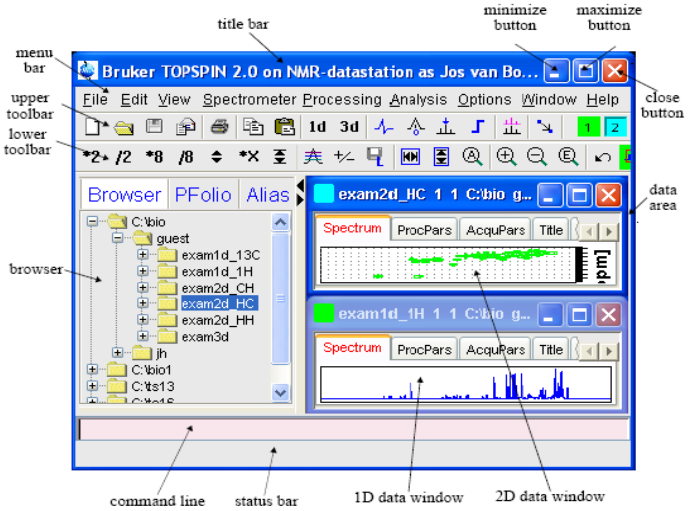
TOPSPIN INSTRUCTIONS

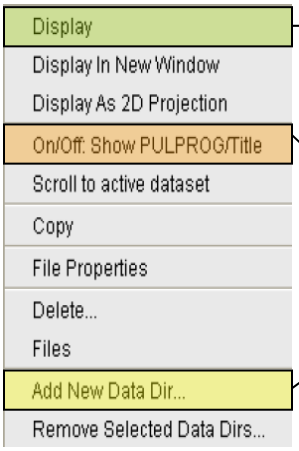
1. **How to start TOPSPIN?**
2. **The TOPSPIN window**
3. **How to open an old dataset?**
4. **How to create a new dataset?**
5. **How to lock and shim?**
6. **How to acquire FID signal and modify acquisition parameters?**
7. **How to process 1D spectrum and modify process parameters?**
8. **How to process a 2D NMR spectrum?**
9. **How to display multiple 1D /2D spectra?**
10. **How to perform multiplet analysis?**

1. **How to start TOPSPIN**
   a. Login using your group ID and password
   b. Double click TOPSPIN icon to start TOPSPIN software

2. **This is the TOPSPIN window:**



3. **How to open an old dataset:**



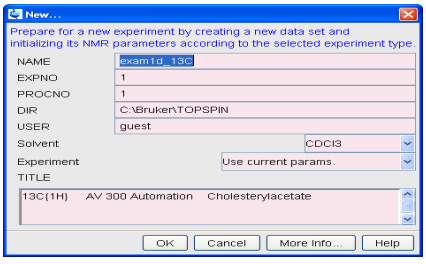
The popup Menu

a) In the Browser window, locate your data, right-click a dataset name, and choose **Display** in the popup menu
b) Or, click a dataset name and hold, then drag it to the data window

The display of title and pulse in the Browser window can be switched on or off by right-clicking anywhere in the Browser window and selecting **On/Off Show PULPROG/Title** in the popup menu

If you have a top level data directory which is not shown in the Browser window (such as D:\ rather then C:\Bruker\Topspin), you can right-click anywhere in the Browser window, and choose **Add New Data Dir** in the popup menu

4. **How to create a new dataset:**
   a. Click **File → New; OR** click the button in the upper toolbar; **OR** type **edc** in the command line
   In the popup dialog box:



b. Specify name, expno, procno, dir and user
c. Click the down-arrow of the **Solvent** box to choose a solvent from the list
d. In **Experiment** box, select **Use current params**
e. Type the dataset title in the **TITLE** box
f. Type **rpar** in the command line to choose a parameter set from the list
For example:
Parameter set name: proton experiment =1_protonstd
Carbon experiment = 1_carbonstd

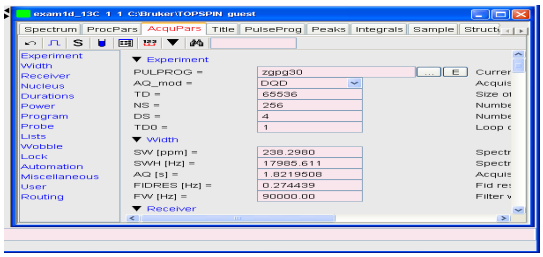
5. How to lock and shim?

a. Type **lockdisp** in the command line OR click the  button in the upper tool menu to open the lock display window
b. Type **lopo** in the command line and select a solvent from the popup list,
c. On the BSMS keyboard:
- Press the **FIELD** button, and move the lock signal to the center of the lock display window
- Press the **PHASE** button, and adjust the lock signal in-phase
- Press the X (or X+Z0), the Y (or Y+Z0), the Z1 (or onaxis+Z1), OR Z2 (or onaxis+Z2) shim buttons, and optimize these shims iteratively to make lock-ring-down pattern observable
- Press the **LOCK** button
- Press the **SPIN** button (for 2D NMR experiments, spin has to be off), and wait for spin indicator to stop blinking
- Optimize Z1 and Z2 shim iteratively by turning the whirl and observing the lock signal level moving up as high as we can
- If necessary, press the **LOCK GAIN** button to decrease/increase lock gain
- Then press the **STDBY** button

d. If shim is messed up, type **rsh currshim** in the command line to read most current shim file in
e. Autoshim: type **topshim**. In the popup window, choose **1D** shim and turn **Z6** off, then click **start** **(only for TOPSPIN 2.0 and newer)**

6. How to acquire FID signal and modify acquisition parameters

a. Type **rga** in the command line, then
b. Type **zg** in the command line
c. Sometimes it is necessary to modify acquisition parameters
- Modify acquisition parameters
  - Clicking **AcquPars** tab in the tab bar of the data window
  - **OR** type **eda** in the command line
- Modify pulse program parameters
  - Click the  button in the toolbar
  - **OR** type **ased** in the command line



Other buttons in AcquPars toolbar

 Set probehead/solvent dependant parameters [getprosol]

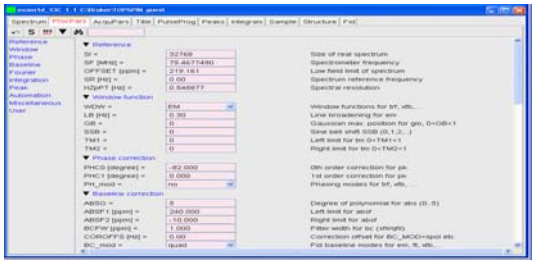
 Set nuclei and routing [edasp]

 Change data dimensionality, which will changes the number of parameter columns and value of the acquisition parameter **PARMODE**

7. How to process 1D spectrum and modify process parameters

a. Modify process parameters

- Click **ProcPars** tab in the tab bar of the data window
- **OR** type **edp** in the command line



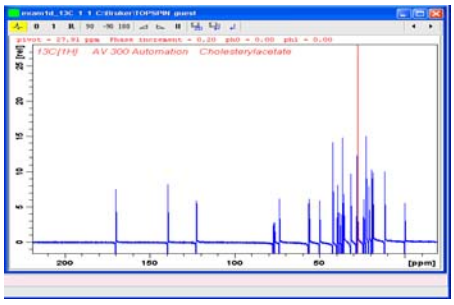
b. Fourier Transform:

- Type **efp** in the command line

c. Phase correction:

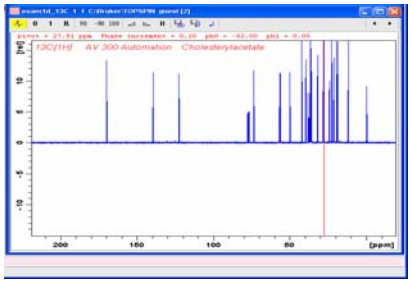
➢ Manual method

- Click phase correction  button in the upper toolbar
- The Tab bar of the active data window will be replaced by the following toolbar



- Left-click-hold the  button and move the mouse until the reference peak is exactly in absorption mode

- Left-click-hold the button and move the mouse until the entire spectrum is exactly in absorption mode
- Click the  button to save and execute the phase correction

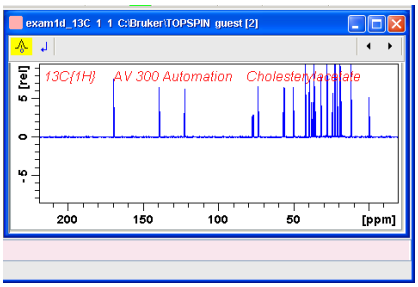


➢ Automatic method:

- Type **apk** in the command line to execute automatic phase correction

d. <u>Chemical shift calibration</u>

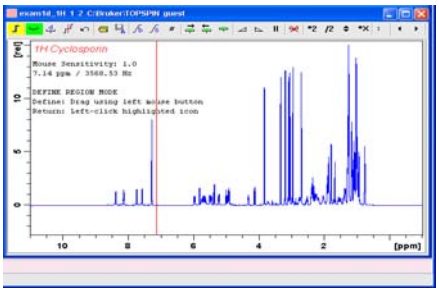
- Click the  button in the upper toolbar, and the Tab bar of the active data window will be replaced by the following toolbar



- Position the red cursor line at the reference peak
- Left-click at that position and enter the chemical shift of the reference peak at the popup dialog box

e. <u>Integration</u>

- Click the  button in the upper toolbar, and the Tab bar of the active data window will be replaced by the following toolbar



- Define integral regions: <u>Note: the active button is highlighted in green</u>

: define integral region interactively

: define integral region via dialog

: cut integral region

- When this button is highlighted in green, put the red cursor line at one edge of a peak or multiplet, then left-click-hold and drag the cursor line to the other edge of the peak or multiplet.
- Use or buttons to modify the integral region.

- Select a single integral region
  - Right-click in the integral region you want to select
  - Choose **Select/Deselect** from the popup menu

: select the next integral region

: select the previous integral region

: select all integrals

: delete selected integral region from the display

- Calibrate integrals
  - Right-click in the reference integral region
  - Choose **Calibrate** from the popup menu
  - Enter the desired value for the reference integral and click **OK**
- Other buttons:

*2 /2 *X : Scale selected integrals

: Move all the integrals up and down

: Change the mouse sensitivity

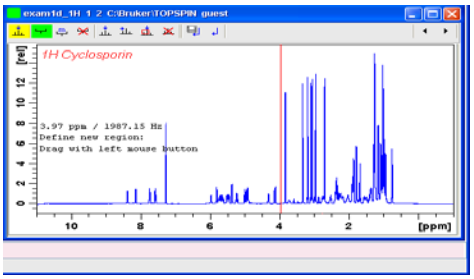
: Perform interactive Bias and Slope correction

: Save integrals and return

: Return, discarding any changes

f. Peak picking:

- Click the button in the upper toolbar, and the Tab bar of the active data window will be replaced by a following toolbar



- Define peak picking regions: Note: the active button is highlighted in green

 : Define peak picking range

 : Change peak picking range

 : delete all peak picking regions

When the  button is green, put the cursor at the upper-left corner of a peak picking range, then left-click-hold and drag the cursor to the low-right corner of the range. You can use this  button to modify the peak picking range.

- Other buttons in the toolbar

 : Define peaks manually

 : Define peaks semi-automatically

 : Delete all peaks

 : Save the peak region and peak list and return

 : Return, discarding any changes

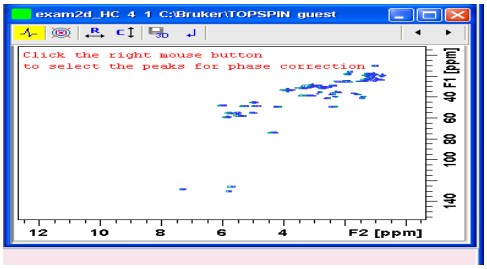
8. How to process a 2D NMR spectrum

a. Fourier transform:

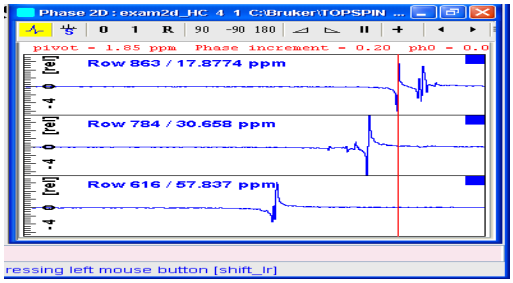
- Type **xfb** in the command line

b. Phase correction:

- Click phase correction  button in upper toolbar
- The Tab bar of the active data window will be replaced by a following toolbar



- Right-click and choose **add** in the popup menu to select three peaks at different parts the spectrum
- Click the  button to display rows of selected peaks under phase row mode



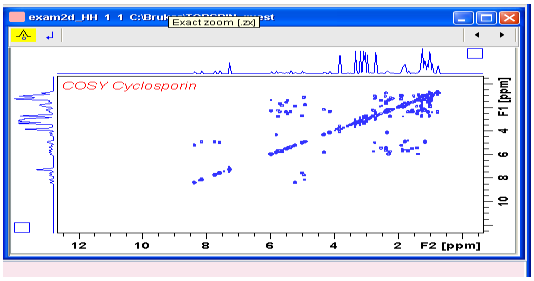
- Perform phase correction by click-holding the 0 button and 1 to make all peaks in three rows in absorption mode
- Click the button to execute, save and return
- Click the button to display columns of selected peaks under phase column mode
- Perform phase correction by click-holding the 0 button and 1 to make all peaks in three rows in absorption mode
- Click the button to execute, save and return
- Other buttons in the tool bar

  + −: show next or previous row/column

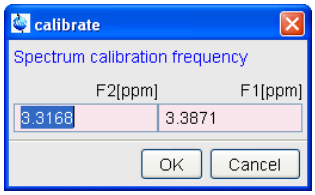
  : arrange row/column horizontally or vertically or vertically in a split window
- Click the button to return from 2D phase mode

c. 2D chemical shift calibration

- Click the button in the upper toolbar, and the Tab bar of the active data window will be replaced by the following toolbar



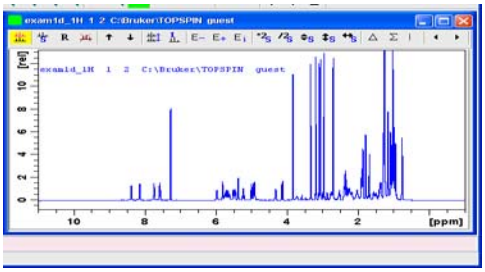
- Left-click at the reference peak in the data window, the dialog box will appear



- Enter the F2 and F1 chemical shifts you want to assign to the reference peak
- Click **ok**

9. How to display multiple 1D /2D spectra

a. Click the button in the upper toolbar, and the Tab bar of the active data window will be replaced by a following toolbar



b. Add a dataset:
   - Enter **re** and specify the additional dataset
   - **OR** left-click-hold the dataset in the browser and drag it into the data window
   - **OR** right-click the dataset in the browser and choose **Display** from the popup menu

c. Select/deselect the datasets
   - The browser is split in two parts and in the lower part you can click one dataset to select it
   - **OR** click in the corresponding area in the data window
   - Click the  button to deselect all the datasets

d. Remove a dataset:
   - Select a dataset you want to remove as step c
   - Click the  button to remove it

e. Other buttons:

 : Toggle between superimposed and stacked display

 : Switch on/off display of datapaths and scaling factors

 : Show the difference between the first and the sum of the other datasets

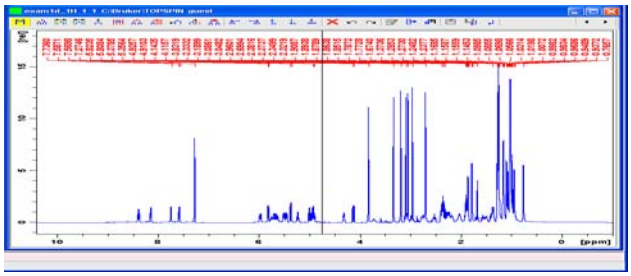
 : Show the sum of all datasets in the multiple display window

10. How to perform multiplet analysis?

a. Perform Peak-picking as Procedure 7(f) (you might need use manual peak-picking  button to pick all peaks)

b. In Menu bar, click **Analysis → Structure Analysis → Multiplet Definition [mana]**

c. The Tab bar of the active data window will be replaced by the following toolbar

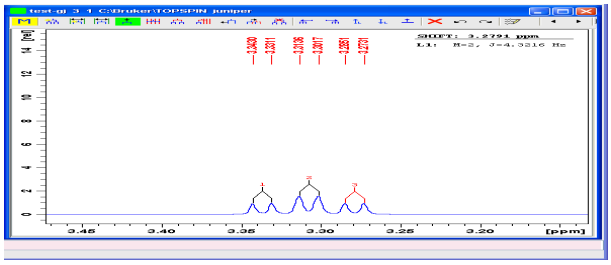


d. Automatically define multiplet

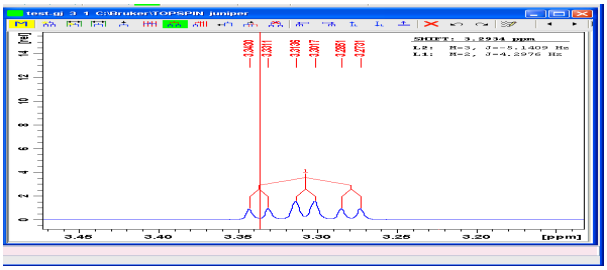
- Click the  button in toolbar to define multiplet in whole sweep width automatically
- Click the  button in toolbar; left-click-hold mouse and drag to define the region, multiplet in this region will be defined automatically.

e. Manually define multiplet

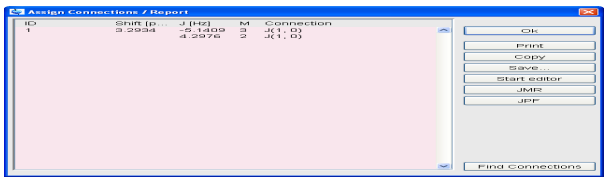
- Click the  button in the toolbar
- Put red cursor line on a peak and left-click to select, repeat to select other peaks, then right-click and select **Define Multiplet** in the popup menu



- Click the  button in the toolbar to couple existing multiplets
  - Left-click to select each multiplet
  - Right-click and select **Define Multiplet** in the popup menu



  - The coupling constants will be listed in the up-right corner of the window
  - Click the  button in the toolbar, the resulting report will show in popup window

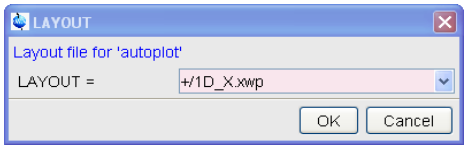


f. Click the  button in the toolbar, and save multiplet assignment and return

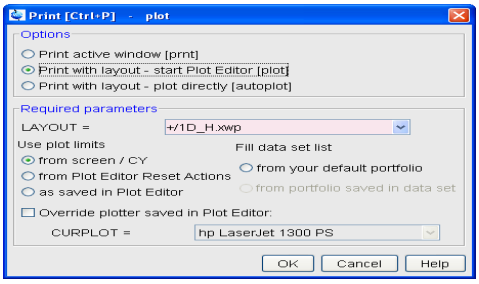
TOPSPIN PLOT EDITOR INSTRUCTIONS

1. **How to use TOPSPIN PLOT EDITOR to plot a spectrum?**
2. **How to plot several 1D spectra in stack mode in Topspin Plot Editor?**
3. **How to export a spectrum as PDF or PNG or EMF format file so you can insert it to your report/thesis?**

1. **How to use TOPSPIN Plot Editor to plot a spectrum**
   a. Type **Layout** in the command line to select the desired layout by clicking down-arrow button of LAYOUT box , then type **plot** in the command line and TOPSPIN Plot Editor will start



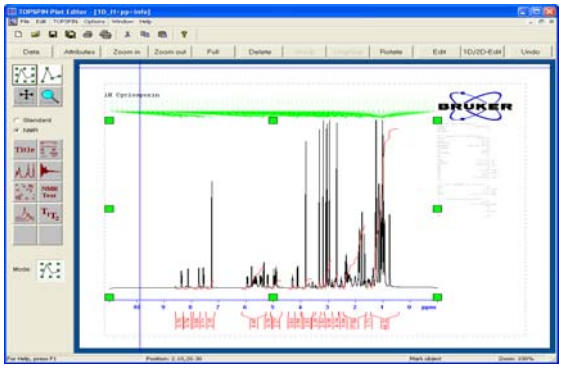
   b. OR **File→Print**, and select **Print with layout-start Plot Editor** in the popup window



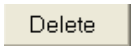
   In the required parameters, select the desired layout by clicking down-arrow button in **LAYOUT** box. After clicking **OK** button, the TOPSPIN Plot Editor will start

   The layout can be specified by using one of the following abbreviations:
   +: the standard layout directory: ../topspin/plot/layout
   ~: the user home directory
   #: current processed data directory

   c. Preview the current plot layout and plot (Click **File→ Print**)



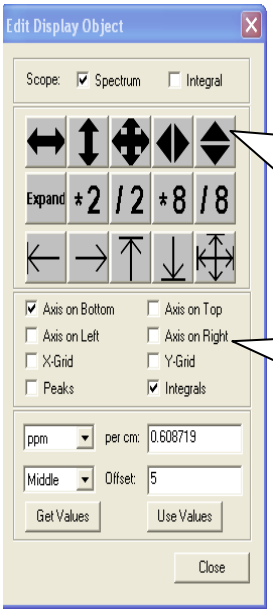
   d. Modify the plot layout
   <u>Move, resize and delete an object (spectrum, title, parameter or logo):</u>

   - Mark an object by clicking the  button and then clicking the object
   - Click-hold the object and move the mouse to move the object
   - Click-hold one of the green markers and move the mouse to resize the object
   - Click the 

button in command bar to delete the object

Modify the spectrum

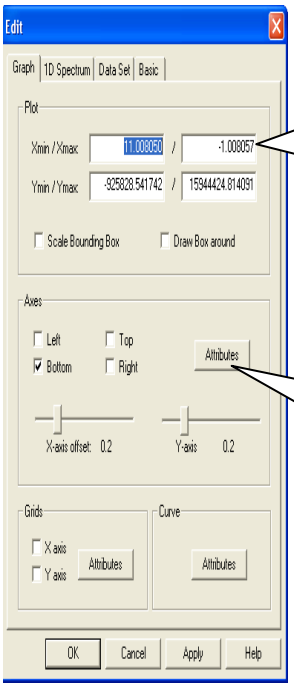
- Mark the spectrum object and click the 1D/2D-Edit button in the command bar



All buttons, which have same functions as in TOPSPIN, are active for spectrum or integral or both by setting the scope

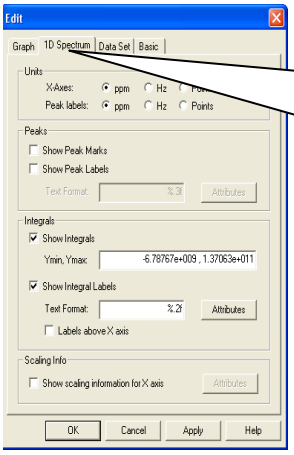
Checking the various buttons in this part to change the spectrum object

- Mark the spectrum object and click the Edit button in the command bar



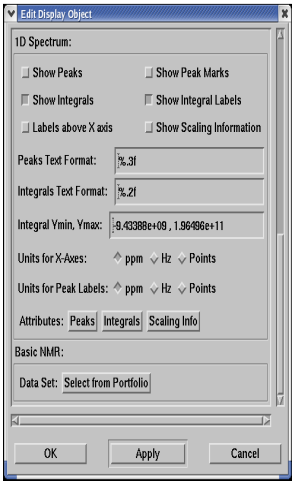
Under **Graph** tab, you can expand a spectrum by entering the exact limits of a certain spectral region

You can modify the attributes of Axes ad Curve

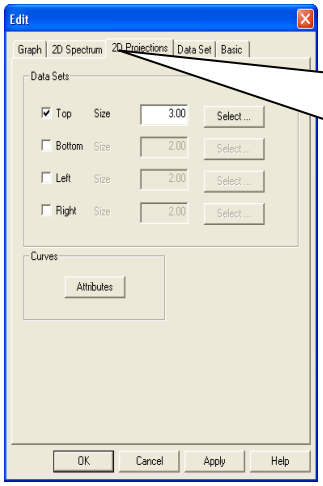


Under **1D Spectrum** tab, you can modify the units of axes and peak (ppm or Hz), attributes of peak labels and integral labels

Under Linux, all parts (Graph, 1D spectrum. DataSet and Basic) are shown simultaneously



If the spectrum is a 2D spectrum, the popup window is



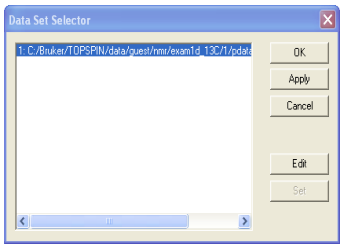
Under **2D Projections** tab, you can define the projections on F1 (left/right) and F2 (top/bottom) dimensions from 1D datasets

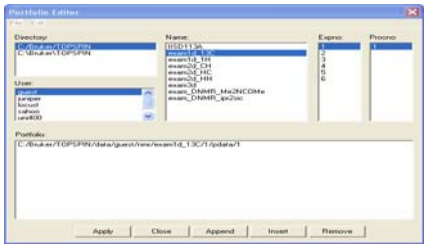
Modify parameters and title

- Right-click the object and choose corresponding buttons in the popup menu to modify the object

2. How to plot several 1D spectra in stack mode in Topspin Plot Editor

a. Click the Data button in the command bar, click **Edit** button in the popup **Data Set Selector** window. The **Portfolio Editor** window will pop up





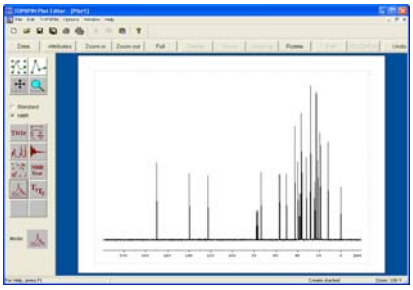
b. In **Portfolio Editor** window, choose right **Directory** and **User**, all datasets will show up.

c. Choose the first spectrum by clicking the respective entries in the sections **Name, Expno** and **Procno.** Then click the **Append** button.

d. Repeat step **c** for the rest of spectra, then click **Apply** back to **Data Set Selector** window, click **OK**

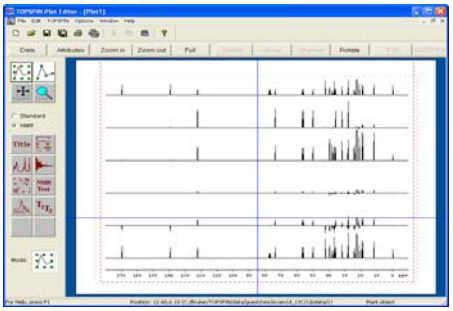
e. In **TOPSPIN Plot Editor**, click **File → New** to open a new layout

f. Click the  button, click-hold left mouse button and drag in the layout area

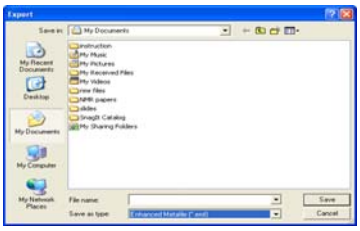


g. Mark the spectrum by click the  button, then click Edit button in command bar. The popup window is

h. Click **Stacked** menu bar, fill the box. In Spectra Offset box, the first number is offset of X-axes, and the second number is offset of Y-axes. By adjusting these two offsets, you will get the desired layout

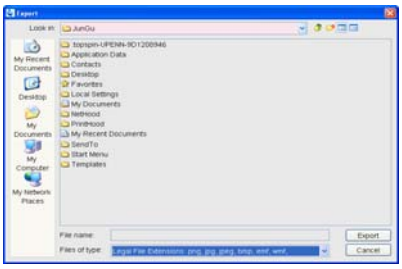


3. **How to export a spectrum as PDF or PNG or EMF format file so you can insert it to your report/thesis?**
    a. <u>From Topspin Plot Editor</u>
        - A spectrum is appeared in the Plot Editor with desired layout
        - Click **File → Export**



        - In the box of **Save as type**, you can choose the type you want, and put filename in box of **File name**, then click **Save** button

    b. <u>From Topspin (**Note: No PDF type is available**)</u>
        - A spectrum is appeared in the data area
        - Click **File → Export**



        - Put filename in the **File name** box with extension
        - Click **Export** button