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 user interface

Plot area
The user interface

Plot functions

Layouts

Printers

View

Objects
The new user interface

Data Browser
The user interface

Portfolio area
The plot and view functions
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.
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
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

Expansions
More on expansions

- Shift – drag
- Ctrl – drag
- Alt - drag
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 vertical 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
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
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 axes or between axis and spectrum
  - Check box to select interactive scaling functions
Manipulating individual objects

- **Axis**
  - Choose ppm, Hz or points
  - Define axis details
  - Choose color
  - Choose display of scaling info on plot
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
Manipulating individual objects

• Curve

• Defines the color and line thickness of the spectrum
That is how you do it.
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
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