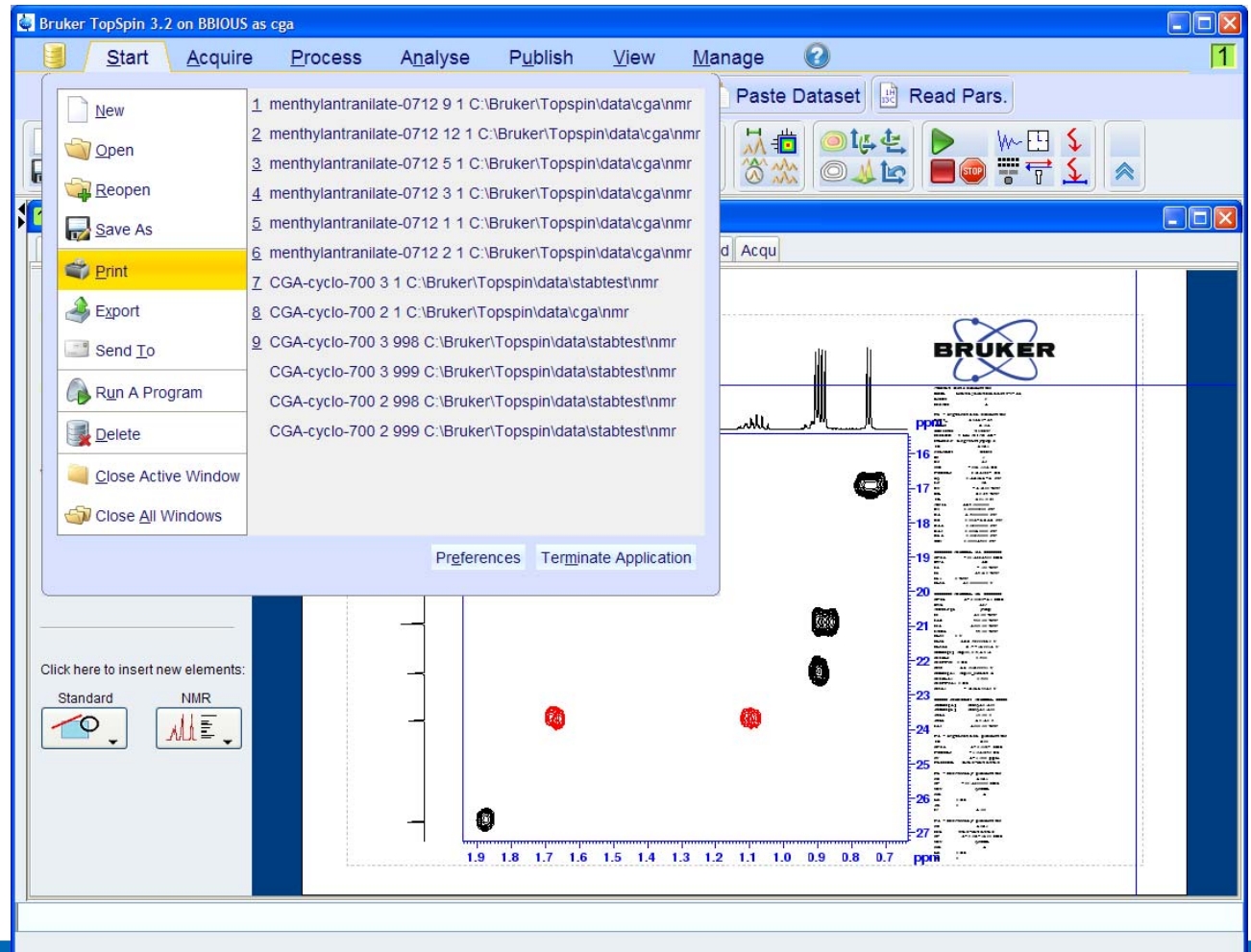
- Curve, Axes, Grids and Plot limits

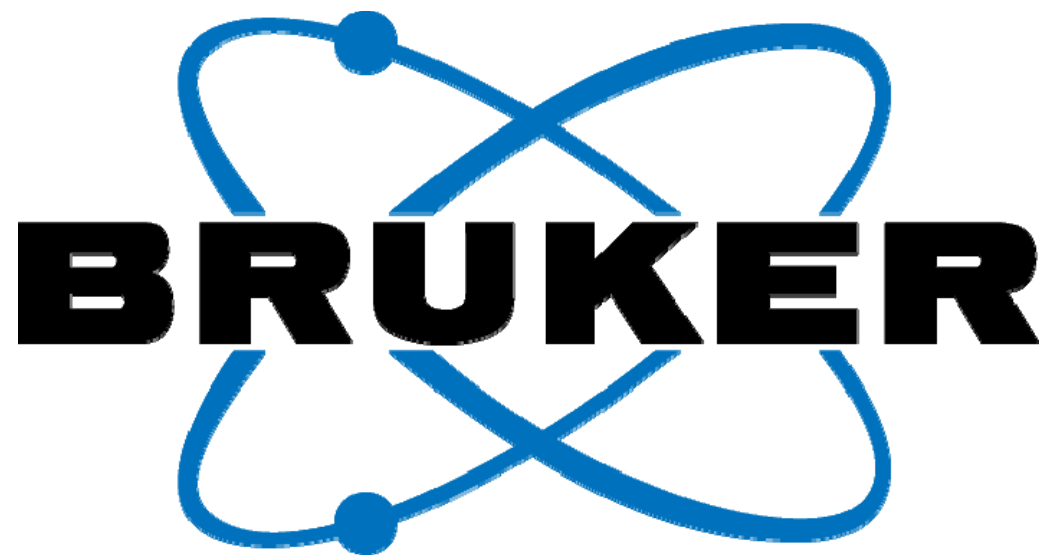


# 2D Plot Editor



- Finishing up
- Print for hardcopies
- Export for digital copies as PDF, PNG, PS, TIF, JPG and BMP





Innovation with Integrity