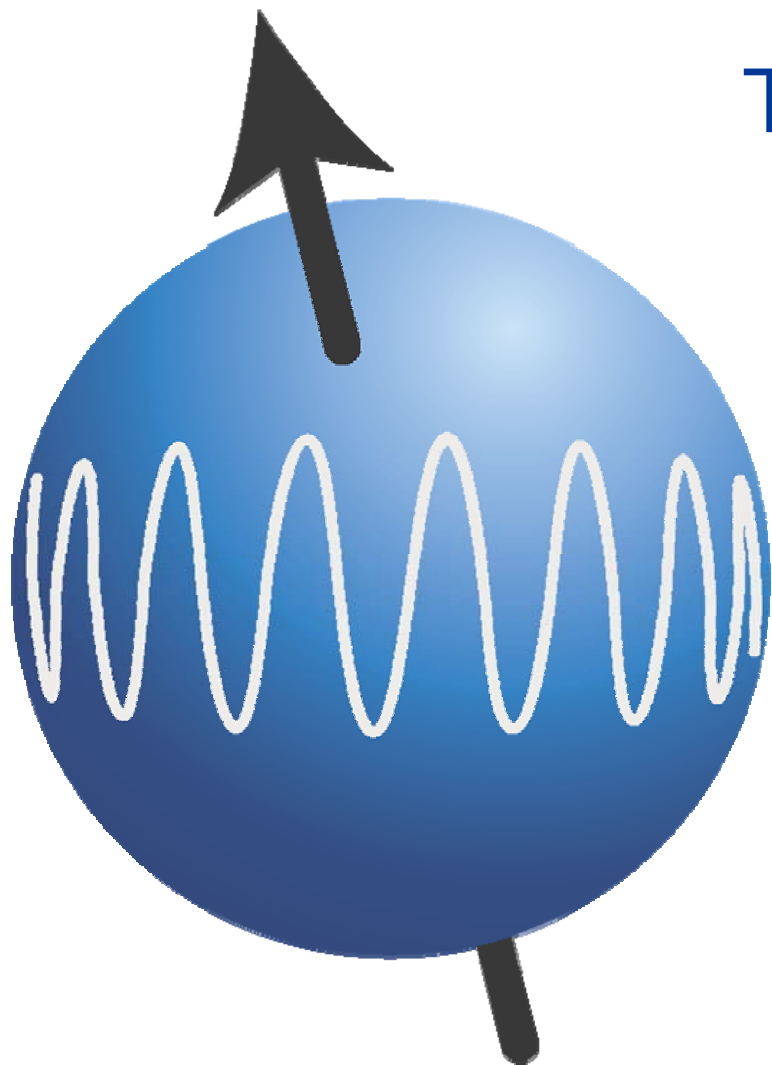


TOPSPINPLOT(XWINPLOT)

Easy and Simple Plotting



Written by:

Mike Brown

Version 01092006.meb

Bruker South Training Center

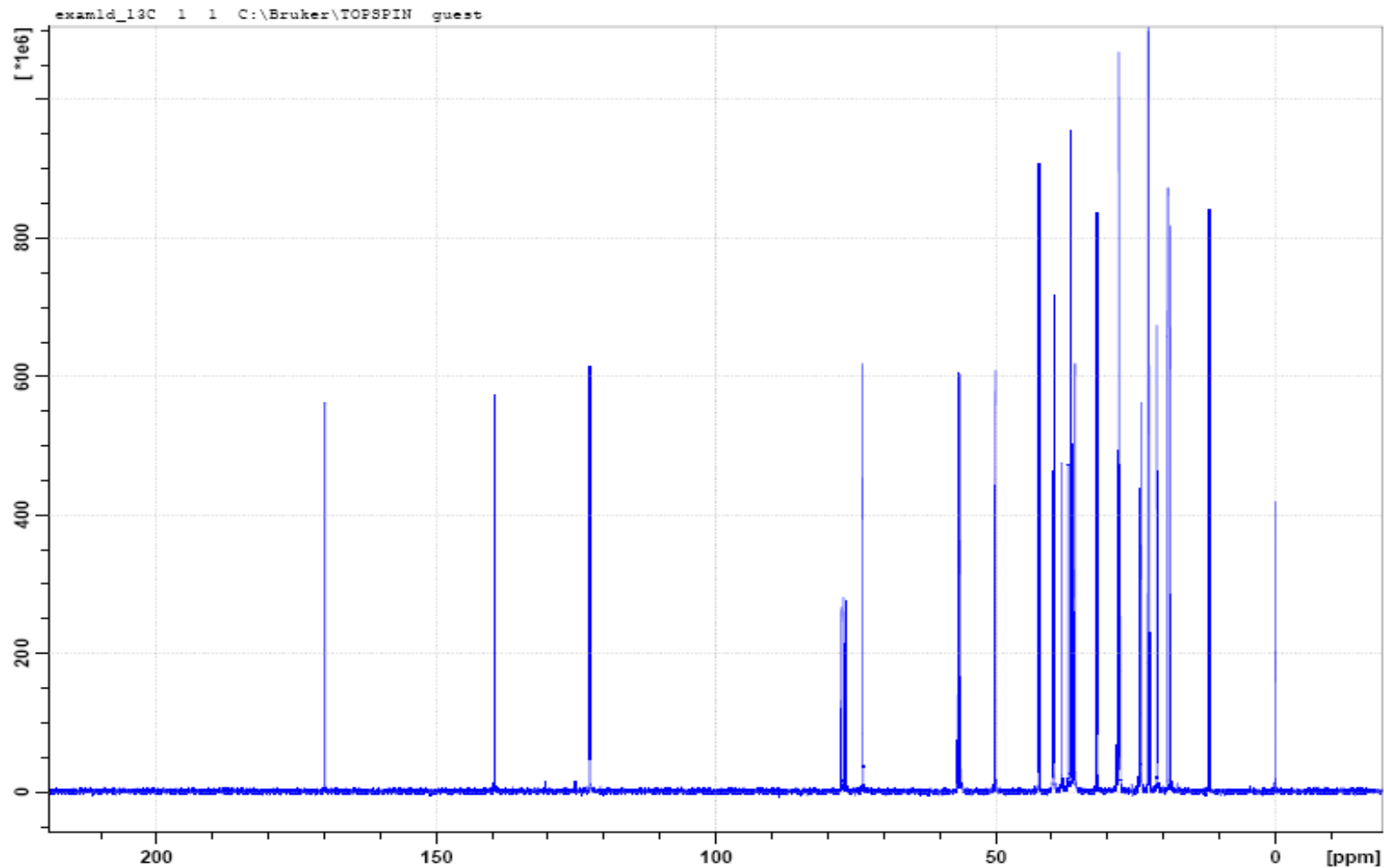
- Definitions
- Starting XWINPLOT
- Layouts
- Plot Limits
- Normal 1D and 2D plots
- Stacked Plots
- Help!

- **autoplot:** Plot data according to Plot Editor layout (1D,2D), with the current limits and scaling
- **plot:** Open the Plot Editor (1D,2D), adjust scaling, limits etc.
- **prnt:** Print the current dataset (1D,2D,3D) exactly as it appears on the screen
- **print:** Open print dialog box (1D,2D,3D)
- **plintfac:** Plot integrals with different scaling factors (au)
- **plot_sino:** Plot spectrum, scaling depends on Signal-to-Noise (au)
- **plot_to_file:** Creates a postscript file of the desired plot (au)
- **plotx:** Plots all integral regions separately with same scaling of x axis. (au)

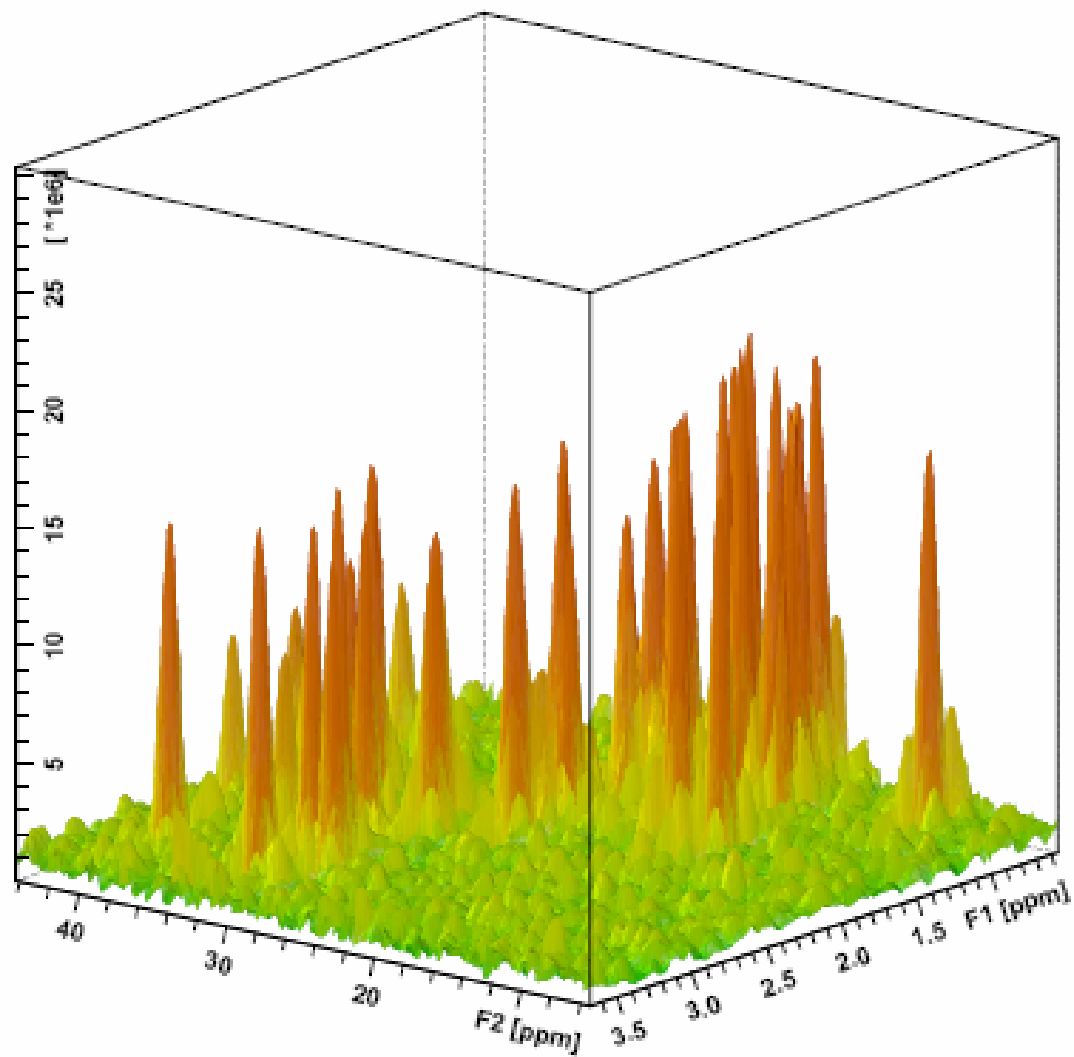
- **plot** : start with TOPSPIN plot limits
- **plot -r** : use plot limits defined by layout settings
- **plot -n** : use the layout without any modification
- **xwp**: For convenience of XWIN-NMR users, the command *xwp* is mapped to *plot*
- **xwpr**: For convenience of XWIN-NMR users, the command *xwpr* is mapped to *plot -r*.

You can also start **XWINPLOT** by typing `Xwinplot` in the command line !

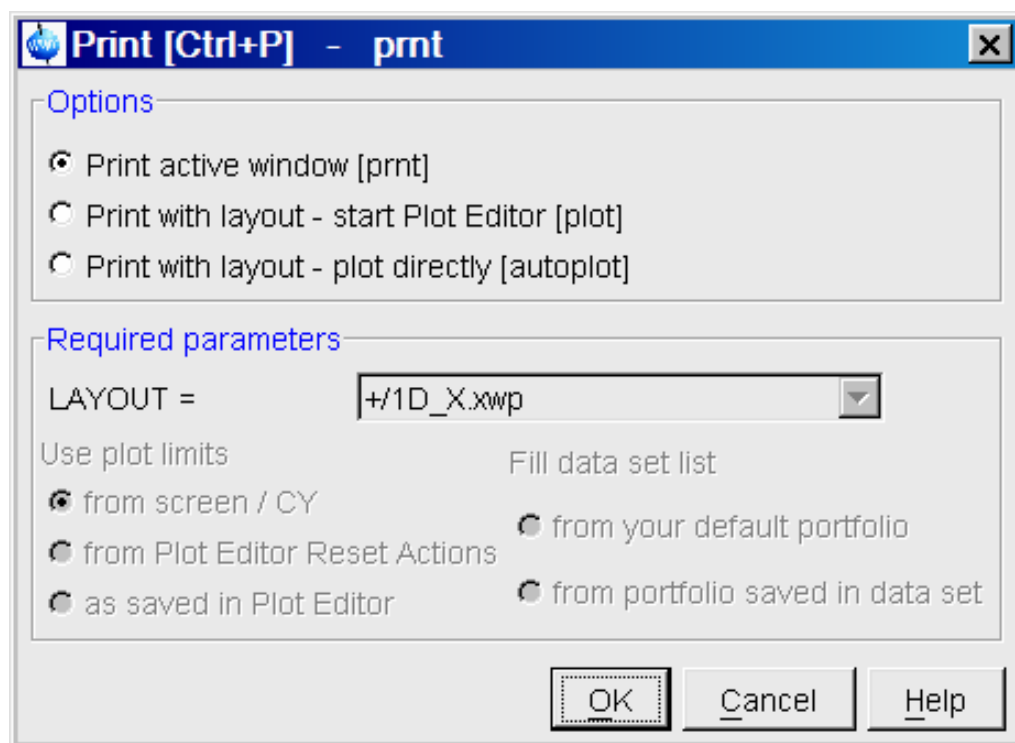
- “prnt” will plot exactly what is in the spectra window of TopSpin



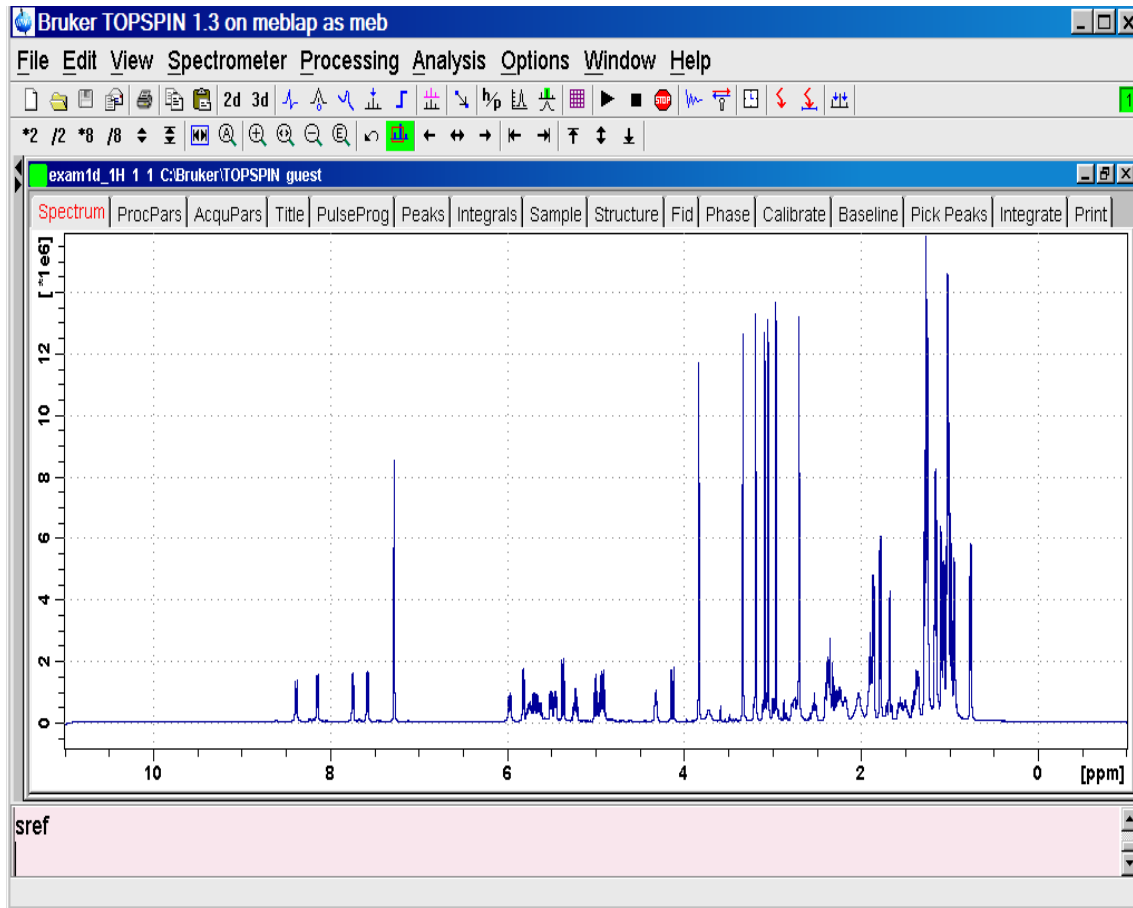
exam2d_CH 1 1 C:\Bruker\TOPSPIN guest



- “print” will open the print dialog box (1D,2D,3D)



Starting Xwinplot



- The plot limits have been set,
- the scaling has been set and
- the layout has been set

- Just type xwp, plot or whichever way you want to start. On the command line.

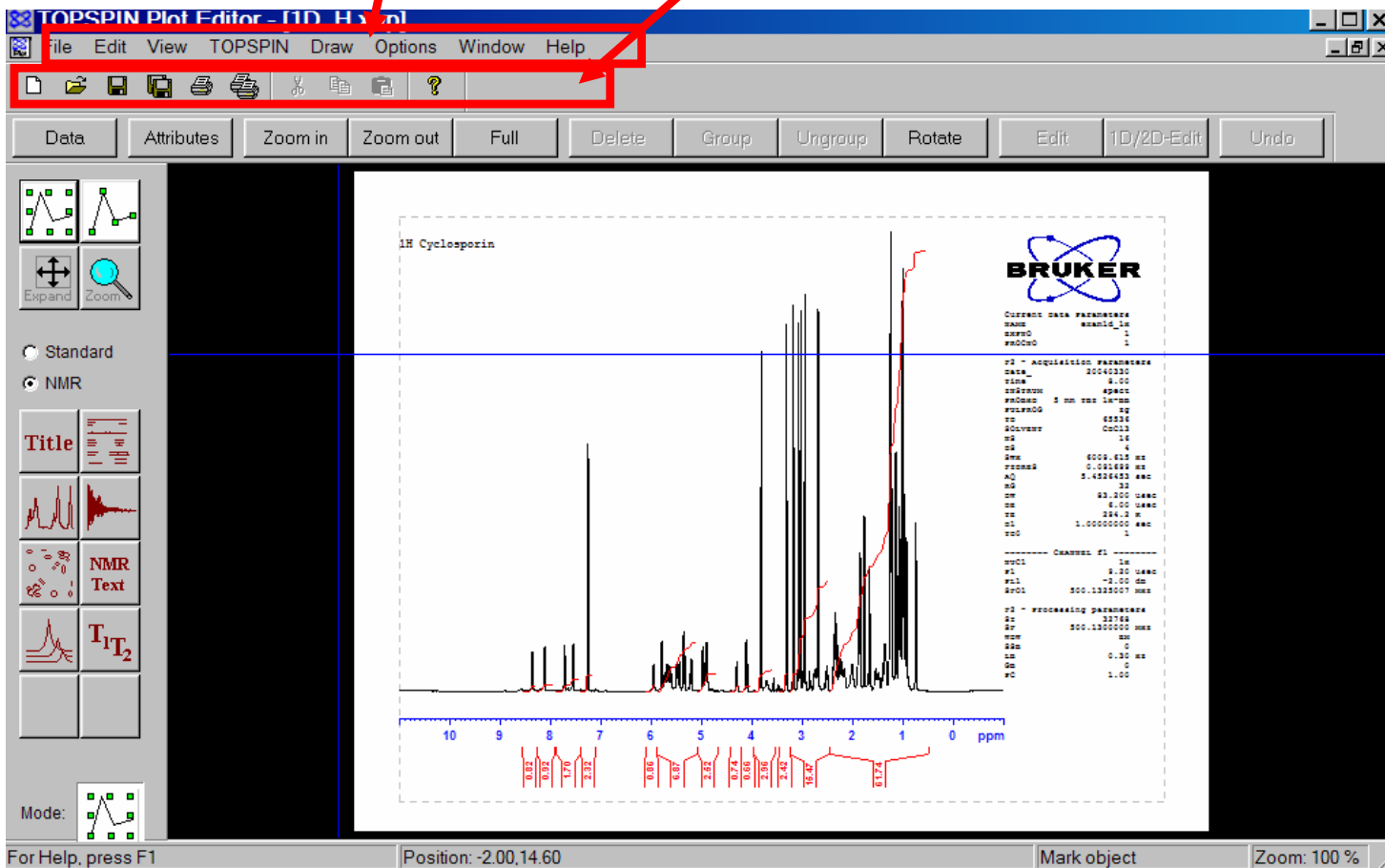


Layout name (from edp)

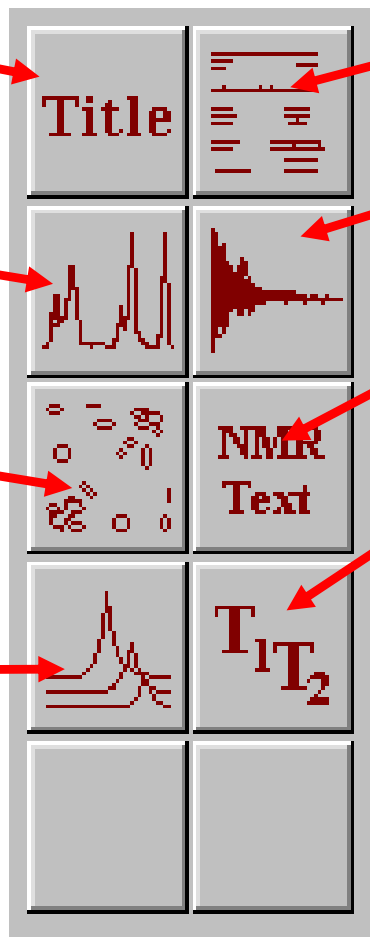
menus

Icons

- If you type xwp (or plot) in TopSpin
- You will use the current layout the current plot limits and scaling



- Use this to insert a title
- Use this to insert a 1D spectra
- Use this to insert a 2D spectra
- Use this to insert a set of stacked spectra



- Use this to insert parameters
- Use this to insert a FID
- Use this to insert text
- Use this to plot T1 and T2 datasets

- You can enter the layout you want to use in edp
- You can start Xwinplot, and then call up a new layout
- Or you can create your own from scratch
- Or you can create a new one from one of the canned layouts.

F1P [ppm] =	11.008	Left limit for pp
F2P [ppm] =	-1.00806	Right limit for pp
CY [rel] =	15	Intensity of reference peak
Automation		
AUNMP =	proc_1d	Processing AU program
LAYOUT =	+1D_H.xwp	Layout file for 'autoplots'
Miscellaneous		

- Choose a layout here in edp
- Don't forget the "+" at the front
- Layouts are stored normally on windows at:
C:\Bruker\TOPSPIN\plot\layouts
- Layouts are stored on Linux at:
\opt\topspin\plot\layouts
- But you can store your layouts any where on any disk

- Every Bruker parameter set has a layout that will usually work with that experiment.
- Others are available
- You can make up your own
- You can also have sub directories of your own
- You can name your layouts anything you want, but you must supply the .xwp extension yourself.

1D+1D+1D.xwp

1D_BB.xwp

1D_H+noint+ppp.xwp

1D_H+pp.xwp

1D_noediff.xwp

1D_X+ppfile.xwp

2D_inv.xwp

t1norm.xwp

1D+1D+int.xwp

1D_H+info.xwp

1D_H+pp+info.xwp

1D_H+zoom.xwp

1D_X+int.xwp

1D_X.xwp

prohump.xwp

1D+1D+pp.xwp

1D_H+lf.xwp

1D_H+pp+lf.xwp

1D_H.xwp

1D_X+nopp.xwp

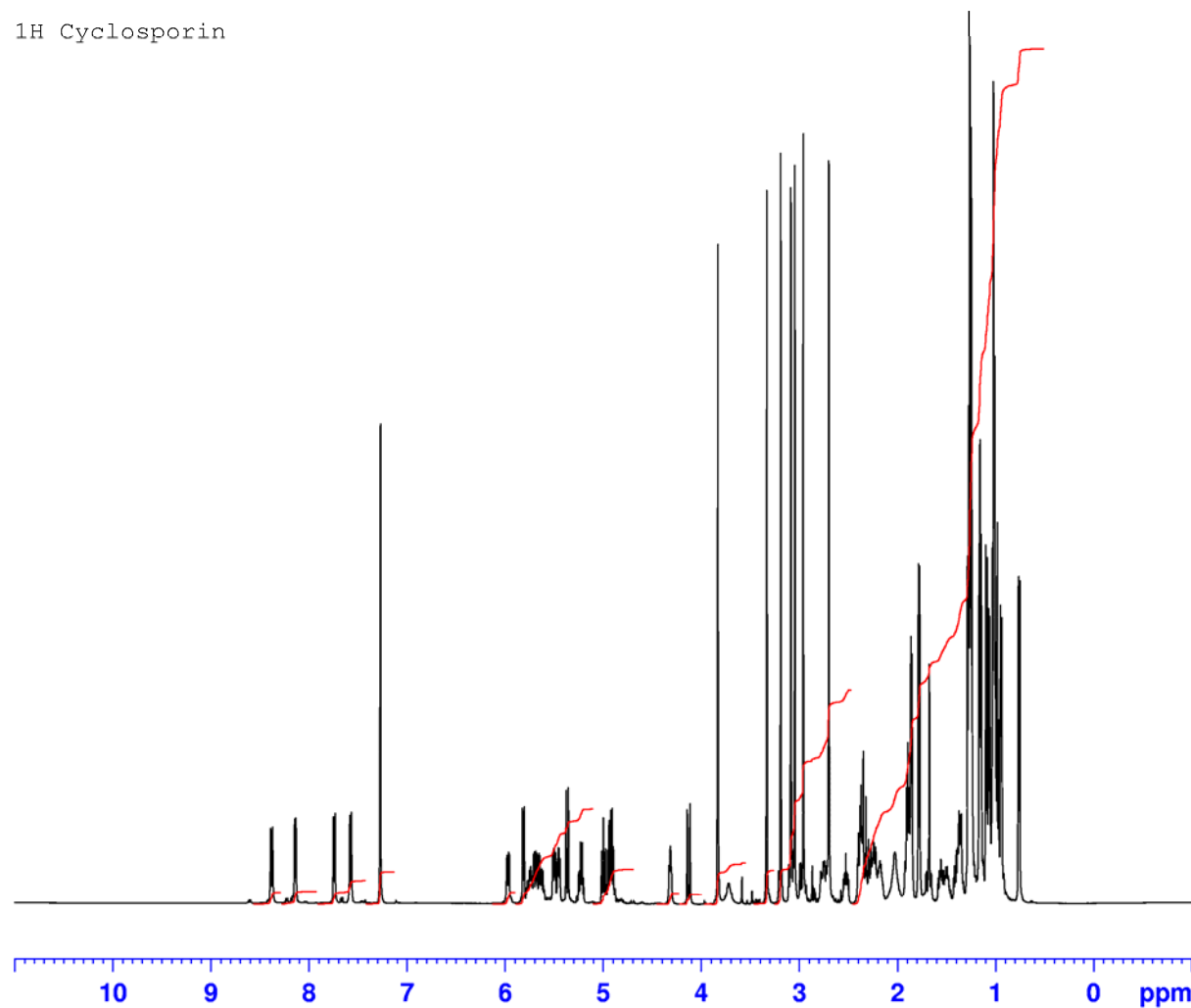
2D_hom.xwp

proresol.xwp

Normal 1D Layout (Proton 1D_H.xwp)



1H Cyclosporin



0.82 0.92 1.70 2.32 0.86 6.87 2.52 0.74 0.66 2.96 2.42 15.47 61.74

```
Current Data Parameters
NAME      exam1d_1H
EXPNO     1
PROCNO    1

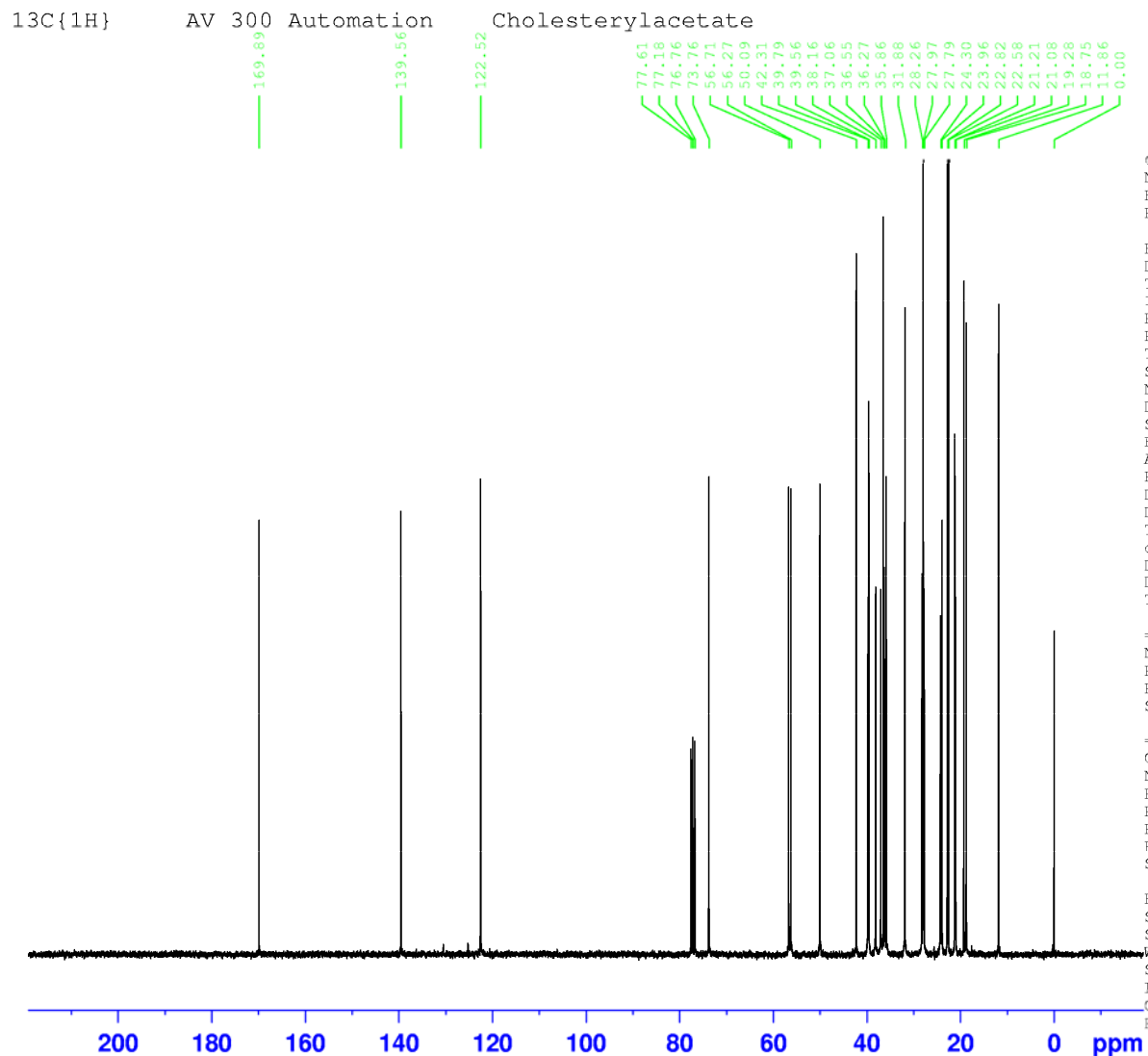
F2 - Acquisition Parameters
Date_     20040330
Time      8.00
INSTRUM   spect
PROBHD    5 mm TBI 1H-BB
PULPROG   zg
TD         65536
SOLVENT   CDC13
NS         16
DS         4
SWH        6009.615 Hz
FIDRES     0.091699 Hz
AQ         5.4526453 sec
RG         32
DW         83.200 usec
DE         6.00 usec
TE         294.2 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1      1H
P1        9.20 usec
PL1       -2.00 dB
SFO1      500.1325007 MHz

F2 - Processing parameters
SI         32768
SF         500.1300000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



Normal 1D Layout (Proton 1D_13C.xwp)



```
Current Data Parameters
NAME      examld_13C
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20040330
Time      3.43
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         256
DS         4
SWH        17985.611 Hz
FIDRES     0.274439 Hz
AQ         1.8219508 sec
RG         32768
DW         27.800 usec
DE         6.00 usec
TE         303.0 K
d11        0.03000000 sec
D1         2.00000000 sec
DELTA     1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         8.00 usec
PL1        0.00 dB
SFO1       75.4752958 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      100.00 usec
PL2        0.00 dB
PL12       20.00 dB
PL13       22.00 dB
SFO2       300.1312005 MHz

F2 - Processing parameters
SI         32768
SF         75.4677448 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

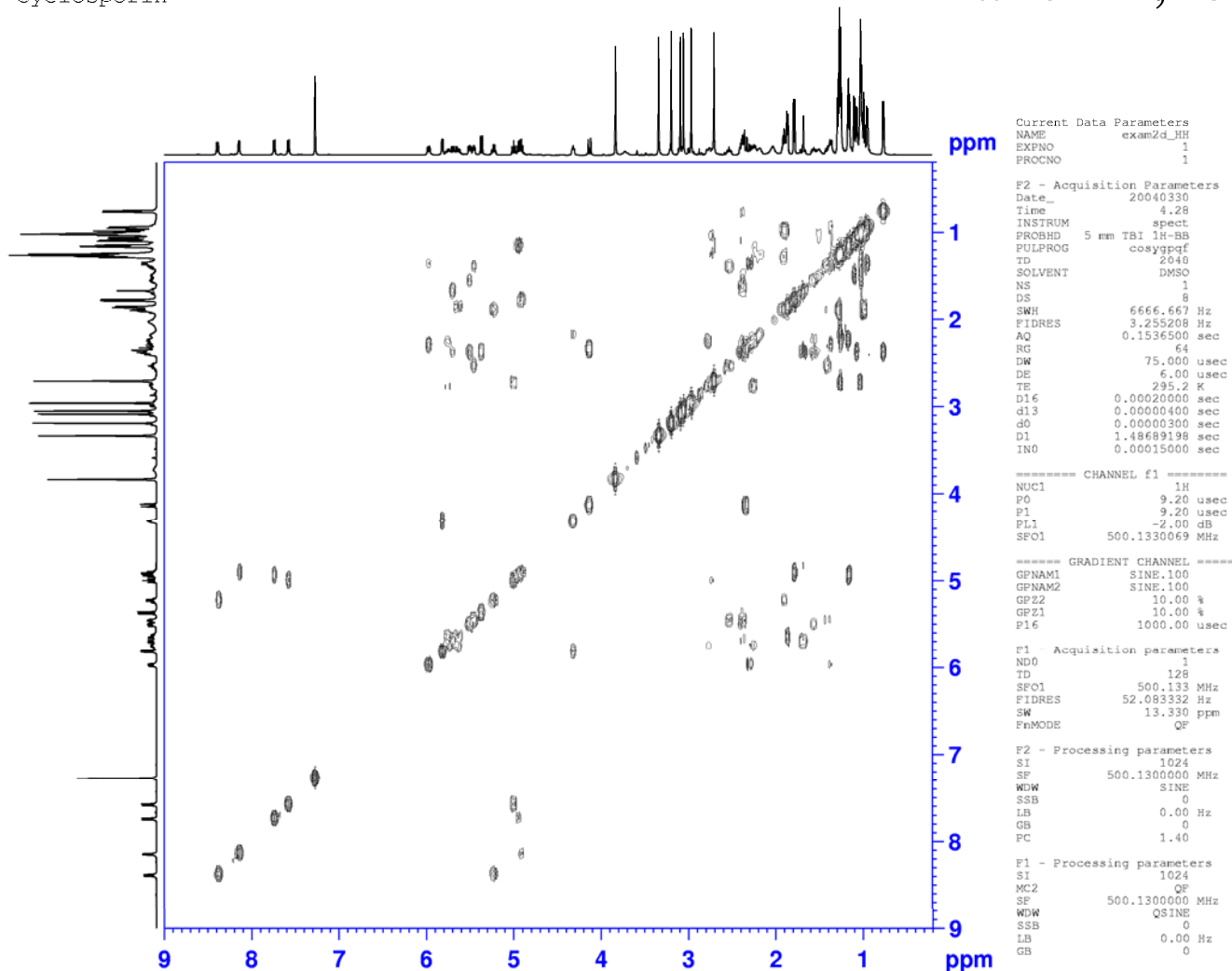


Normal 2D Layout (2D_HOMO.xwp)



Remember, a COSY is usually plotted with the same limits in F1 and F2, it's a square matrix

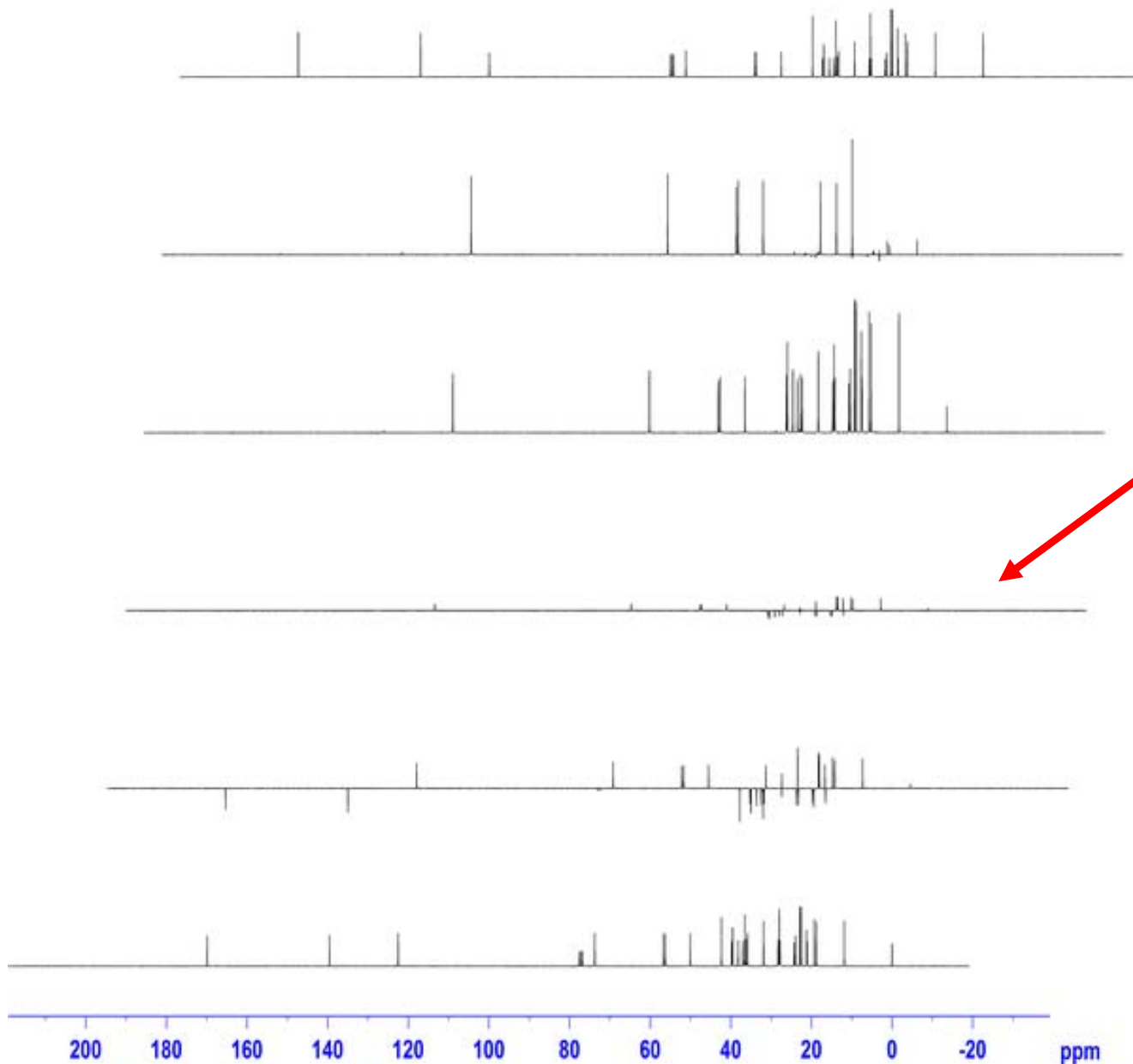
COSY Cyclosporin



Stacked Plots



¹³C{¹H} AV 300 Automation Cholesterylacetate
Stacked plot



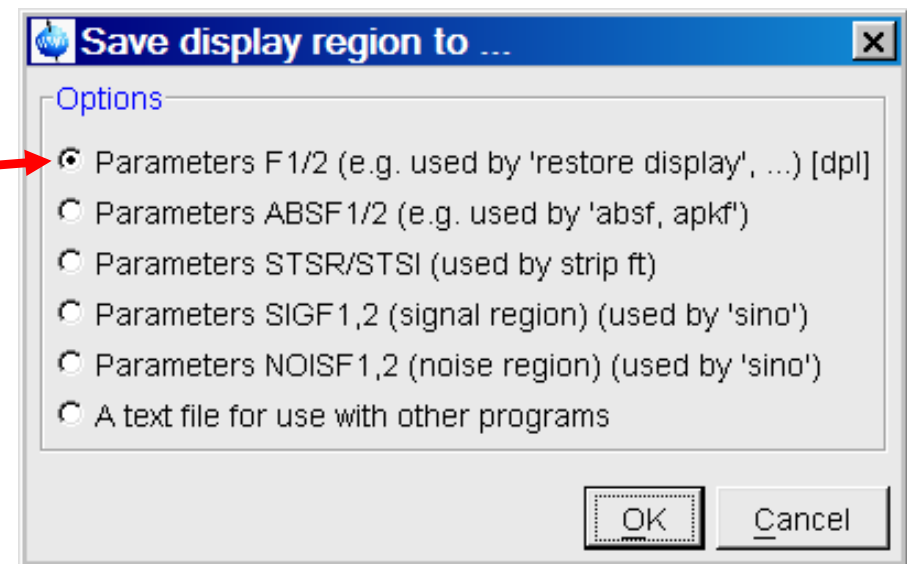
One of the problems with Stacked plots is all of the spectra scale to each other .



Plot Limits (1D)

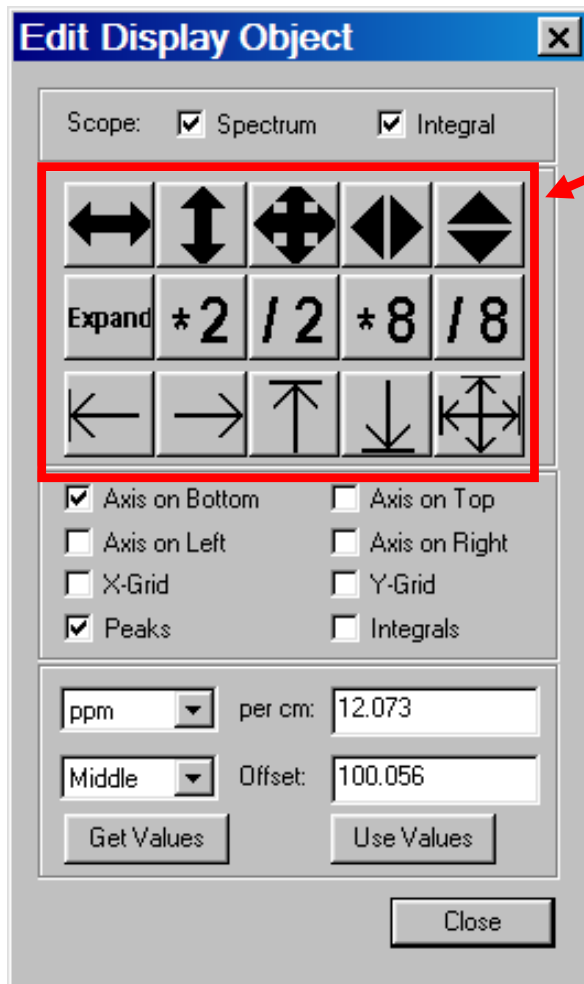


- You can set the plot limits in Topspin with the cursor, right click, and choose save display region to...



- What ever the limits are on the display will be the new plot limits for Xwinplot.

- Or you can choose the plot limits in Xwinplot itself

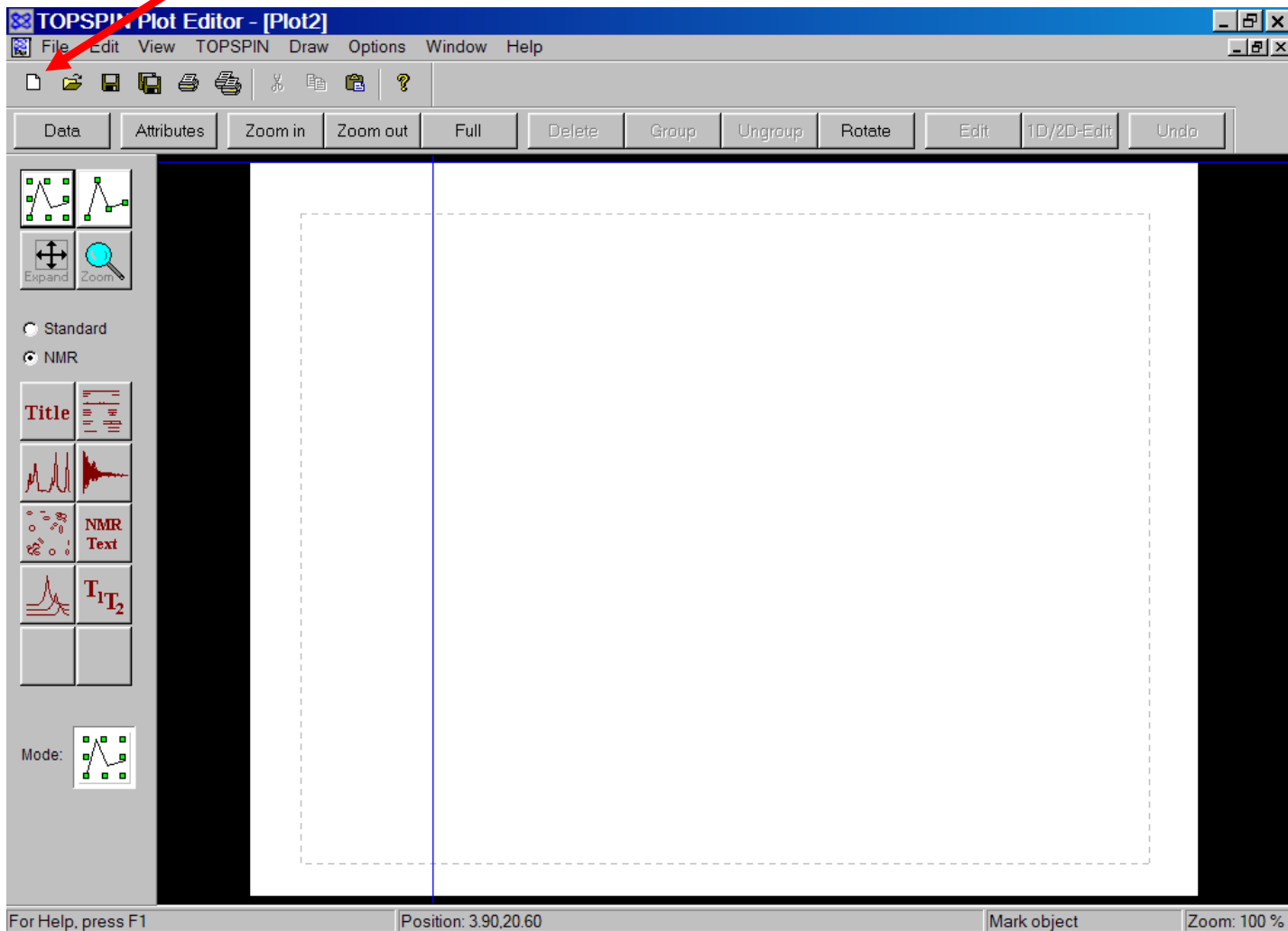


- You can also choose the scaling of the Spectra or the integrals in this window
- You can also add or change the appearance of the axis and integrals

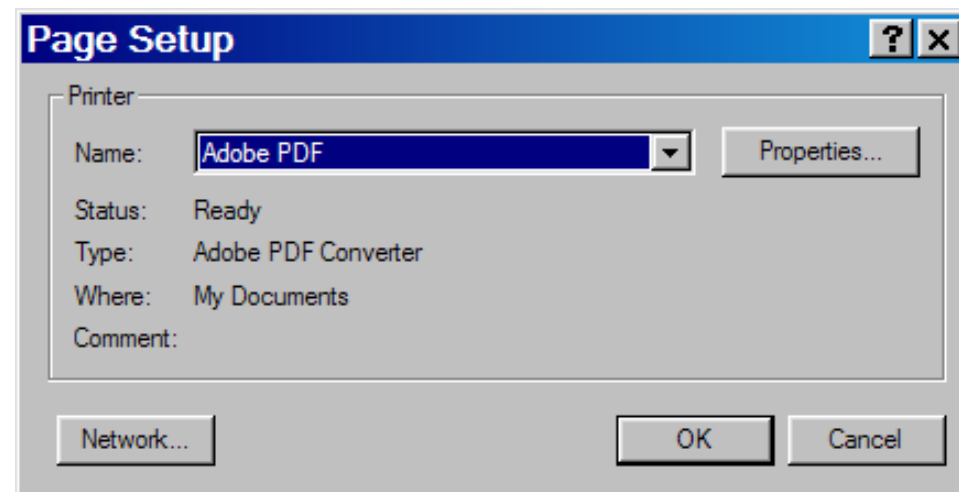
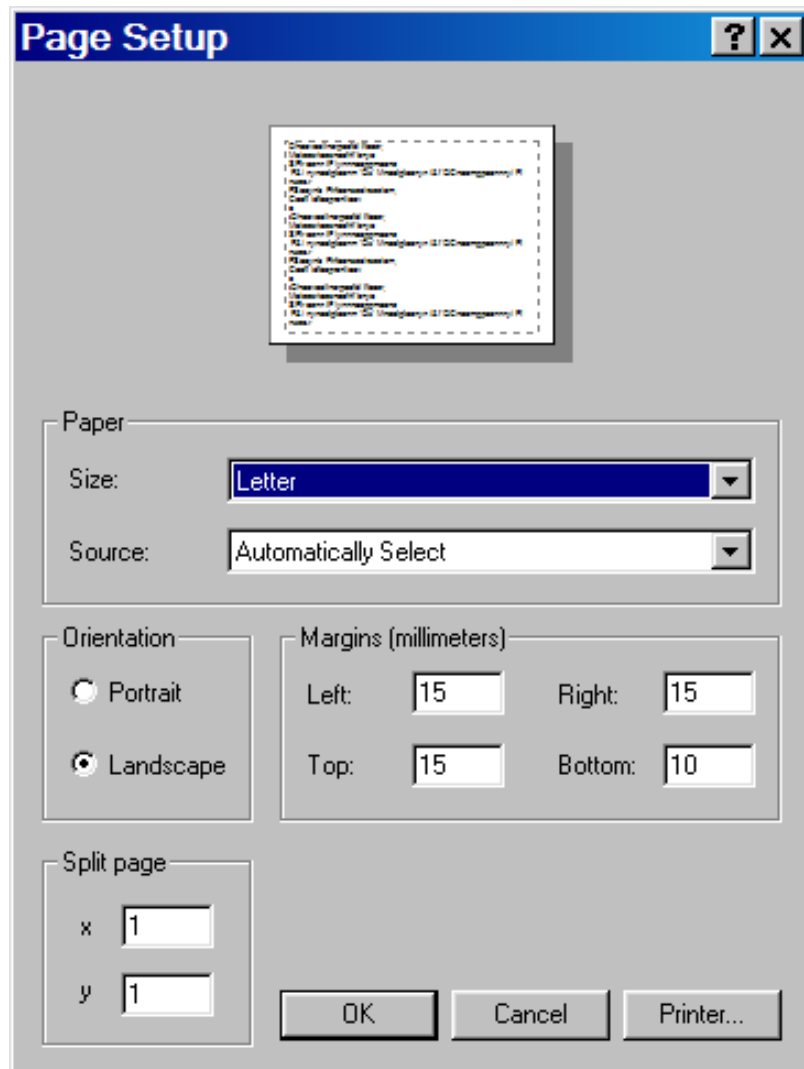
Creating a new layout from scratch



- Click the “new” icon, this blanks the current layout



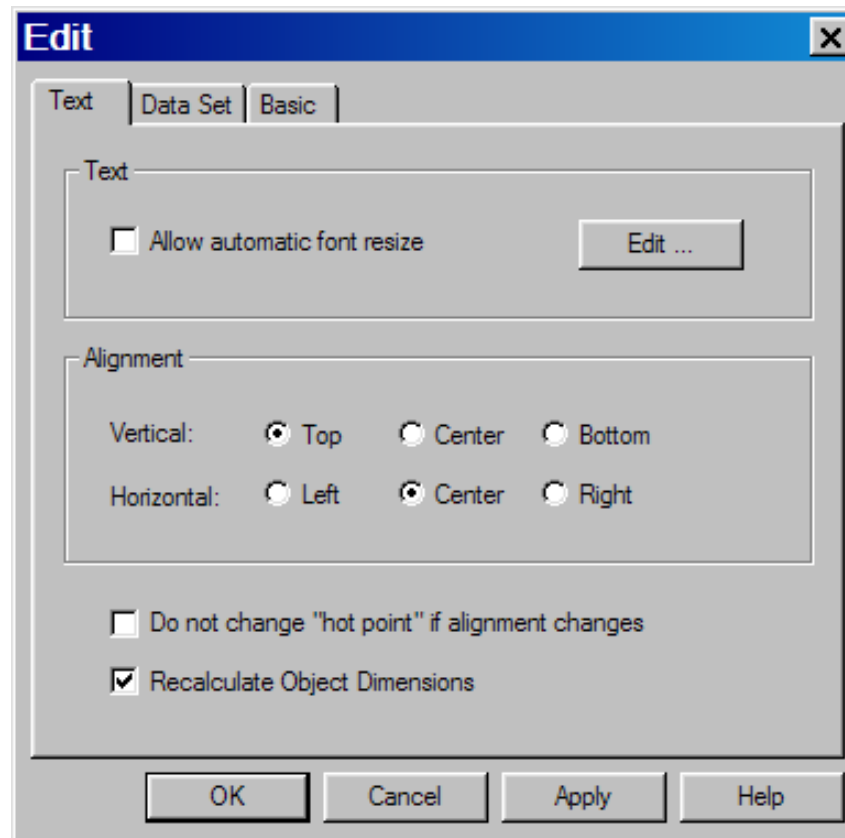
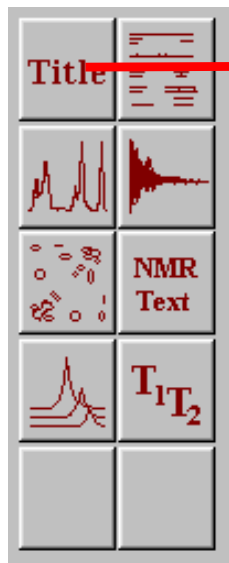
- Check to make sure the printer and print limits are correct



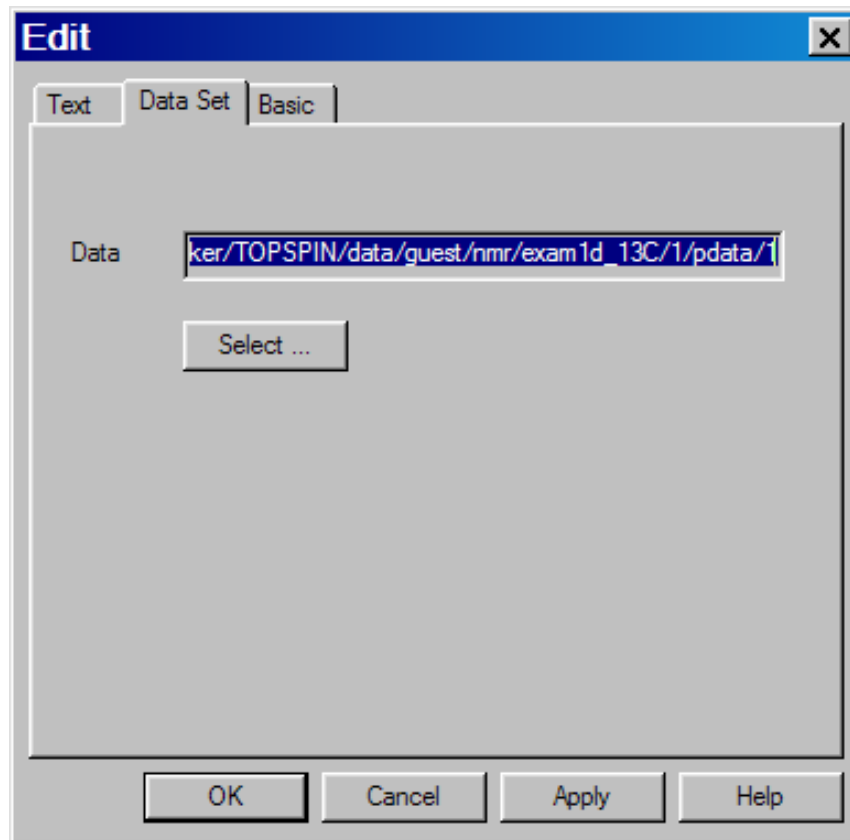
Creating a new layout from scratch



- Click the Title button and add the title where you want it
- Alignment



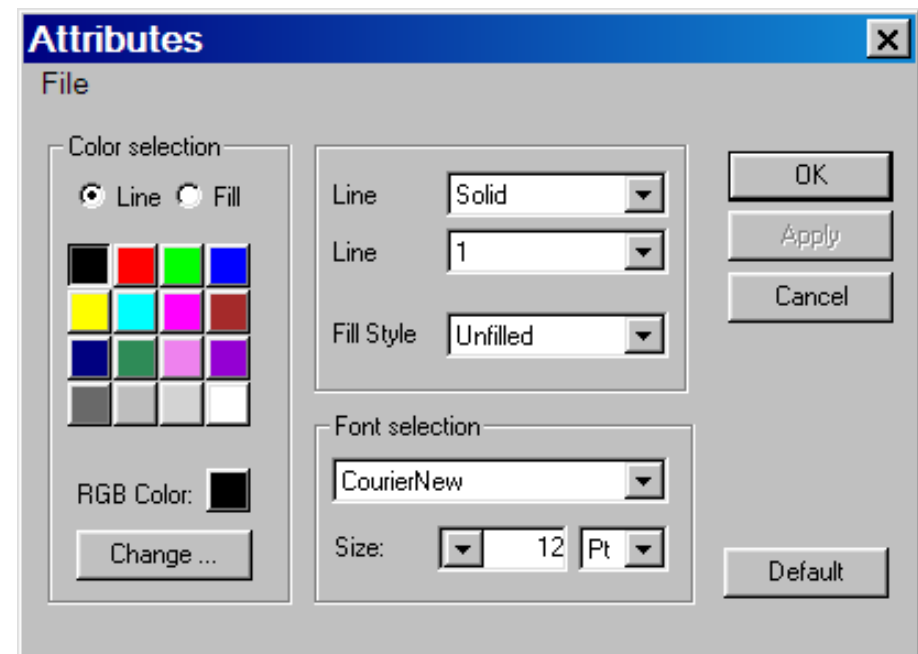
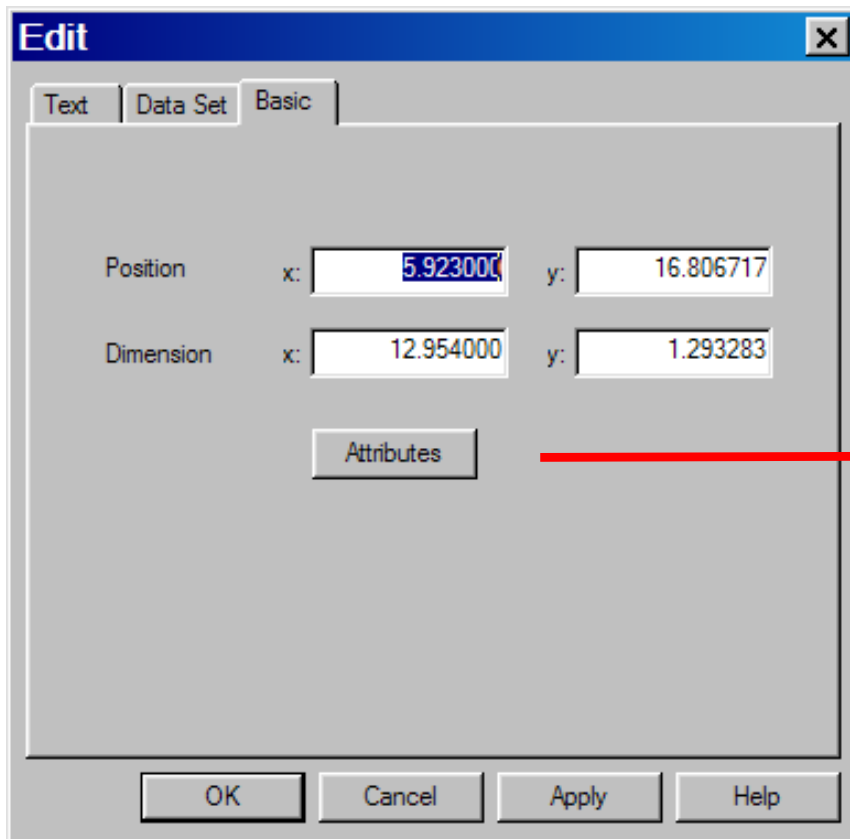
- the data set that has the title you want to use



Creating a new layout from scratch



- Then set the orientation, size, position and attributes (color, font etc.)



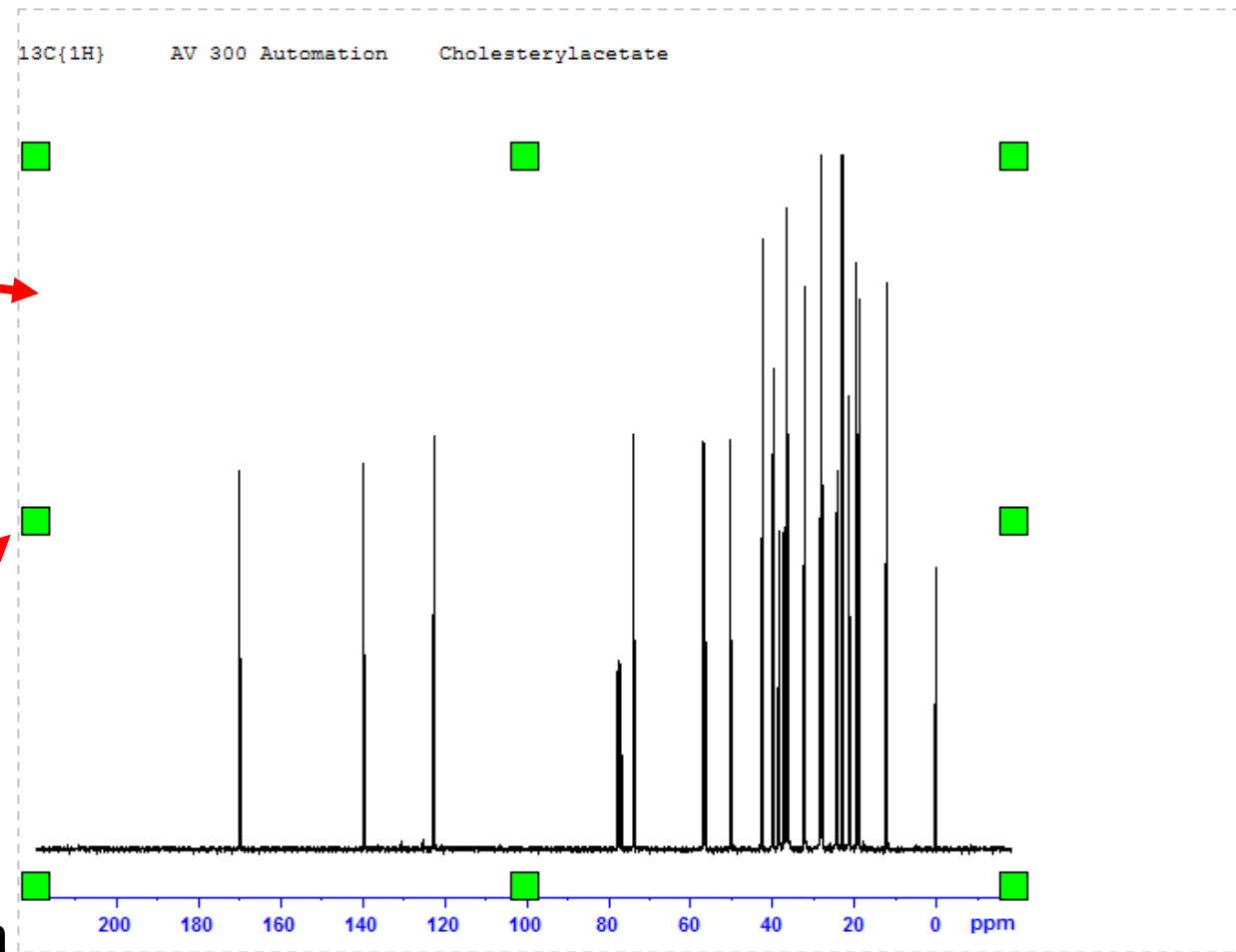
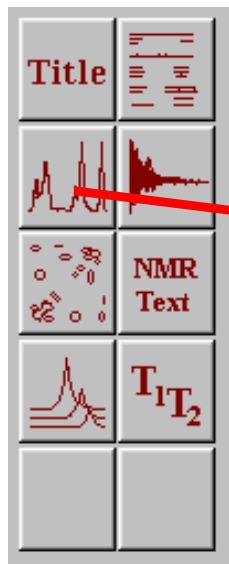
Make sure you hit apply before leaving!



Creating a new layout from scratch



- After you have the title where and how you want it click the spectra button, insert the spectra where you want it on the plot window



You can use the handles to re-size and move the spectra

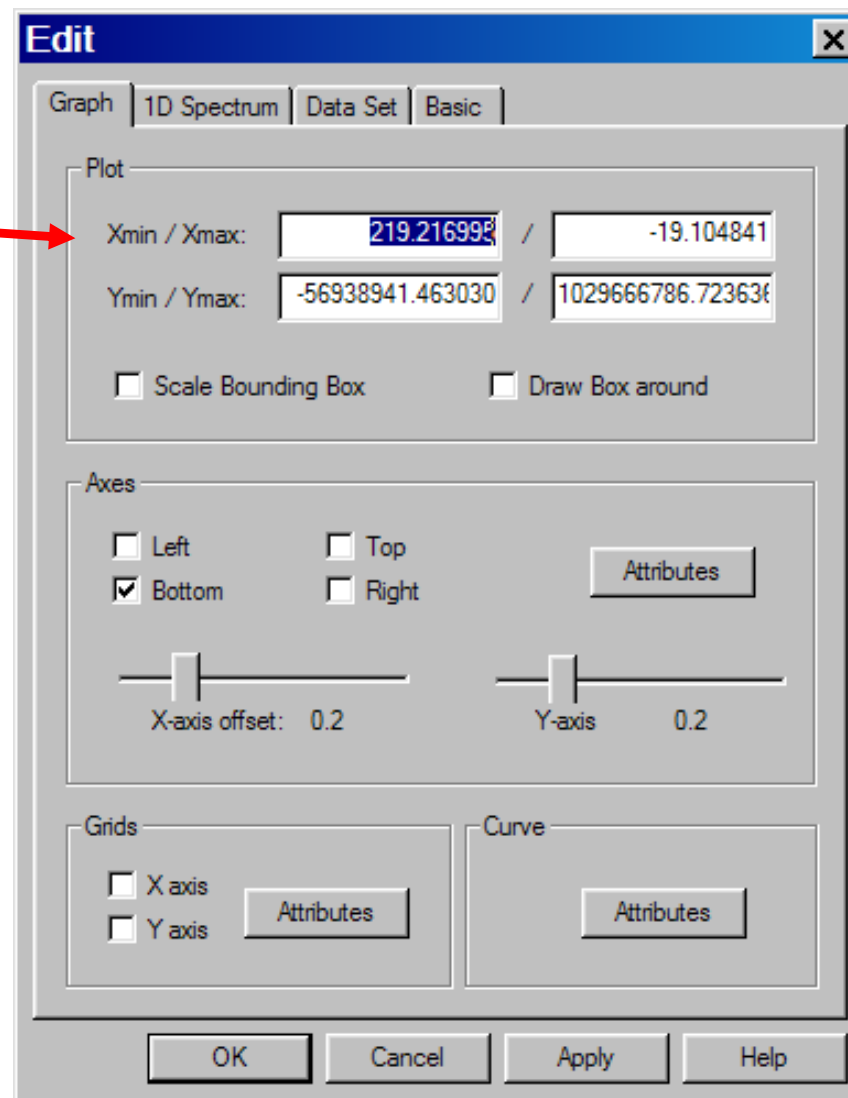


Creating a new layout from scratch



- You can change the plot limits here
- Set the axes and the attributes, offset etc. from here.

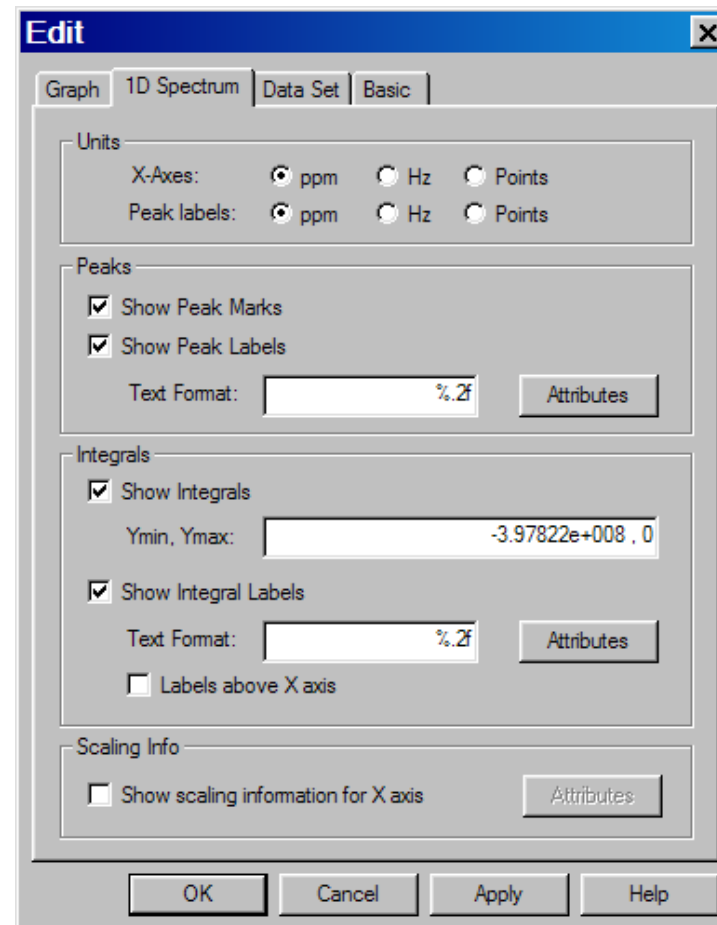
Plot limits in hertz
Or PPM



Creating a new layout from scratch



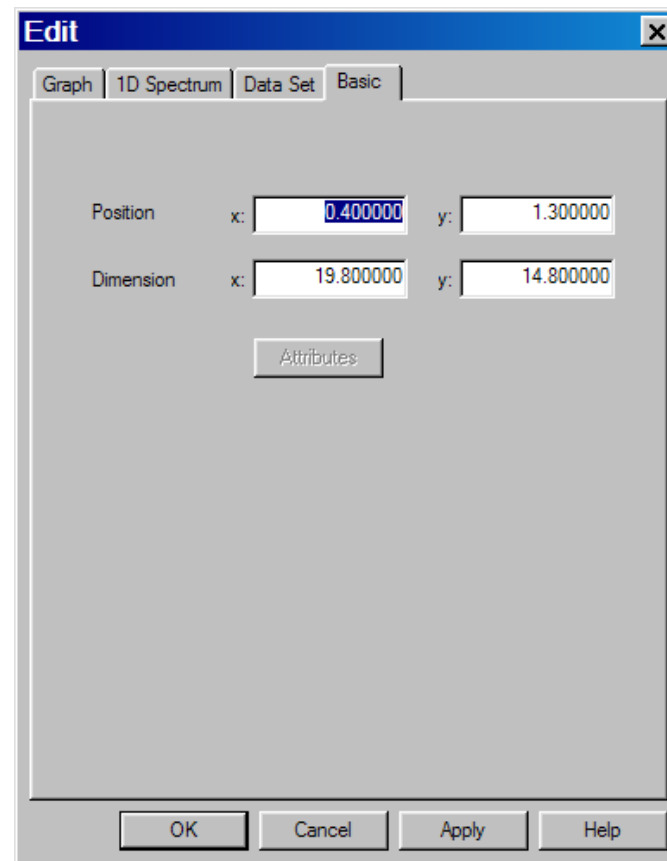
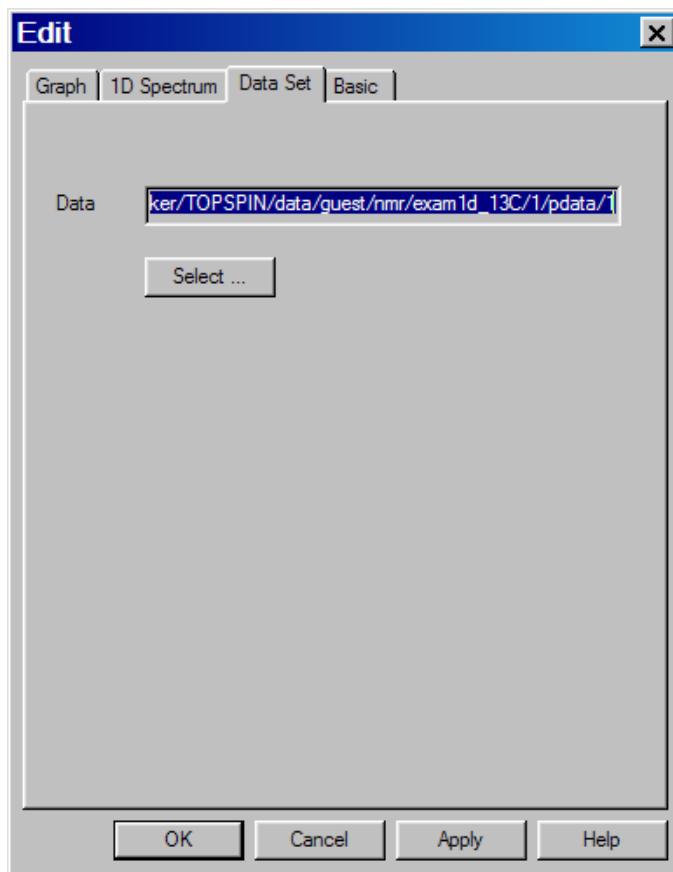
- Set the axis for PPM or Hertz here
- Add peak picking and peak marks
- Add integrals and integral labels here also



Creating a new layout from scratch



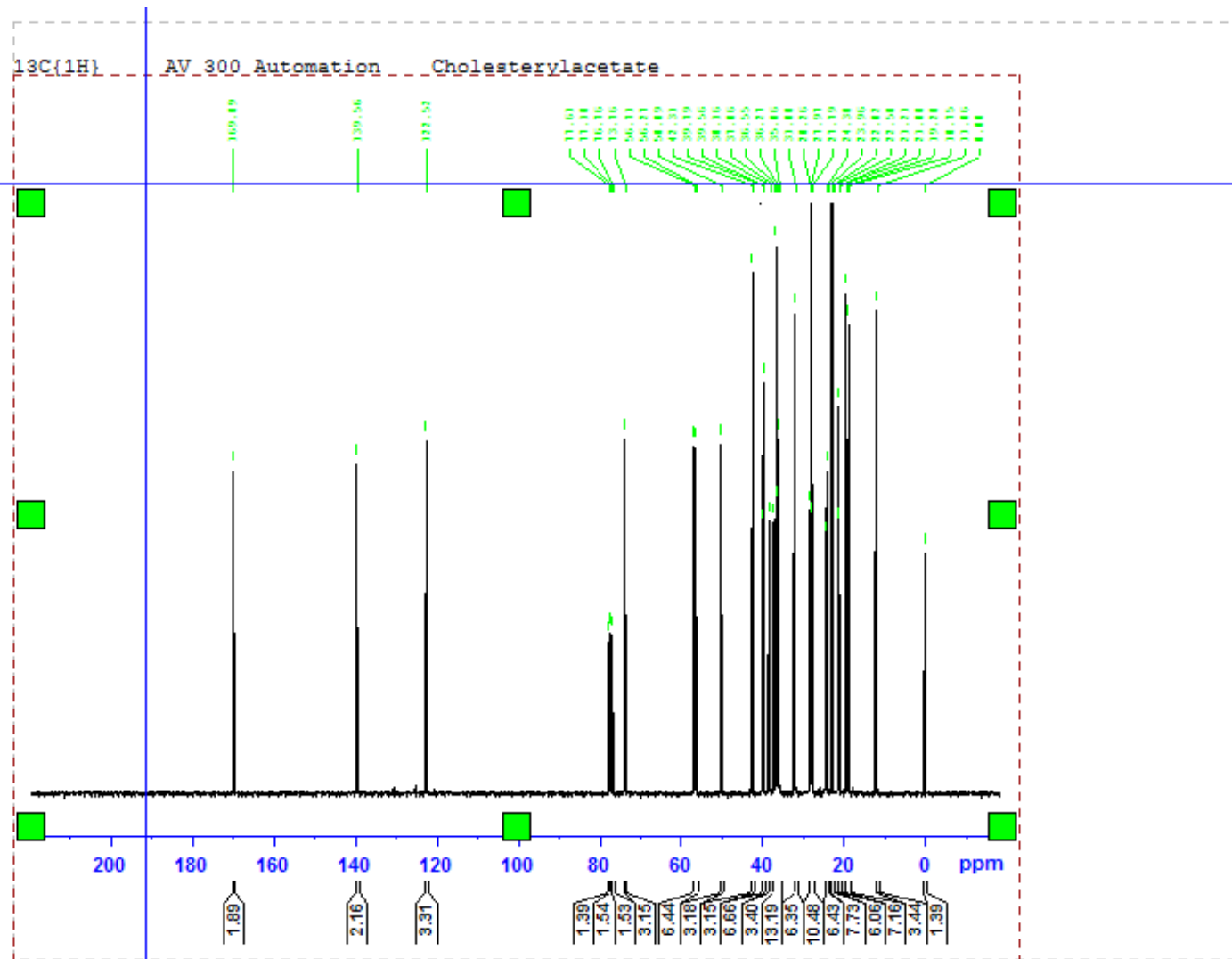
- From here you can choose the data set
- And the position and dimension of the spectra window



Creating a new layout from scratch



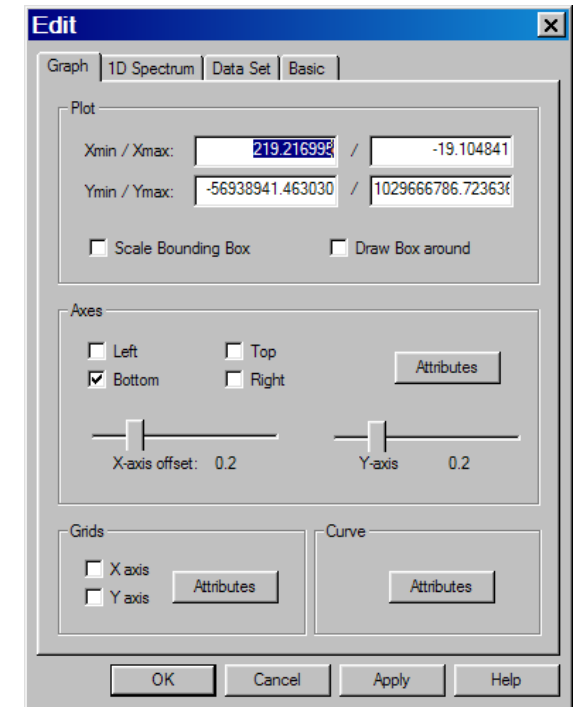
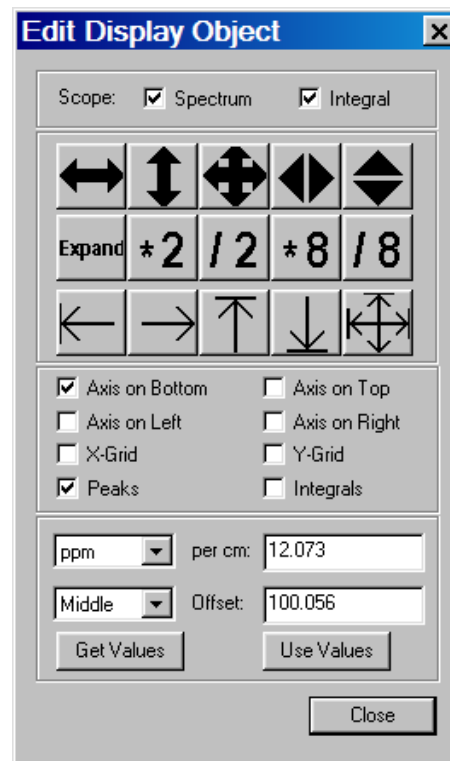
- The blue “cross hairs” indicate the cursor position



Creating a new layout from scratch



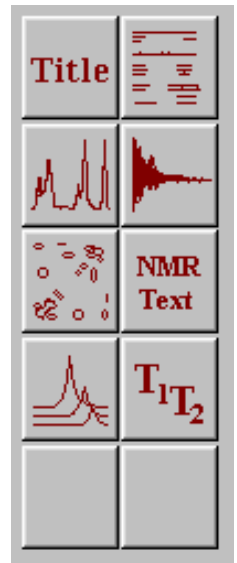
- If you do a right click on the spectra window you will get this menu
- From here you can choose the “Edit Panel”
- Or the “Edit Display Object Panel”



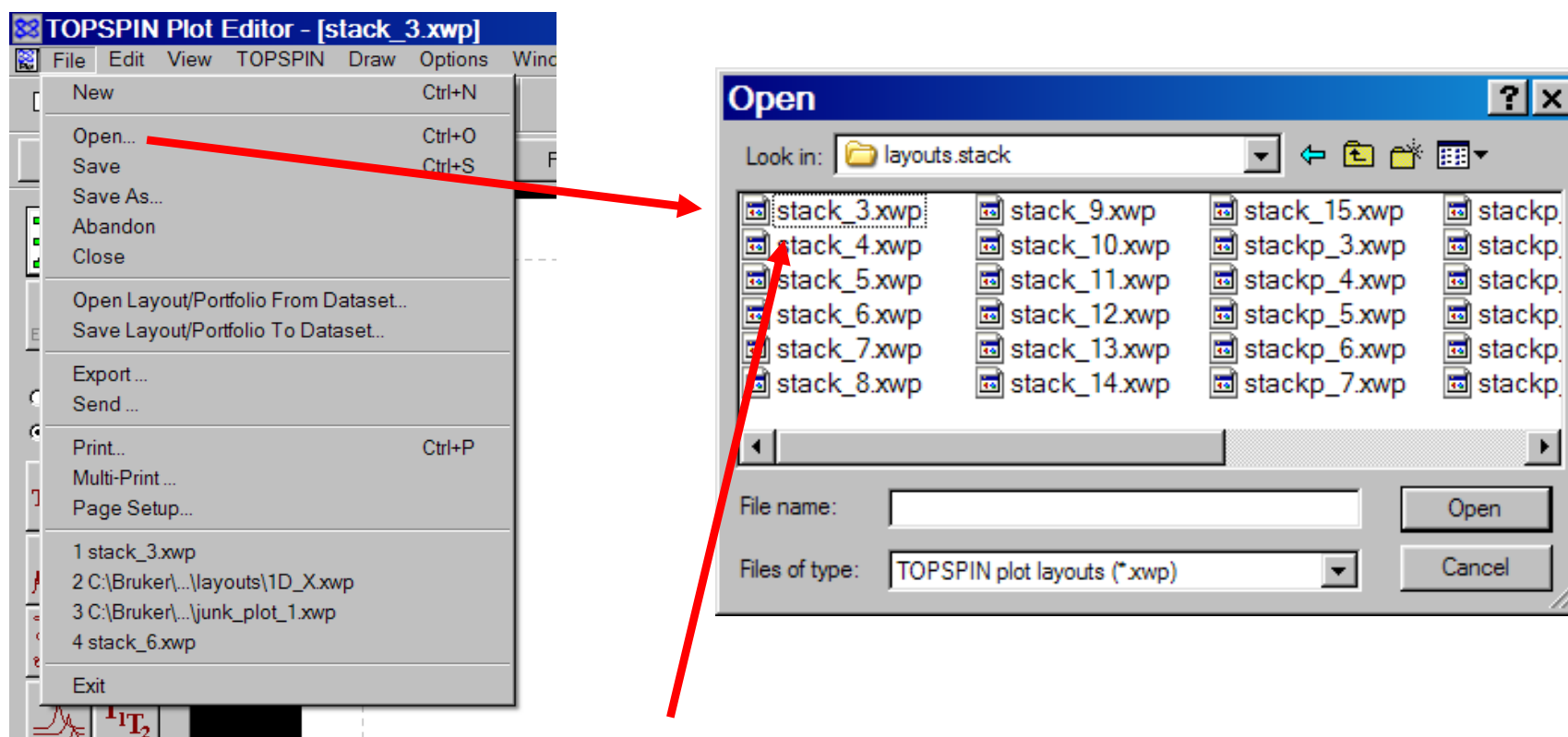
Creating a new layout



- The same principles apply to the parameters or NMR text or any other object you add to the plot layout.
- The same things apply to 2D spectra also
- And you can do the same sort of things for stacked plots.
- And of T1/T2 plots work exactly the same.

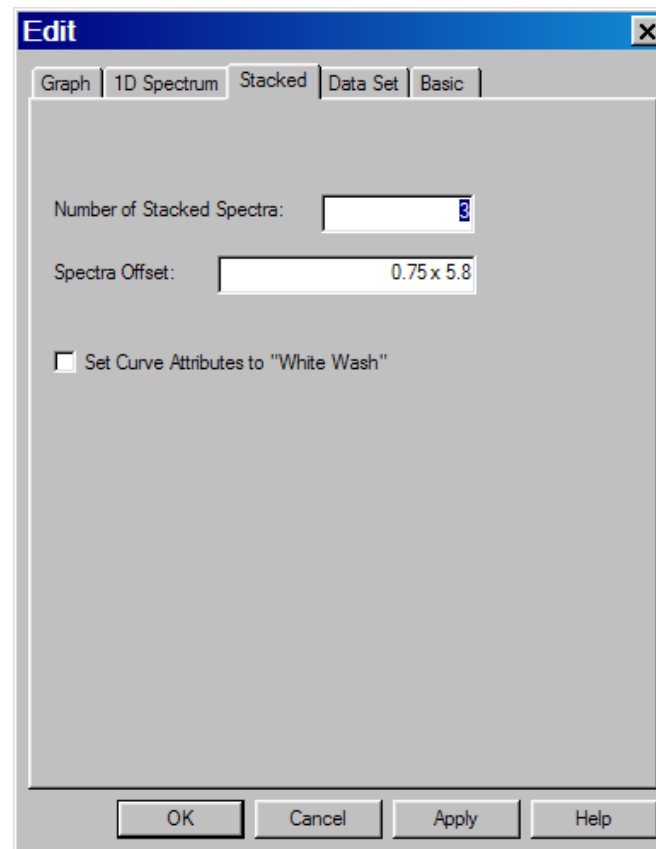


- Go to the first data set of the series of sets you want to plot together, its easier if they are increasing expno's or procno's
- Click file and then open and navigate to the stacked plot directory



Choose the layout with the most appropriate number of spectra
3 in this case

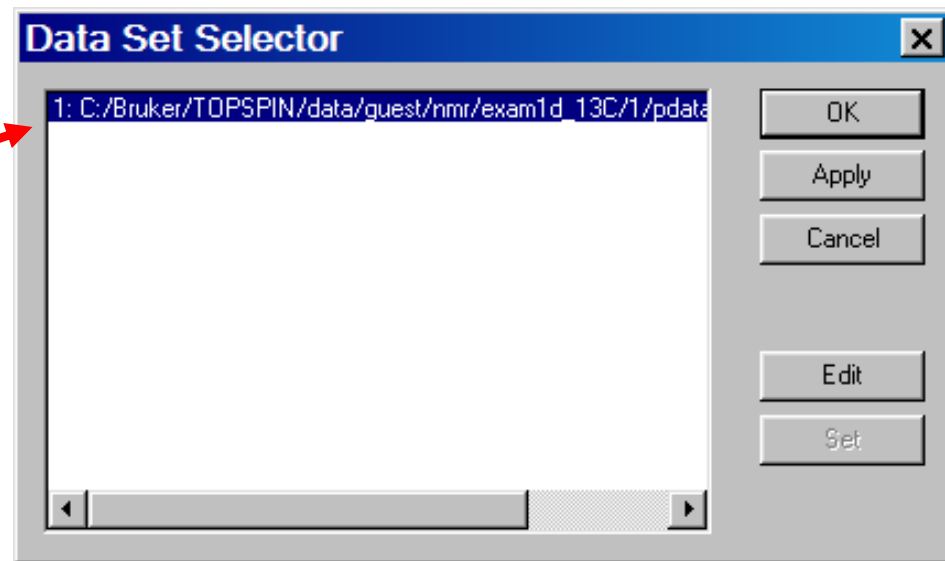
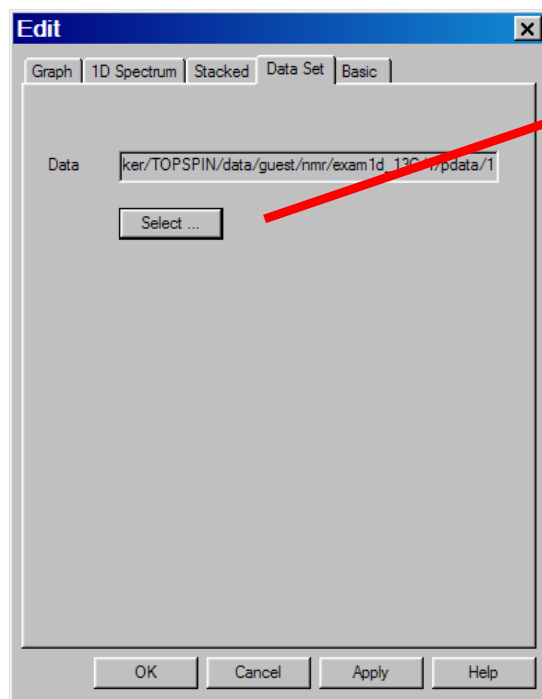
- The right click and choose “edit” navigate to the “stacked” tab
- You can set the X and Y offset if you want and the number of spectra to be used



Stacked Plots



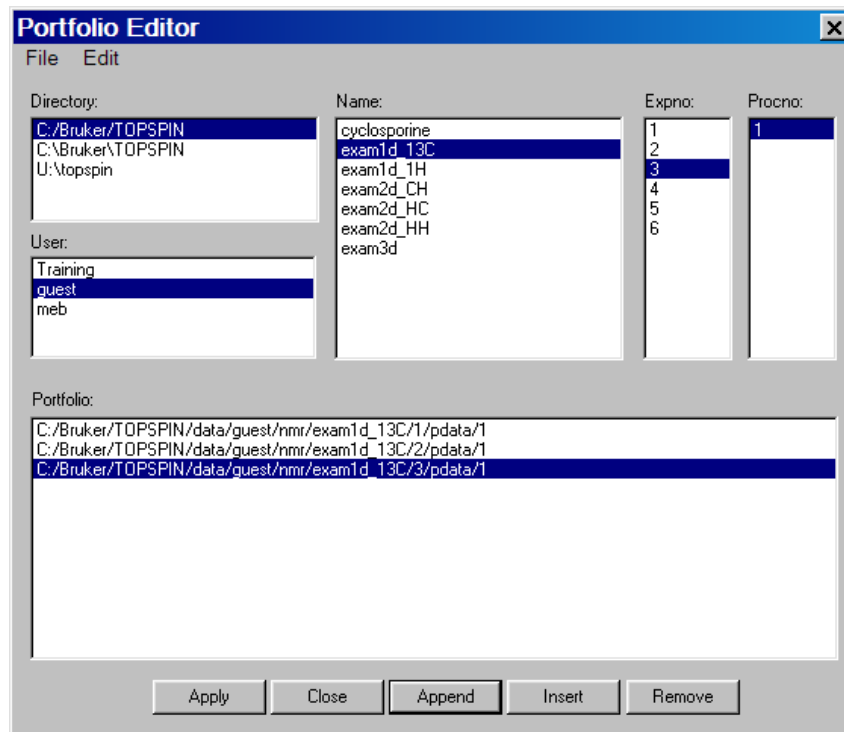
- Navigate to the “Data Set” tab, then click “Select”
- The data set selector will open up
- The click “edit”



Stacked Plots



- The portfolio edit should open up in the correct data set if not, navigate to the correct one
- Choose which data set you want and click “append” after each one



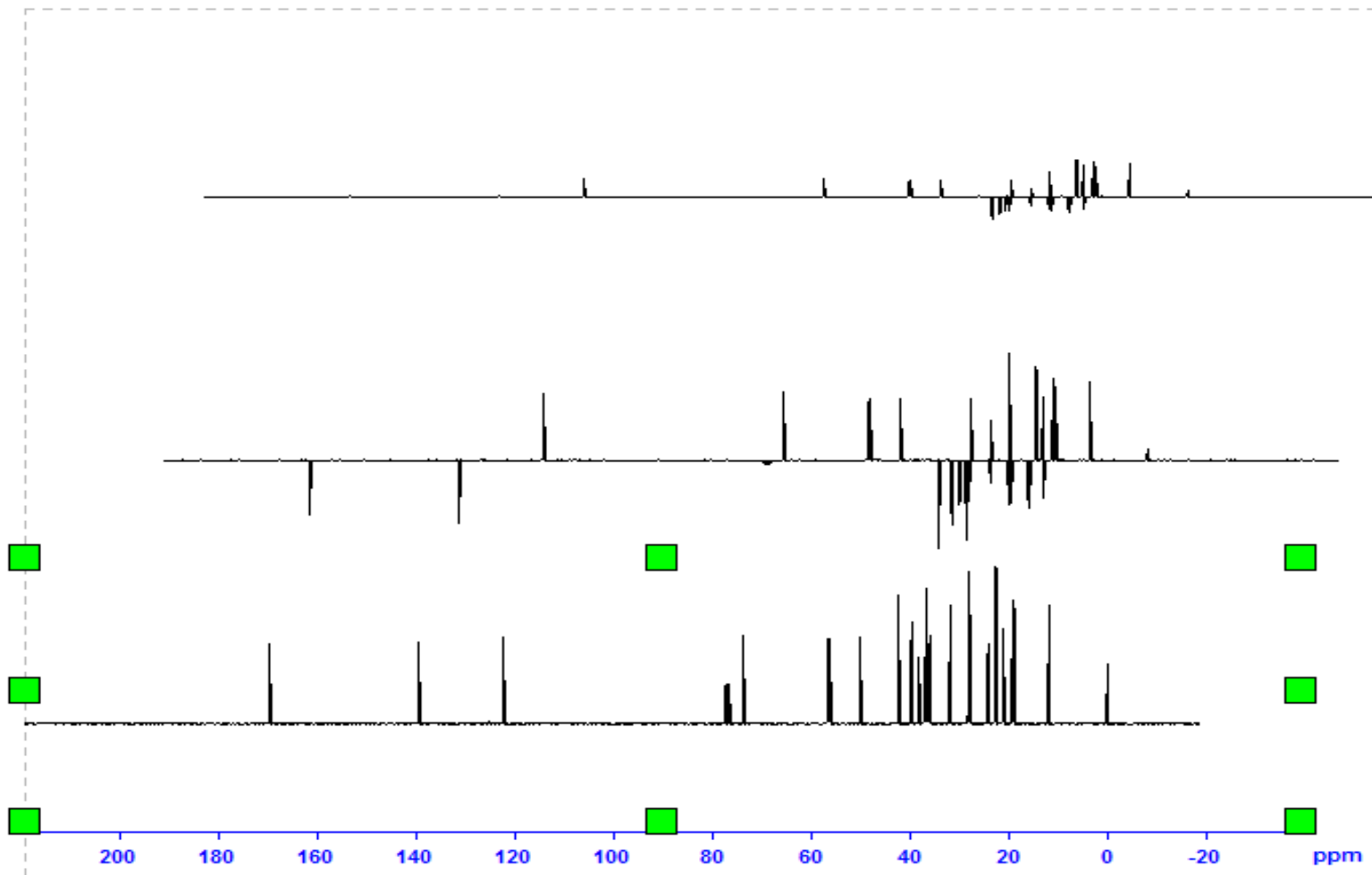
Then click “apply” and “apply” in the “data set selector”



Stacked Plots

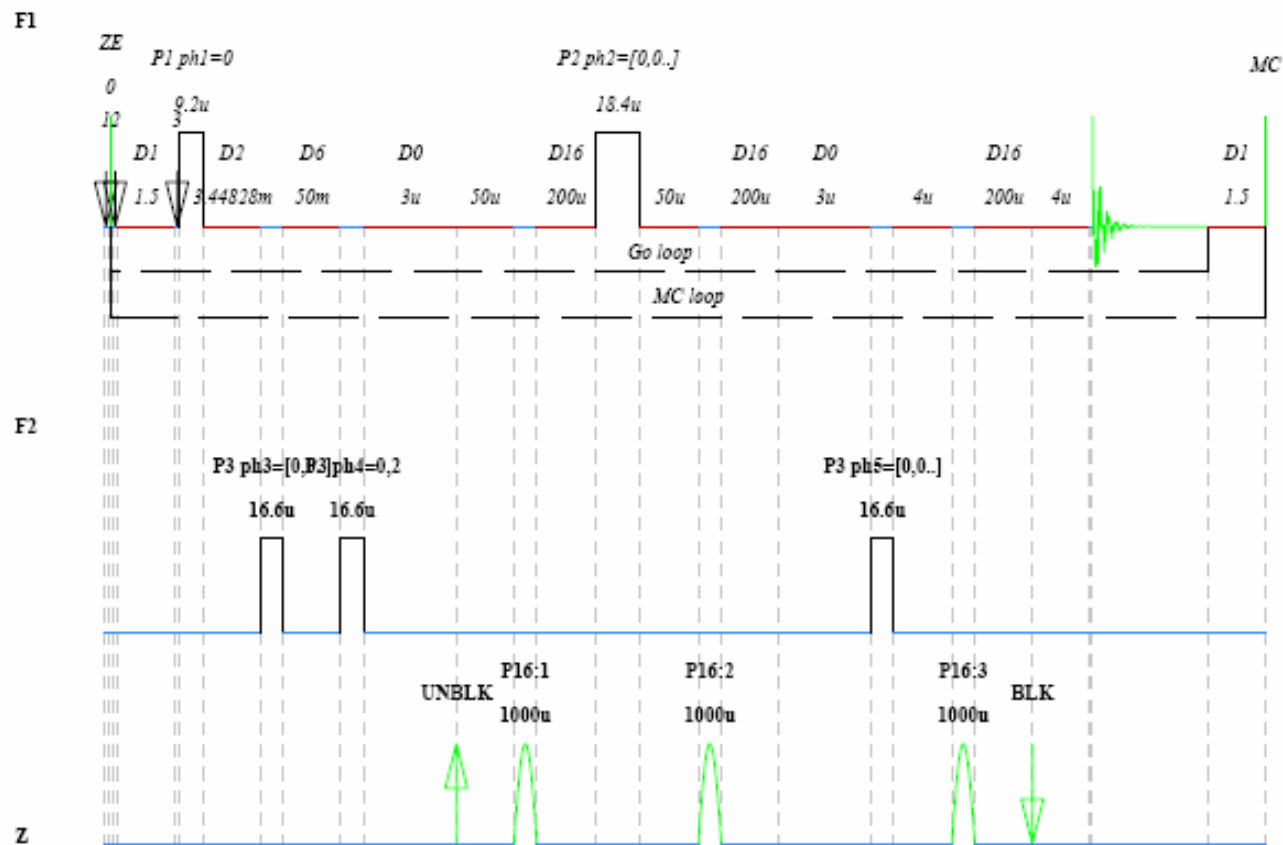


- Adjust the handles, and amplitude of the spectra
- Add a title or parameters or offsets

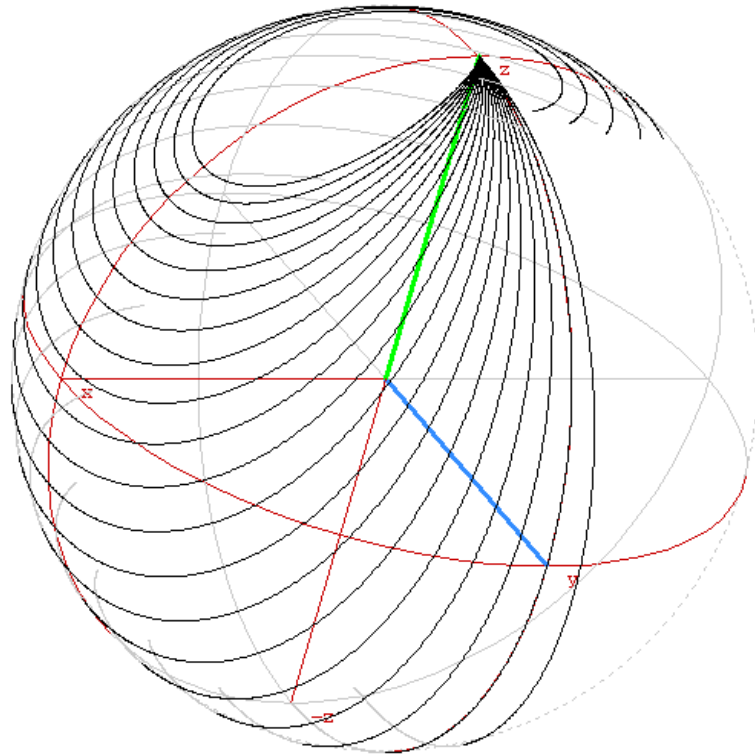


- Showpp

C:\Bruker\TOPSPIN\exp\stan\nmr\lists\pp\hmbcgp1pndqf



- Bloch Simulator from Shape tool and NMRSIM





• Tip of the day

• Complete manual

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- XWINPLOT Manual
- TopSpin Processing Reference Guide
- TopSpin Automation Reference Guide