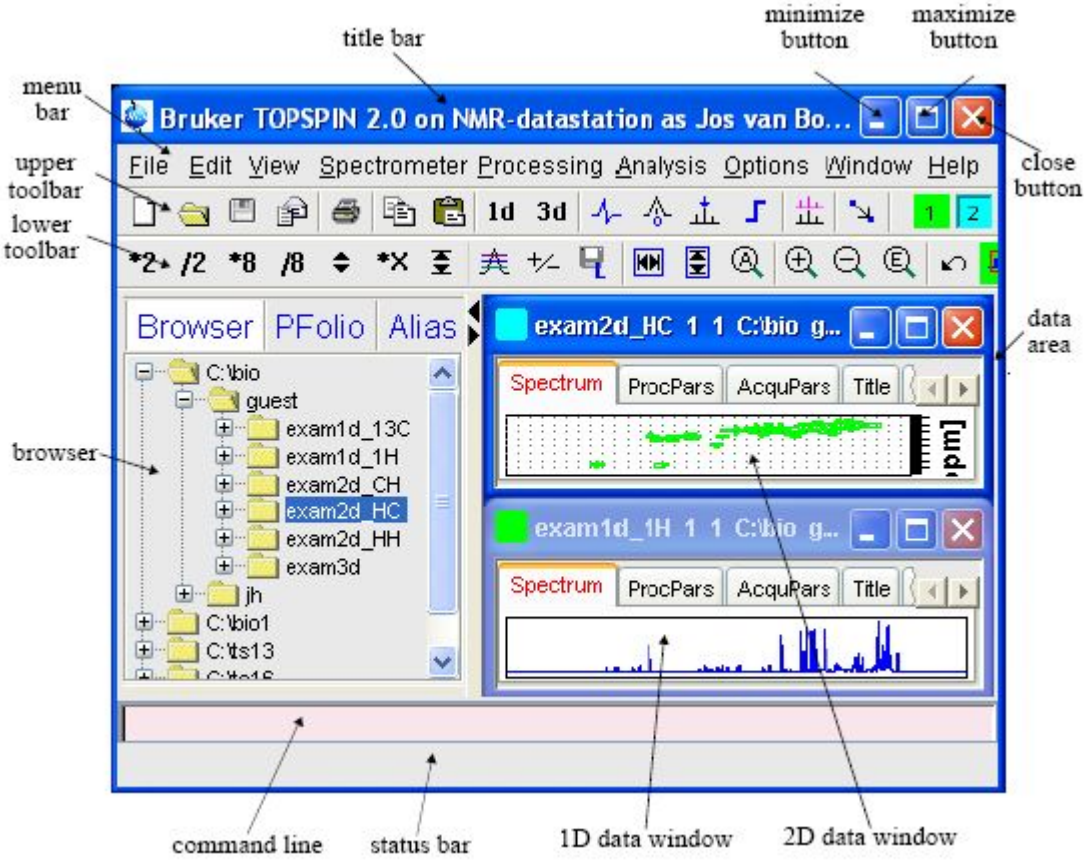
12/05/2013 **1D TOPSPIN INSTRUCTION**

1. Start TOPSPIN

a. Login using your group ID and password

b. Double click TOPSPIN icon to start TOPSPIN software

TOPSPIN window:



2. Insert the sample

blue spinner (temperature 15-35 ºC), white ceramic spinner (other temperature). Replace ONLY with the dummy standby sample ($CDCl_3$) into the magnet when you are done.

a. Type ej in the command line or Press the "lift on/off" (green = on) on BSMS Window, take the dummy sample out, wipe your tube, then insert the sample to Spinner into the depth measure then slide the tube down to the bottom.

b. Type **ej** in the command line or Press the "lift on/off" (green = on) on BSMS Window

Make sure your NMR tube is supported by compressed air before releasing it.

c. Type **ij** in the command line or Press the "lift off" button (no light) on BSMS Window

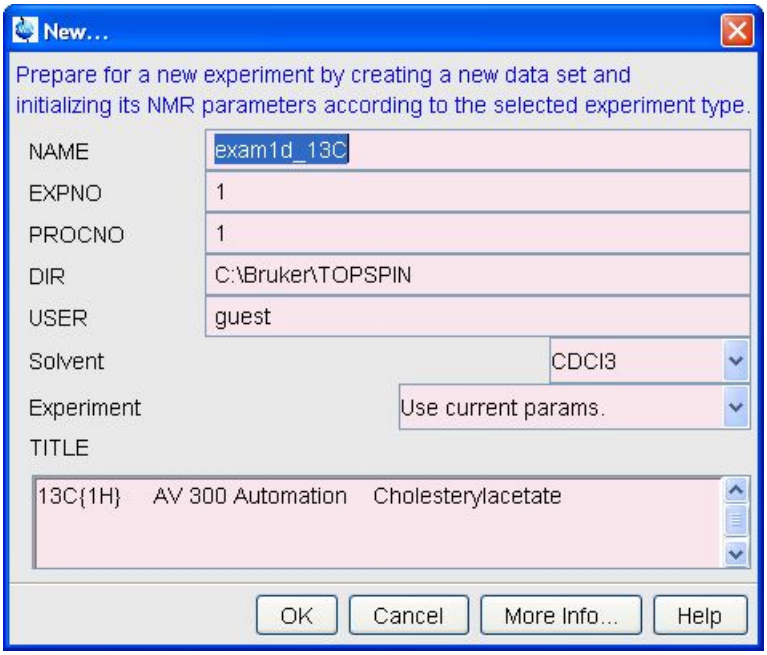
3. Open an old dataset

In the Browser window, locate your data, right-click a dataset name, and choose **Display** in the popup menu

4. Create a new dataset

a. 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. Tune, lock and shim

a. Type **atma** in the command line

b. Type **lock** in the command line and and select a solvent from the popup list

c. Type **topshim** in the command line

*type ro in the command line, then type 20 at rate to the popup box to turn the spin on (not recommended; definitely do not spin for 2D experiments)

d. If shim is messed up, type **rsh** in the command line to select most current shim file from the list, then type **topshim**.

6. 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

7. Process 1D spectrum

a. Type **efp** in the command line

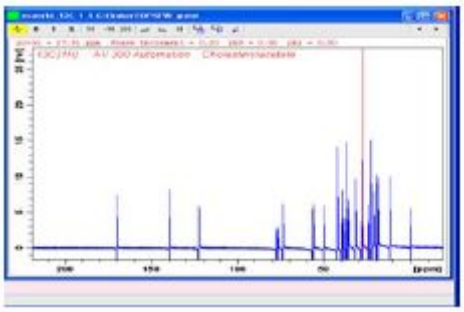
b. phase correction

Automatic method:

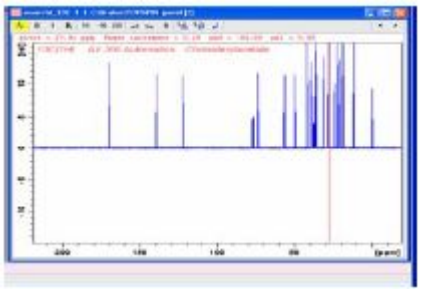
Type **apk** in the command line to execute automatic phase correction

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

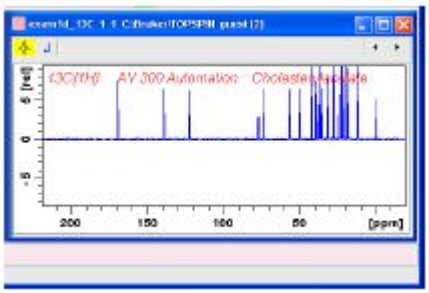


- Left-click-hold the 0 button and move the mouse until the reference peak is exactly in absorption mode
- Left-click-hold the 1 button and move the mouse until the entire spectrum is exactly in absorption mode
- Click the button to save and execute the phase correction



c. Chemical shift calibration

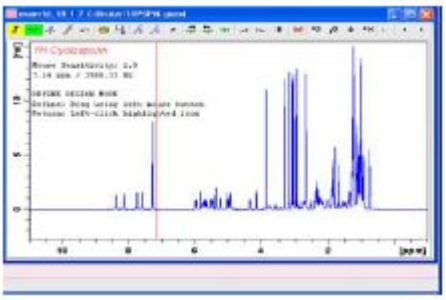
- Click the button in the upper toolbar, and the Tab bar of the active data window will be replaced by the following toolbar



- 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

d. Integration

❖ 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: Note: the active button is highlighted in green

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

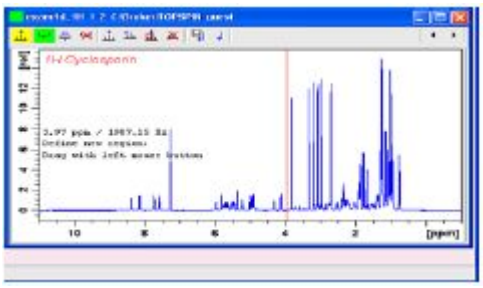
: Perform interactive Bias and Slope correction

: Save integrals and return

: Return, discarding any changes

e. 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. Plot 1D spectrum

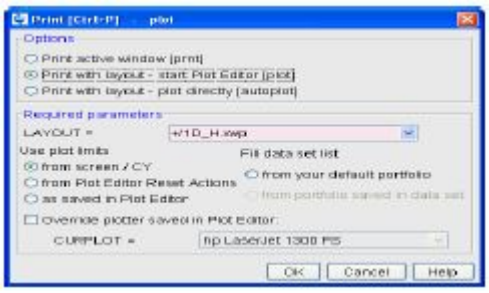
Click **file** in the menu bar, then select **print**, click **OK** in the popup dialog box, then click **print** in the popup dialog box.

TOPSPIN PLOT EDITOR INSTRUCTION

1. 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

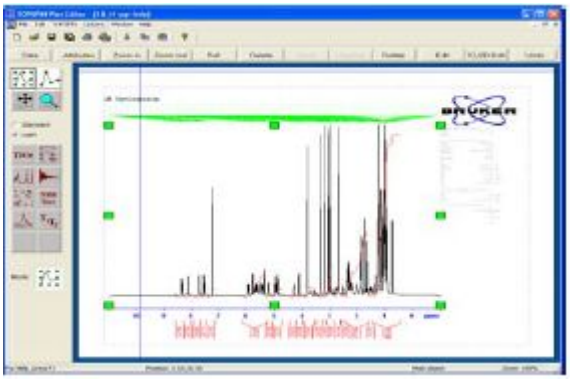
The layout can be specified by using one of the following abbreviations:

+: 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**)



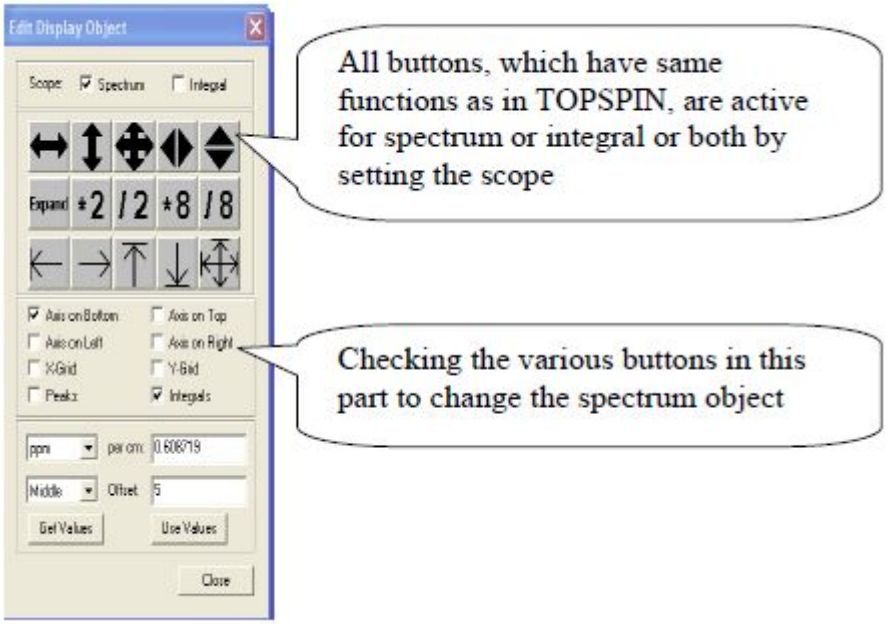
d. Modify the plot layout

Move, resize and delete an object (spectrum, title, parameter or logo):

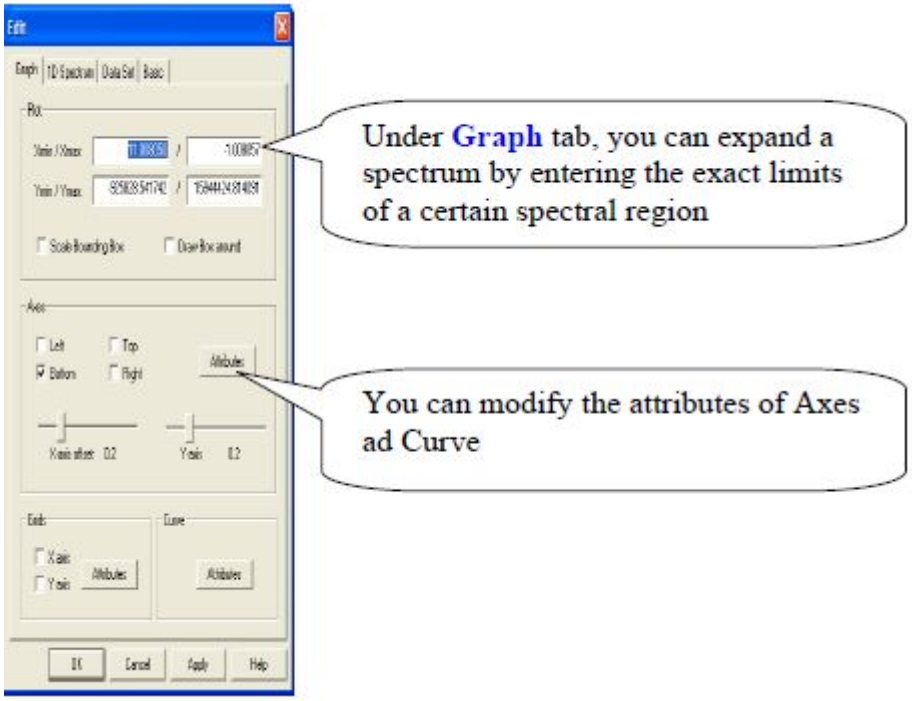
- •Mark an object by clicking the button and then clicking the object
- •Click-hold the object and move the mouse to move the object
- •Click-hold one of the green markers and move the mouse to resize the object
- •Click the Delete button in command bar to delete the object

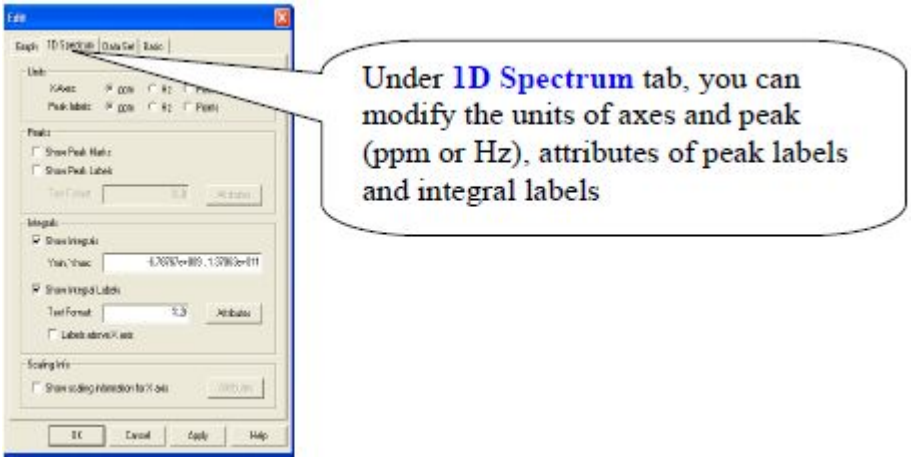
Modify the spectrum

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



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





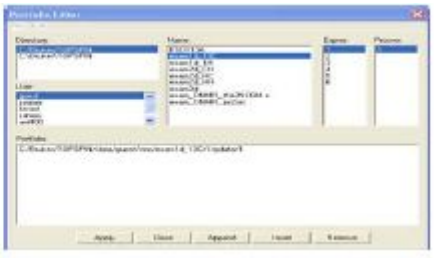
Under Linux, all parts (Graph, 1D spectrum. DataSet and Basic) are shown simultaneously

Modify parameters and title

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

2. 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



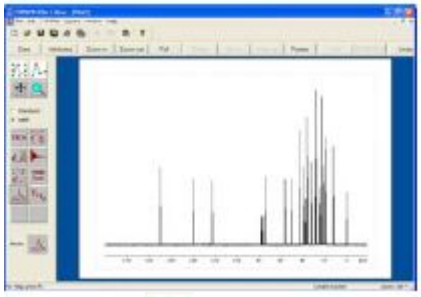
b. In **Portfolio Editor** window, choose right **Directory** and **User**, all datasets will show up.

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**

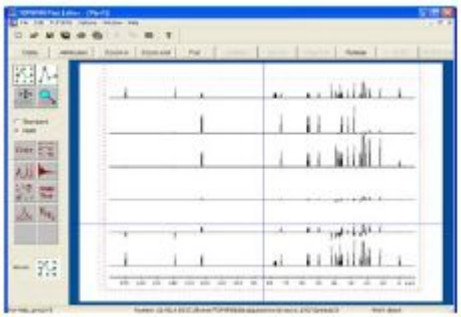
e. In **TOPSPIN Plot Editor**, click **File** → **New** to open a new layout

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. Export a spectrum as PDF or PNG or EMF format file so you can insert it to your report / thesis

a. From Topspin Plot Editor

•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. From Topspin (**Note: No PDF type is available**)

•A spectrum is appeared in the data area

•Click **File** → **Export**

•Put filename in the **File name** box with extension

•Click **Export** button