TopSpin

Users

Guide

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Starting TopSpin

Method (1):

Click on: the TopSpin Icon on the desktop

Method (2):

Open a Linux Shell/Terminal Window

Type: *topspin*

Using the Topspin Browser

The browser appears at the left of the TOPSPIN window and from the browser you can (1) browse datasets, (2) select a dataset, or (3) open a dataset. The following options are offered:

Browser: The browser shows data directory trees and allows you to expand/collapse branches by clicking on the arrow to the left of each entry.

black indicates 1D data

blue indicates 2D data

magenta indicates 3D data.

The browser also shows:

The EXPNO with the pulse program with the dataset EXPNO (e.g. 1 – zg30).

The displayed pulse program is the status pulse program if data acquisition has been completed.

If no data exists the pulse program shown is the setup pulse program.

Last50: Click on the Last50 tab to display the list of the last 50 displayed datasets. Press the *Enter* key to display the highlighted dataset in the current window or Double-click a dataset to display it in the current window.

Groups: Click the Groups tab to display the list of user defined dataset groups. Individual users can create, modify and display groups

of datasets. You may find it useful to define a separate group containing several experiments relating to the same projects.

Alias: Click on the Alias tab to display the list of user defined alias names for datasets. Right-click on an entry to define, remove or interpret alias names. Personally, I don't use this feature.

Opening a Dataset from the Browser

There are several ways to open a dataset. Choose the method that you like from the list below:

- Left-click-hold a dataset *name*, *expno* or *procno* and drag it into the data area. The data will be displayed in a new data window.

- Left-click-hold a dataset *name*, *expno* or *procno* and drag it into an open data window. The data will replace the currently displayed data.

- Left-click-hold a dataset *name*, *expno* or *procno* and drag it into an empty data window created with *Alt+w n*.

- Left-click-hold a dataset *name*, *expno* or *procno* and drag it into a multiple display data window. The data will be superimposed on the currently displayed data.

- Right-click a dataset *name*, *expno* or *procno* and choose Display from the popup menu; the data will be displayed in the current data window.

- Right-click a dataset *name*, *expno* or *procno* and choose Display in new window from the popup menu; the data will be displayed in a new data window.

- Hold the *Ctrl* key and left-click several datasets to select them or hold the *Shift* key
  and left-click two datasets to select these two and all in between. Right-click one of
  the selected datasets and choose Display from the popup menu. A new window will
  open showing the selected datasets in multiple display mode.

  Note: If the current window was already in multiple display mode, the selected spectra will be **superimposed** on the currently displayed spectra.

Opening a dataset from the command line:

Type: ***re***

Enter the dataset name you wish to open in the dialog box and left-click OK.

To open a dataset in a new window:

Type: ***rew***

Enter the dataset name in the dialog box and left-click OK.

To open a new procno of the **current** dataset:

Type: ***rep***

Enter the *procno* in the dialog box and left-click OK.

To open a new procno of the current dataset in a new window:

Type**: *repw***

Enter the procno in the dialog box and left-click OK.

Creating a New Dataset

There are several ways to create a new dataset. Choose the method that you prefer:

Method (1): Let's assume that you have optimized the acquisition parameters for your particular sample and you want to create a new dataset using these parameters. In this case the simplest way to proceed is to:

Type: ***edc***

In the dialog box you can then change the experiment name, experiment number or the user (if you are copying the parameters from another user)

Method (2): Click *File* > *New* [**Ctrl+n**]

Alternatively, Click the button on the upper toolbar.

When the dialog box appears fill in the appropriate boxes to specify:

- dataset *name*
- *expno*

- *procno*
- *dir*
- *user*

Next:

- Left-click the arrow adjacent to the Solvent box and select
  your solvent from the list.

- Left-click the arrow adjacent to the Experiment box and choose
  a parameter set from the list, or type a parameter set name.

- Type the dataset title in the Title box.

- Click OK.

Locking and Shimming the magnet on Your Sample:

1. Type: ***bsmsdisp***
2. Type: ***lockdisp***
3. On the lock panel of the BSMS console left-click on: Lift
4. Adjust sample depth and insert sample atop the magnet
5. Left-click on: Lift
6. Type: ***Lock***
7. Select your solvent from the popup window.
8. Left-click on the shim that you want to optimize. (e.g. "Z")
9. Left-click on Step + or Step – to optimize the shim you selected.
10. Repeat steps 8 and 9 for X-, Y-, Z^2- shims

If the lock signal goes to the top of the window, under "Auto" on the BSMS console click on **Gain** and just the lock level downward by left clicking on **Step -.**

Alternatively, if you are using Topspin 2.0 on the AV-400, you can let the computer optimize all of the shims as follows:

Type: ***topshim*** (or ***topshim gui***)

Wait until the computer prints: topsphim finished at the bottom of the screen.

Checking Data Acquisition Parameters:

After the instrument has been shimmed on your sample click on the Green Square in the upper right-hand corner of the screen to return to the Acquisition Window.

1. Left-click on: **AcquPars** (tab).
2. Review the acquisition parameters and adjust as necessary.
3. Left-Click on: **Spectrum** (tab)

Data Acquisition:

1. Type: ***rga*** (to automatically adjust the receiver gain).
2. Type: ***zg***

Data Processing:

Exponential multiplication and Fourier Transformation:

Left-click on ProcPars

Adjust processing parameters (e.g: lb, si, etc.) as necessary.

Alternatively:

Type: ***lb***

Adjust as necessary.

Type: ***efp***

Phase correction: [***.ph***]

- Left-click on the Phase Correct Icon on the Upper toolbar

(As you place the cursor over each icon a dialog box will appear
to explain the function of that icon.)

- Left-click-and hold the cursor on "0". Move the mouse Up or down to adjust the Zero-order phase.
- Left-click-and hold the cursor on "1" and move the mouse
up and down to adjust the First-order phase.
- Left-click on the save and return Icon

Baseline Correct: [***.basl***]

- Place cursor over the coefficient you want to adjust.
- Left-click-and-drag the mouse to adjust as necessary
- Left-click the save and return icon.

Integration: [***.int***]

- Left-click in Integration Icon.
- Left-click-and -hold on down-field (left) side of selected
resonance.
- Drag cursor to up-field (right) side of selected resonance.
- Repeat for each resonance you wish to integrate.
- Adjust scale (*2, /2)
- Adjust base and slope as necessary.

Integral calibration:

- Right-click to select a particular integral region.
- Select calibration method from the popup window.

Peak picking: [***.pp***]

- Set a value of CY for the reference peak in the dialog box.
- Place cursor down-field of the region wherein you want to pick
  the peaks.
- Left-click-and-hold and drag to create a box enclosing the spectral
  region of interest.

Plotting Data:

Method (1):

- Left-click on the plotter icon.
- Left-click on options.

  check: print with layout – start plot editor
- Left-click on arrow adjacent to Layout.
- Select the layout you wish.
  - eg: 1D_H + info.xwp
- left-click on OK

Method (2):

Type: ***plot*** (to open the plot editor)

Customizing the TopSpin Interface:

- Left-click on: ***Options***
- Left-click on: ***Preferences***
- Check options you wish to turn on.

  eg: Open window with last dataset