

TopSpin

- User Guide
User Manual
Version 014



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Document Number:

P/N: H9469SA4

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1 Introduction

1.1 About the User Manual

About this document

The user manual describes the main aspects of Bruker's integrated software package TopSpin. This manual enables all users who work with Bruker software to get an overview of the various functionalities of TopSpin. The main aspects outlined in here describe the possibilities and features of the TopSpin interface and elucidate working processes for data acquisition and processing.

Target audience

The Bruker user manual for TopSpin supports all Bruker users who already work with Bruker software products or who newly enter the software dimension of TopSpin. The main aspect of this manual is to enable new TopSpin users and experienced TopSpin users to work with this software package.

How to get the User Manual

This manual is available:

- as PDF file in the TopSpin software help menu.
- as the up to date version on the Bruker web server:

<https://www.bruker.com/service/information-communication/user-manuals/nmr.html>

Note: All text messages and graphics shown in this manual are taken from the current version of the respective software products. Small differences to other versions are possible.

How to read the User Manual

The user manual describes especially the TopSpin interface with all its functionalities to acquire, process and interpret spectrometer data. To find information more readily you can read selected chapters, depending on your requirements, or read the user manual in succession for general information.

1.2 Safety Regulations

To work safely in laboratories with NMR-spectrometers all users must follow the safety regulations for magnetic, electrical, cryogenic and chemical safety. For detailed information please refer to the safety instructions in the Beginners Guide manual provided on the TopSpin DVD or in the Safety Considerations manual provided on the BASH DVD.

1.3 User Manual Conventions

The User Manual utilizes different script types in order to make selected text more transparent and explicable to users. Please note that this document contains the following conventions:

Font and Format Conventions

Type of Information	Font	Examples
Shell Command, Commands, “All that you can enter”	Arial bold	Type or enter fromjdx zg
Button, Tab, Pane and Menu Names “All that you can click”	Arial bold, initial letters capitalized	Use the Export To File button. Click OK . Click Process...
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names Data Path Variables Table Column Names Field Names (within Dialog Windows)	Arial Italics	<i>\$tshome/exp/stan/nmr/</i> <i>lists</i> <i>expno, procno,</i>
Parameters	Arial in Capital Letters	VCLIST
Program Code Pulse and AU Program Names Macros Functions Arguments Variables	Courier	go=2 au_zgte edmac CalcExpTime() XAU(prog, arg) disk2, user2
AU Macro	Courier in Capital Letters	REXPNO

Table 1.1: Font and Format Conventions

1.4 TopSpin Overview

Functionality

TopSpin is an integrated software package for:

- Displaying NMR spectra.
- Printing and plotting spectra.
- Exporting displays and plots in various graphics and metafile formats.
- Importing NMR data from files of various formats.
- Archiving spectra in various formats such as JCAMP-DX and ZIP.
- E-mailing data.
- Processing 1D-8D fids and spectra: window multiplication, various transforms (Fourier, Hilbert, DOSY), phase correction, baseline correction, integration, peak picking, linear prediction, smoothing, adding spectra etc.
- Displaying multiple superimposed spectra (1D and 2D).
- Simulating 1D and multi-dimensional fids, given a pulse program and a spin system. See **Help | Manuals (docs) | Analysis and Simulation | NMR-SIM Experiment Simulator**.
- Calculating T1/T2 relaxation times.

- Fitting peaks with Lorentzian and Gaussian line shape models, deconvolve overlapping peaks.
- Multiplet analysis.
- Automatic 1D, 2D and 3D peak picking.
- Automatic 1D, 2D and 3D integration.
- Line shape analysis of solids spectra.
- Data acquisition with Bruker Avance type spectrometers.
- Supporting automated and walk-up spectrometers (IconNMR).
- Remote spectrometer control including web-enabled IconNMR.
- Adding user defined functionalities to TopSpin (AU programs, Macros and Python programs).

Available Documentation

In TopSpin the **Help | Manuals** submenu contains a list of available manuals for the following categories:

General

Acquisition - Users Guides

Acquisition - Application Manuals

Acquisition & Processing References

Automation and Data Publishing

Analysis and Simulation

Programming Manuals

Technical Manuals

Installation Guides

Good Laboratory Practice

Each document is listed with a short description of its contents.

1.5 TopSpin License Management and Product Order

TopSpin uses the new Code Meter license management. A license can be ordered from the Bruker website. Just go to https://www.bruker.com/nmr_license_requests.html and fill out the request form. The License department will process the order details and generate an **activation ticket** and provide it to the customer. A ticket consists of a 25 character code like e.g.:

PH3T4-9D9U9-FNSGP-J9FXP-TTNXC

This code works as an access key to the purchased license package. It authorizes the customer to assign the license package to a computer of personal choice.

Install the software product on the computer system. During installation you may also be requested to install the package **CodeMeter Runtime**. This is the component of the license management system. Most installation routines will perform this task automatically.

A Free TopSpin Evaluation license can be ordered on the following web page:

<https://www.bruker.com/service/support-upgrades/software-downloads/nmr/free-topspin-processing/topspin-demo-licences-generation.html>

A Free TopSpin Processing license for Academia can be ordered on the following web page:

<https://www.bruker.com/service/support-upgrades/software-downloads/nmr/free-topspin-processing/nmr-topspin-license-for-academia.html>

For further information please look up the Code Meter License Management User Manual H162728.

1.6 Packages on the TopSpin DVD

1	TopSpin	Acquisition and Processing Software	3.6.x	4.x
	TopSpin Plot Editor	Object oriented WYSIWYG plot editor. ³	X	X
	Cygwin Tools	Used for compilation of TopSpin AU programs. ³	X	X
	NMR-GUIDE	A web-based training and teaching tool providing a lot of theoretical and practical information on NMR spectroscopy and NMR methods for everybody interested in NMR. ²	X	X
	NMR-Sim	Program for numerical simulation of NMR experiments. ³	X	X
	CMC-q Viewer	Automation & Analysis ³	X	X
2	Central Audit File	Enables a Central Audit File for activity recording in TopSpin.	X	X
3	CMC-a	CMC-assist, a tool for structure verification based on NMR data.	X	X
4	IconNMR	Icon-driven interface for Routine Spectroscopy and Automation.	X	X
5	MICS	Magnet Information & Control System.	X	X
6	NMR-Data	Example datasets	X	X
7	CodeMeter Runtime	License manager required to start TopSpin programs.	X	X
8	AURELIA-AMIX-Viewer	Multiple object viewer ¹ During the installation the program is displayed as <i>AMIX</i> .	X	X
9	SpectrOS	Spectrometer operating system for AVANCE NEO. SpectrOS is needed for workstations controlling a spectrometer.		X
10	Diskless	Spectrometer operating system for AVANCE III. Diskless is needed for workstations controlling a spectrometer.	X	
11	SBASE	Spectra base for AMIX ¹	X	X
12	Dynamics Center	Analysis of NMR data containing non-frequency dimensions (incl. Protein Dynamics) ¹	X	X
13	InsightMR	Reaction Monitoring	X	X

¹ Requires a separate license.

² Package is integrated in TopSpin4.x, package is selectable in TopSpin3.6.x

³ Installed by default together with the TopSpin package.

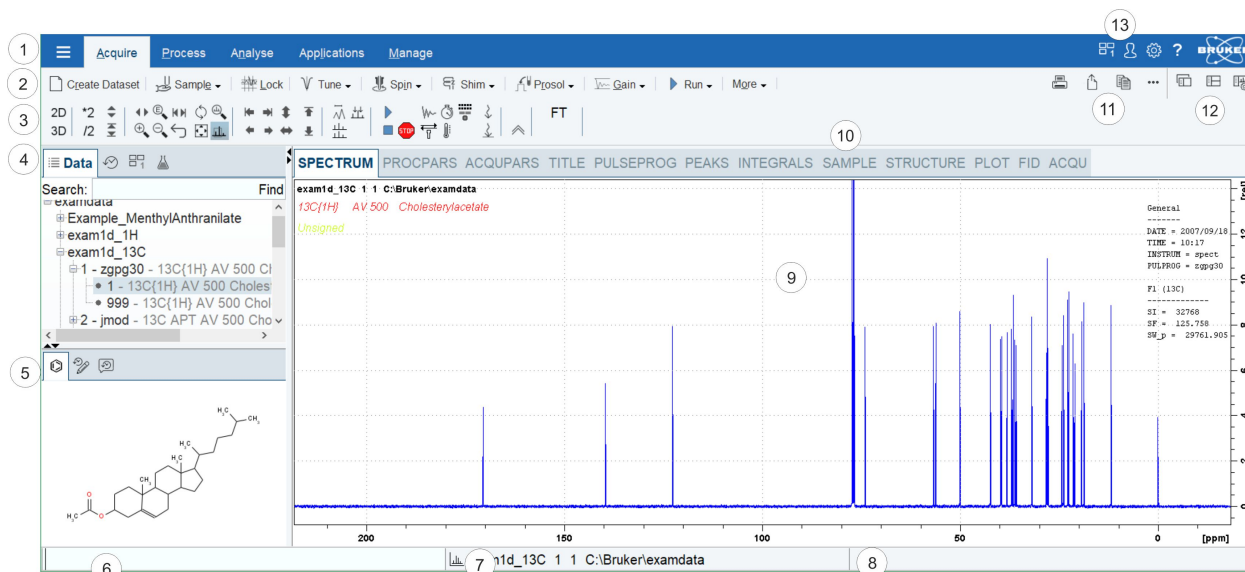
Packages available on a separate DVD:

	TopSpin	Acquisition and Processing Software	3.6.x	4.x
--	----------------	--	--------------	------------

14	AssureNMR	The AssureNMR software provides automated multicomponent identity, quantification, classification, and detection of outliers with spectral databases and System Suitability Tests for GxP compliance. ¹	X	X
15	AssureNMR- Methods	This directory includes Analysis Methods, for use with AssureNMR, that automate the analysis of poloxamers, molar substitution, tire rubber, heparin, Aloe vera and other common materials. Some of these methods may require separate software licenses for use (heparin and Aloe vera).	X	X

¹ Requires a separate license.

2 The TopSpin Interface



1	Menu Bar	8	Status Display Bar
2	Workflow Button Bar	9	Dataset Window
3	Tool Bar	10	Dataset Window Tabs
4	Browser and Search Window	11	Print, Export, Copy and Publish
5	Structure Window, Command Line History, Status Line History	12	Viewing Options
6	Command Line	13	Window Switcher, Login, Setup Preferences and Help
7	Current Dataset Bar		

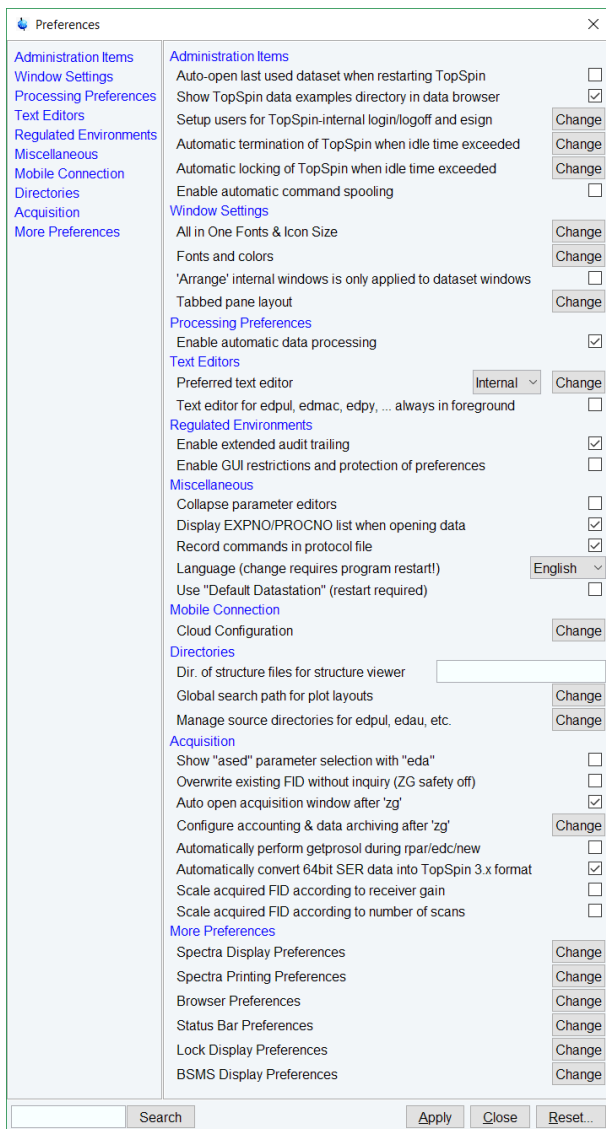
Setup Preferences

For all changes in the TopSpin appearance use the global **Setup preferences** button in the menu bar.

TopSpin can be tailored to your preference in many respects. This ranges from startup options to spectrum objects, menu settings, remote connections, colors and fonts etc. Every standard user can create his own set of preferences.

A dialog box will appear with, at the left side, the categories that can be tailored. Click the category you want to view or change. It will become highlighted and the corresponding objects will be displayed at the right part of the dialog box.

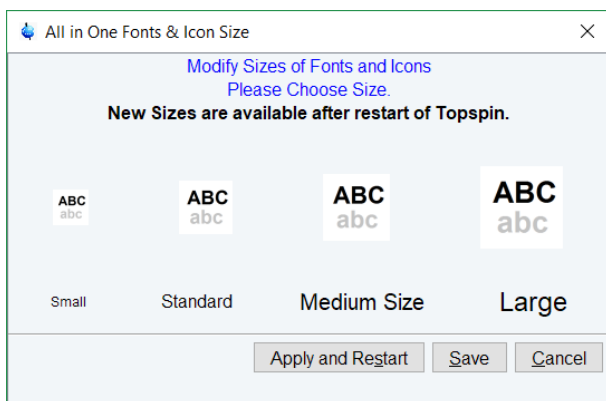
The TopSpin Interface



TopSpin on High Resolution Screens

To adapt the font and icon size to a small/standard/medium or large screen resolution

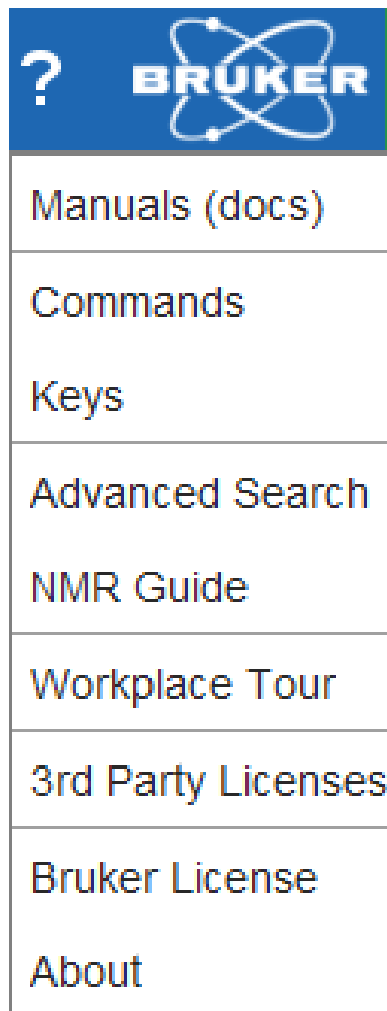
- click **Setup Preferences** and in the category **Window Settings | All In One Fonts & Icon Size** click **Change**.



Help/About TopSpin/Version and License Information



This button gives information about the TopSpin documentation, software version and license.



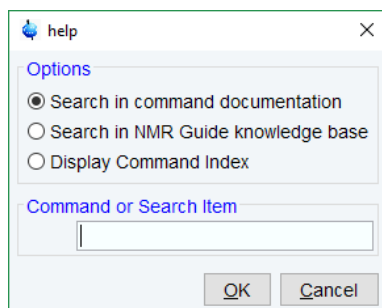
Clicking **Manuals (docs)** or entering **docs** on the command line will open the list of all manuals delivered with TopSpin.

- Click **Help | Manuals | Acquisition Application Manuals | Dosy** will open the DOSY manual, for example.

The TopSpin Interface



Enter **help** to get information for an individual command. Three different sources can be selected for the search:



Tooltips

Pointing to a button with the mouse in the various menus opens a tooltip that describes the button functionality. Example:

▶ Run ▼

Start acquisition (zg)
 Uses the acquisition parameters of the currently active dataset. If a dataset exists, zg will ask to override it, unless this feature was disabled (command "set", ZG safety off). You may also enable "auto-archiving" so as to avoid inadvertent data data loss. (command "set", Configure accounting and data archiving).

Workflow Button Bar

The workflow-based interface with its arrangement of all working processes allows the user to control the workflow intuitively.

Clicking one of the menu buttons opens the corresponding workflow. It contains a horizontal feature list which stays open and provides all functionality for this workflow with one mouse-click.

Furthermore, some of the buttons on the Workflow button bar include a **drop-down** arrow. Click the **drop-down** arrow to see more options.

Proc. Spectrum ▼

- Compute Spectrum from raw data (proc1d y)
- Configure Standard Processing (proc1d)
- Window Multiplication (wm)
- Fourier Transform (ft)
- Fourier Transform Options ... (ftf)
- Start Automation AU Program (xaup)

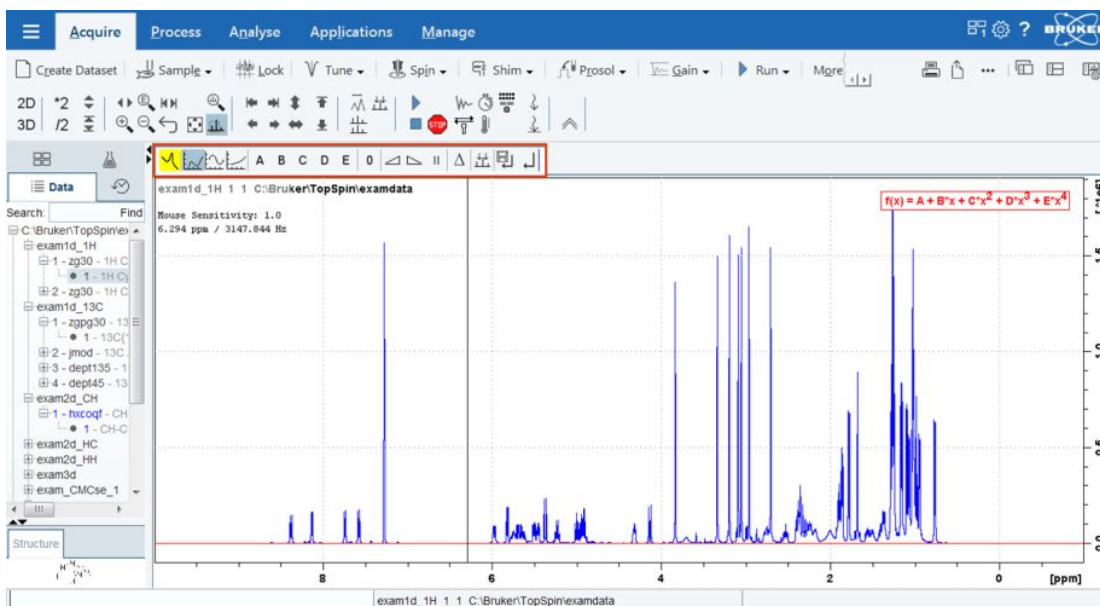
Dataset Toolbar

Depending on which dataset window tab is selected, an individual dataset toolbar is displayed, in the example the ACQU toolbar:



Note: The ACQU window tab is only displayed when TopSpin controls a spectrometer (noticeable through the Acquire tab in the TopSpin menu). When TopSpin is installed for processing-only, the Acquire tab is also not displayed.

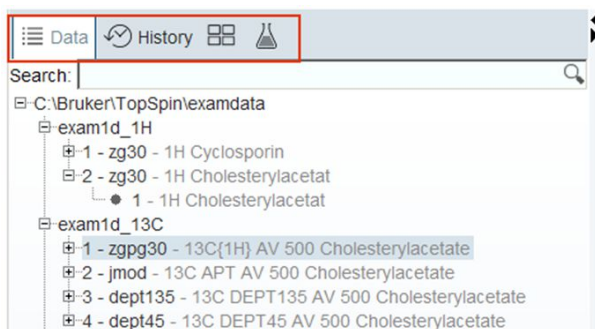
Note: Sometimes the dataset toolbar is displayed without dataset window tabs, e.g. entering a command as **.basl** will display the baseline correction toolbar:




Browse and Search Window

The Browser window provides tabs as:

- Data browser and Search
- History browser
- Dataset Switcher
- Experiment Selector library



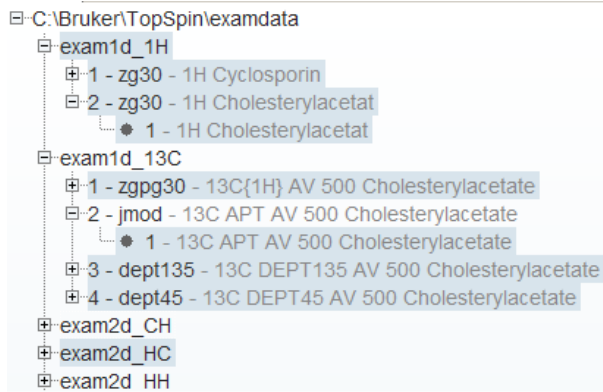
The window can be toggled On or Off with a click on the black **left** or **right** arrow.

Alternatively, the **Toggle Perspective** button on the top-right of the TopSpin window can be clicked. 

The data tree tab includes a search field. Enter a search phrase, for example:

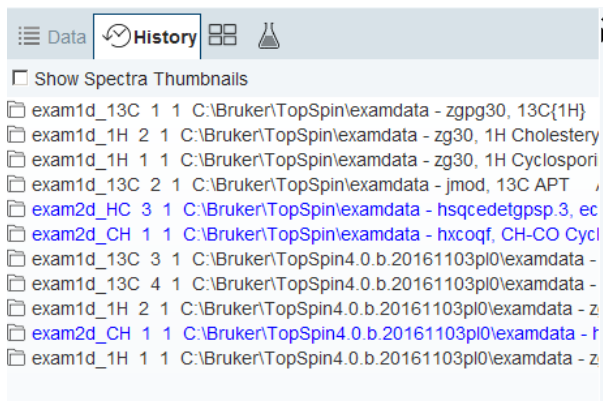
Search: X

To limit the search results, select or deselect the data trees with **SHIFT** click or **CTRL** click.




History Tab

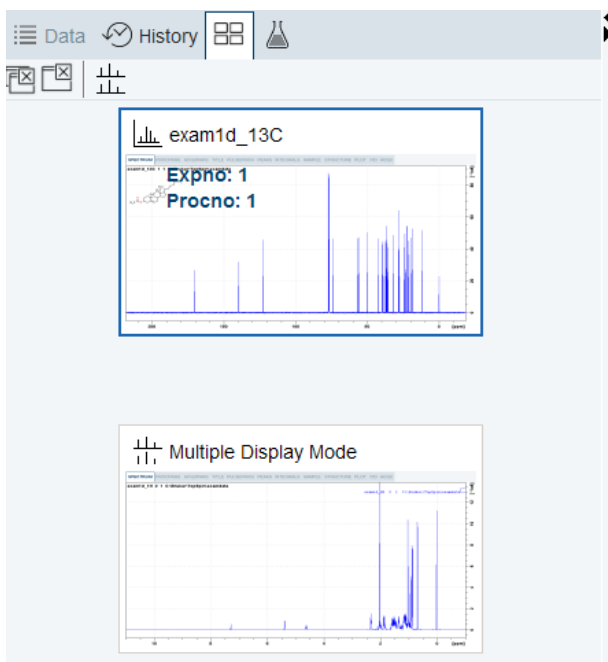
The History tab displays the last opened datasets in a list.



Dataset Switcher Tab

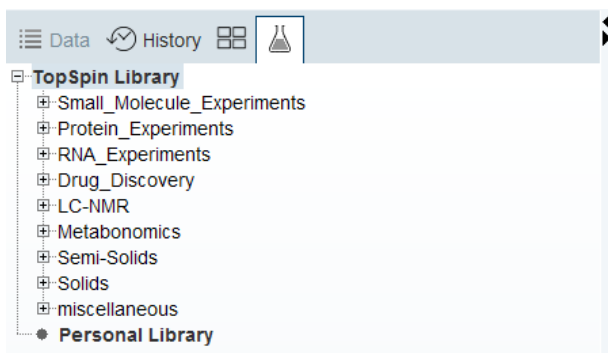
This tab has a similar function as the Window Switcher , see below, but only provides a quick overview of all currently opened datasets.

The TopSpin Interface



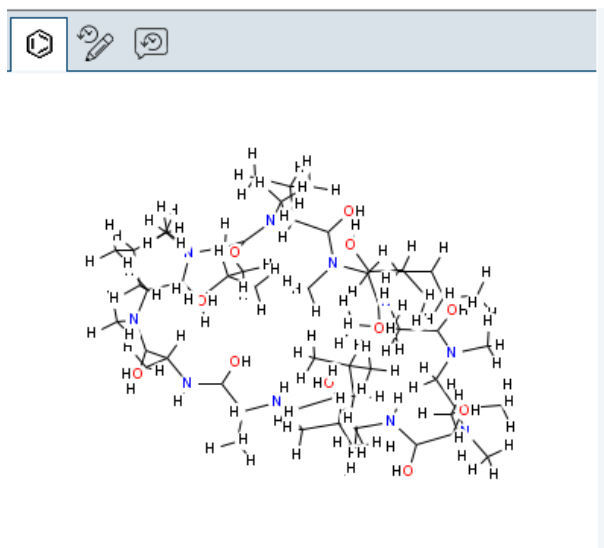
Experiment Library Tab

The Experiment library tab provides easy access to the vast experiment library of standard experiments that is available in the standard release of TopSpin. It is also a tool that allows the user to personalize his most frequently used experiments into a separate library.



Structure Window

Molecular structures as *.mol* or *.pdb* files can be displayed here and are freely resizable. The structure window can be toggled On or Off with a click on the black **up** or **down** arrow ▲▼.

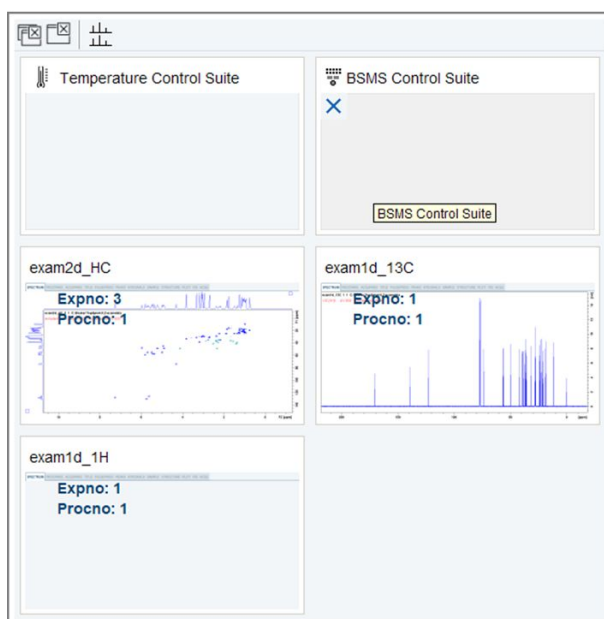



- Drag the vertical or horizontal split bar to resize the structure window.

Window Switcher

The **Window Switcher** button indicates the number of all opened dataset windows plus all opened TopSpin window types like

- Dataset windows.
 - Lock display window.
 - Acquisition display window.
 - BSMS display window.
 - Temperature unit window.
- Click the **Window Switcher** button to switch between these windows.



A dataset can be closed with the **Close** button .

Viewing Integrals, Peaks and other Spectra Components

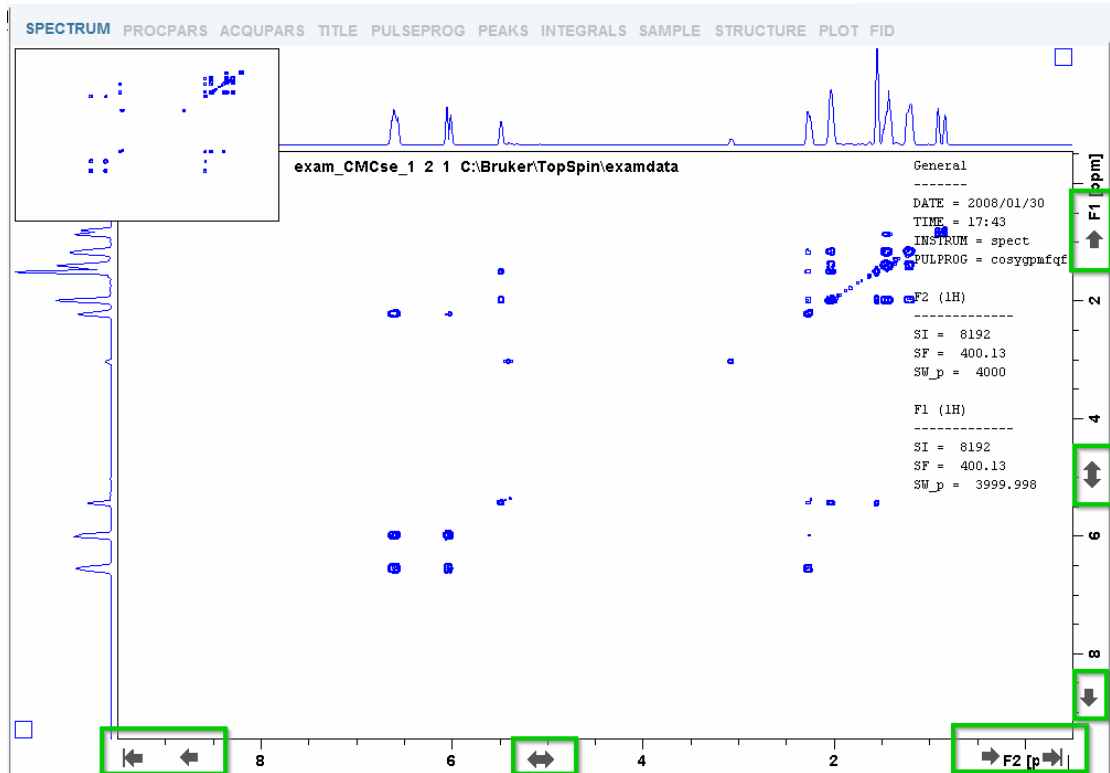
- Click **Spectrum display properties** to toggle the visibility of integrals, peaks and other spectra components. They can only be displayed when available.



Shift, Scroll and Zoom Spectra Axes

Clicking and dragging the spectrum axis allows intuitive scrolling through the spectrum.

- Single Clicks on the end regions of the axes or a click and dragging the mouse shift through the axes depending on the mouse position, see the next figure.
- Double click in the middle of the spectra axes switches to full axes region.
- Double click in the middle of the spectra itself maximizes all axes regions.
- Click on axes to shift left, right, up or down.
- Turn mouse wheel to zoom in or out.



Dataset Windows


The TopSpin window has a dataset area that may contain multiple dataset windows.

To open multiple dataset windows

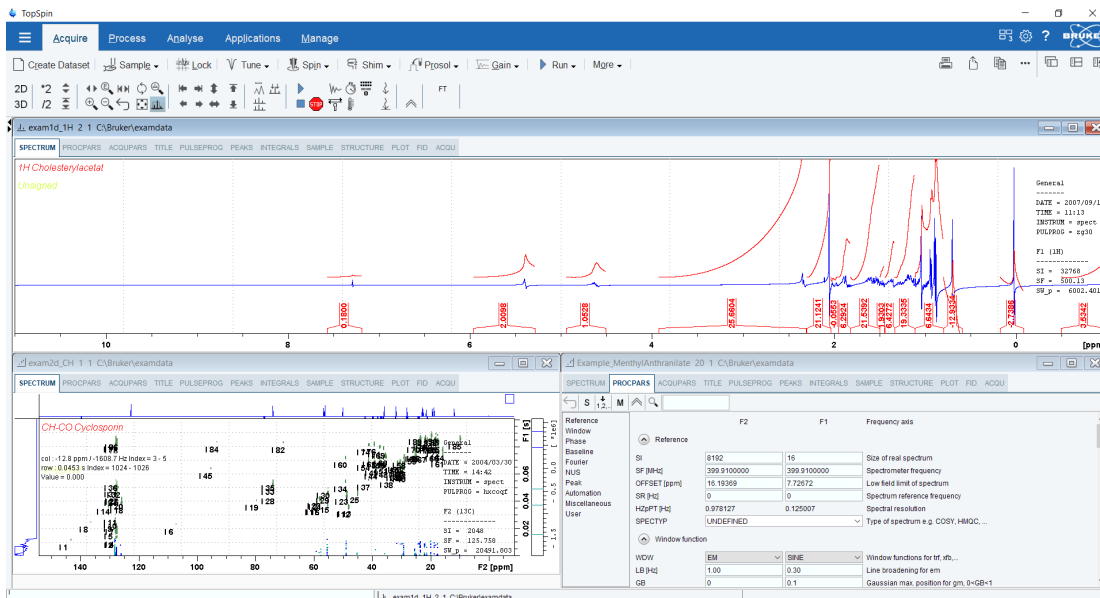
- Right-click in the Browser window and in the list, select **Display in new window**.

Note, that selecting **Display** will override a current dataset.

The size of the data area depends on the overall size of the TopSpin window and on presence of the Browser. Note, that the Browser window can be toggled On or Off with the

Toggle Perspective button . The following figure shows the TopSpin window without the Browser and three dataset windows.

The TopSpin Interface



Note, that the three dataset windows show different data objects: a 1D spectrum, a 2D spectrum and 1D processing parameters.

How to Move a Dataset Window

- Click-hold the title bar and move the mouse.

How to Resize a Dataset Window

- Move the cursor to the window edge until it becomes a double-headed arrow.
- Click-hold that position and move the mouse.

Depending on the position of the double-headed arrow, you can change the window height, width or both.

How to Select (activate) a Dataset Window

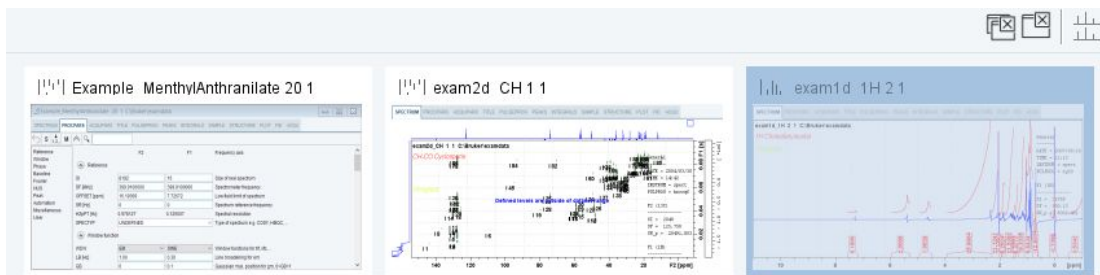
The active dataset window is the window of which the title bar is highlighted. The TopSpin menu, tool bars and command line commands correspond to and act on that window. Only one dataset window is active at a time.

To activate a different dataset window:

- Click in the desired dataset window or click its title bar.

or

- Click the **Window Switcher** button  to switch between the windows.



How to Arrange Dataset Windows

If the data area contains multiple dataset windows, you can arrange them in various ways. All the arrange commands arrange the windows left to right and/or top to bottom in the order in which the windows have been active. The currently active dataset window will therefore be positioned at the top and/or left of the data area.

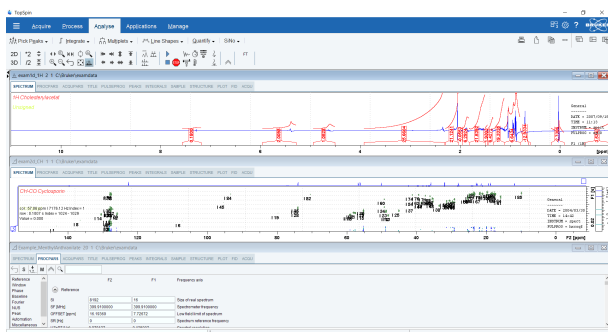
To arrange the dataset windows as a grid:

- Click **Show Layout Options**  and **Show as Grid** .

Depending on the number of windows, they will be arranged vertically and/or horizontally.

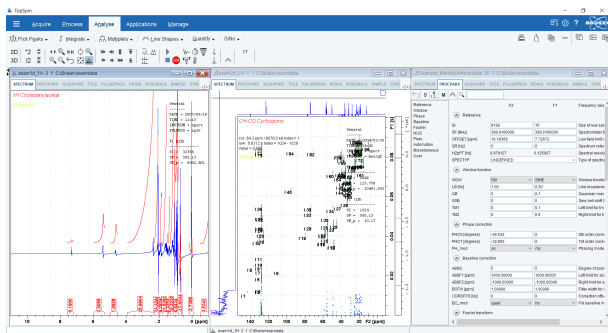
To arrange dataset windows in stack:

- Click **Show Layout Options**  and .



To arrange dataset windows side by side:

- Click **Show Layout Options**  and .



To display a dataset windows as full screen:

- Click **Show Layout Options**  and  or click the **full screen windows button** .

To close the active dataset window:

- Click **File | Close Active Window** or enter **Ctrl-w**.
or

The TopSpin Interface

- Click the  button in the windows title bar.

To close all dataset windows:

- Click **File | Close All Windows** or enter **closeall**.

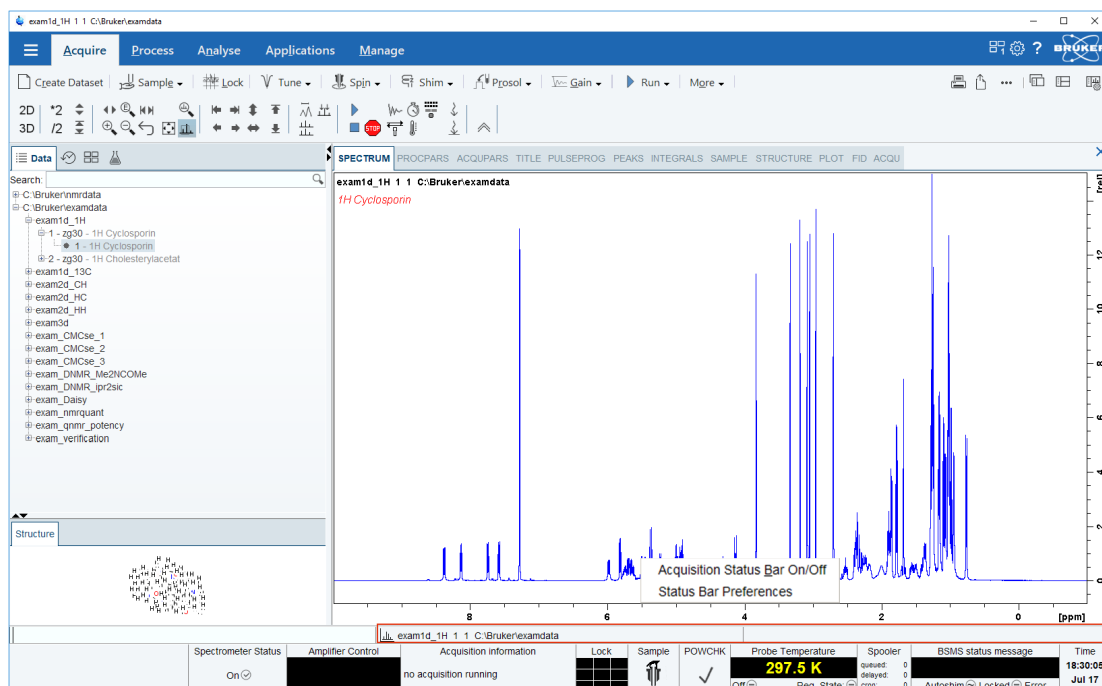
How to Swap Dataset Windows

Within a certain layout, you can easily swap two TopSpin windows with the command **swin**. If the data area contains exactly two windows, **swin** simple swaps their position and geometry.

If it contains more than two dataset windows, **swin** opens a list from which you can select any window to be swapped with the currently selected (active) window.

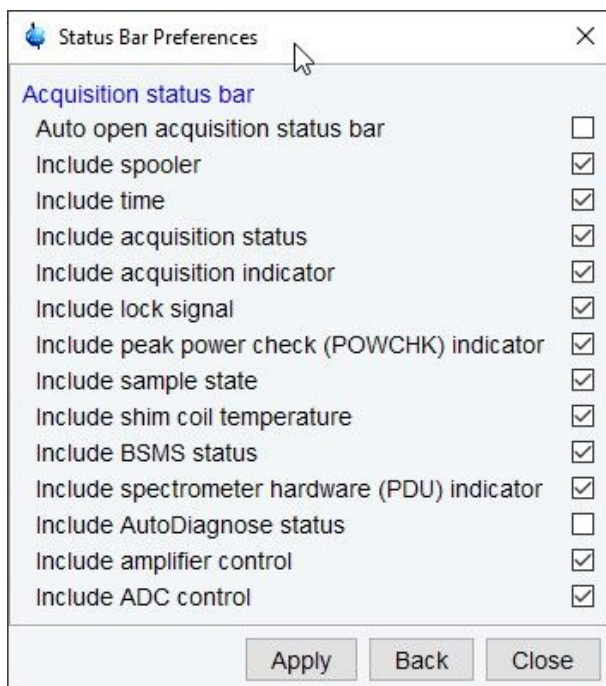
Acquisition Status Bar

- Right-click the Status display or Current dataset bar to toggle the Acquisition status bar On or Off.

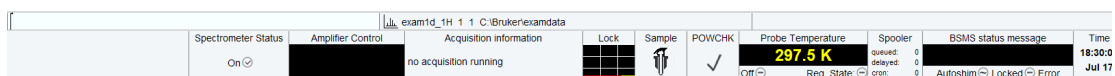


- Click **Status Bar Preferences** to set the *Auto-open the acquisition status bar* option as default.


Acquisition Status Bar On/Off
Status Bar Preferences



The acquisition status bar contains the new Spectrometer Status area to turn the spectrometer On and Off. This functionality is also available in the menu with a click on **Manage | Spectrometer | Spectrometer power On/Off** or the command **pdudisp**.



Print, Export and Publish

Click on any of the 4 icons  to either print the active window, export the active window to a PDF file, copy the active window to the clipboard or, show more publishing options such as E-mailing a dataset, sending a dataset to cloud storage, etc.

- Click **Show More publishing options**, e.g. to copy and paste, E-mail or use shared cloud directories.



3 Getting Started

3.1 Startup TopSpin

Under Windows

- Click the TopSpin icon on the desktop.
or
- Click **Start | Bruker NMR Software | TopSpin<version>**

To start TopSpin from a Command Prompt as follows:

- Open a Shell window with **cmd** and in the Command Prompt enter:
cd <tshome>
topspin
where *<tshome>* is the directory where TopSpin is installed.

Under Linux

- Open a Linux Shell or Terminal Window.
- In the Shell/Terminal enter
cd <tshome>.
./topspin.

Where *<tshome>* is the directory where TopSpin is installed.

Startup TopSpin specifying dataset

TopSpin can be started with a dataset option:

- Open a Windows Command Prompt or Linux Shell.
- Enter **topspin -j TOP_DATA:<dataset path>**.

The specified dataset is automatically displayed after startup.

Examples:

```
topspin -j TOP_DATA=c:\bio\data\guest\nmr\exam1d_1H1\pdata\1
topspin -j TOP_DATA=c:\bio\data\guest\nmr\exam1d_1H1\pdata\1\1r
topspin -j TOP_DATA=c:\jcamp.dx
topspin -j TOP_DATA=c:\data-archive.zip
```

3.2 Configuration

After the installation of TopSpin, it must be configured once. See the TopSpin Installation Guide for a detailed description.

3.3 How to Display Spectra

In this chapter, opening data in standard Bruker format is described. Opening other data formats is described in the chapter [Dataset Handling \[p 41\]](#).

How to locate NMR data

NMR data can be in any arbitrary directory.

The typical directory storage format is:

`<dir>/<name>/<expnos>/pdata/<procnos>`

e.g. `c:\mydir\sucrose\10\pdata\1`

Program versions older than TopSpin 2.5 used a different directory structure where `<dir>` was built up as `<dir>\data\<user>\nmr`.

Example: `c:\bruker\topspin\data\guest\nmr\exam1d_13C\1\pdata\1`

- The old format is still valid because it is a special case of the new storage format.
- The old and new style data storage must not be mixed, this would confuse the TopSpin data browser.
- The browser command **scroll to active dataset** will not work for old style data storage.
- The Bruker example datasets (if installed at all) can be found with TopSpin 2.5 and newer in `<TOPSPIN INSTALLATION DIR>/examdata`.
- This directory is automatically shown in the browser if enabled in the Setup Preferences (command **set**).

How to Open Data from the Windows Explorer

The easiest way to open data set in topspin is to use drag and drop from Windows Explorer (or similar tool on other OS).

You may drag either the data set folder, any subfolder or file (1r, fid...) and drop it into the Topspin data area or dataset Window.

The corresponding data directory is automatically added to the Topspin internal browser.

This considerably simplifies the handling of data directories.

This feature may be switched on or off in the Browser Preferences:

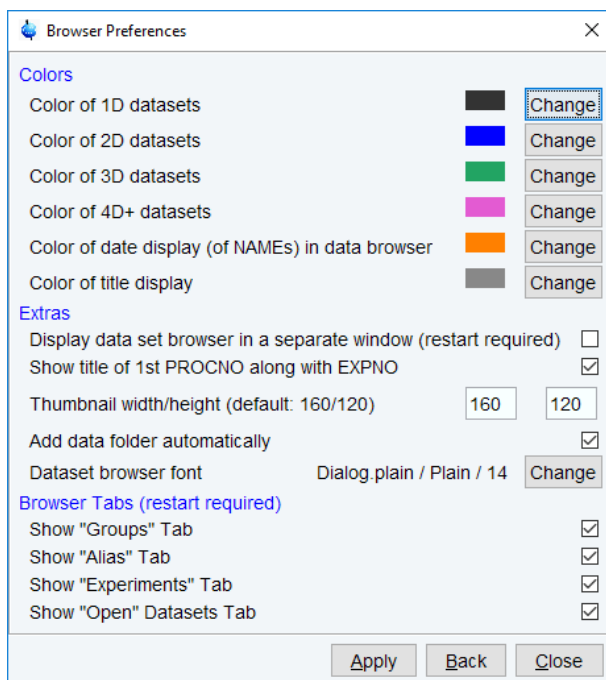
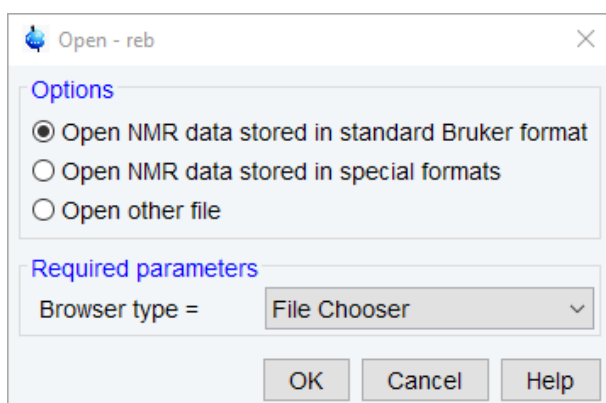


Figure 3.1: Browser Preferences to **Add data folder automatically**.

How to Open Data from the Menu

Open the **File** menu and click **Open...**

A dialog box appears.



Select the first option, the Browser type **File Chooser** and click **OK**.

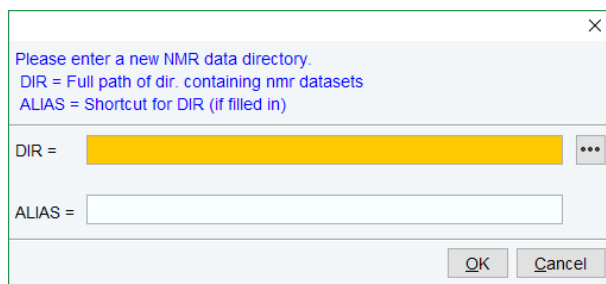
A file browser appears. Navigate to your data directory and expand it to the level of names, expnos, or procnos (double-click a directory to expand it). Select the desired item and click **Display**.

The selected dataset replaces the contents of the currently selected (active) window. If no dataset window was displayed, a new one will be created. The file browser can also be opened by entering **reb** on the command line.

How to Open Data from the Browser Window

TopSpin provides a data browser which, by default, displays the top level data directory (<dir>) with Bruker example data. You can add your own data directories, local or remote, as follows:

- Move the cursor into the browser area.
- Right-click and in the list, select **Add New Data Dir**.



- Enter the desired data directory (<dir>) and optionally an alias name and click **OK**.

Your data directory will now appear in the browser.

To display data from the Browser, proceed as follows:

- Expand your top-level directory (<dir>) in the browser to the level of the *data name*, *expno* or *procno*.
- Select the desired item and drag it into the data area.

How to Open Data in other Ways

TopSpin provides various other ways of displaying data. You can, for example, use command line commands like **re**, **rew**, **rep** and **dir**. Details on these features can be found in chapter [Opening Data \[49\]](#) and in the Processing Reference Manual.

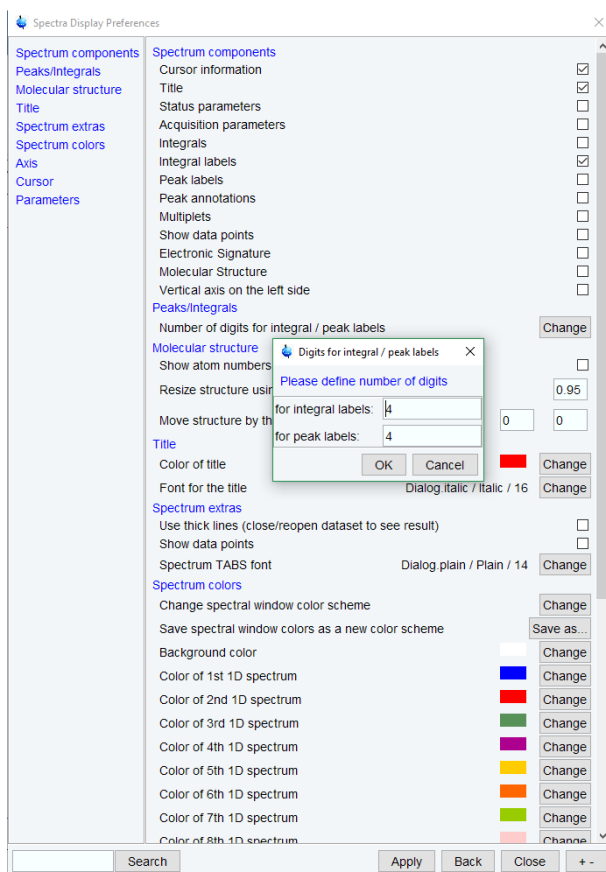
3.4 How to Display Peaks, Integrals, ... together with the Spectrum

When a spectrum is displayed, you can superimpose its title, parameters, integrals, and peaks as follows:

- Move the cursor into the dataset window that contains the spectrum.
- Right-click and select **Spectra Display Preferences**.
- Check the desired items and click **OK**.


Please note that the selected items are only shown if they are available. For example, peaks and integrals are only shown if peak picking and / or integration have been performed (see also [1D Interactive Manipulation \[139\]](#)). The number of displayed digits for the integral and peak labels can be set in the Spectra Display Preferences.

Note: Integrals and peaks etc. can be toggled ON and OFF from the viewing options display.



3.5 How to Display Projections/1D Spectra with 2D Spectra


To display projections or 1D spectra in tandem with a 2D spectrum:

- Open a 2D spectrum.
- If no projections are shown, click **Toggle projection display**  in the Spectrum Display Properties window or enter `.pr` on the command line. Projections can automatically be enabled in the Setup Preferences menu.
- Move the cursor into the F1 or F2 projection area.
- Right-click and choose one of the options. With **External Projection...** an existing 1D spectrum can be read. This can be a regular 1D spectrum or a 2D projection that was stored as a 1D spectrum. With **Internal Projection** the positive projection can be calculated and displayed.

An alternate way to display projections is the following:

- Click **Process | Advanced | Display Projections...[projd]**
- or
- Right-click on a 1D dataset in the browser and choose **Display As 2D Projection**.

3.6 How to Superimpose Spectra in Multiple Display

TopSpin allows to compare multiple spectra in Multiple Display mode. To enter this mode, click the  button in the upper toolbar or enter `.md` on the command line. When you open a dataset now, for example drag one from the browser, it will be superimposed on the current spectrum rather than replacing it. Several multiple display functions are available now in the dataset window toolbar. Most importantly, you can scale and shift each spectrum individually. This allows exact alignment of corresponding peaks of different spectra.

3.7 How to Print or Export the Contents of a Dataset Window

How to Print Data

A TopSpin dataset window may contain various objects like an fid, a spectrum, expansions of a spectrum, superimposed spectra, spectrum components such as parameters, peaks, integrals, cross sections etc. Whatever the content of the dataset window is, it can be printed as follows: type **Ctrl + p** or click **File | Print...**, select **Print active window** in the appearing dialog box and click **OK**.

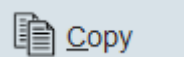
The other options in this dialog box enable you to use or create plot layouts. Details on this can be found in the Data Publishing manual, see **Help | Manuals | Data Publishing**.

The colors of the printed data can be chosen in the User Preferences dialog box. Just enter the command **set** or click **Setup Preferences | More Preferences | Spectra Printing Preferences**.



How to Copy a Dataset Window to Clipboard

Under MS Windows, you can easily copy the dataset window contents to other applications.

To do that, type **copy** or click **Copy to clipboard** . This will copy the dataset window contents to the clipboard. After that you can paste the clipboard contents to any Windows application.

How to Store (Export) a Dataset Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this, TopSpin allows to save the contents of a dataset window in a graphics file of selectable type, e.g. .png, .jpg, .jpeg, .bmp, .emf and .wmf. To do that, click **File | Export...** The resolution of such a screen dump equals the resolution of your screen. Note that when you import a graphics file into another program and resize it you lose information. Therefore, we recommend resampling rather than resize graphics.

3.8 How to Process Data

Since this manual is not a general NMR text book, we assume here that you are familiar with terms like window multiplication, Fourier Transform, phase correction, etc.

Any Fid or a spectrum displayed in a TopSpin window can be processed by:

- Typing a command on the command line, e.g. **ft**.
- Invoking a command from the **Process | Proc. Spectrum** menu.
- Entering an interactive mode by clicking a tool button, e.g. **Process | Adjust Phase**.
- Entering a user defined command (usually an AU or a Python program, see **Help | Manuals | Programming Manuals**).

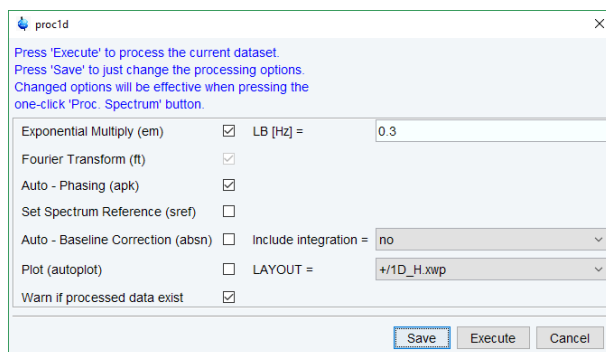
Processing and analysis commands require certain parameters to be set correctly. Most commands in the **Process** or **Analyse** menu, like **wm** and **ftf** open a dialog box showing the available options and required parameters for that command. Other commands such as **em**, **ft**, ... start processing immediately. Before you use them, you must set their parameters from the parameter editor. To do that, enter **edp** or click the **ProcPars** Tab of the dataset window.

If you are a new or occasional user, we recommend processing your data with the TopSpin Processing Guide. This will guide you through the typical sequence of processing steps. To start the Processing Guide, enter **prguide** on the command line.

In *Automatic mode*, the Processing Guide will simply execute each processing command when you click the corresponding button. This requires the processing parameters to be set correctly. In interactive mode (*Automatic mode* unchecked), the Processing Guide will, at each step, open a dialog box offering you the available options and required parameters. For example, the phase correction button offers various automatic algorithms as well as an option to enter interactive phasing mode.

A simple way to process 1D data is the following:

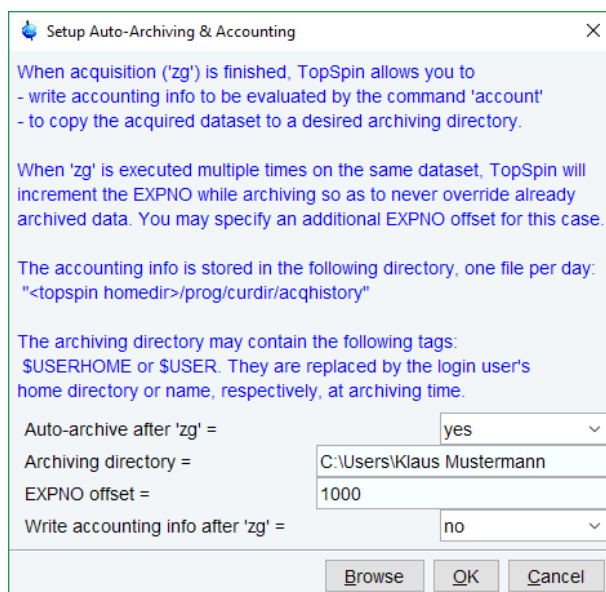
- Click **Process | Proc. Spectrum | Configure Standard Processing** or enter **proc1d** on the command line.
- In the appearing dialog (see below):
 - Enable the desired processing/plotting steps.
 - Set the parameter LB for Exponential multiplication.
 - Select the desired LAYOUT for plotting.
 - Click **Execute**.



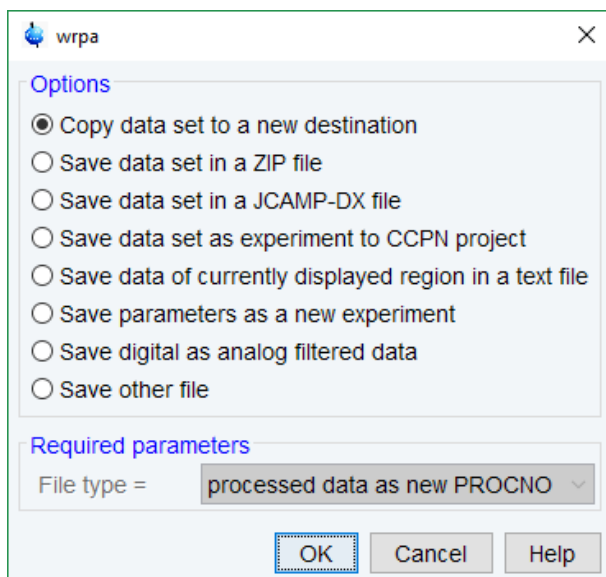
3.9 How to Archive Data

TopSpin provides the following methods for data archiving:

- Automatic archiving of raw data after the acquisition as defined in the setup preferences. Go to **Setup Preferences | Acquisition | Configure accounting & data archiving after zg** and click **Change** to define the archive directory.



- Copying a dataset to a desired destination directory which could for instance be located on a server. Type **wrpa** or click **File | Save As...** or type **Ctrl+ s**.
- Saving a dataset in a ZIP file. A standard Bruker dataset is a directory tree which contains several files. Zipping a dataset stores the entire data directory tree into a single file with the extension **.bnmr.zip**. To zip a dataset, type **tozip** or click **File | Save As...** or type **Ctrl+ s**. To unpack and display a zipped dataset, enter **fromzip**. Note that **.bnmr.zip** files are fully compatible with the well-known PC zip format and can be unpacked with any common unzip utility. Zipping can be applied to 1D, 2D, 3D and 4D data.
- Saving a dataset in JCAMP-DX format. This format is an IUPAC standard, and is available for 1D and 2D datasets. Data and parameters are stored in readable text (ASCII) format. To store data in JCAMP, type **tojdx** or click **File | Save As...** or type **Ctrl+ s**. To convert and display a JCAMP-DX file, type **fromjdx**.



- E-mailing data to a desired destination. Type **smail** or click **File | Send To....** The mailing format is either zip or JCAMP-DX, both of which allow for data compression to keep the transferred data size as small as possible.

3.10 How to Import NMR Data Stored in Special Formats

TopSpin allows to convert various data formats to standard Bruker format for display and processing. Click **File | Open...** and select **Open NMR data stored in special formats**. Then follow the instructions on the screen.

3.11 How to Fit Peaks and Deconvolve Overlapping Peaks

Deconvolution is a useful tool to interpret complex spectra in which the peaks are not fully resolved and clearly visible.

Peaks of a 1D and 2D NMR spectrum can be approximated by a Lorentzian, Gaussian, or a mixture of these line shapes. Overlapping peaks may be deconvolved into a sum of such line shapes.

TopSpin shows the deconvolution result, i.e. peak positions, line widths and integrals on the screen and stores it in the file *dconpeaks.txt*. Furthermore, it switches to multiple display mode to show the original spectrum and the sum of the computed line shapes, superimposed.

To start deconvolution, expand the spectrum on the display to show the peak or peak group of interest. Then type **dcon** or click **Analyse | Line Shapes | Fit Lorentz/Gauss Functions**.

3.12 How to Compute FIDS by Simulating Experiments

TopSpin includes a virtual spectrometer that computes FIDs of any dimension. A real spectrometer excites a sample with high frequency pulses defined by a pulse program and measures the resulting FID. The virtual spectrometer performs this task mathematically by solving the quantum mechanical Liouville equation. The sample must be entered in form of a spin system description. For the computation, the same pulse program and acquisition parameters are taken as for the real experiment. The result is a time domain signal which can

be processed with TopSpin in the same way a measured fid is processed. Techniques such as selective excitation, gradient enhanced spectroscopy, and the handling of mixtures are supported.

To start the virtual spectrometer:

- Enter **nmrsm** on the command line or click **Applications | Simulate | Simulate FID From Pulse Program**.

3.13 How to Add Your Own Functionalities

The TopSpin functionality can be extended with various user defined commands, programs etc.

How to Create Macros

Writing a macro is the simplest way to create a user defined command. Just enter the command **edmac**, create a file, and enter a sequence of regular TopSpin commands and/or Python commands. Save the file under a name of your preference. You have created a new TopSpin command. Just enter its name on the command line to execute it. **edmac** shows a list of all available macros and allows to execute one.

How to Create AU (automation) Programs

Writing an AU program is another way of creating a new TopSpin command. AU programs are more complex and more powerful than macros. They are C-language programs, which may contain C-statements, regular TopSpin commands, and various predefined AU macros and functions. AU programs can perform various tasks such as dataset handling, parameter handling, acquisition, processing, analysis, and printing. Note that AU programs do not support graphics related tasks.

TopSpin is delivered with a large set of Bruker AU programs for data processing and acquisition. Just enter **edau** to see them listed in a dialog box. The easiest way to create a new AU program is to select a Bruker AU program, save it under a new name and modify it to your needs. The chosen name is now available as a new TopSpin command. Alternatively, you can open a new file from the AU dialog box and write your AU program from scratch.

For details on Bruker AU programs and writing your own AU programs, click **Help | Manuals | Programming Manuals | AU Programming**.

How to Create Python Programs

Writing a Python program is yet another way of creating a new TopSpin command. Python is a new generation scripting and object-oriented programming language. Python programs are even more powerful than AU programs. They are easy to use and allow you to execute TopSpin commands, handle NMR data and parameters, generate graphics, and interact with the TopSpin user interface via dialogs, windows etc. To create a Python program, enter the command **edpy**, select a file and insert your Python statements. Graphics and interface features programmed in Python look and work the same as regular TopSpin features.

For details on Python programming, click **Help | Manuals | Programming Manuals | Python Programming**. The examples mentioned there, like **pycmd1**, are delivered with TopSpin. Just enter their names on the command line to execute them.

The Python dialog window is also available from the TopSpin menu:

Click **File | Open...** and select **Open other file | Python program**.

3.14 How to Automate Data Acquisition

TopSpin provides special user interfaces for automation, walk-up, bio-molecular experiments, etc.

To open IconNMR



- Click **Acquire | More | IconNMR Automation**

or







- enter **iconnmr**.

4 Dataset Handling

4.1 The Browse and Search Window

The Browse and Search window appears at the left of the TopSpin window and can be shown/hidden with **Ctrl+d** or by clicking the arrow buttons  at the upper right of the browser or with the **Toggle Perspective** button .

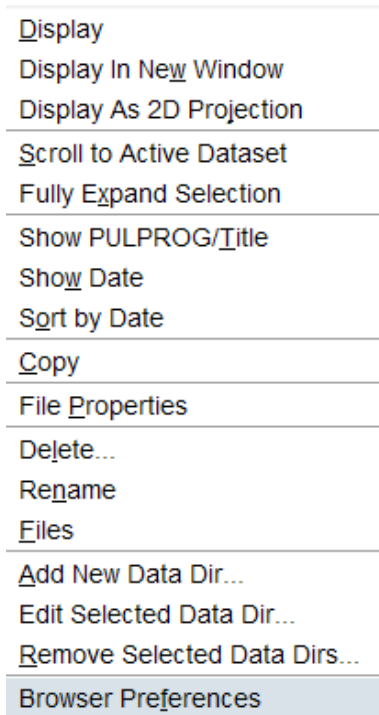
The Browse and Search window provides tabs as:

1. Data Browser tab  **Data**
2. History Browser tab 
3. Groups tab 
4. Alias tab 
5. Dataset Switcher tab 
6. Experiment Selector Library tab 

Note that some of the tabs are visible only when the checkbox option is checked in the preferences window.

Note that the History Browser, Dataset Switcher and Experiment Selector Library tab are already explained in chapter [The TopSpin Interface \[13\]](#).

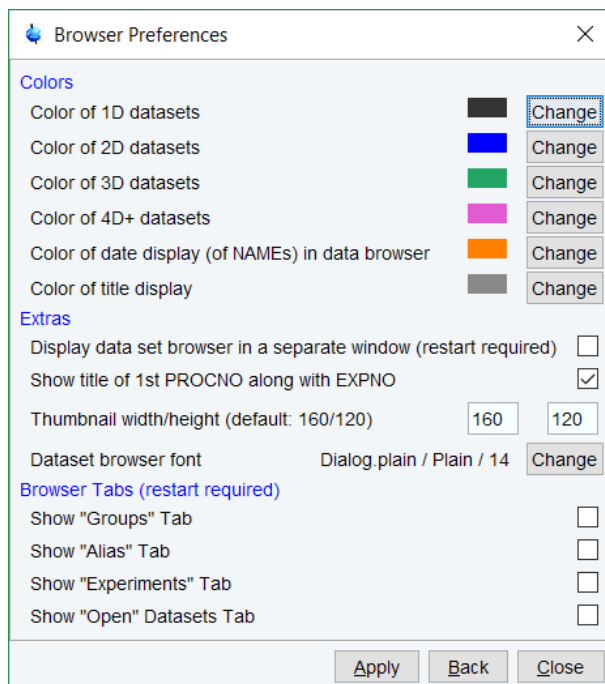
- Right-click in the Browse and Search window and in the list, select **Browser Preferences**.



In the Browser Tabs group check or uncheck

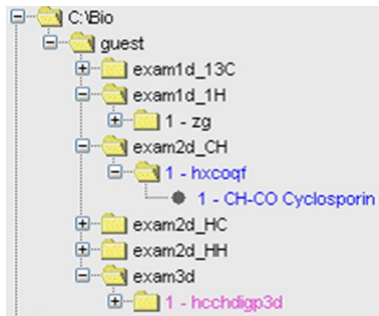
1. Show Groups Tab
2. Show Alias Tab
3. Show Experiments Tab
4. Show Open Datasets Tab.

Then restart TopSpin.



The Data Browser Tab

The browser shows data directory trees and allows to expand and collapse their elements. The figure below shows the browser with three top level data directories and one dataset fully expanded.



The dimensionality of the data is indicated with different colors:

1. *Black* for 1D data.
2. *Blue* for 2D data.
3. *Green* for 3D data.

Note that the colors can be changed in the Browser Preferences window.

Furthermore, the browser displays:

1. The pulse program with the dataset EXPNO (e.g. *1 - hxcoqf* in the figure above).
2. The title with the dataset PROCNO (e.g. *CH-CO Cyclosporin* in the figure above).

Note that the displayed pulse program is the:

1. Status pulse program if an acquisition has been done (raw data exist).
2. Setup pulse program if no acquisition has been done (raw data does not exist).

The display of title and pulse program can be switched off (see table below).

The context menu with right mouse click displays the following list:

Display	=> Display in current dataset window.
Display in New Window	=> Display in new (additional) dataset window.
Display As 2D Projection	=> Display 1D dataset as projection of 2D dataset. Requires that a 2D dataset is loaded in the active dataset window.
Scroll to active dataset	=> Scroll in browser to PROCNO of dataset in active dataset window. This also expands the dataset, see option below.
Fully Expand Selection	=> One or several datasets may be selected and will be expanded.

Show PULPROG/Title	=> Switch pulse program/title display on/off.
Show Date	=> Show acq. date (expno) or last mod. date (name).
Sort by Date	=> Sort data by last modified date.
Copy	=> Copy dataset entry to clipboard.
File Properties	=> Show dataset properties.
Delete...	=> Delete selected entry (name, expno or procno).
Rename	=> Rename dataset name, expno or procno.
Files	=> Show files in selected entry (expno or procno).
Add New Data Dir...	=> Add new top-level data directory.
Edit Selected Data Dir...	=> Displays a window to select a directory and to enter an alias.
Remove Selected Data Dirs...	=> Remove selected top-level data directory.

The Groups Tab

Clicking the **Groups** tab displays the list of user defined dataset groups. Here you can create, modify and display groups of datasets. Defining a group is useful if you work on projects where each project involves multiple datasets. It allows to easily organize your projects and access all data belonging to a certain project.

- Right-click to display the following list:

Display	=> Display selected dataset(s) in active window.
Display In New Window	=> Display selected dataset(s) in new window.
Display Group	=> Display all datasets in group in new windows.
Add Selected Dataset window	=> Add selected dataset window to selected group.
Add all Open Dataset windows	=> Add all open dataset windows to selected group.
Update Window Bounds & Display Limits	=> Update window bounds and display regions.
Remove Selected Datasets From Group	=> Remove selected datasets from group.
Collapse All Groups	=> Collapse all groups.
Toggle Dim/Pulprog./Title	=> Show/hide dimension, pulse program, title.
Add new Dataset Group	=> Add a new (empty) dataset group to the list.
Close All Group Windows	=> Close all dataset windows of selected group.
Process Selected Datasets	=> Process selected dataset with serial processing.
File Properties	=> Show file properties of selected dataset.
Files	=> Show file list of selected dataset.
Copy	=> Copy pathnames of selected data to clipboard.

Note that a group not only defines the datasets involved, but also their dataset window positions and dimensions and the displayed region of each spectrum.

The Alias Tab

Clicking the **Alias** tab displays the list of user defined alias names for datasets. Just right-click any entry to define, remove or interpret alias names.

D <u>is</u> play
Display In New <u>W</u> indow
File <u>P</u> roperties
<u>F</u> iles
Define Alias For Data In Selected Window
List Selected Alias
List All Aliases
Remove Selected Aliases...
List Available Alias Commands

The Experiment Library Tab

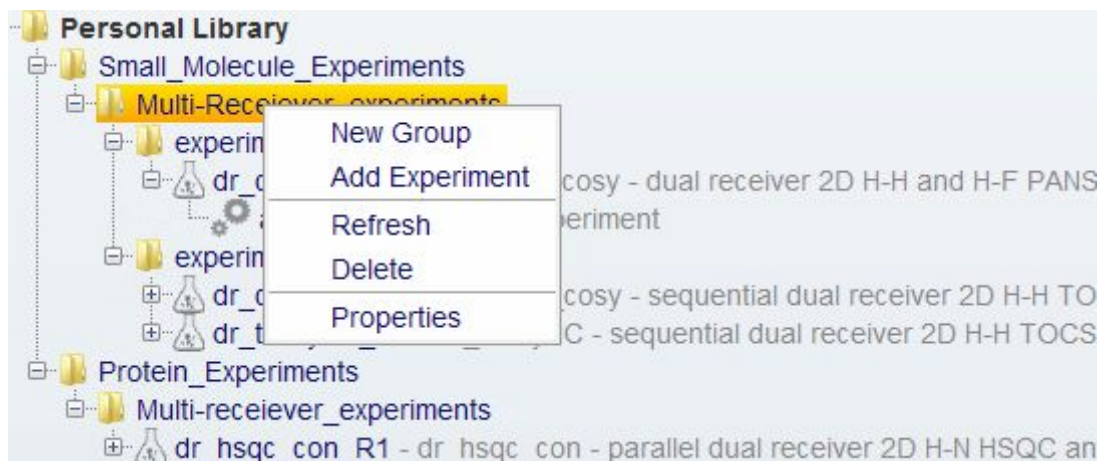
The Experiment library tab provides easy access to the vast experiment library of standard experiments that is available in the standard release of TopSpin. It is also a tool that allows the user to personalize his most frequently used experiments into a separate library.



The experiments are grouped according to their application areas, such as small molecules, proteins or drug discovery. Further grouping into sub-groups according to the type of experiments may occur depending on the number of experiments that is available within a group. For instance, the protein experiments are grouped into backbone experiments, side-chain experiments and similar. Some experiments, for instance the multi-receiver experiments, may also have an associated action item, in this case for adding a child experiment. The action items are au-programs that reside in the standard au-program library.

The Personalized Library initially is empty and can be populated by simply dragging and dropping individual experiments or groups from the standard TopSpin Library. Alternatively, the experiments can be added manually:

- Select the desired group of experiments.
- Right-click and in the list, select **Add Experiment**.



How to Open the Data Browser in a Separate Window

The browser can be opened in a separate window as follows:

- Click **Setup Preferences | More Preferences | Browser Preferences | Change**
- Check **Display dataset browser in a separate window**.

You must restart TopSpin for the change to take effect.

How to Put the Focus in the Data Browser

- Click **F2**
- or
- Click inside the data browser.

How to Select Folders in the Browser

To select a folder:

- Left click the folder button.
- or
- Click arrow-up/down while the focus is in the browser.

To select multiple folders:

- Hold the **Ctrl** key and left-click multiple folders to select them.
- or
- Hold the **Shift** key and left click two folders to select these two and all in between.

How to Expand/Collapse a Folder in the Browser

To expand a collapsed folder:

- Click the **+(plus)** button to the left of the folder button.
- or
- Double-click the folder button.
- or
- Hit the **Right-Arrow** key while the folder is highlighted.

To fully expand a collapsed folder:

- Right-click the DIR, NAME or EXPNO node and choose **Fully Expand Selection**.

To collapse an expanded folder:

- Click the **–(minus)** button to the left of the folder button.

or

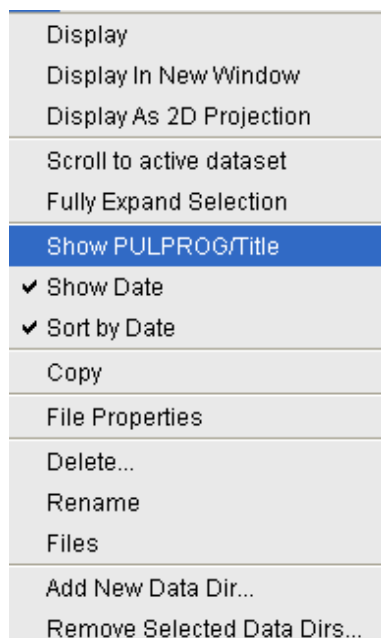
- Double-click the folder button.

or

- Hit the **Left-Arrow** key while the folder is highlighted.

How to Show/Hide Pulse program and Title in the Data Browser

- Right-click the data name folder button and in the list, select **Show PULPROG /Title**.



How to Display Dataset Dates in the Browser.

- Right-click the data name folder button and select **Show Date**.

The last modified date is displayed the right of the dataset NAME, whereas the acquisition date is shown to the right of the dataset EXPNO:



How to Suppress the Display of the TopSpin Data Examples Directory in the Data Browser Window

By default, the browser shows the TopSpin installation directory with the Bruker example datasets. To suppress this feature, click **Setup Preferences | Administration items** and uncheck **Show TopSpin data examples directory in data browser**.

How to Add, Remove or Interpret Alias Names

To add an alias name:

- Click the **Alias** tab in the browser (must be enabled in the Browser Preferences).
- Right-click in the Alias table and in the list, select **Define Alias For Data In Selected Window**.
- Enter an alias name in the appearing dialog box and click **OK**. Note that alias names must begin with a letter.


To remove an alias name:

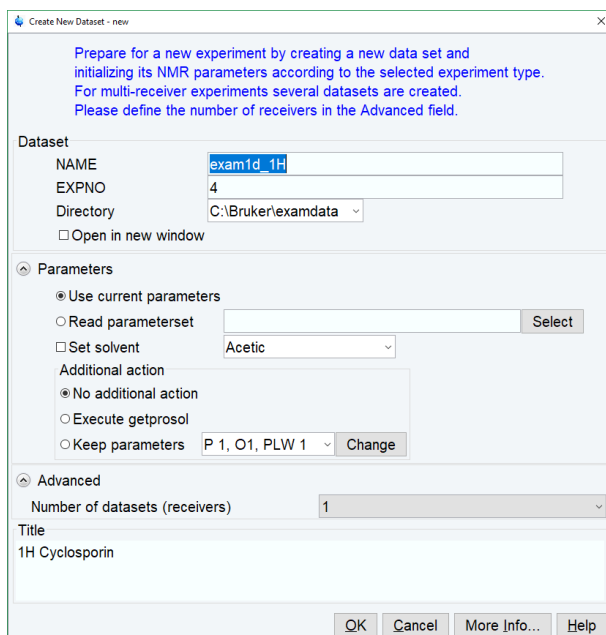
- Right-click the alias name.
- In the list select **Remove selected aliases...** from the popup menu (see the figure below).

Furthermore, the popup menu offers entries to display the dataset, list its properties and display the full dataset specification.

4.2 Creating Data

How to Create a New Dataset

- Click **File | New [new, Ctrl+ n]** or click the  Create Dataset button in the upper toolbar.
- Specify the dataset *name*, *expno*, *dir* and *user* in the appearing dialog box. If one or more datasets are open, the fields are initialized with the current dataset (see the figure below).
- Click the **down-arrow** of the **Solvent** box and choose a solvent from the list or type a solvent name.
- Click the down-arrow of 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**.



A dataset will be created and initialized with the parameters of the chosen experiment. No FID or spectrum is available yet. They can be created by data acquisition and data processing, respectively.

4.3 Opening Data

TopSpin allows to open data in several ways, from the browser, the menu, the Windows Explorer or the command line. Furthermore, data can be opened:

1. In an existing dataset window replacing the current dataset.
2. In a dataset window which is in multiple display mode, being superimposed on the current spectra.
3. In a new dataset window, which becomes the active window.

Note that if a dataset is already displayed in one window and it is opened in a second existing window, it still replaces the dataset in the latter one. As a result, the same dataset will be displayed in two windows (see also command **reopen**).

How to Open Data from the Browser

In the browser:

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

or

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

or

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

or

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

or

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

or

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

or

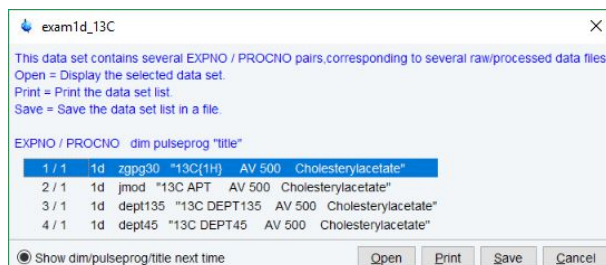
- Hold the **Ctrl** key and left-click several datasets to select them or hold the **Shift** key and left-click two datasets to select these two and all in between. Then right-click one of the selected datasets and choose **Display** from the popup menu. A new window will be opened showing the selected datasets in multiple display mode. However, if the current window was already in multiple display mode, the selected spectra will be superimposed on the currently displayed spectra.

How to Automatically Select the first expno/ procno of a dataset

If you open a dataset from the Browser by clicking a data *name*, there might be more than one *expno* and/or *procno* available. By default, TopSpin then opens a dialog box from which you can select the desired *expno/procno* combination (see the figure below). Clicking *Open* will open the selected dataset, whereas clicking *Print* will print the displayed dataset list.

You can, however, configure TopSpin to automatically open the first available *expno/procno* combination:

- Click **Preferences [set]**.
- Click **Miscellaneous** in the left part of the dialog box.
- Uncheck the item **Display EXPNO/PROCNO list when opening data..**
- Click **Apply** and **Close**.



Note that the command **rel** also opens the dialog shown in the figure above, showing the available EXPNO's under the current dataset. Similarly, **repl** shows the available PROCNO's under the current dataset EXPNO.

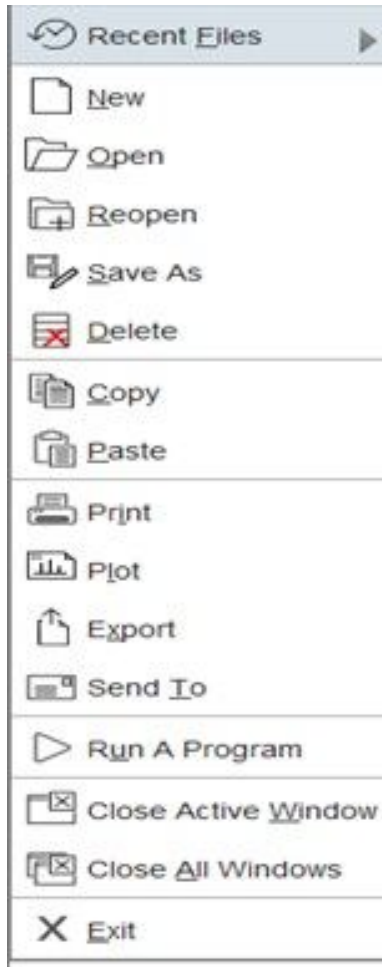
How to Open Data from the TopSpin menu

To open a dataset:

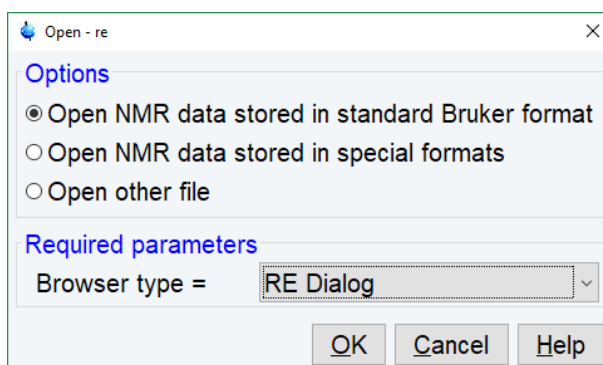
- Click the **File** button in the upper toolbar.

or

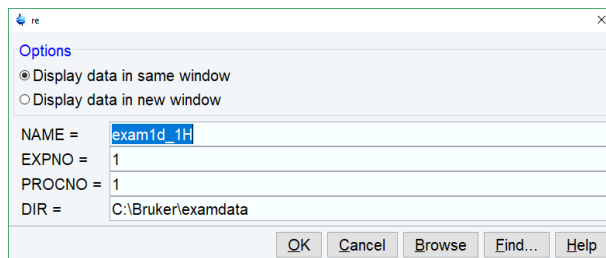
- Click **File | Open [open, Ctrl+ o]**.



- Select the option **Open NMR data stored in standard Bruker format**.
- Select the browser type **RE Dialog**.
- Click **OK**.



- Specify the dataset *name*, *expno* etc.
- Click **OK**.



Note that the dataset specification consists of the five variable parts of the data directory tree, in this case:

```
C:\bio\data\guest\nmr\ exam1d_1H\ 1\data\ 1
```

The text boxes are initialized with the dataset in the current dataset window.

How to Open Data from the Explorer, Konqueror or Nautilus

You can open a dataset from the Windows Explorer as follows:

1. From the Windows **Start** button. Navigate to the data *name*, expno or procno.
or
2. By entering the command **expl** in TopSpin. The Explorer shows the contents of the current dataset procno directory. Navigate to the desired data *name*, expno or procno.
expl can also be used with the argument **top** to open the TopSpin installation directory, **home** to open user home directory or with an absolute pathname to open that directory.
 - The command **expl spect** opens the Explorer in **<tshome>/conf/instr/ current instrument>**
 - The command **expl prop** opens the Explorer in the user's properties directory **User-HOME/topspin<name_of_PC>/prop** By entering **expl <illegal argument>** all available options are shown.

Now you can open a dataset with:

Drag & Drop:

- Click-hold a dataset *name* or any of its sub-folders or files and drag it into the TopSpin data area or dataset window

or

Copy & Paste:

- Right-click a dataset and in the list, select **Copy**.



- Click **File | Paste [paste]**: 

How to Open Datasets from the Command Line

- Enter **re**.
- Specify a dataset in the appearing dialog box.
- Click **OK**.

To open a new procno of the current dataset:

- Enter **rep**.
- Specify a *procno* in the appearing dialog box.
- Click **OK**.

To open a dataset in a new window:

- Enter **rew**.
- Specify a dataset in the appearing dialog box.
- Click **OK**.

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

- Enter **repw**.
- Specify a *procno* in the appearing dialog box.
- Click **OK**.

To open a data browser and read a dataset from there:

- Enter **reb**.
- Select a dataset from the appearing dialog box.
- Click **Display**.

Note that **re**, **rep** and **reb**:

1. Replace the data in the currently selected dataset window.
2. Open the data in a new window when they are used after typing **Alt+ w n**.
3. Add the data in the currently selected window if this is in multiple display mode, whereas **rew** and **repw** always open the dataset in a new window.

TopSpin allows to open datasets stored in the following directories structures:

```
<mydata>/<dataname>/<expno>/pdata/<procno>
```

- Enter **reb** on the command line, browse to the desired dataset and click **Display**.

Open the Operating System File Browser, browse to the desired dataset and open it in TopSpin with **Copy & Paste** or **Drag & Drop**.

Note that this will create a copy of the dataset in the standard TopSpin data path:

```
<tshome>/data/<user>/nmr/<dataname>/<expno>/pdata/<procno>
```

where <user> is the current internal TopSpin user. This copy can be processed, deleted or overwritten, even if the original dataset is write-protected. The original dataset is left unchanged.

How to Open Special Format Data

Apart from the standard Bruker data format, TopSpin can read and display various other formats:

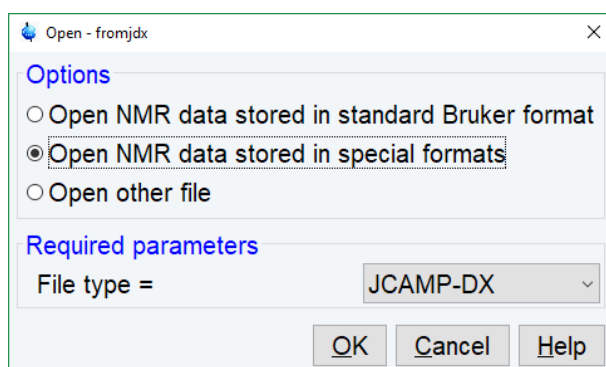
- Click **File | Open [open, Ctrl+ o]**.
- Select the option **Open NMR data stored in special formats**, select the desired file type (see the figure below) and click **OK**.

A dialog will appear which depends on the chosen file type. Just follow the instructions on the screen.

The following file types are supported:

1. JCAMP-DX - Bruker TopSpin data stored in JCAMP-DX format. Note that the TopSpin data format is identical to the XWIN-NMR data format.
2. Zipped TopSpin - Bruker TopSpin data stored in ZIP format.
3. WINNMR - Bruker WINNMR data.
4. A3000 - Bruker Aspect 3000 data.
5. VNMR - data acquired on a Varian spectrometer.
6. JNMR - data acquired on a Jeol spectrometer.
7. Felix - 1D data, FID or spectrum, which are stored in FELIX format.

Note that in all cases, the data are stored in a single data file which is unpacked/converted to standard Bruker format, i.e. to a data directory tree.



How to Open a ZIP or JCAMP-DX file from the Windows Explorer

Data stored in ZIP or JCAMP-DX format can also be opened directly from the Windows Explorer. You can do that in one of the three following ways:

Drag & drop

- Click-hold a file with the extension *.dx* or *.zip* and drag it into the TopSpin data area or dataset window.

Copy & paste

- Right-click a file with the extension *.dx* or *.zip* and in the list, select **copy**.
- Click **File | Paste [paste]**.

Associate JCAMP-DX files with a script

- Create a file with the extension *.cmd* (e.g. *jcamp.cmd*) with a text editor.
- Enter `<tshome>\prog\bin\sendgui.cmd fromjdx %1`
- Store the file.
- Open the Explorer and find the JCAMP-DX file.
- Right-click the filename and choose **Open with | Choose program | Browse**.
- Find and select the script and click **OK**.

Now, every file with the extension *.dx* will automatically be opened in TopSpin when double clicked.

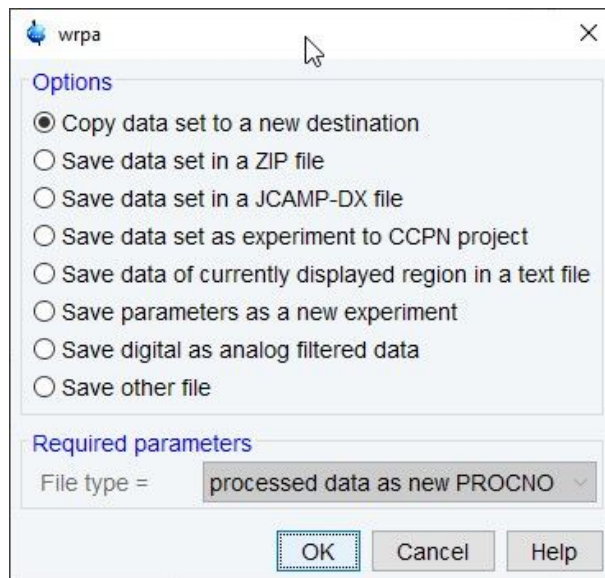
4.4 Saving/Copying Data

How to Save or Copy Data

You can save the current dataset as follows:

- Click **File | Save [Ctrl+ s]**.

This will open a dialog box:



- Select an option and, if applicable, a file type.
- Click **OK** to execute the option.

The options correspond to the following command line commands:

wrpa - copies the current data to a new data *name* or *expno*.

toccpn - convert experiment information to ccpn format.

tozip - convert a dataset of any dimension to ZIP format.

tojdx - convert a 1D or 2D dataset to JCAMP-DX format.

totxt - convert a 1D or 2D dataset text format.

wpar - write parameter set.

convdta - save digitally filtered data as analog filtered data.

wrp , **wra** , **genfid** , **wmisc** - write various files.

How to Save an Entire Dataset

- Click **File | Save [Ctrl+ s]**.
- Select the option **Copy dataset to a new destination [wrpa]** and click **OK**.
- Specify the dataset variables and click **OK**.

How to Save Processed Data

- Click **File | Save [Ctrl+ s]**.
- Select the option **Save other file**.

- Select File type **Processed data as new procno** [wrp] and click **OK**.
- Enter a processing number (procno) and click **OK**.

How to Save Acquisition Data

- Click **File** | **Save** [Ctrl+ s].
- Select the option **Save other file**.
- Select File type **Acqu. data as new expno** [wra] and click **OK**.
- Enter an experiment number (expno) and click **OK**.

How to Save Processed Data as Pseudo Raw Data

- Click **File** | **Save** [Ctrl+ s].
- Select the option **Save other file**.
- Select File type **1r/1i as fid** [genfid] or **2rr/2ii as ser** [genser].
- Click **OK**.
- Enter a destination expno.
- Click **OK** (optionally, you can specify further data path specifications).

4.5 Deleting Data

How to Delete a Specific Dataset

- Right-click the data *name*, *expno* or *procno* in the browser, then click **Delete...**

A confirmation dialog will appear. Just click **OK**, if you are sure you want to delete.

Note that TopSpin does not allow you to delete the last available dataset, e.g. the last *procno* under an *expno*, the last *expno* under a *name* or the last *name* under a *user*.

How to Delete Types of Datasets

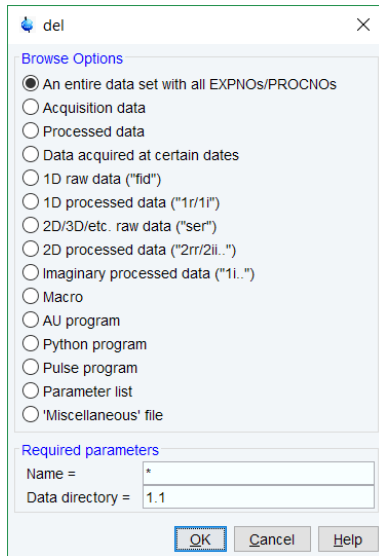
To delete certain types of data like 1D raw data, 2D processed data etc.:

- Click **File** | **Delete...**

or

- Enter **delete** on the command line.

Note: To use this function at least one dataset must be open!



- Select a data type option

For each option, the corresponding command appears in the title of the dialog box. These commands (**del**, **dela**, **delp**, **deldat**, **delf**, **dels**, **delser**, **del2d**, **deli**, **delmac**, **delau**, **delpy**, **delpul**, **delist**, **delmisc**) can also be used to delete data from the command line.

- Specify the **Required parameters**

Note that you can use the wildcards:

- Asterix (*) for any character and any number of characters.
- Question mark (?) for any single character.

- Click **OK**

A dialog box will appear showing the matching datasets. For example, if you select the option **An entire dataset ...**:

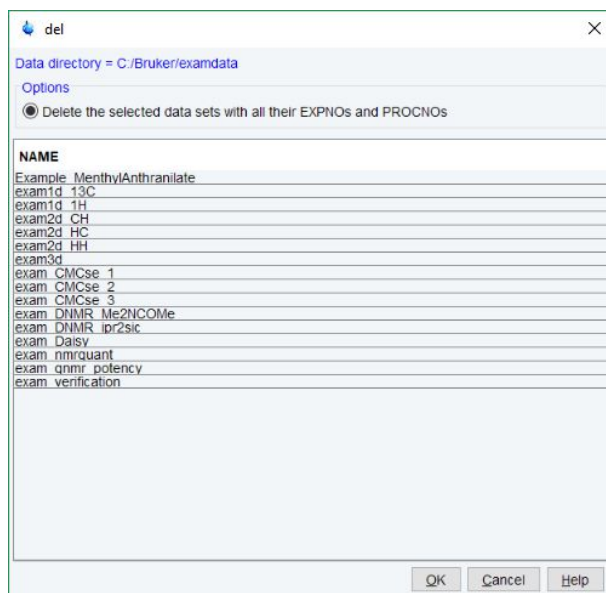
- Select dataset entries for deletion (selected entries are highlighted). To select multiple entries: click them holding the **Shift** or **Ctrl** key.
- Click **OK** to delete the entire data directory.

If you select the option **Acquisition data** or **Processed data**, you can choose between deleting the data files only and deleting the entire expno or procno directory, respectively:

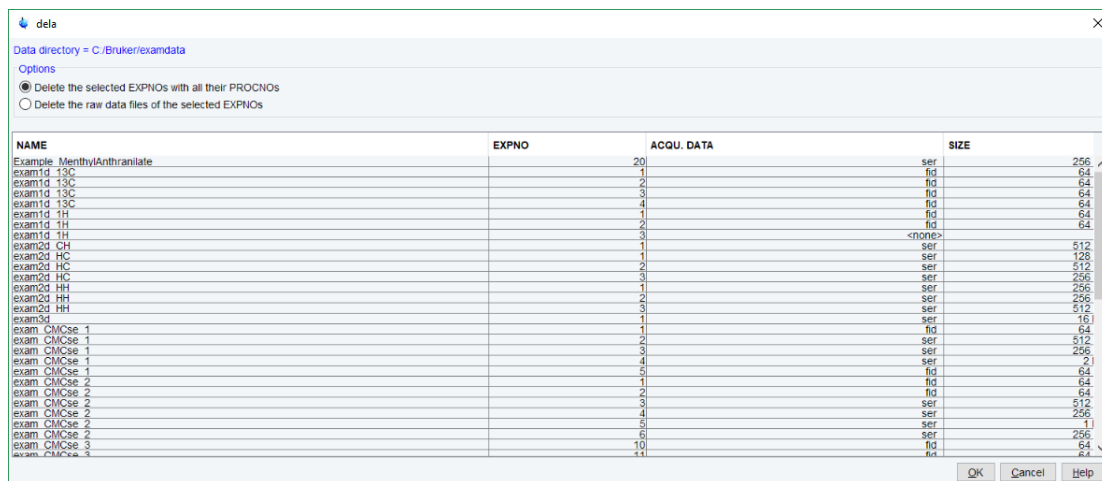
Browse option	Command
An entire dataset with all EXPNOs/PROCNOs	del
Acquisition data	dela
Processed data	delp
Data acquired at certain dates	deldat
1D raw data	delf
1D processed data	dels
2D/3D/etc. raw data	delser

Browse option	Command
2D processed data	del2d
Imaginary processed data	deli
Macro	delmac
AU program	delau
Python program	delpy
Pulse program	delpul
Parameter list	delist
Miscellaneous file	delmisc

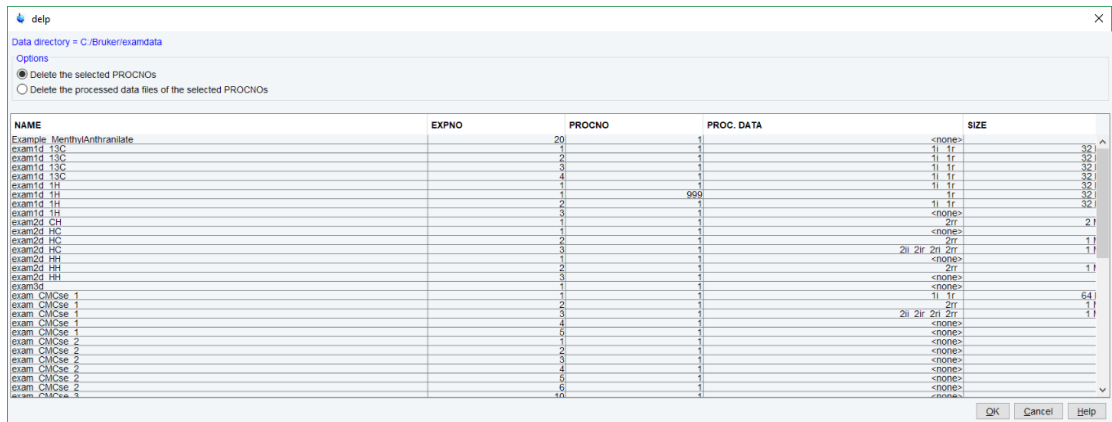
Selection **An entire dataset with all EXPNOs/PROCNOs** opens the del window:



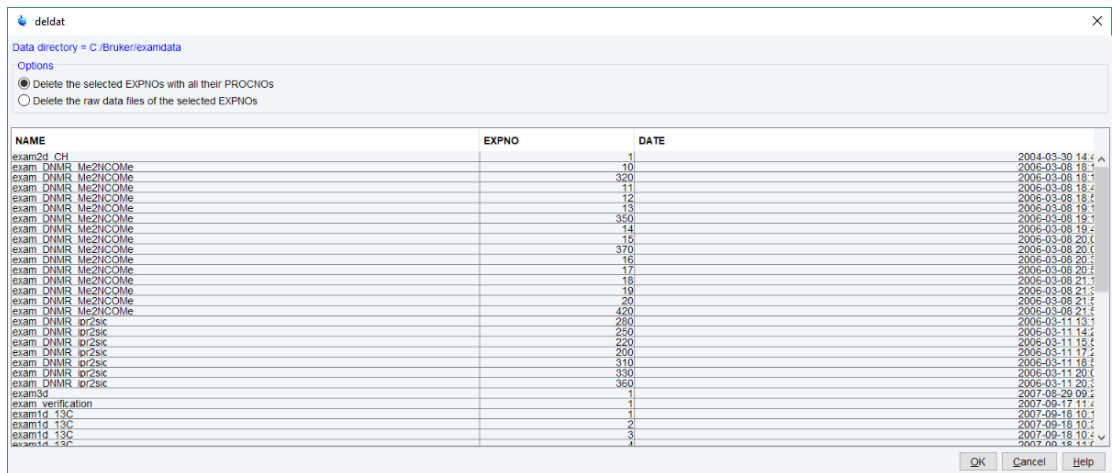
Selection **Acquisition data** will open the dela window:



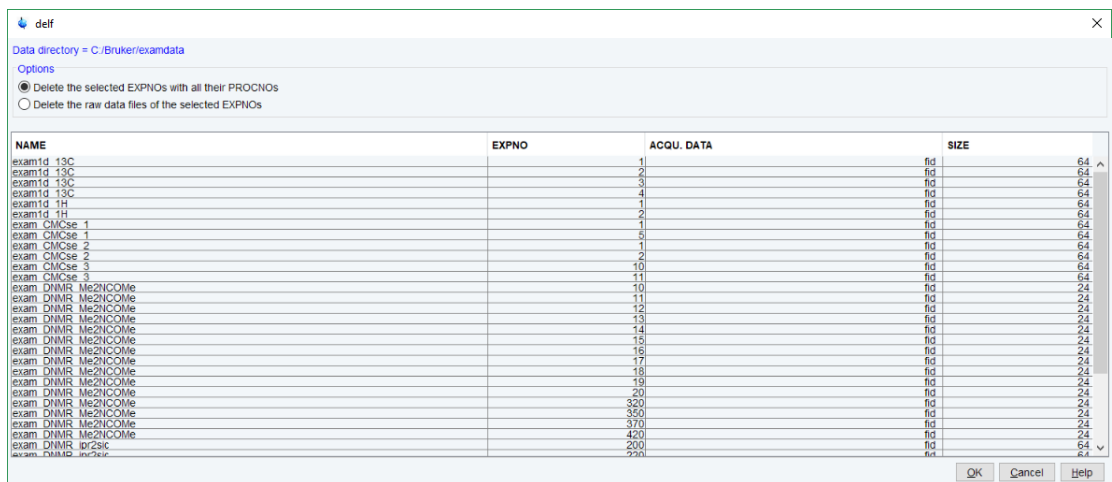
Processed Data will open the delp dialog:



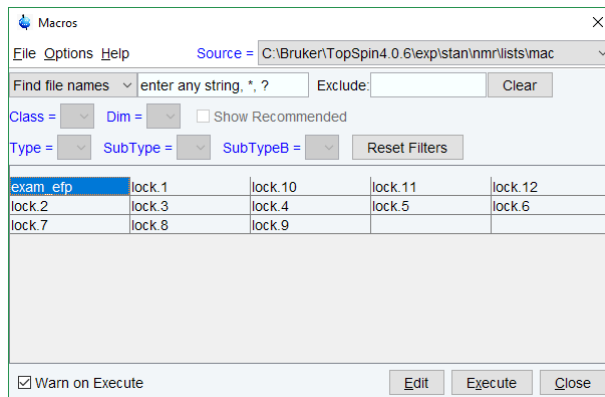
Data acquired at certain dates:



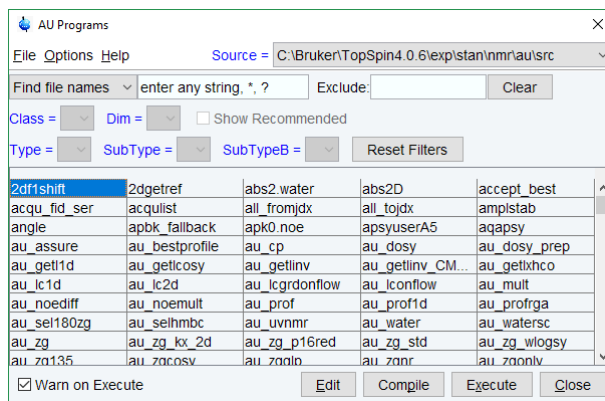
Delete 1D raw data will open the delf dialogue:



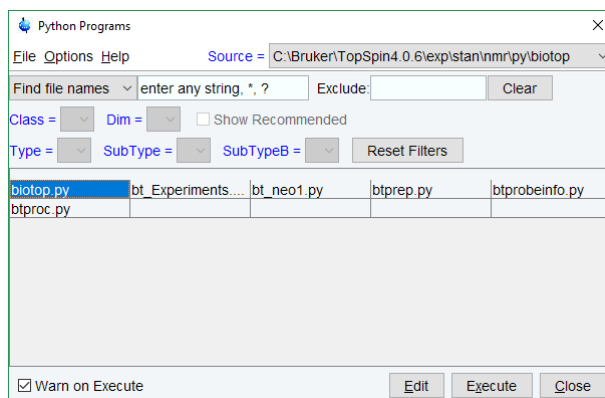
Macros



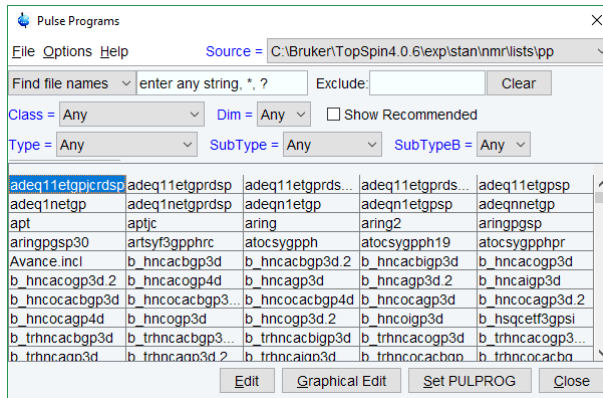
AU Programs



Python Programs



Pulse Programs



4.6 Renaming Data

How to Rename a Specific Dataset

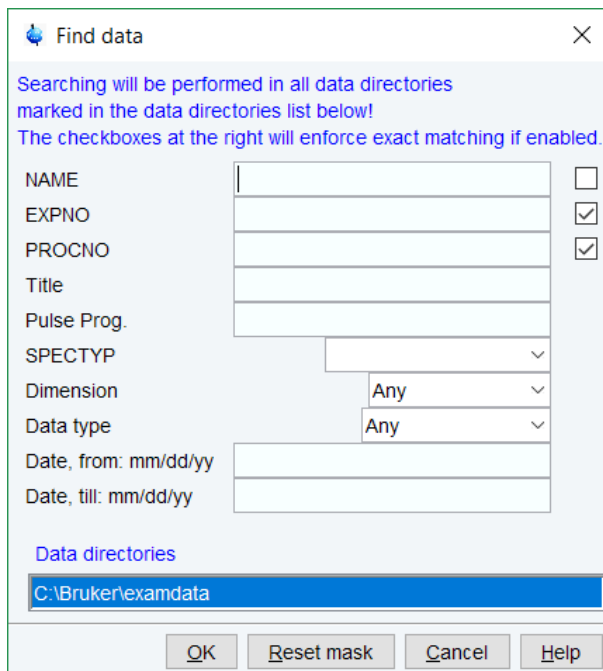
- Right-click the dataset name, expno or procno in the data browser, then click **Rename...**
- In the appearing dialog: Enter the new dataset name, expno or procno.
- Click **OK**.

4.7 Searching/Finding Data

How to Find Data

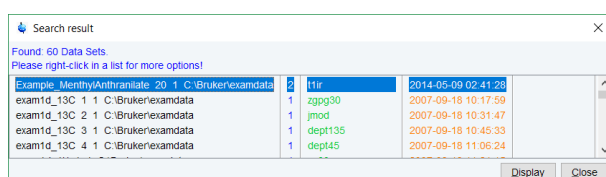
You can find TopSpin data according to various criteria. To start searching:

- Enter **Ctrl+f** to open the **Find data** window:



- Enter the search items in the upper part of the dialog. Note that:

1. There will be searched for items containing the specified string.
 2. Exact matching is performed for dataset variables, NAME, EXPNO, PROCNO and USER, if the checkboxes at the right are enabled.
 3. The search is restricted to data created between the specified dates. Note that this refers to the acquisition date.
 4. The **Reset mask** button allows to reset the default criteria.
- Select the **Data directories** to be searched in the lower part of the dialog. If no directories are selected, all will be searched.
 - Click **OK** to start the search. A list of data that fulfill the defined criteria will appear:



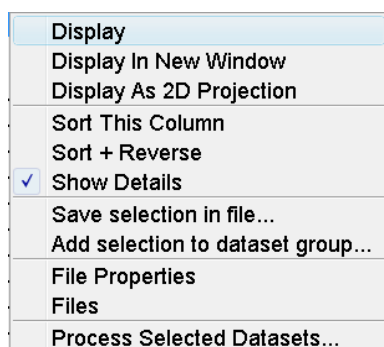
Note that on exiting TopSpin, the search criteria will be reset to default.

How to Display one of the Found Datasets

In the search result window (see figure above):

- Click one or more datasets to select them.
- Click **Display** to display the selected dataset(s) in the current dataset window. If multiple datasets are selected, they are displayed in a new dataset window in multiple display mode.

The search result window offers a right-click context menu with various options:



Display

Display the selected dataset(s) in the current dataset window. If multiple datasets are selected, they are displayed in the same dataset window in multiple display mode. Equivalent to clicking the **Display** button or pressing **Enter**.

Display in New Window

Display the selected dataset(s) in a new window. If multiple datasets are selected, they are displayed in the one new dataset window in multiple display mode.

Display as 2D Projection

Display the selected dataset as a projection of the current 2D dataset. A dialog will appear allowing you to choose F1-projection, F2-projection or both. If multiple datasets are selected, only the first one is considered. If the current dataset is not a 2D dataset, nothing happens.

Sort this Column

Sort the selected column in ascending order.

Sort + Reverse

Sort the selected column in descending order.

Save Selection in file...

Save the list of selected datasets in a text file. First opens a file dialog where you can select or specify a filename. The saved dataset list can, for example, be used for serial processing (command **serial**, see also **Process Selected Datasets** below).

Add selection to dataset group...

Selected datasets can be defined as dataset group.

File properties

Show main dataset parameters like *Dimension*, *Pulse program*, *Acquisition Date*, *Nuclei*, *Spectrometer frequency* and *Solvent*.

Files

Show the files in the processed data directory of the selected dataset.

Process Selected Datasets

Perform serial processing on the selected datasets. Opens a dialog where you can change or edit the dataset list and specify the command, macro or Python program to be executed (starts the command **serial**).

The **Close** button allows to close the search result dialog.

4.8 Handling Data Files

How to List/Open the Current Dataset Files

A Bruker dataset is represented by a directory tree which contains files in the *expno* and *procno* subdirectories. These files contain the actual data, parameters, lists etc.

- Right-click inside the dataset window and in the list, select **Files**.

If the spectrum is displayed, the files in the *procno* subdirectory are shown. If the **Fid** is displayed, the files in the *expno* subdirectory are shown.

- Select a file and click **Open** to view its contents.

Note that this only makes sense for ascii files.

How to List/Open the current Dataset Files in the Windows Explorer

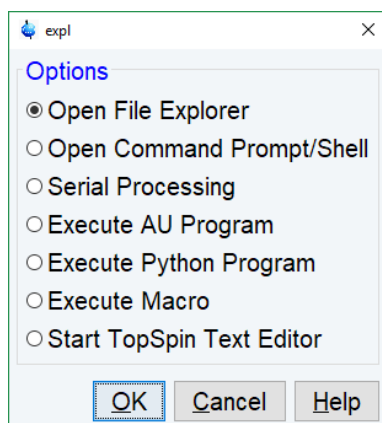
To list the current dataset files in the Windows Explorer:

- Click **File | Run a Program**
- Select **Open file explorer [expl]** in the appearing dialog box.
- Click **OK**.

Alternatively, you can enter the command **expl** on the command line. The Windows Explorer will be opened showing the processed data files (the files in the procno directory) of the current dataset. Under Linux a Web browser like KDE Konqueror or Gnome Mozilla will be opened.

To open a file:

- Double-click the file or right-click the folder icon and select **Open**.



If TopSpin data area contains no datasets, the **expl** command opens the Explorer showing the users home directory. When entered on the command line, **expl** can also be used with the argument **top** to open the TopSpin installation directory, **home** to open user home directory or with an absolute pathname to open that directory.

5 Parameter Handling

5.1 Processing Parameters

Processing parameters can be set/changed in three different ways:

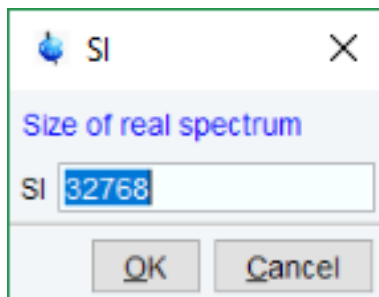
1. From the parameter editor: click the **ProcPars** tab or enter **edp**.
2. From the command line: e.g. enter **si**.
3. From a command dialog box: e.g. **wm**.

How to Set a Processing Parameter from the Command Line

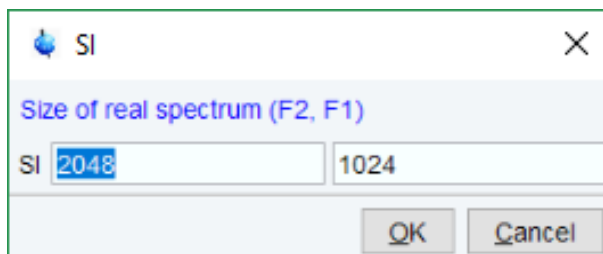
Enter the parameter name on the command line. For example, to set the size:

- Enter **si**.

For 1D data, the following dialog box will appear:



For 2D data, the following dialog box will appear:



- Specify the desired value(s), e.g. **32768** or **32k**.
- Click **OK**.

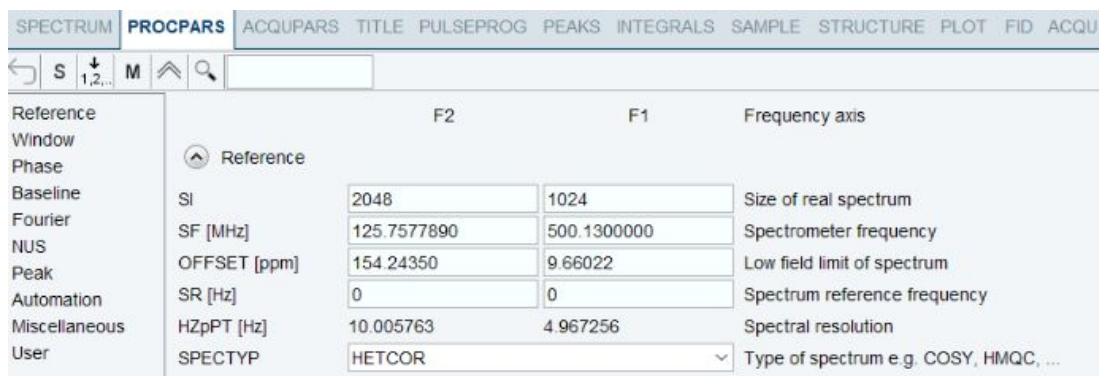
How to Set Processing Parameters from the Parameter Editor

To open the processing parameter editor:

- Click the **ProcPars** tab in the Tab bar of the dataset window.






or

- Enter **edp** on the command line.




At the left of the parameter editor window you will see a list of parameter sections.

The processing parameter editor supports the following functions:

- Collapse/expand a parameter section by clicking the  button. Note that the section Window function is collapsed.
- Collapse/expand all parameter sections by clicking the large  button of the dataset window toolbar.
- Enter (part of) a parameter name in the search field and click .
- Click a parameter section, e.g. Phase at the left of the dialog box. The section becomes highlighted and the corresponding parameters will appear in the right part of the dialog box.
- Click in a parameter field, e.g. PHC0, to set the parameter value.
- Click  right of parameters like AUNMP to open a list of the corresponding programs/lists.
- Click **Edit Processing AU program**  to open the current program/list with an editor
- Hit the **Tab** key to jump to the next parameter field.
- Hit **Shift + Tab** to jump to the previous parameter field.
- Use the scroll bar at the right of the dialog box to move to parameters further up or down in the dialog box.

How to Undo the Last Processing Parameter Change


- Click  Undo last parameter change.

How to Display Processing Status Parameters


- Click  Show processing status parameters.

Note that the command **dpp** opens the parameter editor and automatically shows the status parameters.

How to Switch to Maxent parameters

- Click  Switch to Maxent parameters.

How to Change Processed Data Dimensionality

- Click  1,2,... Change data dimensionality.

This changes the number of parameter columns and value of the processing parameter PPARMOD. TopSpin supports data dimensionalities up to 8D.

The parameter editor does not allow you to modify status parameters. Processing status parameters reflect the status of the processed data and are used for further processing, display or plotting. Changing them can make the dataset inconsistent. In rare cases, however, it can be useful to change a status parameter and TopSpin allows to do that from the command line. If, for instance, you want to change the F1 status parameter MC2 of a 2D dataset, enter:

s mc2

Note that the command **s** is used for 1D, 2D and 3D dataset. TopSpin automatically recognizes the dimensionality of the data and displays the parameter in all relevant dimensions. Note that, for example, the parameter MC2 only exists in F1.

5.2 Acquisition Parameters

How to Set Acquisition Parameters

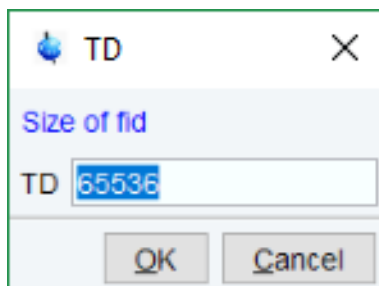
Acquisition parameters can be set/changed as follows:

1. From the parameter editor: click the **AcquPars** tab or enter **eda**.
2. From the command line: e.g. enter **td**.
3. From the interactive parameter adjustment window (enter **gs**).

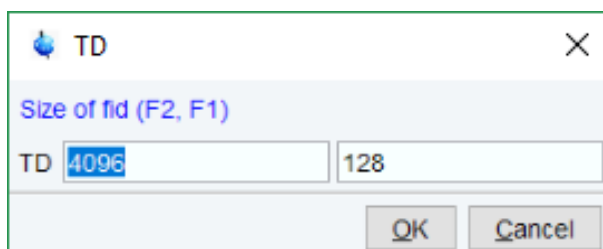
How to Set an Acquisition Parameter from the Command Line

Enter the parameter name on the command line. For example, to set the time domain size:

- Enter **td** for 1D data, the following dialog box will appear:



For 2D data, the following dialog box will appear:



- Specify the desired value(s), e.g. **65536** or **64k**.
- Click **OK**.

How to Set Acquisition Parameters from the Parameter Editor

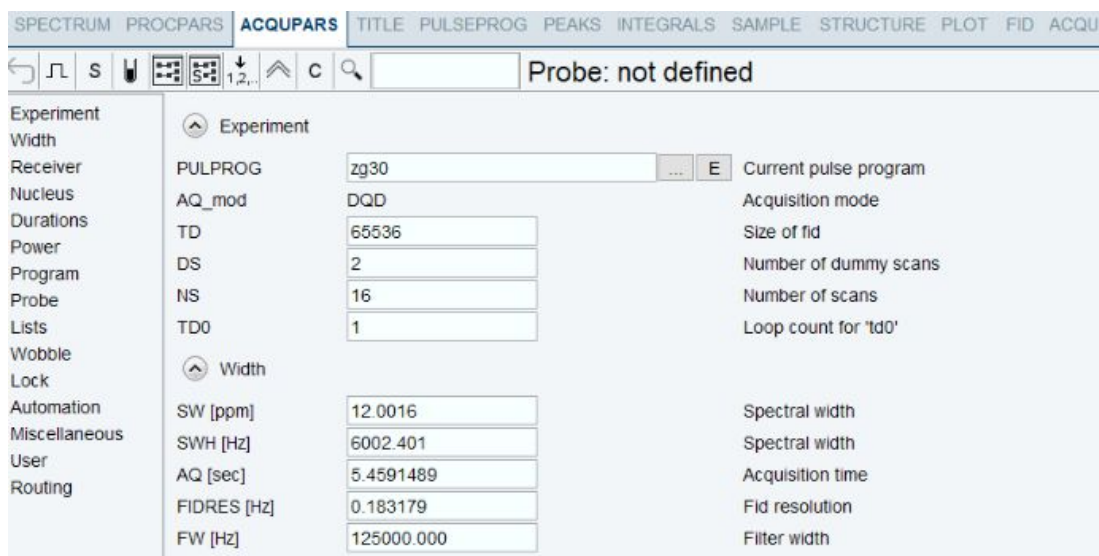
To open the acquisition parameter editor:

- Click the **AcquPars** tab in the Tab bar of the dataset window.






or

- Enter **eda** on the command line.


The figure below shows an example of the acquisition parameter editor with the Experiment parameters displayed.




The processing parameter editor supports the following functions:


- Collapse/expand a parameter section by clicking the  button. Note that the section Width is collapsed.
- Collapse/expand all parameter sections by clicking the large  button of the dataset window toolbar.
- Enter (part of) a parameter name in the search field and click .
- Click a parameter section, e.g. Experiment at the left of the dialog box. The section becomes highlighted and the corresponding parameters will appear in the right part of the dialog box.
- Click in a parameter field, e.g. TD, to set the parameter value.
- Click the  button to the right of parameters like PULPROG to open a list of the corresponding programs/lists.
- Click **Edit pulse program**  to open the current program/list with an editor.
- Hit the **Tab** key to jump to the next parameter field.
- Hit **Shift + Tab** to jump to the previous parameter field.
- Use the scroll bar at the right of the dialog box to move to parameters further up or down in the dialog box.

How to Undo the Last Acquisition Parameter Change

- Click  Undo last acquisition parameter change.

How to Set Pulse Program Parameters


- Click  Show pulse program parameters [**ased**].

The button will change to  .

To make this the default setting:

- Click **Setup Preferences | Acquisition**, check **Show ased parameter selection with eda** and click **Apply**.

How to Display Acquisition Status Parameters

- Click  Show acquisition status parameters.


Note that the command **dpa** opens the acquisition parameter editor and automatically shows the status parameters.

How to Get Probe/Solvent Dependent Parameters

- Click  Set probe/solvent dependant parameters [**getprosol**].

Probe and solvent dependent parameters can be set up with the command **edprosol**.

How to Change Acquisition Data Dimensionality

- Click  Change data dimensionality.

This changes the number of parameter columns and value of the acquisition parameter **PARMODE**.

How to Set Lock Parameters

- Enter the command **edlock** and set the lock parameters in the appearing dialog box.

For a detailed description of **edlock**, please

- refer to the Acquisition Reference manual

or

- enter **edlock?** on the command line.

How to Set Routing Parameters

- Enter the command **edasp** and set the routing parameters in the appearing dialog box.

For a detailed description of **edasp**, please

- refer to the Acquisition Reference manual

or

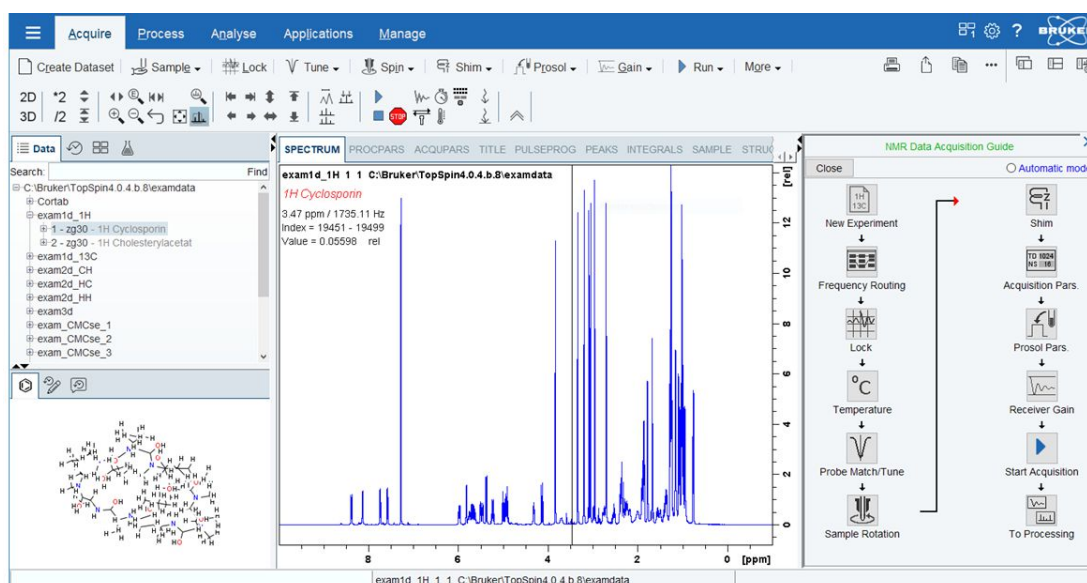
- enter **edasp?** on the command line.

6 Acquisition

This chapter describes TopSpin acquisition as far as the interface is concerned. Individual acquisition commands are described in the Acquisition Reference manual.

6.1 Acquisition Guide

If you are a new or occasional user, we recommend acquiring your data with the *NMR Data Acquisition Guide* flowchart. This will guide you through the typical sequence of acquisition steps. To start the *NMR Data Acquisition Guide*, enter **aqguide**.



In **Automatic mode**, the Acquisition Flowchart will simply execute each command when you click the respective button. This requires the acquisition parameters to be set correctly. In interactive mode (**Automatic mode** unchecked **Automatic mode**), the Acquisition Flowchart will, at each step, open a dialog box offering you the available options and required parameters. Note that the last button **To Processing** will open the processing equivalent of the Acquisition Flowchart, the Processing Guide [prguide].

6.2 Acquisition Setup and Toolbar Buttons

Acquisition can be prepared and controlled from the Manage menu.

- Click **Manage | Spectrometer | Experiments/Parameters**.

Spectrometer power on/off (pdudisp)	Install Standard Experiments (expinstall)
Hardware Detection	Convert Parameter Set (paracon)
Experiments/Parameters	Shape Tool (stdisp)
Manage temporary acquisition data	Probe/Solvent Dependent Params (edprosol)
BSMS Control	Edit Solvent Table (edsolv)
Cryo Display	Edit Lock Table (edlock)
ProdigyDisplay	Edit Nuclei Table (ednuc)
Save/Restore Installation	Edit customer/system information (edcstm)
Spectrometer Usage (account)	

Here you find several categories of acquisition related commands. Each entry gives access to a submenu with various commands.

For most entries, the command line command, for example **expinstall**, is specified in brackets.

Common acquisition commands can also be started from the TopSpin toolbar. The toolbar displays the following buttons:



- Click one of the following buttons:



Start the acquisition. Acquires NS scans in the current dataset, over writing possibly existing data. Equivalent to the command **zg**.



Halt the acquisition. This stops the acquisition after the current scan has finished. All data acquired so far are saved. Equivalent to the command **halt**.



Stop the acquisition. This stops the acquisition immediately. Data acquired after the last disk write (if any) are lost. Equivalent to the command **stop**.



Open the online FID display window. Shows the currently acquired FID. Only works during acquisition. Equivalent to the command **acqu**.



Open the Lock display window. Shows the lock signal. Equivalent to the command **lockdisp**.



Calculate the experiment time. Shows the total experiment time and file size of the raw data. Equivalent to the command **expt**.



EVTU Control Suite [vtudisp].



BSMS Control Suite [bsmsdisp].



Set SFO1, O1, O2 and O3 interactively. Puts a red cursor line in the dataset window. A click at the desired frequency opens a dialog box where you can set O1, O2 and/or O3.



Set the sweep width to the current region and the spectrometer frequency to the center of the current region. Update the parameters SW and SFO1, respectively.

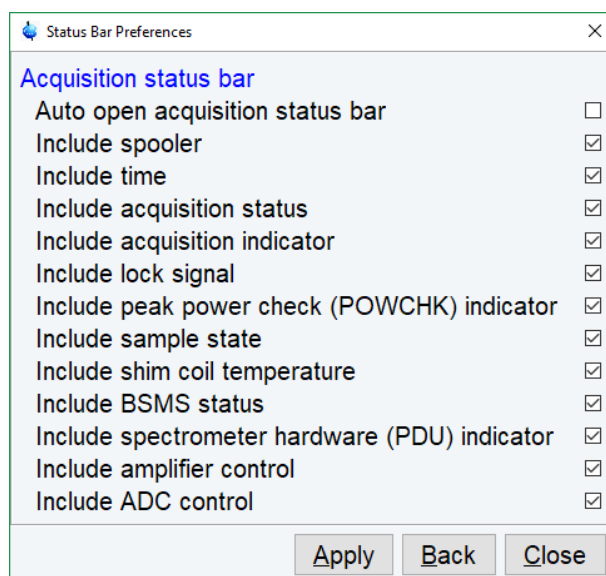


Setup a frequency list interactively.

6.3 Acquisition Status Bar

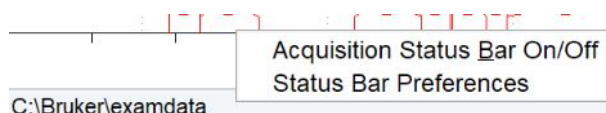
The acquisition can be followed and controlled from the acquisition status bar. Before you use the acquisition status bar, it must be configured from the Setup Preferences window.

- Click **Setup Preferences | More Preference | Status Bar Preferences | Change**.
- Check the items to be displayed.



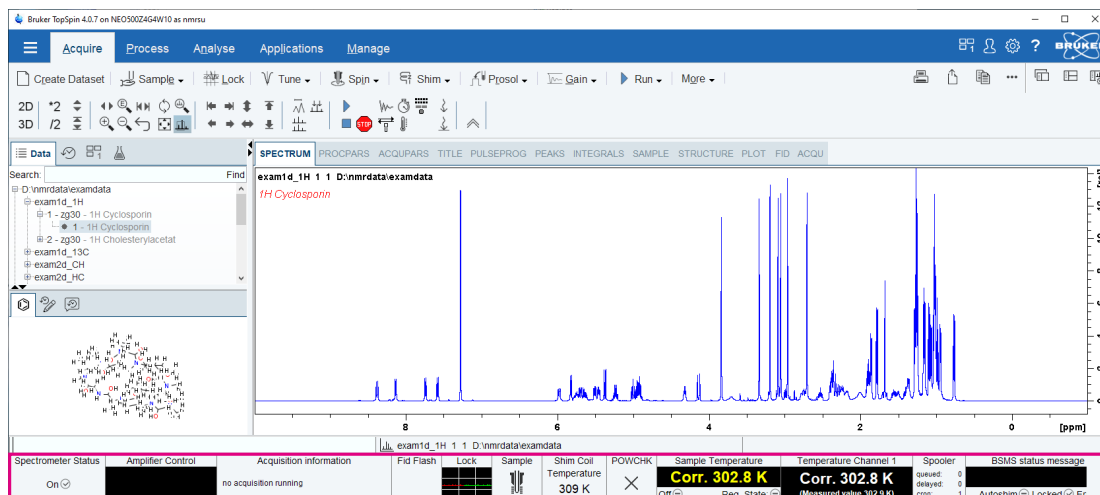
or

- Right-click in the status display bar at the bottom of the TopSpin window and in the list, select **Status Bar Preferences**.



To switch the acquisition status bar On or Off:

- Right-click in the status display bar at the bottom of the TopSpin window and in the list, select **Acquisition Status Bar On/Off**.



The Sample field iconifies the status of the sample:

Sample



Sample is in the magnet.

Sample



Sample ejected, no sample in magnet.

Sample



Sample eject in progress, status unsure.

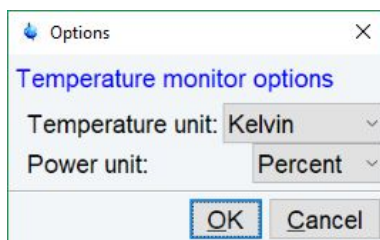
The acquisition status bar not only displays information, it also allows to perform various actions, e.g.:

- Double-click the **Time** field to view detailed time and date information.
- Double-click the **Lock** field to open the lock display.
- Click the **Spooler /queued /delayed /cron** field to open the spooler main window.
- Double-click on sample field to open BSMS control suite.
- Double-click on VTU opens the edte window.
- Right-click the **Fid Flash** field to switch on/off FID flashing or to stop the acquisition.
- For more information about peak power check (POWCHK) please look up the Acquisition Commands and Parameters manual, Chapter 3 - Spectrometer configuration commands. Within the command explanation of **cf** you will find the functionality of POWCHK.
- Right-click the Probe Temperature **VTU** field and in the list, select **Options**.

Options...

Toggle VTU state (on/off)

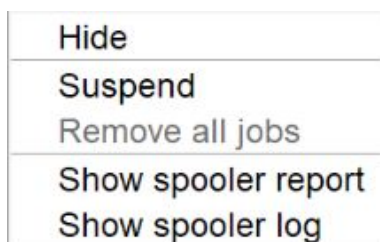
This will open the following window:



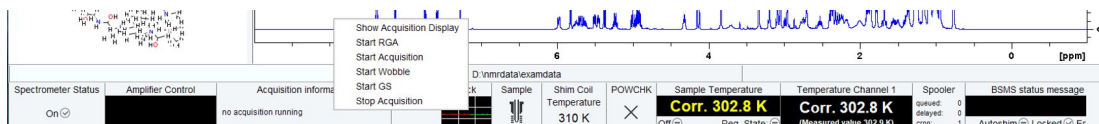
- Right click the Lock field to open the following list:



- Right click the Spooler field to open the following list:



- Right-click the Acquisition Information field to open the following popup menu:



From this list, you can start various acquisition commands as

- Show Acquisition Display
- Start RGA
- Start Acquisition
- Start Wobble
- Start GS
- Stop Acquisition

Data specific acquisition display allows you to open multiple acquisition display windows, one for each dataset.

Note that the **Acqu** tab is automatically activated when the acquisition is started from the TopSpin menu, toolbar or command line.

6.4 Command Queuing and Scheduling

TopSpin supports command queuing (spooling) and scheduling. Acquisition commands like **zg**, **go**, **rga** and **atma** are automatically queued, if this feature is On (default Off). This allows you, for example, to enter multiple **zg** commands on different datasets. Automatic queuing can be switched on as follows:

- Check **Setup Preferences | Processing Preferences | Enable automatic data processing**.

Processing commands can be queued with the command **qu**. For example, the command sequence **zg ; qu xfb** on a 2D dataset, will start an acquisition and, when this has finished, process the data.

Acquisition and processing commands can be scheduled with the command **at**. Enter **help qu** or **help at**, for more details on the respective commands.

Queued commands can be viewed in the Spooling field of the acquisition status bar. Note that the spooling field must be activated in the User Preferences window (command **set**).

6.5 Tuning and Matching the Probe

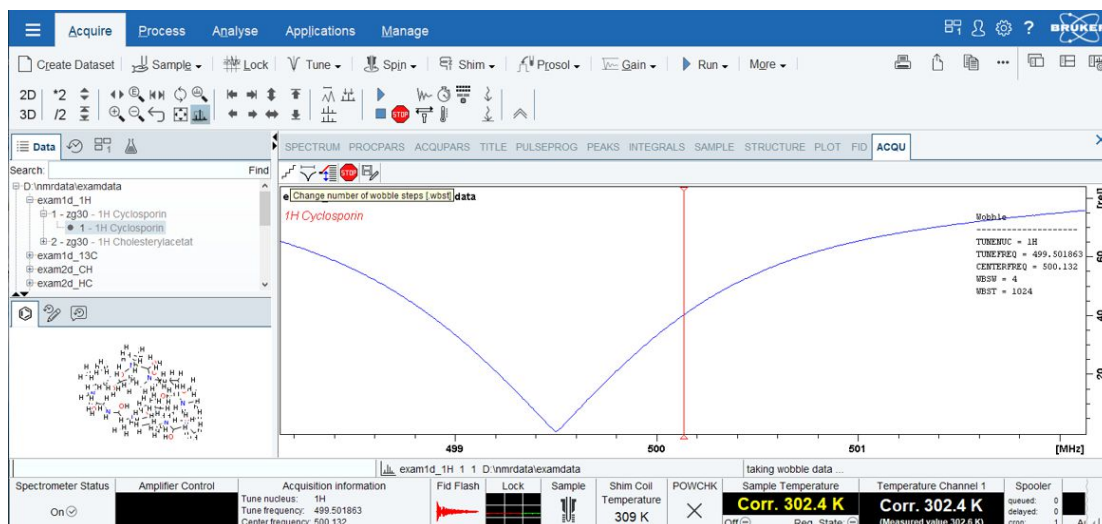
Tuning and matching of conventional probes, (non-ATM), is performed with the wobble procedure:

- Enter **wobb** on the command line.

or

- Click **Acquire | Tune | Display wobble curve (wobb)**.

The dataset window toolbar switches to the **Acqu** tab and the wobble window is displayed:



The buttons of the wobble toolbar have the following functions:



Change the number of wobble steps [**.wbst**].



Change the wobble sweep width [**.wbsw**].



Switch to the next channel/nucleus (if available) [.nuc].



Emergency Stop acquisition, fid not saved [stop].



Save wobb curve to disk [wbwr].

- Turn the tuning and matching knobs on the probe until the wobble curve is exactly in the middle and its minimum reaches the zero line.

Automatic tuning and matching of ATM probe can be performed with the command **atma**.

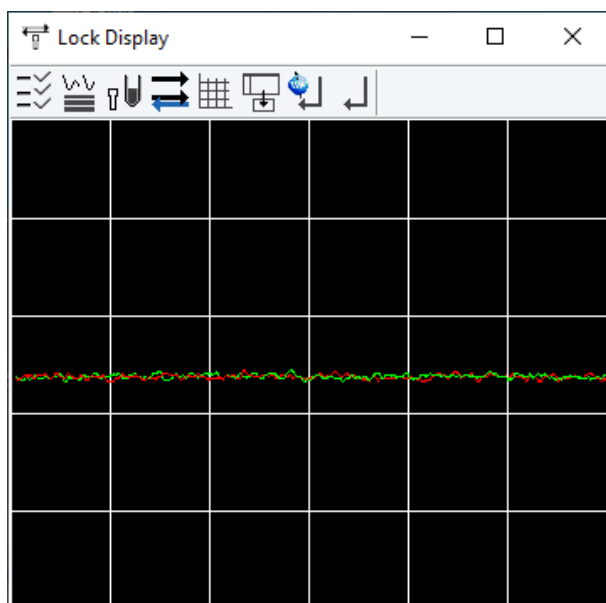
6.6 Locking

To open lock display

- Click **Acquire | Lock**

or

- enter **lockdisp**
- or on the Acquisition Status bar, in the Lock field right-click and in the list, select **Lock Signal Display**
- or
- Double-click the lock field in the Acquisition Status bar.

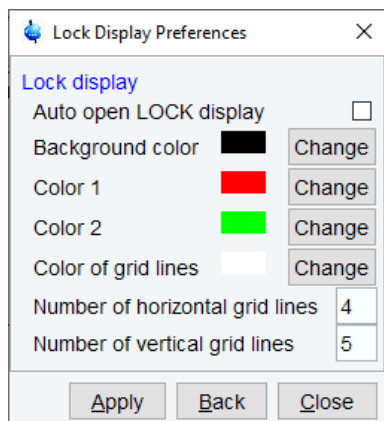


Here, you can view the lock signal, either during the lock-in procedure or, as shown above, after lock-in has been successful. At the top of the lock window the following buttons are available:



Open the Lock Display Preferences window [set].

Here colors and numbers of grid lines can be defined.



The Lock Display Toolbar Buttons:



Toggle lock monitor mode.



Lock current sample [**lock**].



Toggle display mode between *single* and *dual* color. Colors can be set in the Lock Display Preferences window.



Toggle grid mode between *both*, *vertical*, *horizontal*, *off*, *single*.



Detach lock window from main TopSpin window.



Set focus on TopSpin main window.



Close window.

Note that an external lock display window is independent from the TopSpin window. You can for example, minimize TopSpin while keeping the lock display open.

The lock process can be started by entering **lock** on the command line. This command is described in the Acquisition Commands and Parameters manual.

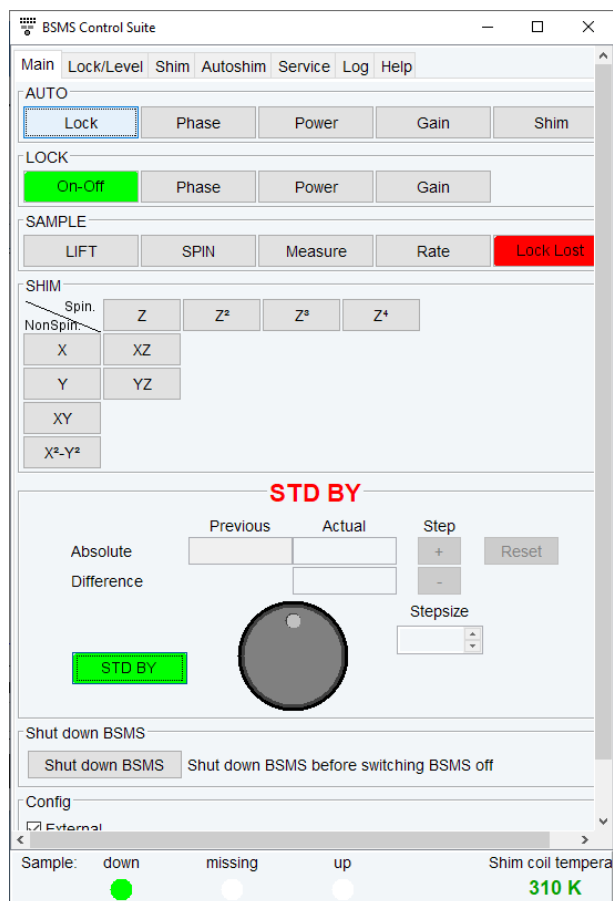
6.7 BSMS Control Panel

The BSMS control panel allows shimming, locking, sample handling and helium level measurement. To open this panel:

- Click **Acquire | Shim | Shim manually using BSMS panel (bsmsdisp)**

or

- Enter **bsmsdisp** on the command line



The individual function of the BSMS control panel are described in detail in the Acquisition Commands and Parameters manual.

6.8 Interactive Parameter Adjustment (GS)

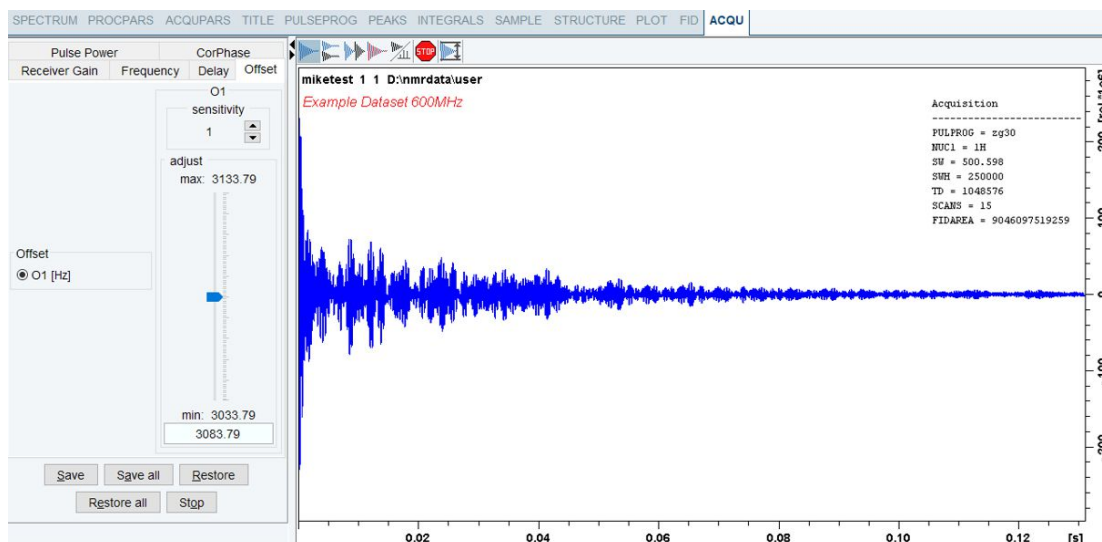
Several parameters can be adjusted interactively, while observing the acquired FID. To start this:

- Click **Acquire | Run | Real-Time Go Setup**

or

- Enter **gs** .

A split window displays the FID:



The GS parameter adjustment dialog

The buttons of the FID display are the same as for the acquisition command **zg**.

The GS parameter adjustment dialog offers tabs at the top of the window to select power, frequency, delay etc. The selected parameter is shown in the middle of the window. The slider at the right of the window allows you to change the selected parameter. The current value can be viewed and modified in the field below the slider. The sensitivity of the slider can be set in the field **Sensitivity** above the slider.

The effect of the change can be viewed in the FID display, the right part of the window. This can be manipulated with the FID display buttons as described in the next chapter.

At the bottom of the window you find the following buttons:

Save: Save the value of the current parameter.

Save all: Save the values of all changed parameters.

Restore: Restore the value of the current parameter.

Restore all: Restore the value of all changed parameters.



Stop: Stop the acquisition and quit the GS window.


6.9 Running an Acquisition

A typical acquisition is performed as follows:

- Click **File| New [new, Ctrl+ n]** to create a new dataset.
- Specify the data path variables *name*, *expno*, *dir* and *user*, select the desired **Solvent** and **Experiment**, enter the **Title** and click **OK**.

The dataset will appear in the data field with no raw and no processed data available.

- Click the **AcquPars** tab to display the acquisition parameters.
- Optionally: click  to show the pulse program parameters only.
- Click the  button to read the prosol parameters or set the relevant parameters manually.

- As an alternative, you can set the acquisition parameters interactively in the GS window (see [Interactive Parameter Adjustment \(GS\)](#) [▶ 79]).
- To start the acquisition, click  in the upper toolbar or enter **zg** on the command line.

The dataset window toolbar will automatically switch to the Acq tab and the FID display window will appear.



For further explanations or for a description of the toolbar buttons enter

- **help zg**

or

- Click **Help | Manuals | Acquisition & Processing Parameters | Acq. Commands and Parameters** and read the chapter *Acquisition Commands*.

When the acquisition has finished:

- Enter **efp** to process the FID.

The processed spectrum will be displayed in the dataset.

From here, the processed data can be analyzed, printed and/or archived.

6.10 Shape Tool

The Shape tool interface allows to create/manipulate RF shapes and wave format.

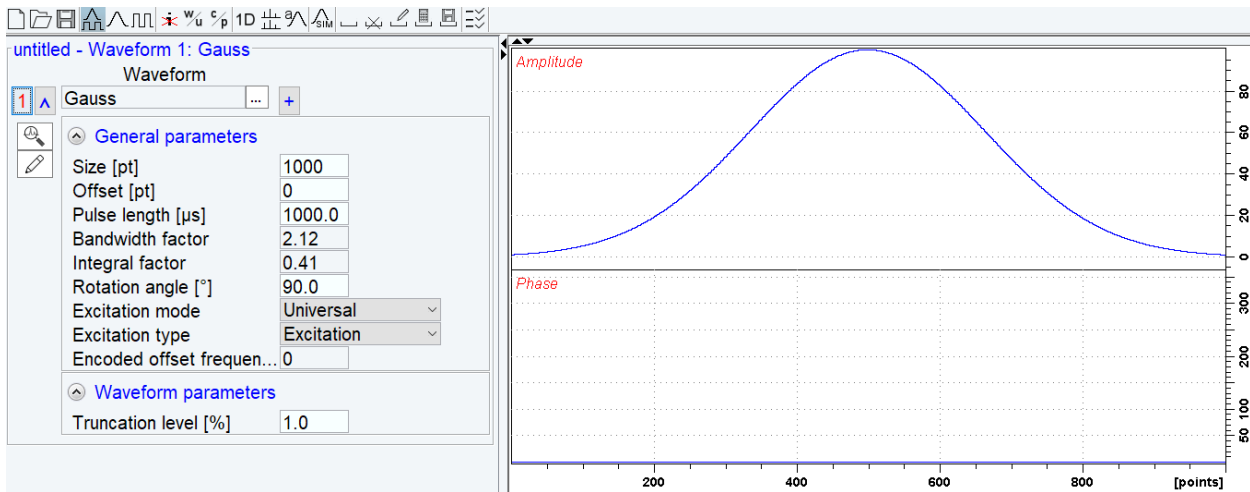
To start the Shape Tool interface:

- Click **Manage | Spectrometer | Experiment/Parameters | Shape Tool**

or

- Enter **stdisp** on the command line.

The Shape Tool window will be displayed:



This consists of a toolbar, a command line and a split pane with a data section at the right and a parameter section at the left.

If Shape Tool is opened with a dataset the current dataset will be displayed.

By default, a 1000-point Gauss shape is displayed with Truncation level 1.0.

Note that all functions of the interactive Shape Tool can also be performed non-interactively with the TopSpin command `st`. This command must be entered with the appropriate arguments on the command line while the associated dataset is displayed and selected.

A full description of the interactive and non-interactive Shape tool can be found under:

- Click **Help | Manuals | Acquisition Application Manuals | Shapetool**

7 Data Processing

7.1 Interactive Processing

Interactive processing allows full control over the processing sequence. However, it requires detailed knowledge about the required parameters (see chapter [Startup TopSpin \[29\]](#)) and commands. Therefore, it is only suitable for the advanced user. New or intermediate users are recommended to use the Processing Guide for semi-automatic processing.

How to Process Data with Single Commands

Data can be processed by entering single commands on the command line. A typical 1D processing sequence would be:

- em**: exponential window multiplication.
- ft**: Fourier transform.
- apk**: automatic phase correction.
- sref**: automatic calibration (referencing) .
- abs**: automatic baseline correction.

This allows full control over each individual processing step.

How to Process Data with Composite Commands

Data can also be processed with so called composite commands. These are combinations of single processing commands. The following composite commands are available.

- ef**: Exponential multiplication + Fourier transform.
- efp**: Exponential multiplication + Fourier transform + phase correction.
- fmc**: Fourier transform + magnitude calculation.
- fp**: Fourier transform + phase correction.
- gf**: Gaussian multiplication + Fourier transform .
- gfp**: Gaussian multiplication + Fourier transform + phase correction.

They can be entered on the command line or clicked from the menu. For the latter option:

- Click **Process | Advanced | Special Transforms**

Advanced ▾	
Process Dataset List (serial)	Hilbert (ht)
Integrate Spectra List (intser)	Inverse Fourier (ift)
ROI View of Spectra List (vregs)	User Defined Processing of Raw Data (trf)
Add/Sub./Mult. Spectra (adsu)	User Defined Processing of Pre-Processed Data (trfp)
Reference Deconvolution (.refdcon)	em + ft (ef)
Special Transforms ▶	ft + pk (fp)
Miscellaneous Operations ▶	em + ft + pk (efp)
	gm + ft (gf)
	gm + ft + pk (gfp)
	ft + mc (fmc)

Just like single commands, composite commands can be used in Macros, AU programs and Python programs.

7.2 Semi-automatic Processing

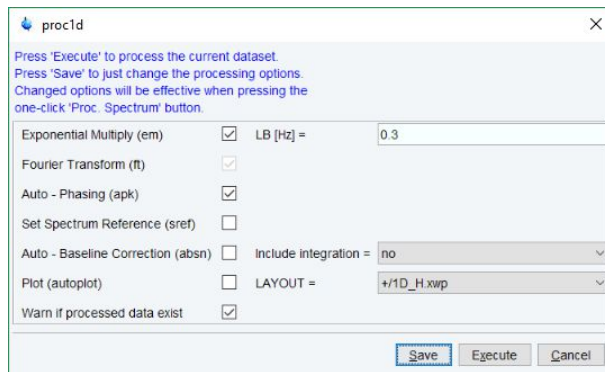
How to Use the 1D Processing Dialog

1D data processing often involves the same sequence of steps, which can easily be performed as follows:

- Click **Process | Proc Spectrum | Configure Standard Processing** or enter **proc1d**.

In the appearing dialog (see the figure below):

- Enable the desired processing/plotting steps.
- Set the parameter LB for exponential multiplication.
- Select the desired LAYOUT for plotting.
- Click **OK**.

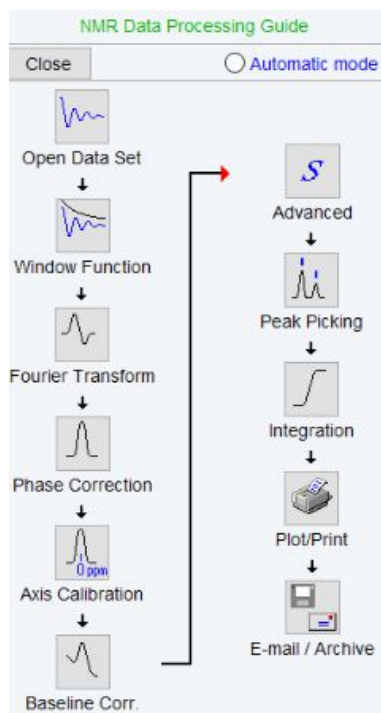


How to Use the Processing Guide in Automatic mode

The Processing Guide in automatic mode guides you through the entire processing sequence of data selection, processing, printing and archiving with minimum user interaction.

- Enter **prguide**.

The Processing Guide window will appear as an integral part of the current dataset window.



In the Processing Guide window:

- Check **Automatic mode** on the upper right part of the window to perform complete automatic processing.
- Click **Open Data Set** and click **OK** to open a dataset manually, e.g. from the browser or click **Browse** to open the File Chooser.
- Click **Window function** | **Fourier Transform** | **etc.**

Each processing step will be executed without user interaction.

How to Use the Processing Guide in Interactive mode

The Processing Guide in interactive mode guides you through the entire processing sequence of data selection, processing, printing and archiving requiring some user interaction.

- Enter **prguide**.

The Processing Guide window will appear as an integral part of the current dataset window.

In the Processing Guide window:

- Uncheck **Automatic mode**.
- Click **Open Data Set** and click **OK** to open a dataset manually, e.g. from the browser or click **Browse** to open the File Chooser.
- Click **Window function** | **Fourier Transform** | **etc.**

For each step a dialog box will appear where you can enter options, parameters etc. For details on these items, please refer to the corresponding commands in the Processing Reference Guide.

7.3 Processing Data with AU programs

Data processing can be performed by using AU programs. An AU program is actually a C-program which contains TopSpin commands (macros) and/or C-language statements. Various standard AU programs are delivered with TopSpin. A typical 1D processing AU program is **proc1d**. A simplified version of this AU program is:

```
EF
APK
SREF
ABS
AUTO PLOT
QUIT
```

It executes the commands **ef**, **apk**, **sref**, **abs** and **autoplot**. To run this AU program, just enter **proc_1d** on the command line. Before you can use any Bruker AU program, **expinstall** must have been executed once. You can create your own AU programs with the command **edau**. Note that an AU program must end with QUIT or QUITMSG("your message"), and that all statements must be specified in capital letters. For more information on AU programs, please refer to the AU programming manual:

Click [Help](#) | [Manuals](#) | [Programming Manuals](#) | [AU Programming](#)

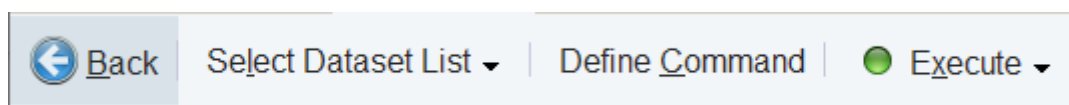
As an alternative to AU programs, you can also write Python programs, which allow you to use TopSpin commands, User Interface functions and Graphic functions. For more information:

Click [Help](#) | [Manuals](#) | [Programming Manuals](#) | [Python Programming](#)

7.4 Serial Processing

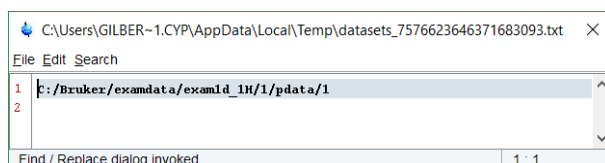
TopSpin allows you to process a series of datasets using serial scripts. The dataset list and command(s) to be used can be easily setup from the TopSpin interface as follows. Enter **serial** on the command line or click **Process** | **Advanced** | **Process Dataset List**.

This will open the Serial Processing flow bar:



- Click **Select Dataset List** | **Edit Dataset List**

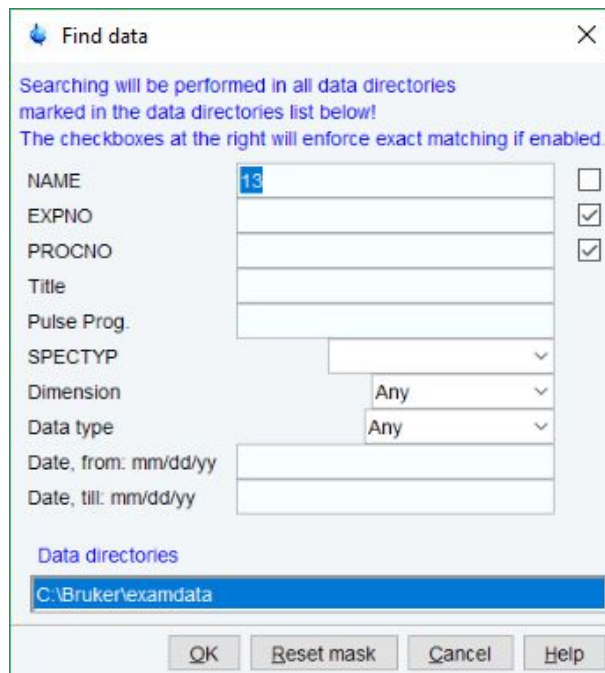
This opens a text file for editing and search datasets.



OR

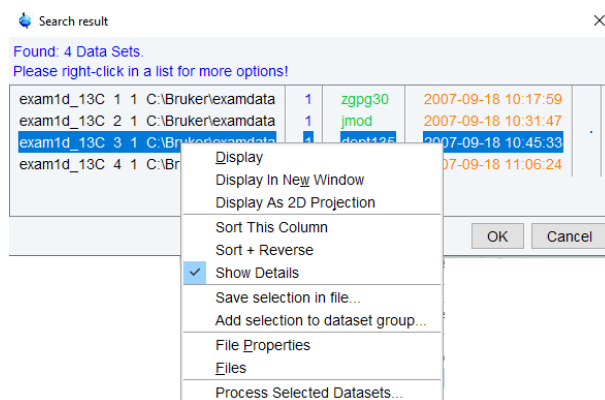
- Click **Select Dataset List** | **Build dataset list using Find**

You can find datasets in all data directories marked in the appearing dialog window list:

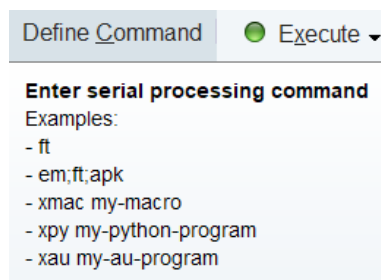


Search result example:

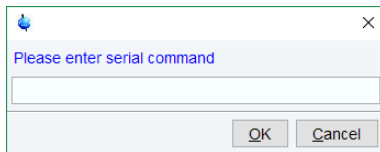
- Right-click a dataset for more options.



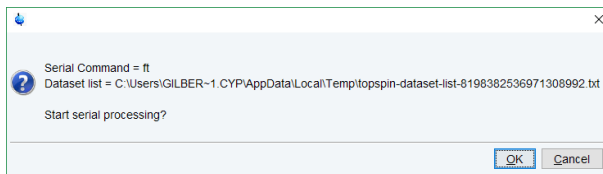
- In the Serial Processing flow bar click **Define Command**.



- As indicated above, several commands can be entered separated by semicolon. Also, macros, python scripts, and AU programs can be selected.



- In the Serial Processing flow bar click **Execute** or click the down arrow and select **Execute in background**.



- In the Serial Processing flow bar click **Back**.

8 1D Display

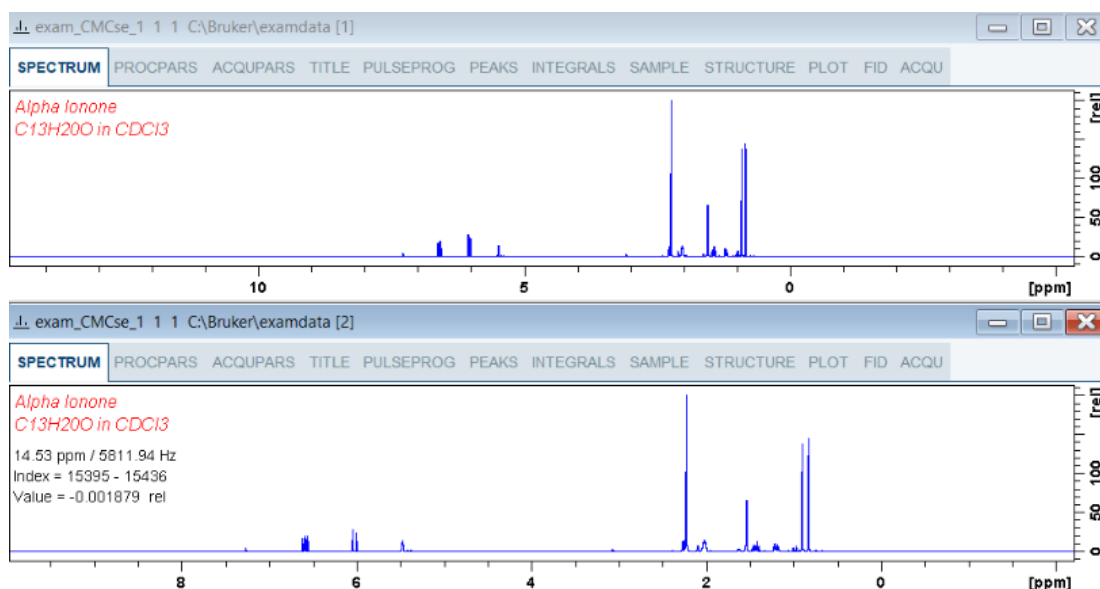
8.1 Displaying one Dataset in Multiple Windows

TopSpin allows to display one dataset in multiple dataset windows. This is, for example, convenient to view various regions or various objects (spectrum, fid, parameters etc.) of the same dataset.

How to Reopen a Dataset in a Second/Third etc. Window

- Select (activate) the desired dataset.
- Click **File | Reopen [reopen]**.

Multiple dataset windows with the same dataset are indicated with a number in square brackets, e.g. [1], in the title bar:



How to Rescale or Shift one Dataset in Multiple windows

Display buttons like ***2** and **▲** only work on the active dataset window. The same counts for the keys **Alt+ PageUP** and **Alt+ PageDown**. However, when used with the control key, they work on all windows, for example:

- Enter **Ctrl+ *2** Ctrl+Alt+PageUp or Ctrl+Alt+PageDown.

8.2 Changing the Display of a 1D Spectrum or FID

TopSpin offers buttons to scale or shift the spectrum vertically and horizontally.





How to Change the Vertical Scaling of the FID or Spectrum

- Turn the mouse wheel while the cursor is in the dataset window.

or

- Hit one of the following the keys:
Alt+ PageUp: Increase the intensity by a factor of 2.
Alt+ PageDown: Decrease the intensity by a factor of 2.
Alt + Enter: Reset the intensity.

or

- Click one of the following buttons:
 Increase the intensity by a factor of 2 [***2**].
 Decrease the intensity by a factor of 2 [**/2**].
 Click and move the mouse for smooth vertical scaling.
 Reset the intensity [**.vr**].




Alternatively, you can enter the corresponding commands as specified between square brackets [].

To manipulate all dataset windows, press the **Ctrl** key while clicking one of the above buttons.

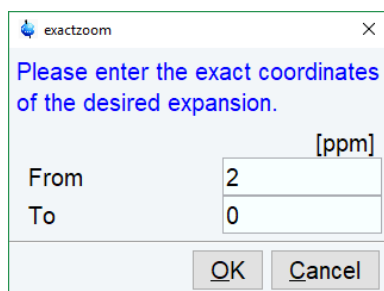
How to Change the Horizontal Scaling of the FID or Spectrum

- Click  and move the mouse for smooth horizontal scaling.

or

- Click one of the following buttons:
 Zoom in to the center (spectrum) or left edge (FID) of the displayed region, increasing the horizontal scaling. [**.zi**].
 Zoom out from the center (spectrum) or left edge (FID) of the displayed region, decreasing horizontal scaling) [**.zo**].
 Perform an exact zoom via a dialog box [**.zx**].

Enter the coordinates of the desired region in the dialog box:



The dialog box titled "exactzoom" contains the following text and fields:


Please enter the exact coordinates of the desired expansion.





[ppm]

From

To

Buttons:


- Click **OK**
- Click one of the buttons:
 Undo last zoom [**.zl**].

-  Reset horizontal scaling to show the full spectrum **[.hr]**.
-  Display the entire spectrum (baseline position and intensity scaling are adjusted if necessary) **[.all]**
-  Toggle interactive zoom mode. When switched off, interactive zooming only selects an horizontal region; baseline position and intensity scaling remain the same. When switched on, interactive zooming draws a box selecting the corresponding area.
-  Retain horizontal and vertical scaling when modifying dataset or changing to different dataset **[.keep]**. Effects all dataset windows.

Alternatively, you can enter the corresponding commands as specified between square brackets [].


How to Shift a Spectral Region to the Left or to the Right

- Click-hold the following button and move the mouse:

 Smoothly shift to left or right.


or

- Click one of the following buttons:

 Shift to the left, half of the displayed region **[.sl]**.

 Shift to the right, half of the displayed region **[.sr]**.

 Shift to the extreme left edge of the spectrum **[.sl0]**.

 Shift to the extreme right edge of the spectrum **[.sr0]**.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

This functionality also becomes available when you move the mouse cursor into the horizontal axis area.

How to Shift the Spectrum Up or Down


To shift the FID or spectrum display up or down:


- Click-hold the button and move the mouse:

 Smoothly shift the spectrum baseline up/down.

or

- click one of the following buttons:

 Shift the spectrum baseline to the middle of the data field **[.su]**.

 Shift the spectrum baseline to the bottom of the data field **[.sd]**.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

This functionality also becomes available when you move the mouse cursor into the vertical axis area.

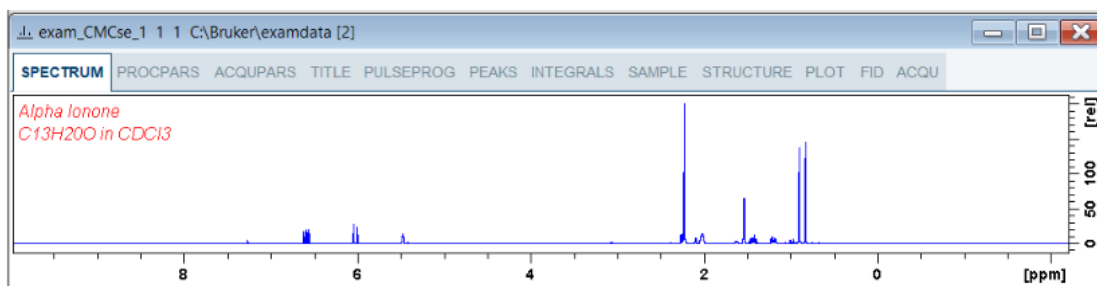
8.3 Using the Tab Bar

Tabs of the dataset window can be activated by clicking them or by entering the corresponding commands, as specified between square brackets, on the command line. Note that command line commands always work on the currently selected (active) dataset window.

The Tab bar can be configured from the User Preference box (command **set**).

How to Display the Spectrum

- Click the **Spectrum** tab [**spec**].



This displays the processed data. If these do not exist, the text *No processed data available* is displayed.

How to Set Processing Parameters

- Click the **ProcPars** tab [**edp**].

This opens the processing parameter editor (see also chapter [Startup TopSpin \[29\]](#)).

- Click one of the following buttons:



Undo last value change. Can be used to undo multiple changes.



Toggle status parameters view. The button turns gray when activated [**dpp**].



Switch to Maxent parameters.



Show eretic parameters.



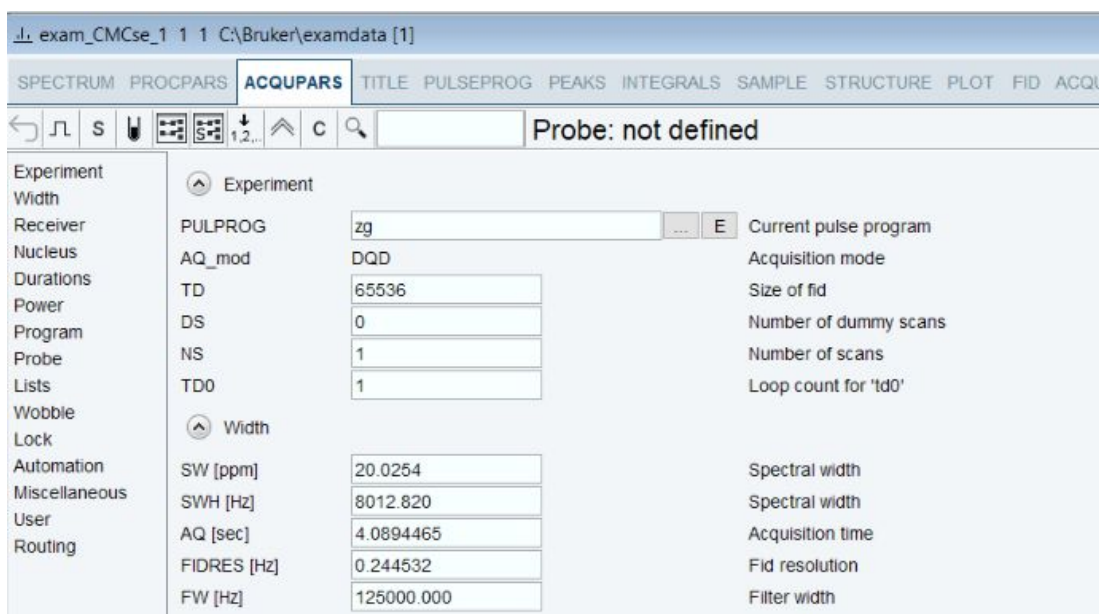
Collapse/expand all parameter sections.

 Search for specified parameter.

Changed parameters are automatically saved.

How to Set Acquisition Parameters


- Click the **AcquPars** tab [**eda**].



Parameter	Value	Description
Experiment		
PULPROG	zg	Current pulse program
AQ_mod	DQD	Acquisition mode
TD	65536	Size of fid
DS	0	Number of dummy scans
NS	1	Number of scans
TD0	1	Loop count for 'td0'
Width		
SW [ppm]	20.0254	Spectral width
SWH [Hz]	8012.820	Spectral width
AQ [sec]	4.0894465	Acquisition time
FIDRES [Hz]	0.244532	Fid resolution
FW [Hz]	125000.000	Filter width


This opens the acquisition parameter editor (see also chapter [Startup TopSpin \[29 \]](#)).


- Click one of the following buttons:


 Undo last value change. Can be used to undo multiple changes.

 Show pulse program parameters [**ased**].


 Status parameter display. The button turns gray when activated [**dpa**].

 Set probe/solvent dependent parameters [**getprosol**].


 Set nuclei and routing [**edasp**]

 Set nuclei and routing [**edasp -s**]

 Change raw dataset dimensionality (parameter PARMODE).

 Collapse/expand all parameter sections.

 Read shim values from current dataset.

 Search for specified parameter.

Changed parameters are automatically saved.

Note that the ... and **E** button to the right of the PULPROG parameter allow to display the pulse program list or edit the current pulse program, respectively.

How to Edit the Title

- Click the **Title** tab [edit].



- Edit the title that appears in the dataset window and on the plot.



Save the title file under its current name.



Save the title file under a new name.



Reload the title file. Undo modifications since the last save.



Open the title file with the external editor (defined in User Preferences).

How to Edit the Pulse Program

- Click the **PulsProg** tab.



This allows to edit the current pulse program.

- Click one of the following buttons:



Toggle status pulse program.




Start the graphical pulse program display with foreground parameters.



Start the graphical pulse program display with status parameters.

E Start the external editor.

 Search for more info in the knowledge base.

How to Display the Peak list

- Click the **Peaks** tab.

exam_CMCse_1 1 1 C:\Bruker\examdata [1]			
SPECTRUM PROCPARS ACQUPARS TITLE PULSEPROG PEAKS INTEGRALS SAMPLE STRUCTURE PLOT FID ACQU			
Peak	v(F1) [ppm]	Intensity [abs]	Annotation
1	7.5311	397.61	
2	7.2828	648.03	
3	7.2719	85421.67	
4	7.0076	426.80	
5	6.9481	2257.34	
6	6.9233	2215.37	
7	6.9086	2511.49	
8	6.8838	2553.65	
9	6.8685	849.27	

This displays the peak list. By default, the peak list shows the following entries:

Peak: the peak number.

v(F1) [ppm]: the chemical shift.

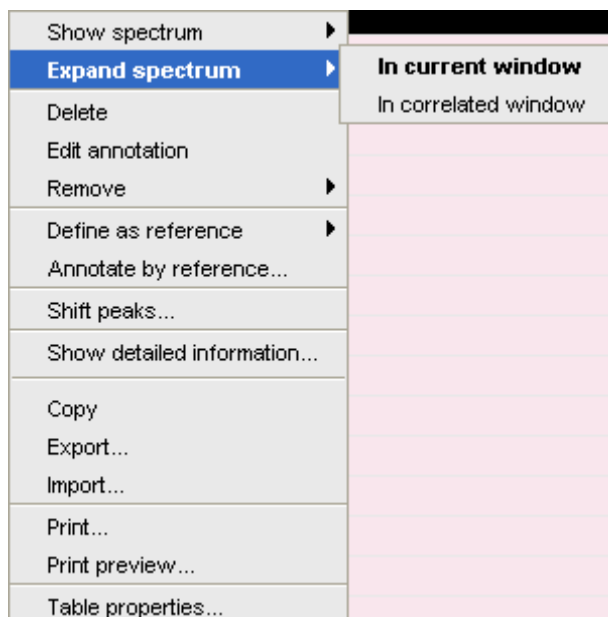
Intensity [abs]: the absolute peak intensity.

Intensity [rel]: the relative peak intensity.

Half width [ppm]: the peak width at half-height.

Display the spectral region around a peak

- Right-click the desired peak and in the list, select one of the following options:
 - **Show spectrum | In correlated window** to open a new dataset window showing the full correlated spectrum.
 - **Expand spectrum | In current window** to change the current dataset window to spectrum display, showing the region around the selected peak.
 - **Expand spectrum | In correlated window** to open a new dataset window showing the region around the selected peak.
 - **Edit Annotation** Edit the annotation of the current peak.
 - **Define as reference | Complete table** Define the entire peak table as a reference for annotation.
 - **Define as reference | Selection** Define the selected peaks as a reference for annotation.
 - **Annotate by reference...** Create annotations according to the peak list of the reference dataset. You will be prompted for the allowed variation in chemical shift.
 - **Shift peaks...** Shift all peaks. You will be prompted for the number of ppm to be shifted.
 - **Show detailed information** Show peak information, dataset information and peak picking parameters.



Export entries of the peak list

Entries of the peak list can easily be exported to Excel or any other program as follows:

- For multiple peaks select the desired entries while pressing the **Ctrl** or **Shift** key.
- Right-click a peak entry to open the popup menu.
- Click **Export...** to export the selected peaks.

This opens a dialog box where you can specify the filename and file type.

- For the latter select from:
 - Auremol peaklist (.ml).
 - Comma Separated Values (.csv).
 - Mixed Shape deconvolution peak list (peaklist).
 - TOPSPIN peak list (.xml).
 - XEASY peak list (.peaks).
 - XWIN-NMR peak list (.txt).

Important: Check the box in the lower-left corner to export the selected peaks only or uncheck it to export the entire list. Then click **Export**.

Delete/remove peaks from the peak list

To delete one peak:

- Right-click the peak and in the list, select **Delete**.

To delete multiple peaks:

- Select the peaks while pressing the **Ctrl** or **Shift** key.
- Right-click one of the peaks and in the list, select **Delete**.

To remove possible duplicate peaks:

- Right-click any entry and select **Remove | Duplicate peaks**.

To remove possible peaks outside of the spectrum:

- Right-click any entry and select **Remove | Peaks positioned outside of the spectrum**.

To remove solvent peaks:

- Right-click any entry and select **Remove | Solvent Peaks**.

Copy the peak list

Instead of exporting entries of the peak list, they can also be copied to the Clipboard and pasted to another application like Excel.

For multiple peaks:

- Select the desired entries while pressing the **Ctrl** or **Shift** key.
- Right-click a peak entry to open the popup menu.
- Click **Copy...** to copy the selected peaks to the Clipboard.

Print the peak list

- Right-click a peak entry and select **Print...**

or

- Enter **print** on the command line.

or

- Press **Ctrl-p**.

All actions will print the entire peak list.

To preview a print:

Right-click a peak entry and select **Print preview...**

Import a Peak List

To import a peak list from a different dataset or program

- Right-click an entry and in the list, select **Import...**
- In the appearing dialog box, navigate to the directory where the list resides and select one of the file types:
 - Auremol peaklist (.ml).
 - MULABEL peak list (labels).
 - TOPSPIN peak list (.xml).
 - XEASY peak list (.peaks).
 - XWIN-NMR peak list (.txt).

Peak lists can be imported from a different dataset or even different program or from a previously exported list from the current dataset.

Note that peak picking commands store the peak list in the processed data directory under the name *peak.xml* (TopSpin 2.1 or newer) or *peak.txt* (XWIN-NMR and TopSpin 2.0 or older).

Shortcuts

- Double-click a peak: zoom into spectrum, i.e. show region around that peak.

- **Enter** key: zoom into spectrum, i.e. show region around selected peak(s).
- **Delete** key: delete the selected peak(s) from the peak list.
- **Ctrl+ c**: copy selected peaks to the Clipboard.
- **Ctrl+ a**: select all peaks.
- **Home**: select the first peak.
- **End**: select the last peak.
- **Shift+ Home**: select current and first peak and all in between.
- **Shift+ End**: select current and last peak and all in between.

Note that these keys only work when the cursor focus is in the dataset window.

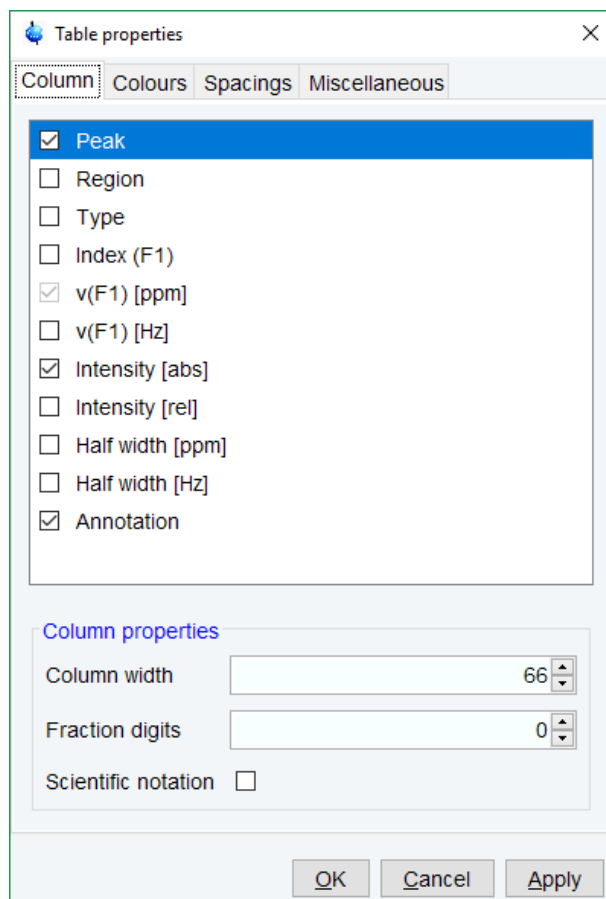
Table properties

Various properties of the peak table can be configured.

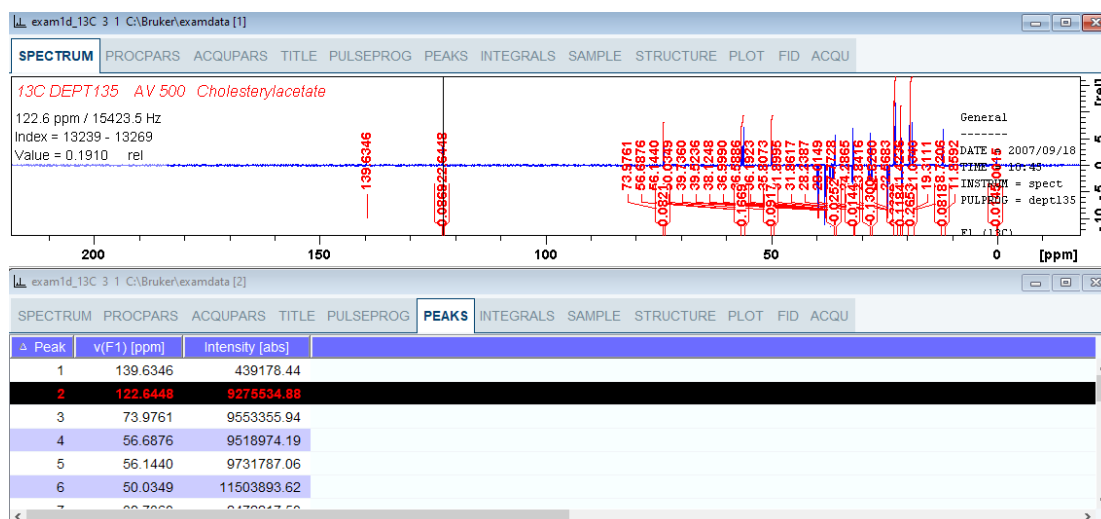
- Right-click an entry and in the list, select **Table properties...**

The Table properties window provides 4 tabs:

1. **Column**: Select the columns to be displayed, set the column width and the number of fraction digits. Furthermore, you can switch on/off scientific notation of values for each column individually.
2. **Colors**: Set various colors of the table.
3. **Spacings**: Set various spacings of the table.
4. **Miscellaneous**: Set grid, printer and font style settings.



When you move the cursor over the peak list, the active peak will, by default, be highlighted in blue (see peak 3 in the figure below). If the correlated spectrum is also displayed, a vertical line moves along, showing corresponding position in the spectrum.



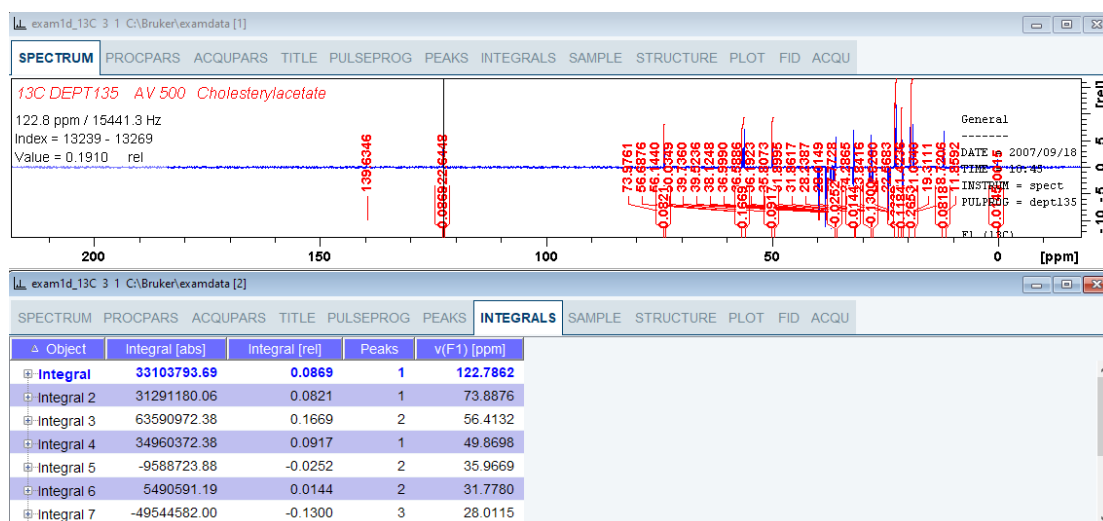
As soon as you click a peak, it is selected and, by default, displayed in red (see figure below). Note that this peak remains selected, i.e. is used by **Enter** and **Delete**, until a different peak is selected.

- To extend the peak list, for example with *Regions*, *Type* and *Index* entries, right-click any part of the header bar.
- To sort the peaks according to peak number, ppm value or intensity, click the header of the respective entry.

Peaks are only available if peak picking has been done (command **pp**). The peak list can be printed with **print [Ctrl+ p]**. List items can be selected with the mouse, copied with **Ctrl + c** and pasted to other applications, e.g. a text editor.

How to Display the Integral list

- Click the **Integrals** tab [**li**, **lipp**, **lippi**].



This displays the integral list (upper part of figure). By default, this shows the following items:

Object: the integral number.

Integral [abs]: the absolute integral value.

Integral [rel]: the relative integral value.

Peaks: the number of peaks within the integral range.

Range (F1) from: the left edge of the integral range.

Range (F1) to: the right edge of the integral range.

Please note the difference between the following items:

1. Selected integral: the entry that has been clicked last (Integral 3 in the figure above). If you right-click an entry, it is selected, and you can execute one of the commands from the popup menu (see figure below). The keys **Enter** and **Delete** work on the selected entry.
2. Active integral: the entry on which the cursor resides (Integral 1 in the figure above). The active integral is also marked in the correlated spectrum by a black vertical line (see lower part of the figure above and description below). When you move the cursor over the integral list, the vertical line in the correlated spectrum moves along with it and vice versa.

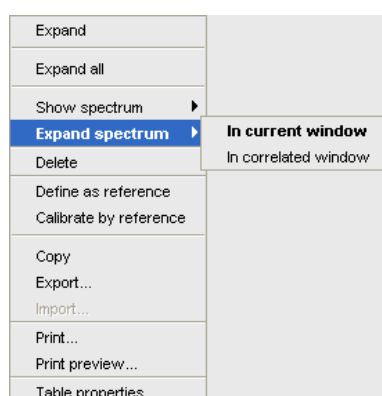
Note that the colors of the selected and active integral can be set in the table properties (see below).

Display the spectral region around an integral

To display the spectral region around a particular integral:

- Right-click the desired integral and in the list, select one of from the following options:
 - **Show spectrum | In correlated spectrum** to open a new dataset window showing the full correlated spectrum.
 - **Expand spectrum | In current window** to change the current dataset window to spectrum display, showing the region around the selected integral.
 - **Expand spectrum | In correlated window** to open a new dataset window showing the region around the selected integral (lower part of the figure above).

Note that clicking the marked entry in the right-click popup menu is equivalent to pressing the **Enter** key.



Export/Import Entries of the Integral List

Entries of the integral list can easily be exported to Excel or any other program as follows:

- For multiple integrals select the desired entries while pressing the **Ctrl** or **Shift** key.
- Right-click an entry and in the list, select one of from the following options (see the figure above):
 - **Copy** Copy the selected integral(s) entry to the Clipboard. Equivalent to clicking **Edit | Copy** or hitting **Ctrl+c**. Copied integrals can easily be pasted in any other application such as Excel.
 - **Export...** Export selected integrals. Check the box in the lower-left corner to export the selected integrals only or uncheck it to export the entire list. Then click **Export**.

Calibrate Integrals to Compare Spectra

Integrals from the current and other spectra can be calibrated with respect to a reference integral.

- Right-click the reference integral and in the list, select **Define as reference**. This will determine the calibration constant.
- Right-click any integral and select **Calibrate by reference**. This will divide all integrals by the calibration constant, setting the reference integral to 1.0.

Now read any other spectrum and calibrate its integrals with respect to the reference integral defined above:

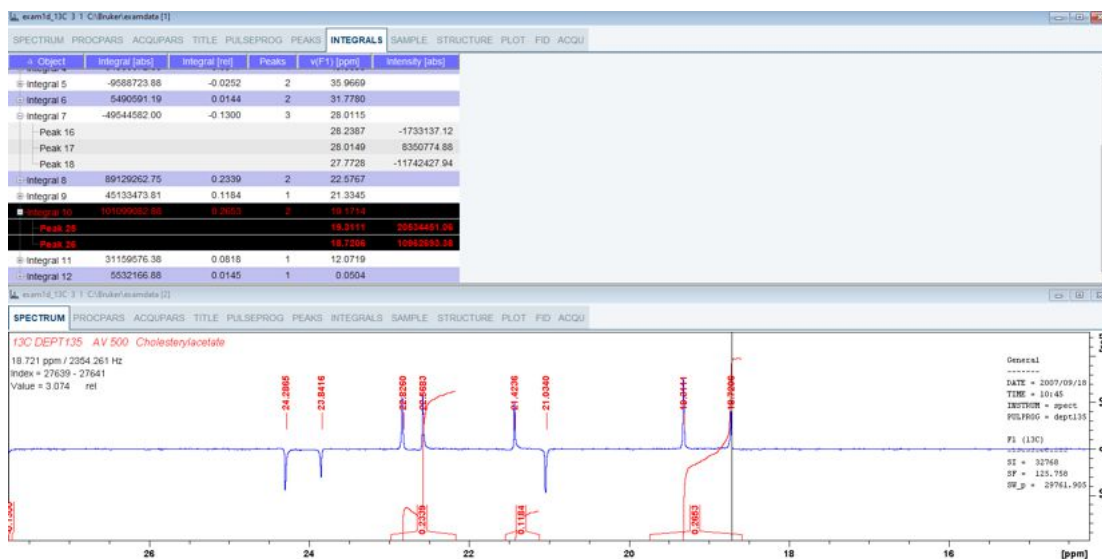
- Read the spectrum.
- Enter **int** to define the integral ranges (if this has not been done yet).

- Click the **Integrals** tab.
- Right-click any integral in the list and select **Calibrate by reference**.

Note that the calibration constant is lost when TopSpin is restarted.

Display the integral list with peaks

The integral list in the figure above shows only integrals. However, if peak picking has been done, the integral list also shows the peaks within each integral range:



Note that the integral entries can be collapsed, (hiding the peaks) or expanded (showing the peaks). As soon as one or more integrals entries are expanded, two extra columns appear showing:

v(F1) [ppm]: the chemical shift of the peak.

Intensity: the peak intensity

Depending on whether integrals are expanded, the right-click list contains the following extra items:

1. **Expand:** Expand the current integral showing all peaks within it.
2. **Expand all:** Expand all integrals showing all peaks within them.
3. **Collapse all:** Collapse all integrals hiding all peaks within them.

In addition to the integral entry, an individual peak within an integral can be activated (by placing the cursor on it) or selected (by clicking it). In the figure above, peak 7 is selected and the correlated spectrum is displayed. Peak 5 is active which is also shown by the vertical line in the correlated spectrum.

Delete an Integral from the Integral List

To delete one integral:

- Right-click the integral and in the list, select **Delete**.

To delete multiple integrals:

- Select the integrals while pressing the **Ctrl** or **Shift** key.
- Right-click one of the integrals and choose **Delete** from the popup menu.

Note that these keys only work when the cursor focus is in the dataset window.

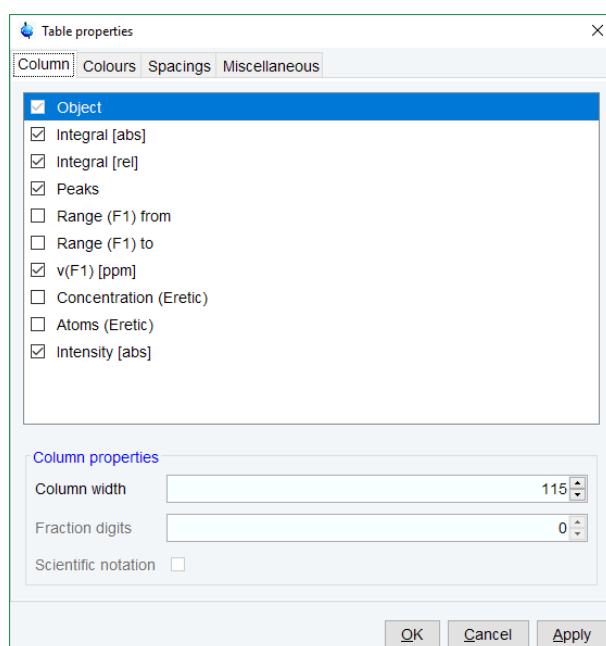
Table properties

Various properties of the integral table can be configured. To do that:

- Right-click an entry to open the popup menu (see figure below).
- Click **Table properties...**

In the appearing dialog box, with 4 tabs:

1. **Column:** Select the columns to be displayed. Set the column width and the number of fraction digits. Furthermore, you can switch on/off scientific notation of values for each individual column.
2. **Colors:** Set various colors of the table.
3. **Spacings:** Set various spacings of the table.
4. **Miscellaneous:** Set grid, printer and font style settings.



Shortcuts

The following shortcuts are available:

Enter key: zoom into spectrum, i.e. show region around selected integral(s).

Delete key: delete the selected integral(s) from the integral list.

Ctrl+c: copy selected integrals to the Clipboard.

Ctrl+ a: select all integrals.

Home: select the first integral.

End: select the last integral.

Shift+ Home: select current and first integral and all in between.

Shift+ End: select current and last integral and all in between.

Double-clicking an integral will show the peaks within the integral region if they exist. If they do not exist; it will zoom into spectrum showing the integral region.

Note that these keys only work when the cursor focus is in the dataset window.

How to view Sample Information

- Click the **Sample** tab [**edsam**].

Sample Description	
Sample ID	<input type="text"/>
Origin	<input type="text"/>
Chemical formula	<input type="text"/>
Concentration	<input type="text"/>
Date Prepared	<input type="text"/>
Buffer	<input type="text"/>
Contact	<input type="text"/>
Comment	<input type="text"/>

This table can be used to fill out any sample information you want to store with the dataset. The table can easily be modified or extended with the following functions:

- To select an item: double-click it!
- Click one of the following buttons:



Save the sample information table with the dataset.



Save the sample information table as default.



Reload the original table discarding any changes.



Add a new item to the table. You will be prompted for an identification name and the desired number of lines.



Remove the selected item from the table.



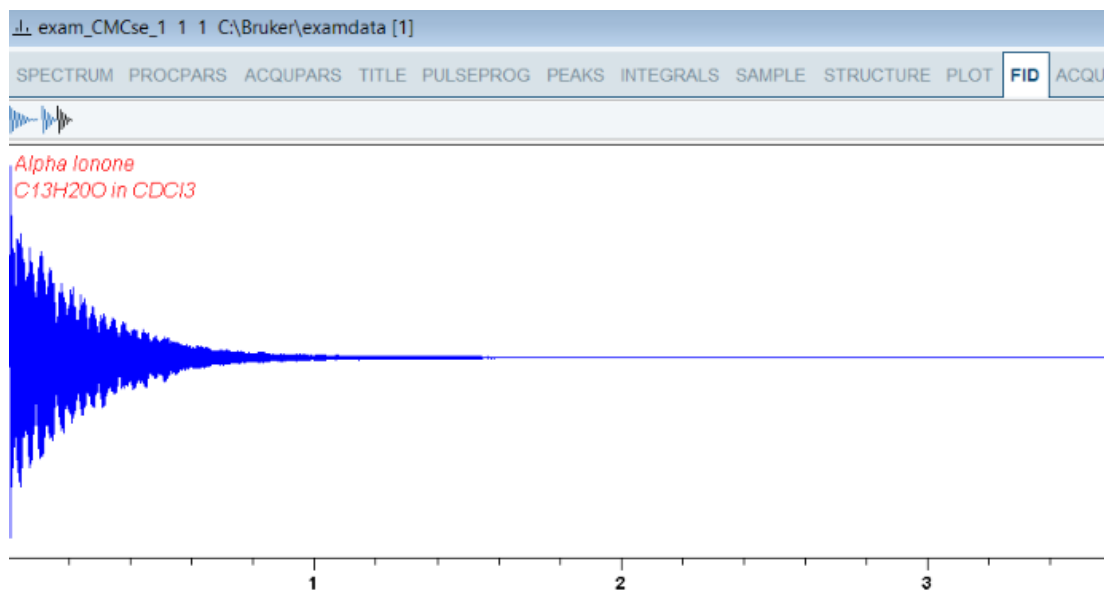
Move the selected item one place up in the table.



Move the selected item one place down in the table.

How to Display the FID

- Click the **Fid** tab [**fid**].



Displays the raw data. If these do not exist, the text *No raw data available* is displayed.

- Click one of the following buttons:



Show FID in shuffled mode.



Show FID in unshuffled mode.

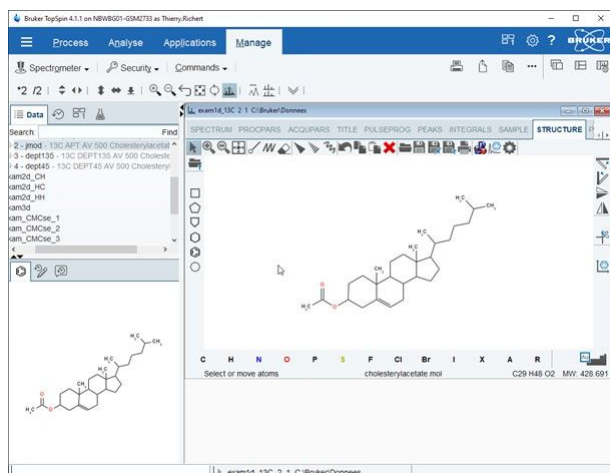
If you open a new dataset, the **Spectrum** tab is activated, no matter which tab was selected before. If you enter any interactive mode, for example phase correction mode, the Tab bar is replaced by a toolbar for that mode.

8.3.1 2D Molecule Structure Editor

The new 2D molecule structure editor is integrated into the Structure tab of the TopSpin spectrum window.


The user interface of the editor consists of several main parts:

1. The top horizontal quick access toolbar contains buttons to activate the main features of the editor like drawing structures, selection and rotation capabilities, undo/redo support, file features, editing of the structure properties etc.
2. Other toolbars allow selection of an element from the periodic table of elements to be used in a drawing. The user may also use a template to draw the structure more quickly.
3. The drawing area: Used to draw and visualize the structure.
4. The popup menu: Provides access to the same features as the toolbar in an alternative way.
5. The status bar: Displays the full path and file name of the opened file.
6. The user interface was designed to follow these criteria:
 - State of the art UI.
 - Simplified use, one click adds an atom (defined bond angle and length).
 - Smart utilization of Drag & Drop.





The editor is like other chemical structure drawing programs, but a brief description of the key buttons is included here.


- Click one of the following buttons:


 - Used to activate selection mode where object can be selected and moved.


 - Used to control the zoom level.

 - Used to scale the structure to its actual size.

 - Activates the drawing mode for normal bonds or chains.


 - Activates erase mode and deletes all touched bonds or atoms (highlighted in red before deleting).


 - Deletes the selection.


 - Used for stereo bond definition (note that at this time CMC-se ignores the stereo chemistry).


 - Used to undo the last step.


 - Simple ring templates.

 - Used to save or open a user defined template.

 - Used to open a structure or save changes.

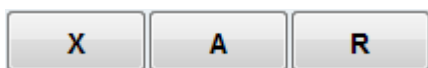
 - Used to copy and paste a selection.

 - Used to rotate or flip structures.

 - Used to clean a structure.



- Use to add an atom.



- Used to add a pseudo atom.

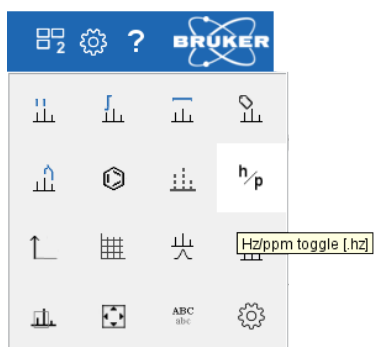


- Used to open the periodic table to select additional elements. Refer to the CMC-se User Manual for a list of the atoms that are supported in CMC-se.

8.4 1D Display Options

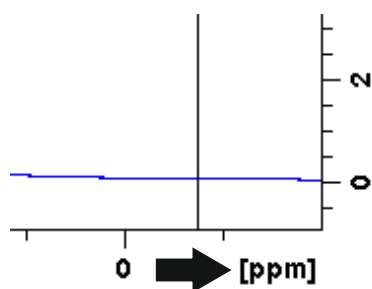
How to Toggle between Hertz and ppm Axis Units

- Click **Spectrum display properties**  and in the popup window toggle .

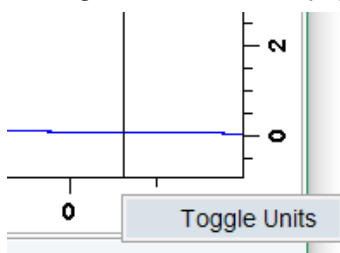


or

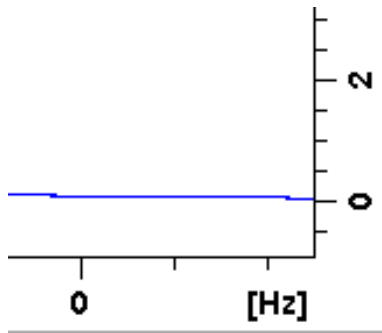
- Move the cursor to the unit info. The cursor changes to an arrow pointing to the right.



- Right-click and in the popup window, click **Toggle Units** or enter **.hz**.

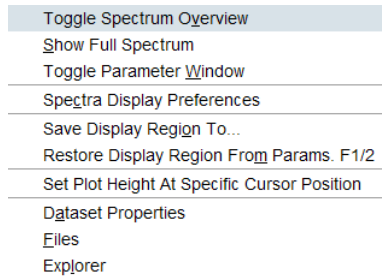


The display will change from ppm to Hz axis units [.hz].



How to Switch on/off the Spectrum Overview display

- Right-click in the dataset window and in the list, select **Toggle Spectrum Overview** or enter **.ov**.



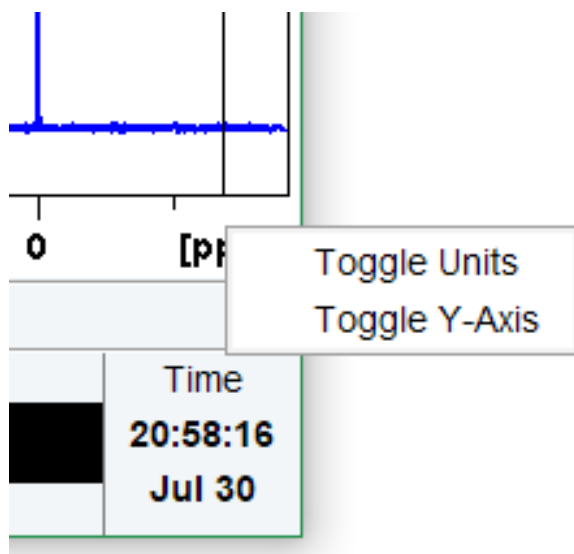
The spectrum overview shows the entire spectrum at the top of the dataset window. It is useful when only a certain region of the spectrum is displayed. In the overview, the displayed region is marked as a gray area. The default color is gray, it can be set in **Preferences | More Preferences | Spectra Display Preferences | Change | Color of zoom area**.

To shift the displayed region,

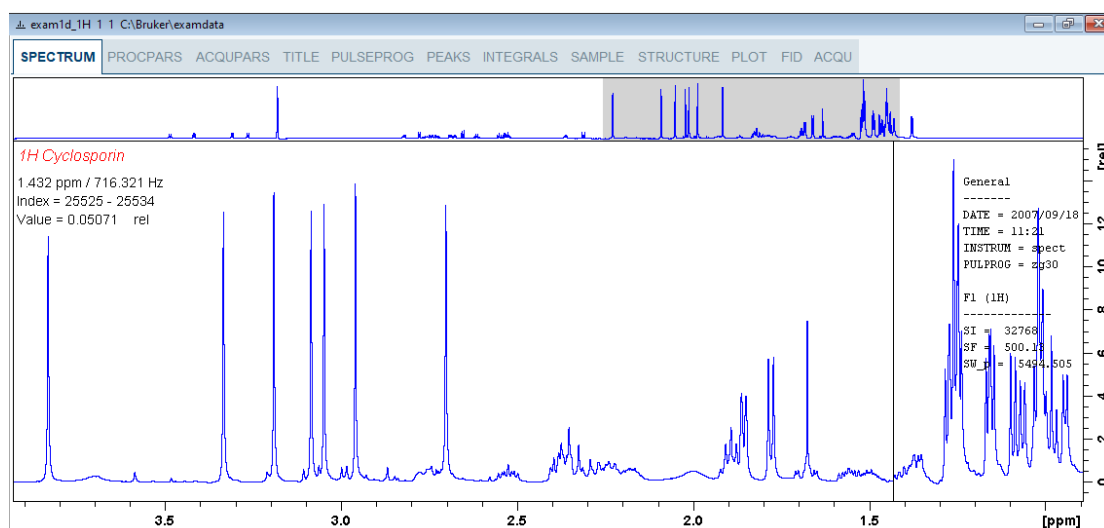
- simply click-hold the gray area in the overview spectrum and move the mouse (see figure below).

How to Toggle the Y-axis Display

- Move the cursor to the unit info.
- Right-click and in the popup window, select **Toggle Y-Axis** or enter **.y**.

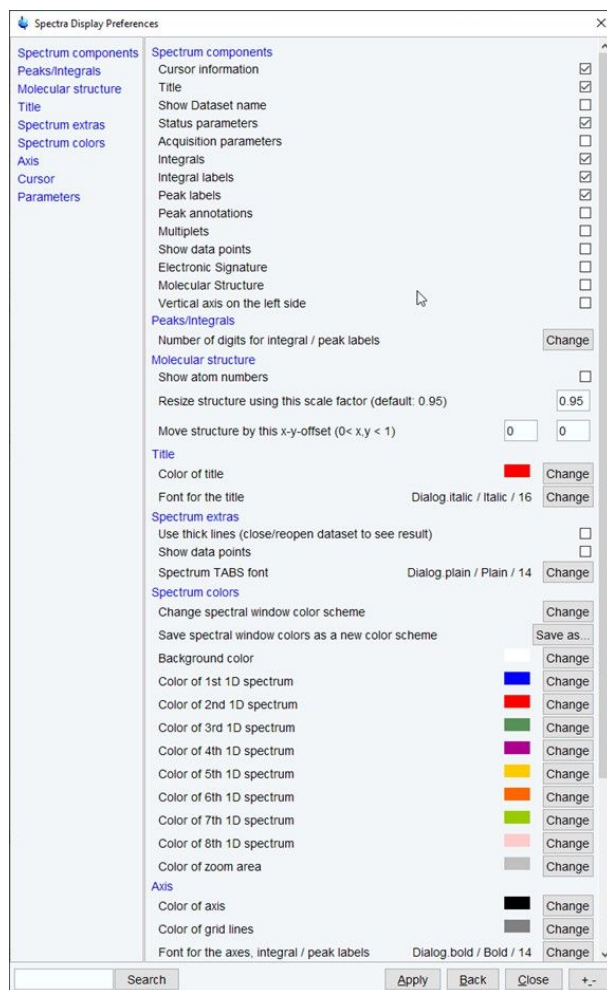


The following figure shows a dataset window with the spectrum overview on, ppm axis units, and relative [cm] Y-axis display.



8.5 Spectra Display Preferences

- Right-click inside the dataset window. In the list, select **Spectra Display Preferences** or enter **.dopt**.



- Check or uncheck the spectrum components and click **Apply** to be displayed in the dataset window.
 - To display the cursor information check **Cursor information**.
 - To display the title check **Title**.
 - To display the main status parameters, check **Status parameters**. These are the status parameters that also appear on the plot.
 - To display the integral trails/labels on the spectrum check **Integrals** and, if desired, **Integral labels**. If no integrals appear, the integral regions have not been determined yet. This can be done with the **int** command.
 - To display the peak labels, check **Peak labels**. Peak annotations appear, on peaks for which annotations have been defined, instead of regular peak labels showing chemical shift values. If no peak labels or annotations appear, peak picking has not been done yet. This can be done with the **pp** command.
 - To display the peak annotations, check **Peak Annotations**. Peak annotations appear, on peaks for which annotations have been defined, instead of regular peak labels showing chemical shift values. If no peak labels or annotations appear, peak picking has not been done yet. This can be done with the **pp** command.
 - To display the multiplets check **Multiplets**.
 - To display the data points, check **Show data points**. Expand the spectral region where you want to see individual points.

- To display the electronic signature, check **Electronic Signature**. The electronic signature, entered with **esign**, will appear below the title.
- To display the molecular structure, check **Molecular structure**.
- To display the vertical axis on the left side of the dataset window check **Vertical axis on the left side**.

Note that the **Spectra Display Preferences** dialog can also be opened in **Setup Preferences**.

How to Display the Main Dataset Properties

- Right-click inside the dataset window and select **Dataset Properties**.

The Properties window is displayed:

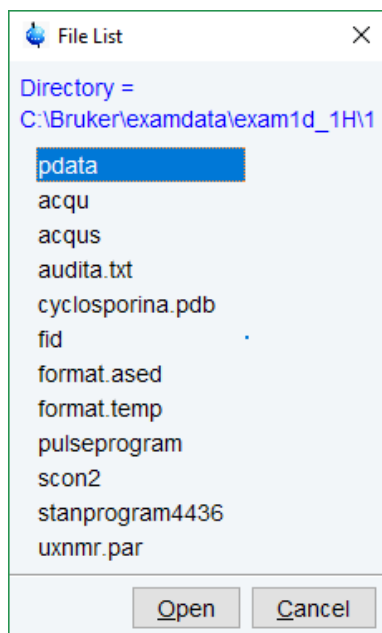


Note: this status information cannot be modified.

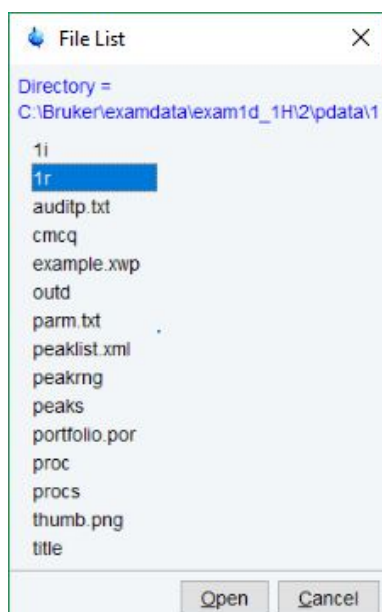
How to Display a List of Files of a Dataset

- Right-click inside the dataset window and in the list, select **Files**.

The following figure displays the file list when the **Fid** tab is active, i.e. when the raw data are displayed. It is the contents of the expno directory.



The next figure shows the file list that appears when the **Spectrum** tab is active, i.e. when the processed data are displayed. It is the contents of the `procno` directory.



The contents of any file in the list can be displayed as follows:

- Select a filename (it will be highlighted).
- Click **Open**.

Note: this is provided for ascii files, e.g. *acqu**, *proc** or files with the extension *.txt*.

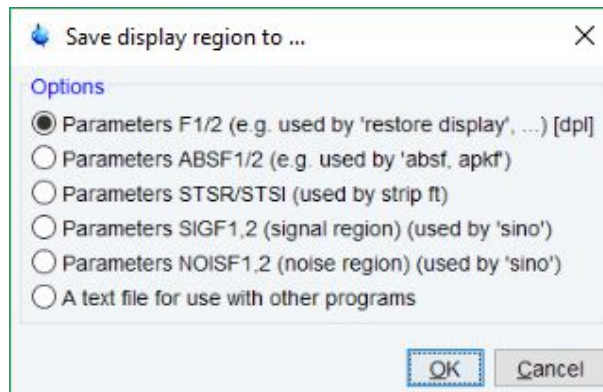
Dataset files can also be displayed/opened with the command **expl**. This opens the Windows Explorer, or under Linux, the Konqueror or Mozilla, showing the contents of the `procno` directory.

8.6 Saving Display Region

The currently displayed spectral region can be stored as follows:

- Right-click in the dataset window and select **Save Display Region To...**

This will open the following dialog:



Here the following options are available:

Parameters F1/2 [dpl] to save the displayed region for restoring the display later. The region is stored in the parameters F1P and F2P.

To restore the saved region,

- Right-click in the dataset window and select **Restore Display Region from Params F1/2**

- Click

Parameters ABSF1/2 to save the displayed region for baseline correction (command **absf**) or phase correction (command **apkf**). The region is stored in the processing parameters ABSF1 and ABSF2.

Parameters STSR/STSI to save the displayed region for Strip FT (commands like **ft** and **trf**). The region is stored in the processing parameters STSR and STSI.


Parameters NOISF1/2 to save the displayed region as the signal region for Signal to Noise calculation (command **sino**). The region is stored in the processing parameters SIGF1 and SIGF2.

Parameters SIGF1/2 to save the displayed region as the noise region for Signal to Noise calculation (command **sino**). The region is stored in the processing parameters NOISF1 and NOISF2.

A text file for use with other programs to save the displayed region in a text file. This file can be viewed with any editor or used by external programs.

8.7 Synchronize Visible Region of all Dataset Windows

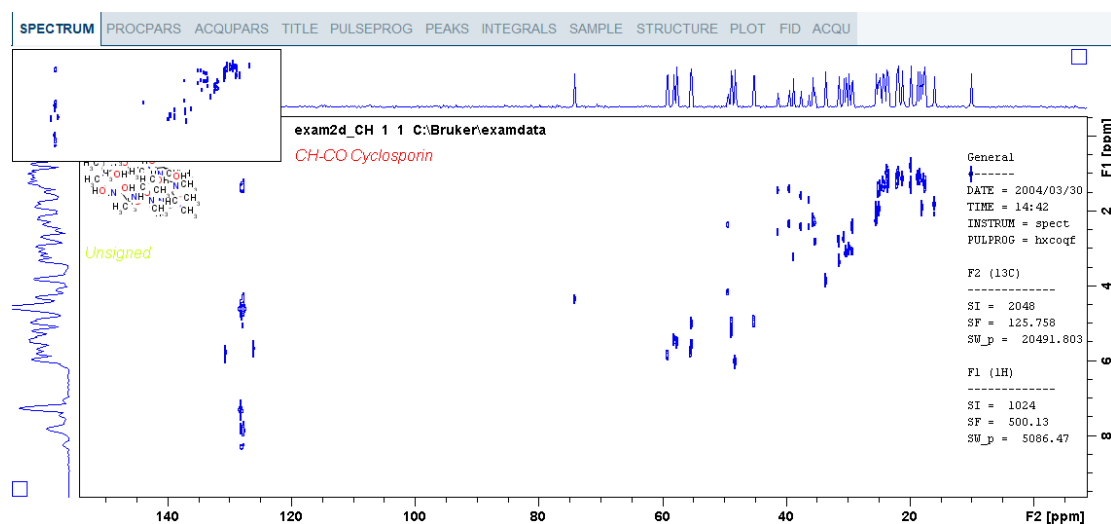
The visible region of all dataset windows can be synchronized as follows.

- Zoom in or out one dataset and then click  or enter **.sync**.

9 2D Display

9.1 The 2D Dataset Window


The following figure provides a dataset with a 2D spectrum.

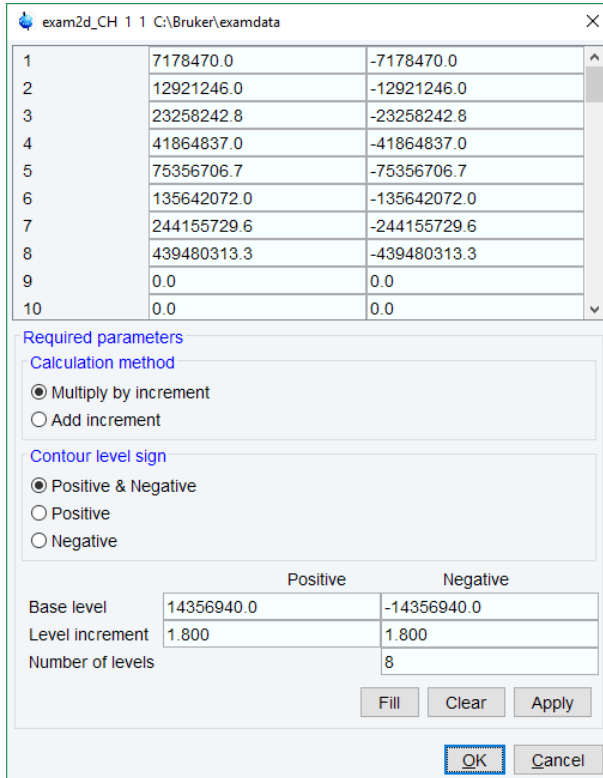


9.2 Changing the Display of a 2D Spectrum

TopSpin offers various buttons to scale or shift a 2D spectrum both vertically and horizontally.

How to Change the Intensity Scaling (contour levels)

- Click **Edit contour levels**  to change the intensity scaling (contour levels) [edlev].



or

- Hit one of the keys:
 - Alt+ PageUp:** Increase the intensity by a factor of 2.
 - Alt+ PageDown:** Decrease the intensity by a factor of 2.
 - Alt + Enter:** Reset the intensity.

or

- Click one of the following buttons:
 - Increase the intensity (decrease the levels) by 2 [***2**].
 - Decrease the intensity (increase the levels) by 2 [**/2**].
 - Reset the intensity to the last saved intensity (contour levels) [**.vr**].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

To manipulate all dataset windows, press the **Ctrl** key while clicking one of the above buttons.

How to Smoothly Change the Vertical Scaling (contour levels)

To change levels, multiplying all levels with the same factor:

- Click-hold the button and move the mouse.

or

- Turn the mouse wheel while the cursor is in the dataset window.

To change the level distance (increment), leaving the base level the same:

- Click-hold the  button and move the mouse.

How to Display a Contour Levels Bar in the Dataset Window




- Right-click in the dataset window and in the list, select **Spectra Display Preferences**. [.dopt]
- In the group **Contour display** check **Contour Levels Bar** and click **Apply**.

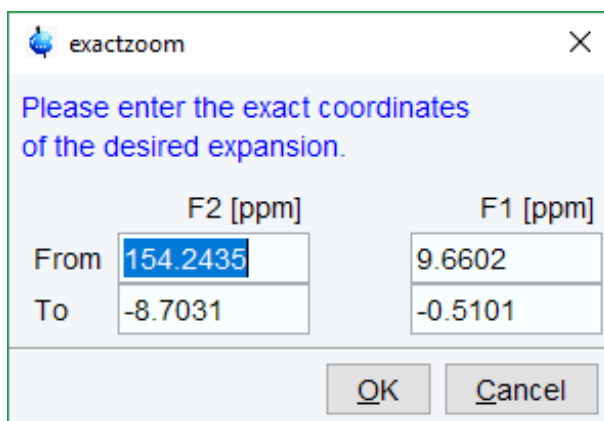
How to Switch on/off Square 2D layout





- Right-click inside the dataset window field and in the list, select **Square Layout On/Off**.

The F2 scaling will be adjusted to reach a square display.

How to Zoom a 2D Spectrum In/Out

- Click one of the following buttons:
 -  Zoom in to the center (spectrum) or left edge (FID) of the displayed region, increasing the horizontal scaling [.zi].
 -  Zoom out from the center (spectrum) or left edge (FID) of the displayed region, decreasing horizontal scaling) [.zo].
 -  Perform an exact zoom via a dialog box [.zx].
- Enter the coordinates of the desired region in the dialog box.
- Click **OK**



- Click one of the following buttons:
 -  Undo last zoom [.zl].
 -  Show full spectral width in F2 [.f2r].
 -  Show full spectral width in F1 [.f1r].
 -  Show full spectrum [.all].



Retain horizontal and vertical scaling when modifying dataset or changing to different dataset. Effects all dataset windows [.keep].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

How to Shift a Spectral Region in the F2 direction (left/right)

- Click one of the following buttons:



Shift to the left, half of the displayed region [.sl].



Shift to the right, half of the displayed region [.sr].

or



- Click-hold the button and move the mouse to smoothly shift in any direction.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

How to Shift a Spectral Region in the F1 direction (up/down)

- Click one of the following buttons:



Shift the spectrum baseline to the middle of the data field [.su].



Shift the spectrum baseline to the bottom of the data field [.sd].

or

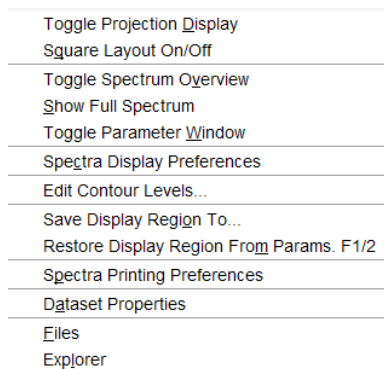


- Click-hold and smoothly shift the mouse up/down and left/right.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

9.3 Show Spectra Display Preferences/Regions/Files

- Right-click in the dataset window and in the list, select **Spectra Display Preferences**.



Here you can set various display options including parameters, integrals, peaks, contours, projections and electronic signature. The number of displayed digits for the integral and peak labels can also be set in the group **Peaks/Integrals**.



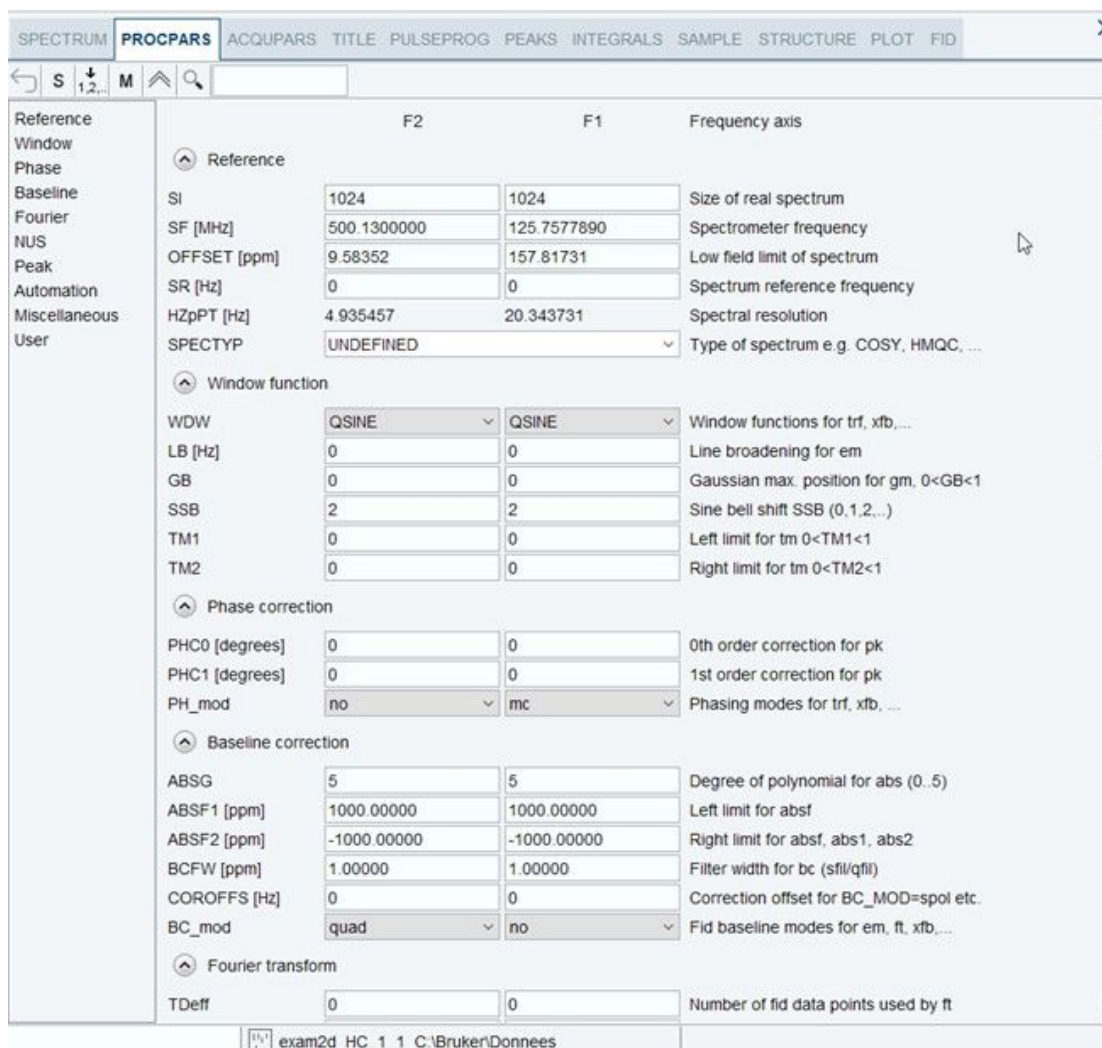
9.4 Using the Tab Bar

The 2D dataset window is a tabbed pane. This means its content depends on the currently active tab in the Tab bar. The individual tabs are basically the same as for 1D display (see chapter How to Expand a Spectral Region). There are, however, some differences, which are discussed below.

How to Set Processing Parameters

- Click the **ProcPars** tab [edp].

The 2D processing parameter editor contains a column for each of the two dimensions F2 and F1. Note that not all parameters exist in both dimensions.



How to Set Acquisition Parameters

- Click the **AcquPars** tab [eda].

The 2D acquisition parameter editor contains a column for each of the two dimensions F2 and F1. Note that not all parameters exist in both dimensions.

ACQPARS		TITLE	PULSEPROG	PEAKS	INTEGRALS	SAMPLE	STRUCTURE	PLOT	FID
F2 F1 Frequency axis									
Experiment									
PULPROG	hmzgpgqf		E		Current pulse program				
AQ_mod	DQD		Acquisition mode						
FnTYPE	traditional(planes)		nD acquisition mode for 3D etc.						
FnMODE	QF		Acquisition mode for 2D, 3D etc.						
TD	1024	128	Size of fid						
DS	16	Number of dummy scans							
NS	4	Number of scans							
TD0	1	Loop count for '3D'							
TDav	0	Average loop counter for nD experiments							
Width									
SW [ppm]	10.1051	165.6392	Spectral width						
SWH [Hz]	5053.908	20831.980	Spectral width						
RL_F [usec]			Increment for delay						
AQ [sec]	0.1013077	0.0061444	Acquisition time						
FIDRES [Hz]	9.870914	162.749847	Fid resolution						
FW [Hz]	125000.000	Filter width							
Nucleus 1									
NUC1	1H	13C	Observe nucleus						
O1 [Hz]	2266.05	9430.77	Transmitter frequency offset						
O1P [ppm]	4.531	74.992	Transmitter frequency offset						
SFO1 [MHz]	500.1322661	125.7672198	Transmitter frequency						
BF1 [MHz]	500.1300000	125.7577890	Basic transmitter frequency						
Nucleus 2									
NUC2	13C	2nd nucleus							
O2 [Hz]	9430.77	Frequency offset of 2nd nucleus							
O2P [ppm]	74.992	Frequency offset of 2nd nucleus							
SFO2 [MHz]	125.7672198	Frequency of 2nd nucleus							

How to Display the Peak list

- Click the **Peaks** tab.

Peak picking [_pp2d append noduplicates] ✕

Options

- Append peaks to list
- Discard new peak(s) if already in list
- Export results as XWinNMR peak list

Parameters

Region

	From (F1P)	To (F2P)	Set to ▶
F2 [ppm]	10.7111	-1.3051	
F1 [ppm]	152.8275	-12.8349	

Sensitivity

Minimum intensity [rel] (MI)	0.1000	Set to ▶
Maximum intensity [rel] (MAXI)	1.0000	
Diagonal gap [points] (PPDIAG)	0	
Resolution [points] (PPRESOL)	1	

Miscellaneous

Maximum # of peaks (PPMPNUM)	100
Interpolation type (PPIPTYP)	None ▼
Pick peaks of sign (PSIGN)	Positive ▼

Reset all to ▶

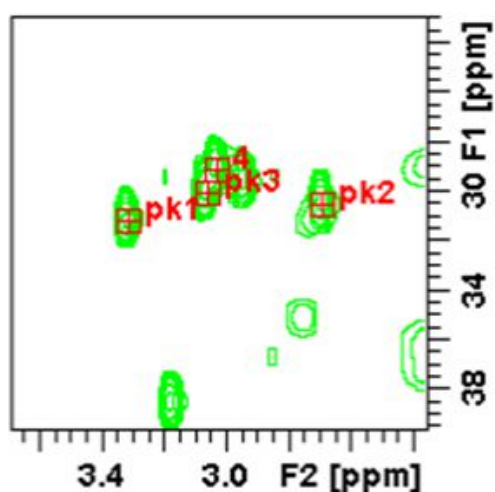
Peak	v(F2) [ppm]	v(F1) [ppm]	Intensity [abs]	Annotation
20	7.2728	128.0752	7316983.44	
11	5.9703	48.1561	5697658.06	
19	5.8178	59.1571	7060454.88	
1	5.7474	130.5019	3474121.12	
9	5.6887	55.4361	5171107.75	
3	5.6418	125.9721	3673180.69	
16	5.5009	55.2744	6283238.12	
18	5.4540	57.5393	6828276.94	
15	5.3719	58.0246	6123020.62	
12	5.2310	48.8032	5795426.88	
13	4.9964	55.2744	5842008.25	
14	4.9377	45.0822	5855596.00	
10	4.9025	48.8032	5367032.50	
17	4.3158	74.2026	6757091.69	
37	3.8346	33.5959	21692679.12	
38	3.3301	31.3310	22937250.94	
40	3.1892	38.7728	23728422.31	
42	3.0836	30.1985	25617898.25	
41	3.0484	29.2278	24970031.12	

This displays list of peaks if these have been calculated (command **pp**). The list is basically the same as for 1D spectra. The only difference is that there are two columns for the two directions:

v(F2) [ppm]: the chemical shift in the F2 direction.

v(F1) [ppm]: the chemical shift in the F1 direction.

To specify or edit an annotation, click inside the **Annotation** field and enter a character string. The peak annotations are shown in the correlated spectrum:



How to Display the Integral list

- Click the **Integrals** tab.

Object	Integral [abs]	Integral [rel]	Type	Peaks	v(F2) [ppm]	v(F1) [ppm]
Integral 1	9256210.25	0.0019	Automatic	1	143.3433	8.4485
Integral 2	105879246.25	0.0216	Automatic	2	128.0287	8.2716
Integral 3	71284449.50	0.0146	Automatic	1	127.8096	8.2686
Integral 4	62213796.50	0.0127	Automatic	1	127.6177	8.2148
Integral 5	2656892732.25	0.5423	Automatic	11	127.9367	7.6181
Integral 6	6120164.25	0.0012	Automatic	1	107.3009	7.2915
Integral 7	12617947.25	0.0026	Automatic	1	127.6692	7.2815
Integral 8	15729719.25	0.0032	Automatic	1	136.5803	7.1276
Integral 9	107315183.50	0.0219	Automatic	1	128.1116	7.0740

This displays the list of integrals if these have been calculated (command **int**). The list is basically the same as for 1D spectra. The only difference is that, when peaks are shown, there are two columns for the chemical shift:

v(F2) [ppm]: the chemical shift in the F2 direction.

v(F1) [ppm]: the chemical shift in the F1 direction.


Furthermore, a stored or exported 2D integral list can be imported as follows:

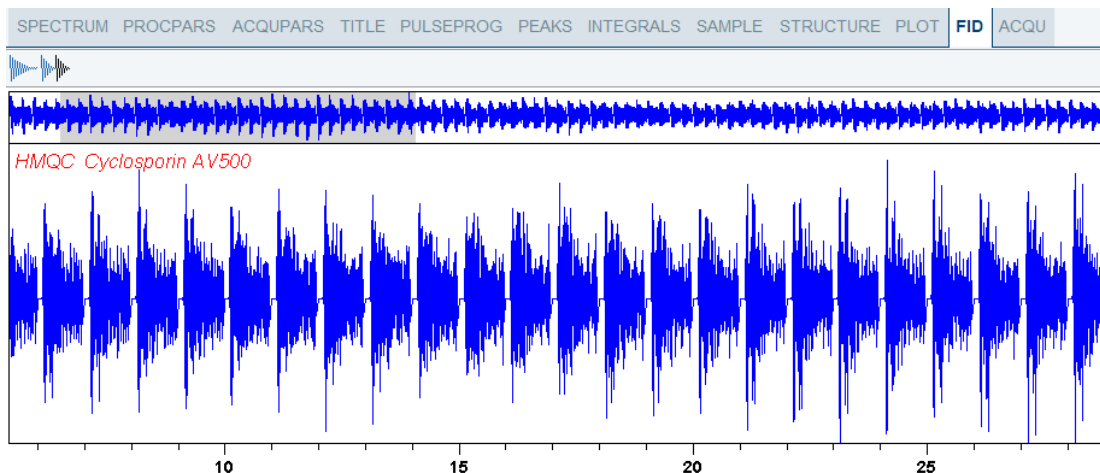
- Right-click an entry in the list, select **Import...**
- In the appearing dialog box, navigate to the directory where the list resides and select the integral list.

As such you can import an integral list from a different dataset or a previously exported list from the current dataset. Note that integration commands store the integral list in the processed data directory under the name *integrals.txt*. Exported integrals are stored in the files *<name>.txt* and *<name>.reg*, where *<name>* is the name specified by the user.

How to Display the FID

- Click the **Fid** tab [fid].

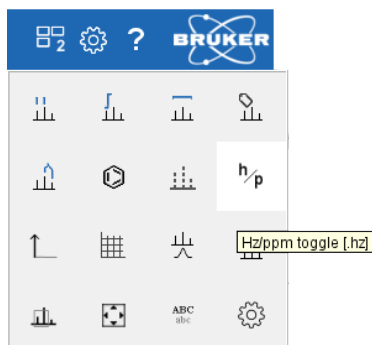
2D raw data consist of a series of FIDs which are displayed in a row. Individual FIDs can be displayed by zooming in. To do that, click  repeatedly. Now you can shift and zoom in/out the data to display different FIDs:



9.5 2D Display Options

How to Switch between Hertz and ppm Axis Units in F2 and F1

- Click **Spectrum display properties**  and in the popup window toggle .



or

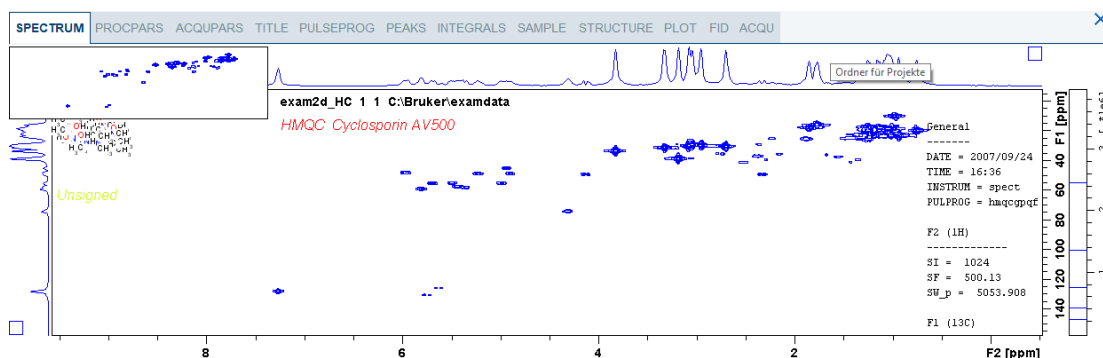
- Move the cursor to the unit info. The cursor changes to an arrow pointing to the right.
- Right-click and in the popup window, click **Toggle Units** or enter **.hz**.

The display will change from ppm to Hz axis units [.hz].

How to Switch On/Off the Spectrum Overview Display

- Right-click in the dataset window and select **Toggle Spectrum Overview** or enter **.ov**.

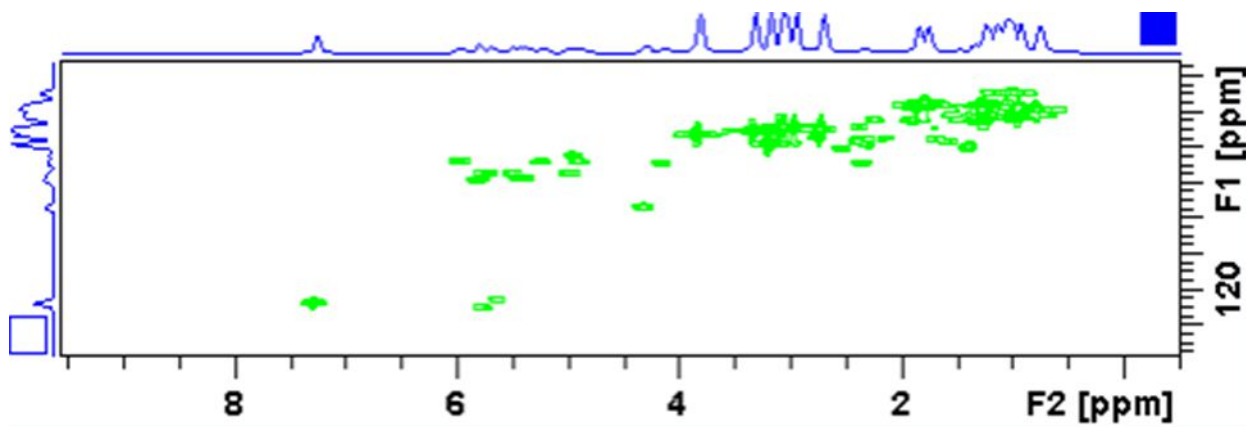
With the spectrum overview on, the dataset window will, for example, look like this:



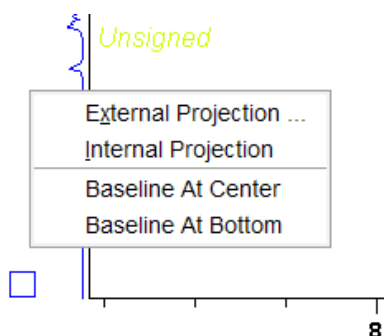
How to Switch On/Off the Projection Display

- Right-click in the dataset window and select **Toggle Projection Display** or enter **.pr**.

With the projections displayed, a 2D dataset looks like this:



In this example, the F1 projection is selected as indicated by the filled blue square whereas the F2 projection is not selected. A selected projection can be rescaled using the toolbar rescale buttons of function keys. If you right-click inside the projection area of the dataset window, the following list appears:



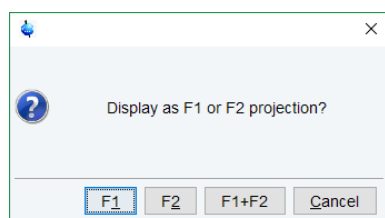
External Projection opens a dialog box where you can specify or search for a 1D dataset and display this as a projection of the current 2D dataset.

Internal Projection calculates and displays the positive projection and displays it along with the 2D spectrum.

Baseline at Bottom or **Baseline at Center** allows to put the projection baseline at the respective positions.

Alternative ways to calculate/display projections are:

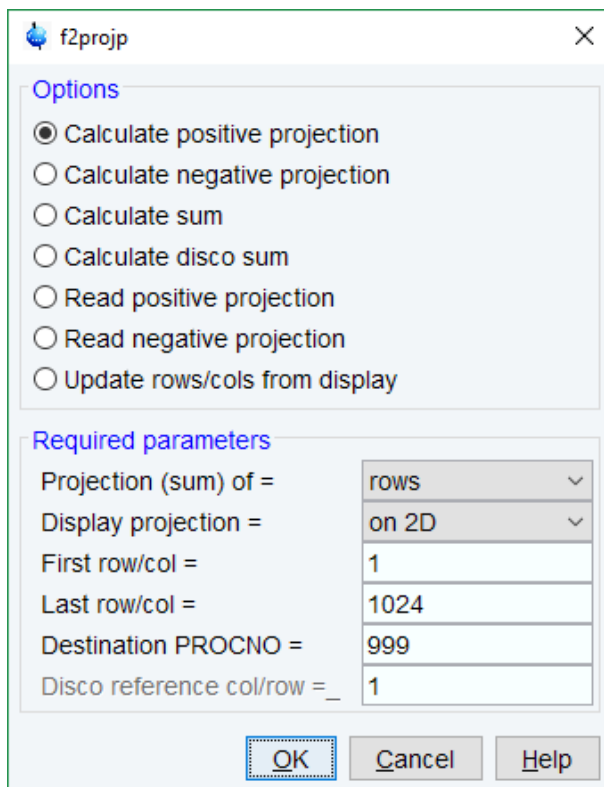
- Right-click on a 1D dataset in the browser and in the list, select **Display As 2D Projection**.



or

- Click **Process | Advanced | Calc. projections [proj]** or enter **proj**.

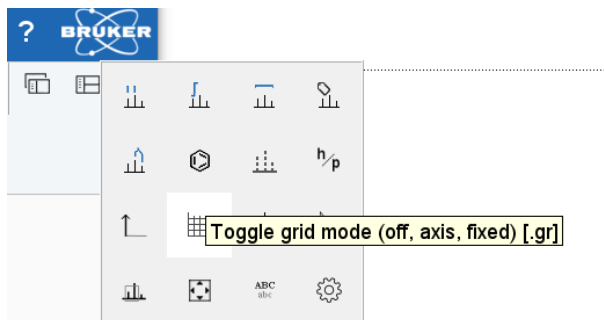
This will open the dialog box:



From here, you can calculate positive, negative, sum and disco projections and either show them with the 2D spectrum or display them in separate dataset window as a 1D data. For more details on the corresponding commands (as shown in the header of the dialog box), please refer to the Processing Reference Manual.

How to Switch On/Off the Grid display

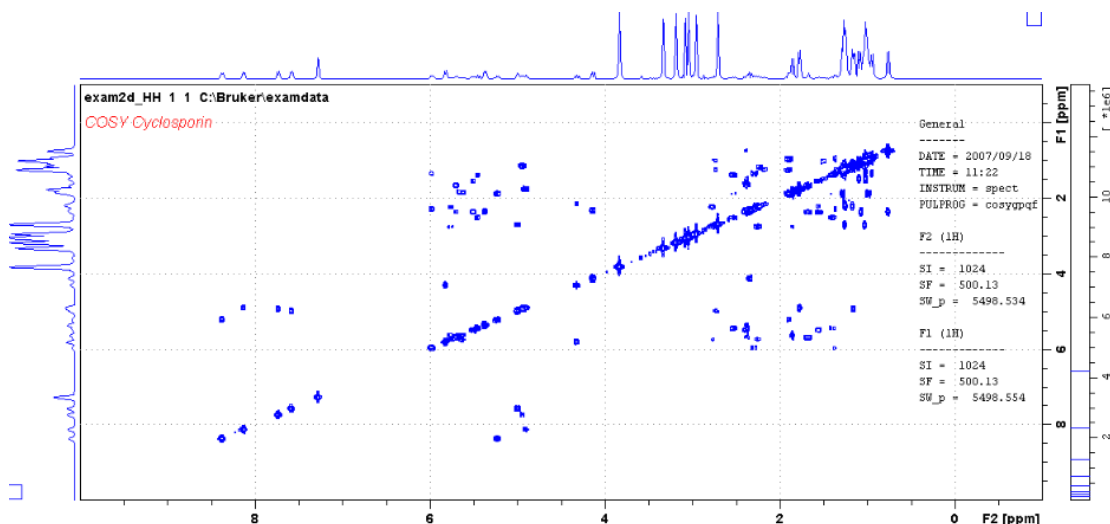
- Click **Spectrum display properties | Toggle grid mode (off, axis, fixed)** to display the grid *axis aligned* or enter `.gr`.



To switch between *no grid*, *axis aligned grid* and *fixed grid*,

- click again **Spectrum display properties | Toggle grid mode (off, axis, fixed)**.

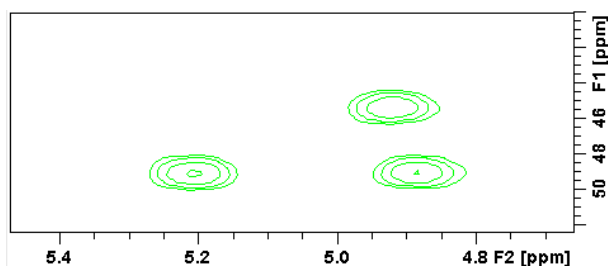
The following figure shows an example of axis aligned grid display.





How to Display a 2D Spectrum in Contour Mode

- In the upper toolbar click  Switch to contour display mode [.co].

In contour mode, a spectral region looks like this:



How to Set the 2D Contour Levels

- Click-hold **Change the level distance**  and move the cursor up or down
- or
- Enter **Alt+ PageUp** respectively **Alt+ PageDown**
- or
- Right-click in the dataset window and select **Edit contour levels [edlev, .lv]**
- or
- Click **Edit contour levels** .

The last two methods will open the following dialog box shown in the next figure. Contour levels can be entered manually, or they can be calculated.

The dialog box 'exam2d_HC 1 1' contains a table with 10 rows and 3 columns. The first two columns contain numerical values, and the third column contains a small upward-pointing arrow icon. Below the table are configuration options for 'Required parameters'.

1	232901.8	-232901.8
2	419223.2	-419223.2
3	754601.7	-754601.7
4	1358283.0	-1358283.0
5	2444909.5	-2444909.5
6	4400837.0	-4400837.0
7	7921506.6	-7921506.6
8	14258712.0	-14258712.0
9	0.0	0.0
10	0.0	0.0

Required parameters

Calculation method

Multiply by increment
 Add increment

Contour level sign

Positive & Negative
 Positive
 Negative

	Positive	Negative
Base level	173794.9	-173794.9
Level increment	1.800	1.800
Number of levels	8	

Buttons: Fill, Clear, Apply, OK, Cancel

Manual setup

This allows to create an arbitrary sequence of levels:

- Enter the level values in the fields 1, 2... at the top of the dialog box.
- Click **Apply** to update the display or **OK** to store the levels, update the display and close the dialog box.

Calculation

This allows to easily create a geometric or equidistant sequence of levels.

- Click one of the following items:
 - **Multiply with increment** to create a geometric sequence of levels.
 - **Add increment** to create a equidistant sequence of levels.
- Enter the desired *Base level*, *Level increment* and *Number of levels*.
- Click **Fill** to display and activate the sequence.
- Click **Apply** to update the display or **OK** to store the levels, update the display and close the dialog box.

The Contour level sign allows to select positive levels, negative levels or both.

How to Store interactively set Contour Levels

To store contour levels that were set interactively

- Click **Save the contour levels to disk**  [..Is].

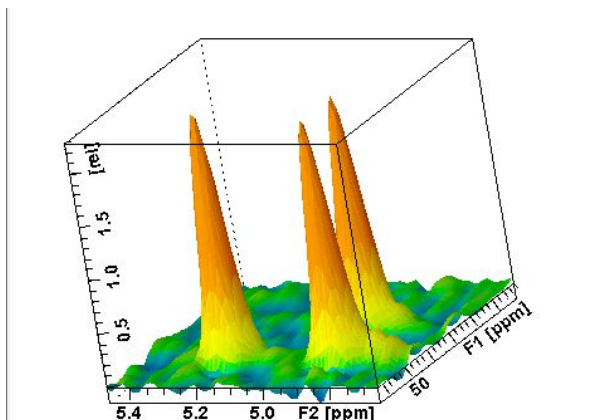
The levels are stored in the file:

```
/< dir>/data/<user>/nmr/< name>/<expno>/pdata/<procno>/clevels
```

How to Display a 2D Spectrum in Oblique Mode

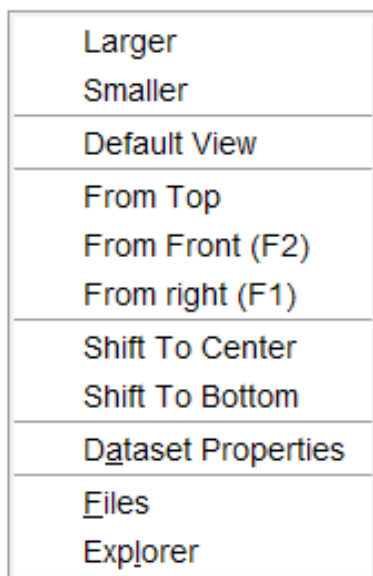
- Click **Oblique mode**  [.st]

In oblique mode, a spectral region looks like that in the following figure:



In this mode you can manipulate the display in various ways.


- Right-click inside the dataset window and select one of the options in the list:




How to Rotate a 2D Spectrum in Oblique Mode

- Click-hold one of the following buttons and move the mouse up/down:

 Rotate around x-axis.

 Rotate around y-axis.

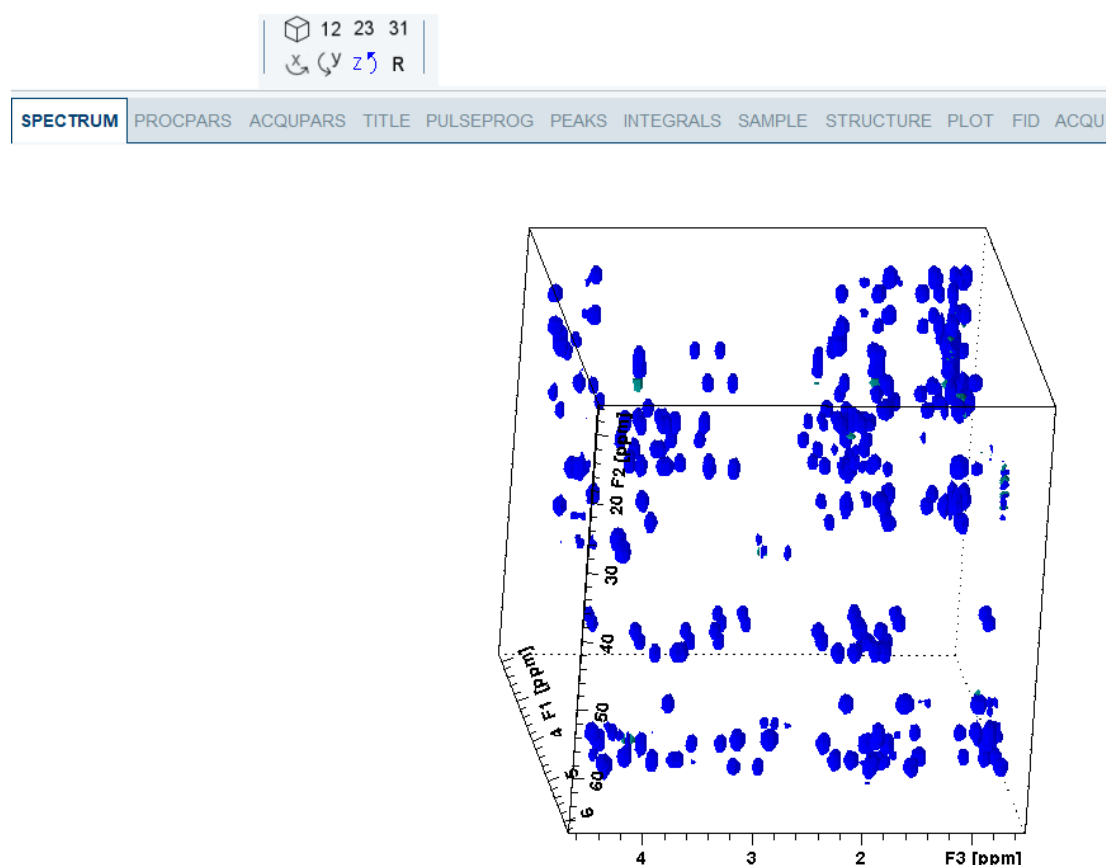
How to Switch between Displaying Positive and Negative levels

- Click  to toggle between positive and negative levels [.It].

10 nD Display

10.1 Display Planes of 3D Datasets

3D datasets can be displayed as 2D planes or as a 3D cube. By default, the first F3-F1 plane is displayed (see the figure below) The plane orientation and number is displayed. The cube in the lower left corner graphically indicates which plane is displayed. The full 2D display functionality is available (see chapter [Getting Started](#) [29]).



How to Switch to 2D Plane Display

If the 3D cube is displayed, you can switch to 2D plane display.

- Click one of the following buttons:



Switch to 2D contour display.



Switch to 2D oblique display.

How to Display various Plane Orientations

- Click one of the following buttons:



Display F1-F2 planes.

23 Display F2-F3 planes.

31 Display F3-F1 planes.

How to Display various Plane Positions (numbers)

- Click one of the following buttons:

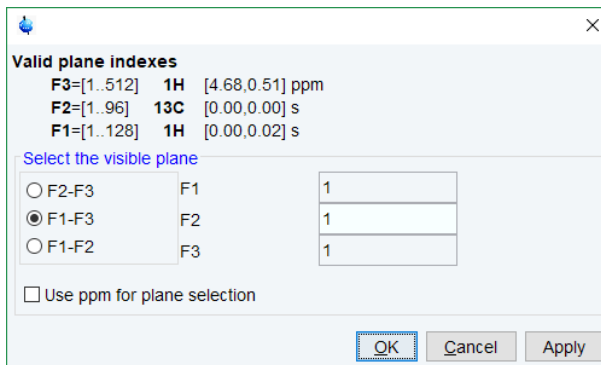
+ Display the next plane.

- Display the previous plane.

↕ Scan planes smoothly.

E Enter the exact plane number.


This will open a dialog, see the next figure. Here, you can specify the desired plane number as well as switch to a different plane orientation.

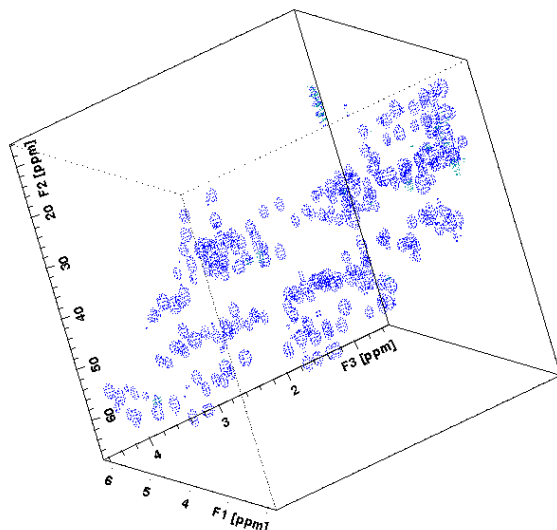


10.2 3D Cube Display Mode

How to Display the 3D Cube

- Click the following button:

 Display 3D cube:



How to Rotate the 3D Cube

- Click-hold one of the following buttons and move the mouse up/down:



Rotate cube around x-axis.



Rotate cube around y-axis.



Rotate cube around z-axis.

How to Scale Up/Down the 3D Cube

- Right-click inside the dataset window and in the list, select **Larger** or **Smaller**.

How to Reset the Cube Size and Orientation

- Click **R** Reset to default size and orientation.

How to Switch Depth Cueing On/Off

- Right-click inside the dataset window and in the list, select **Depth Cueing On/Off**.

Larger
Smaller
Default View
Depth Cueing On/Off
Toggle Parameter Window
Spectra Display Preferences
Spectra Printing Preferences
Dataset Properties
Files
Explorer

Depth cueing makes data points which are closer to the viewer appear brighter and those that are further away appear dimmer. This increases the depth effect of the 3D image.

How to Display a Cube Front or Side view

- Click one of the following buttons:

12 Show F1-F2 planes.

23 Show F2-F3 planes.

31 Show F3-F1 planes.

10.3 nD Parameter Display

TopSpin supports parameter display of up to 8D data. To display processing parameters:

- Click the **ProcPars** tab of the dataset window.

or

- Enter **edp** on the command line.

Parameters of each direction are displayed in a separate column.

The figure below displays the processing parameter display of a 3D dataset.

	F3	F2	F1	Frequency axis
Reference				
SI	2048	128	128	Size of real spectrum
SF [MHz]	600.1300119	150.9027490	600.1300000	Spectrometer frequency
OFFSET [ppm]	4.68016	67.76508	6.28076	Low field limit of spectrum
SR [Hz]	11.90	0	0	Spectrum reference frequency
HZpPT [Hz]	1.220703	73.242188	20.926340	Spectral resolution
AQORDER	3-2-1			Order of fids in ser file
SPECTYP	UNDEFINED			Type of spectrum e.g. COSY, HMQC, ...
Window function				
WDW	QSINE	QSINE	QSINE	Window functions for trf, xfb, ...
LB [Hz]	0.40	0.30	0.30	Line broadening for em
GB	0	0.1	0.1	Gaussian max. position for gm, 0<GB<1
SSB	2	2	2	Sine bell shift SSB (0.1,2,...)
TM1	0	0.1	0.1	Left limit for tm 0<TM1<1
TM2	0	0.9	0.9	Right limit for tm 0<TM2<1
Phase correction				
PHC0 [degrees]	122.535	0	0	0th order correction for pk
PHC1 [degrees]	-101.400	0	0	1st order correction for pk
PH_mod	pk	pk	pk	Phasing modes for trf, xfb, ...
Baseline correction				
ABSG	5	5	5	Degree of polynomial for abs (0..5)
ABSF1 [ppm]	1000.00000	1000.00000	1000.00000	Left limit for absf
ABSF2 [ppm]	-1000.00000	-1000.00000	-1000.00000	Right limit for absf, abs1, abs2
BCFW [ppm]	1.00000	1.00000	1.00000	Filter width for bc (sfll/qfl)
COROFFS [Hz]	0	0	0	Correction offset for BC_MOD=spol etc.
BC_mod	quad	no	no	Fid baseline modes for em, ft, xfb, ...
Fourier transform				
TDef	0	0	0	Number of fid data points used by ft

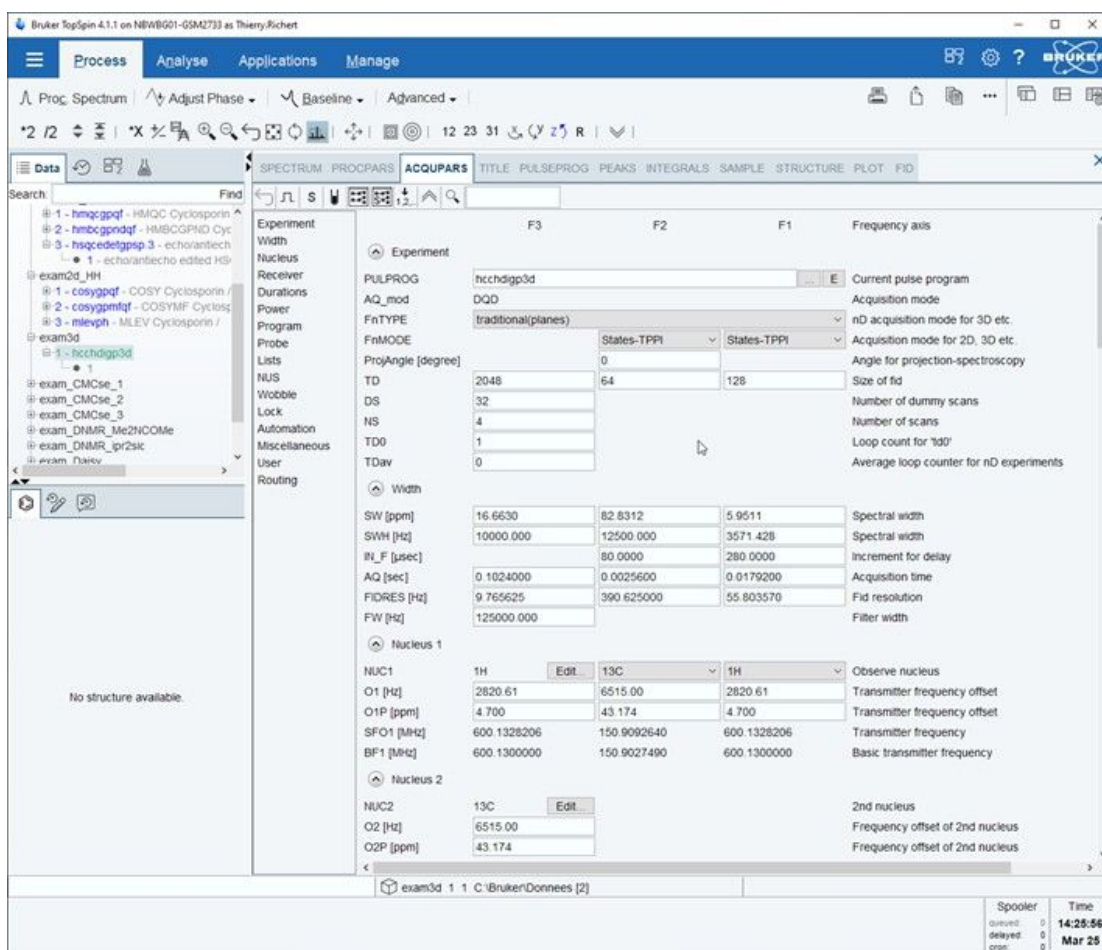
To display acquisition parameters:

- Click the **AcqPars** tab of the dataset window.

or

- Enter **eda** on the command line.

Parameters of each direction are displayed in a separate column. The following figure displays the acquisition parameter display of a 3D dataset.



10.4 nD FID Display

nD raw data can be displayed as a series of 1D FIDs:

- Click the **FID** tab of the dataset window.

or

- Enter **fid** on the command line.

10.5 nD Peak and Integral Display

TopSpin supports peak and integral display of up to 8D data.

To display the nD peak list:

- Click the **Peaks** tab of the dataset window.

or

- Enter **peaks** on the command line.

Peak picking [_pp3d append noduplicates]

Options

- Append peaks to list
- Discard new peak(s) if already in list
- Export results as XWinNMR peak list

Parameters

Region

	From (F1P)	To (F2P)	
F3 [ppm]	4.6802	0.5144	Set to ▶
F2 [ppm]	67.7651	5.6390	
F1 [ppm]	6.2808	1.8174	

Sensitivity

Minimum intensity [rel] (MI)	0.1000	Set to ▶
Maximum intensity [rel] (MAXI)	1.0000	
Resolution [points] (PPRESOL)	1	

Miscellaneous

Maximum # of peaks (PPMPNUM)	100
Interpolation type (PPIPTYP)	None ▼
Pick peaks of sign (PSIGN)	Positive ▼

Reset all to ▶

OK Cancel Help Start manual picker

The following figure displays the peak list of a 3D dataset.

Peak	v(F3) [ppm]	v(F2) [ppm]	v(F1) [ppm]	Intensity [abs]	Annotation
35	4.4768	37.3492	3.3982	17002535.00	
44	4.4768	54.8221	6.0018	18171794.00	
55	4.4768	12.7576	2.3754	21518231.00	
77	4.4768	16.6405	2.5148	30512881.00	
23	4.3954	32.1720	3.3982	14061680.00	
53	4.3954	56.1164	5.9088	20971480.00	
58	4.3954	19.8762	2.4218	22475741.00	
5	4.3140	47.0564	4.6535	11251946.00	
9	4.3140	47.0564	4.4210	11611408.00	
17	4.3140	21.8177	3.0263	12380779.00	
19	4.3140	21.8177	2.2359	13047012.00	
61	4.3140	32.1720	3.4447	23169332.00	
84	4.3140	60.6465	5.8158	35322721.00	
15	4.1025	38.6435	2.9333	12280194.00	
52	4.1025	60.6465	5.6299	20881797.00	
68	4.1025	15.9933	2.3754	24840581.00	
72	4.0781	36.7020	4.3281	27287385.00	
88	4.0781	36.7020	4.6070	43388739.00	
7	3.9398	47.7035	4.9790	11396389.00	
28	3.9398	28.9363	3.2122	14714260.00	

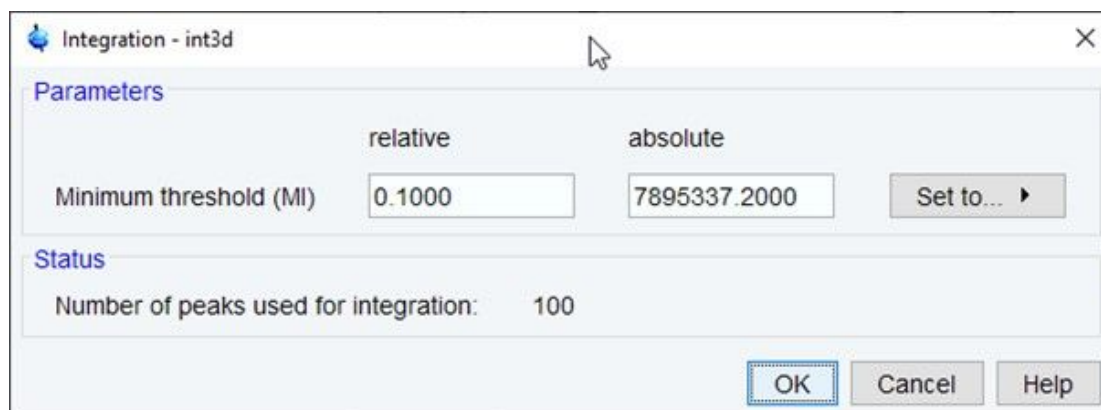
The chemical shift in each of the three dimensions is displayed in a separate column.

To display the nD integral list:

- Click the **Integrals** tab of the dataset window.

or

- Enter **ints** on the command line.



The following figure displays the integral list of a 3D dataset.

SPECTRUM	PROCPARS	ACQUPARS	TITLE	PULSEPROG	PEAKS	INTEGRALS	SAMPLE	STRUCTURE	PLOT
△ Object	Integral [abs]	Integral [rel]	Peaks	v(F3) [ppm]	v(F2) [ppm]	v(F1) [ppm]			
⊕ Integral 1	325428.25	0.1048	1	4.3100	0.0000	0.0000			
⊕ Integral 2	812881.75	0.2618	1	1.5274	0.0000	0.0000			
⊕ Integral 3	417812.75	0.1346	1	0.9985	0.0000	0.0000			
⊕ Integral 4	663838.00	0.2138	1	0.7585	0.0000	0.0000			
⊕ Integral 5	1599482.50	0.5152	1	1.8935	0.0000	0.0000			
⊕ Integral 6	2694168.25	0.8678	1	0.8724	0.0000	0.0000			
⊕ Integral 7	1138637.25	0.3667	2	0.8683	0.0001	0.0000			
⊕ Integral 8	1045436.00	0.3367	2	0.8602	0.0004	0.0000			
⊕ Integral 9	535344.00	0.1724	1	0.8602	0.0009	0.0000			
⊕ Integral 10	992781.00	0.3198	1	0.8683	0.0011	0.0000			
⊕ Integral 11	362501.25	0.1168	1	0.8521	0.0014	0.0000			

The chemical shift in each of the three dimensions is displayed in a separate column.

Peaks and integrals only appear if they have been calculated (commands **pp** and **int**, respectively).

11 1D Interactive Manipulation

The upper toolbar of the 1D menu offers various buttons for interactive manipulation. If you click such a button, the active dataset window will switch to the corresponding mode. An interactive manipulation mode is dataset window specific, i.e. it only applies to the active window.

11.1 1D Interactive Window Multiplication

TopSpin supports 1D interactive window multiplication.

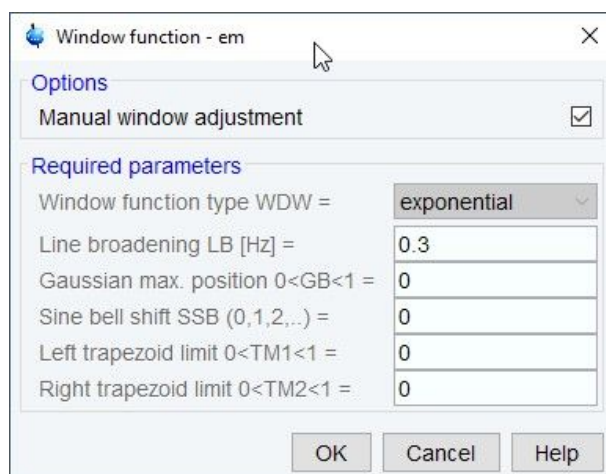
11.1.1 1D Interactive Window Multiplication Procedure

How to Switch to Window Multiplication Mode

- Open a 1D dataset and click **Process | Proc. Spectrum | Window Multiplication [wm]**,
- Enable **Manual window adjustment** in the appearing dialog and click **OK**.

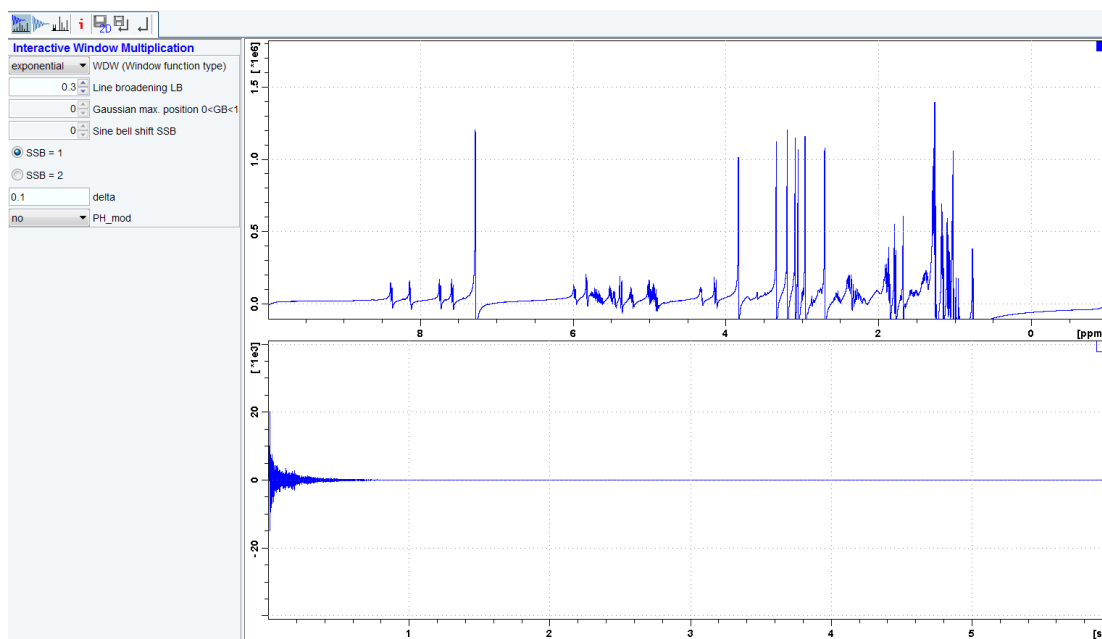
or

- Enter **.winf** on the command line.



The tab bar of the active dataset window will be replaced by a toolbar (see figure below) and the dataset window itself will be divided into three parts:

1. A parameter part at the left.
2. A spectrum part at the upper right.
3. An FID part at the lower right.



Toolbar Buttons

- Click one of the following buttons:



Display both spectrum and FID.



Display FID only.



Display spectrum only.



Switch cursor information on/off (toggle).



Save windows settings to source 2D dataset (see note below) and return.



Save window settings and return.



Return without save.

Note: 2D from which current 1D dataset was extracted, e.g. with *rser*.

Perform interactive window manipulation as follows:

- In the WDW dropdown list select the window function type (parameter WDW).

Interactive Window Multiplication

exponential ▼	WDW (Window function type)
exponential	Line broadening LB
gaussian	Gaussian max. position $0 < GB < 1$
sine bell	Sine bell shift SSB
squared sine	
<input checked="" type="radio"/> SSB = 1	
<input type="radio"/> SSB = 2	
0.1	delta
no ▼	PH_mod

- Set the corresponding parameter(s), e.g.
 - LB for exponential.
 - LB and GB for Gaussian.
 - SSB for sine bell and squared sine.

The displayed spectrum and/or FID will be automatically adjusted as you change the window function and parameters.

- Click **Save** to store the window settings and return.

Now you can perform further processing steps like Fourier transform, phase correction etc.

11.2 1D Interactive Phase Correction

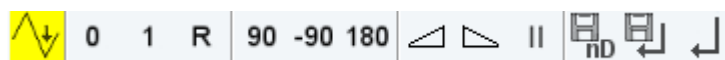
Manually acquired spectra can be phase corrected automatically, with commands like **apk** or **apks** or, interactively, in phase correction mode.


11.2.1 1D Interactive Phase Correction Procedure

How to Switch to Phase Correction Mode

- Open a 1D dataset and click **Process** | **Adjust Phase** or enter **.ph**.

The Phase Correction toolbar is displayed:



The yellow button  indicates that you are in phase correction mode.

Some buttons will turn gray when they are clicked. If a button is gray, it is active.

How to Perform a Typical 1D Interactive Phase Correction

For a typical 1D phase correction, take the following steps:

- Click-hold and move the mouse until the reference peak is exactly in absorption mode.
- Click-hold and move the mouse until the entire spectrum is exactly in absorption mode.
- Click to save and execute the phase correction and return.

11.2.2 1D Interactive Phase Correction Details

How to Set the Phase Pivot Point

By default, the phase pivot point is set to the biggest magnitude intensity of the displayed region of the spectrum. To change the pivot point:

- Right-click on the desired pivot point position and in the list, select **Set pivot point** (see previous figure).

How to Perform Default Zero Order Phase Correction

- Right-click in the dataset window and in the list, select **Calculate ph0** (see previous figure).

The spectrum will automatically be corrected according to the calculated value.

How to Perform Interactive Zero Order Phase Correction

- Click-hold Zero order phase correction (parameter PHC0). The button turns gray.
- Move the mouse until the reference peak is exactly in absorption mode.
- Release the mouse.

How to Perform Interactive First Order Phase Correction

- Click-hold First order phase correction (parameter PHC1).
- Move the mouse until the entire spectrum is exactly in absorption mode.
- Release the mouse (button turns gray).

How to Perform 90, -90 or 180° Zero Order Phase Correction

- Click one of the following buttons:

Perform 90 zero order phase correction [**.ph90**].

Perform -90° zero order phase correction [**.phm90**].




Perform 180° zero order phase correction [**.ph180**].

How to Reset the Phase to the Original Values

- Click Reset zero and first order phase values [**.phr**].


How to Change the Mouse Sensitivity

- Click one of the following buttons:

-  Increase (double) the mouse sensitivity [**.inc**].
-  Decrease (halve) the mouse sensitivity [**.dec**].
-  Reset the mouse sensitivity.

How to Return from Phase Correction Mode with/without Save


To return while saving the phase correction to the current dataset:

- Click  Save, execute and return [**.sret**].

This will perform the following tasks:

- Execute phase correction (command **pk**).
- Save the current phase correction values.
- Leave the phase correction mode.

To return without save:

- Click  Return, discarding any changes [**.ret**].

To return while saving the phase correction to the source 2D dataset:

- Click  Save to 2D [**.s2d**].

This is only applicable on rows or columns extracted from 2D data. The phase values will be saved to the 2D dataset from which the current 1D dataset was extracted.

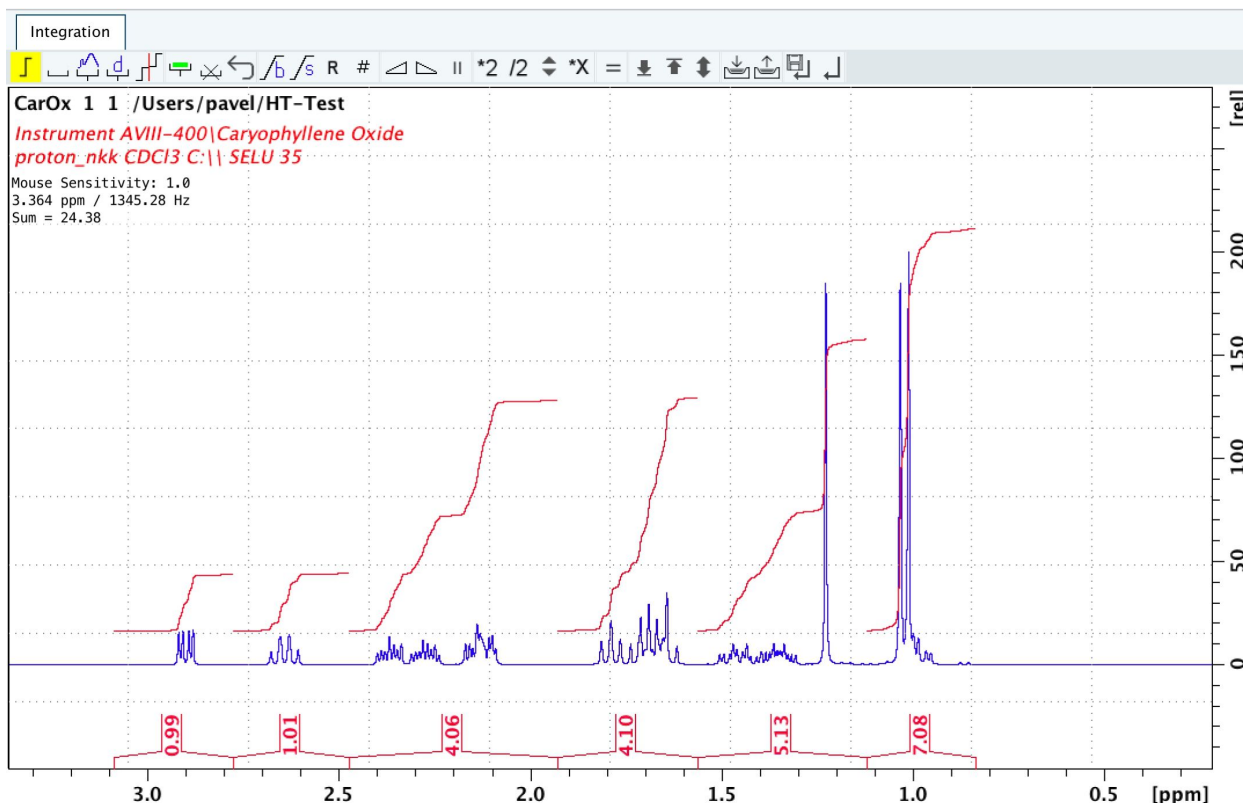
11.3 1D Interactive Integration


Integration of 1D data can be done automatically, with the commands **abs** and **li** or, interactively, as described in this paragraph.

How to Switch to Integration Mode

- Click **Analyse | Integrate** or enter **.int**.

The active dataset window tabs will be replaced by the Integration toolbar.





 The yellow color indicates that the dataset window is in integration mode.

If integral regions have already been determined, for example with **abs** or with a previous interactive integration, these regions are displayed in the dataset window, along with the integral values. You can remove them, change them or add to them, as described below.


How to Define Integral Regions

- For a manual definition click one of the two following buttons:

 : Define new region in the given spectra with manual selection (toggle)

 : Define new integral with automated baseline correction in the selected region (toggle)

To define a new integral with exact coordinates via a dialog

- Click  Define region via dialog (see the following figure).

add ×

Exact coordinates of integrated area

[ppm]

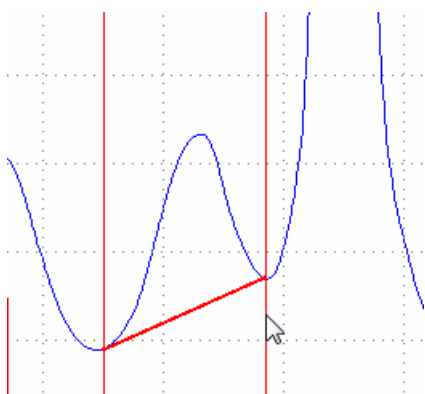
From

To

- Enter the exact values for the region limits and click **OK**.

Follow the next steps for a manual definition:

- Put the red cursor line at one edge of a peak or multiplet.
- Left-click-hold and drag the cursor line to the other edge of the peak or multiplet. In case of a baseline correction the interpolated baseline will be displayed automatically on screen (see the next figure). The integral is calculated considering the new baseline.




- Repeat the last 2 steps for all regions to be defined.
- Click the button again to leave the *Define region* mode.

How to Read Integral Regions from Disk

You can read integrals regions from disk which have been stored by automatic integration (command **abs**) or by a previous interactive integration.

To read integrals:

- Click **Read / import integration regions**  and in the list, select one of the following entries:
 - **Read intrng**: To read the last saved integral regions and apply the saved slope and bias correction values.
 - **Read intrng no slope & bias corr**: To read the last saved integral regions but do not apply the saved slope and bias correction values.
 - **Read intrng use last slope & bias**: To read the last saved integral regions applying the last slope and bias correction values.
 - **Import integration regions**: To read integral regions from external file.
 - **Import intrng from Relaxation Experiment**: To read the last stored integral regions of the T1/T2 relaxation experiment.
 - **Edit intrng**: To edit the file (intrng) that contains the integral regions and slope and bias correction values. Changes in this file are automatically shown on the screen, when the file is saved.

Read 'intrng'
Read 'intrng' No Slope & Bias Corr.
Read 'intrng' Use Last Slope & Bias
Import integration regions
Import 'intrng' from Relaxation Experiment
Edit 'intrng'

How to Select / Deselect Integrals

The integrals may be selected by mouse click in the integration region area:

- Hold down the Shift key or the Ctrl key to select multiple intervals.


Alternative option:

- Right-click in the integral region and in the list, click **Select / Deselect** to toggle the selection.




How to Perform Interactive Bias and Slope Correction

To perform interactive bias correction:

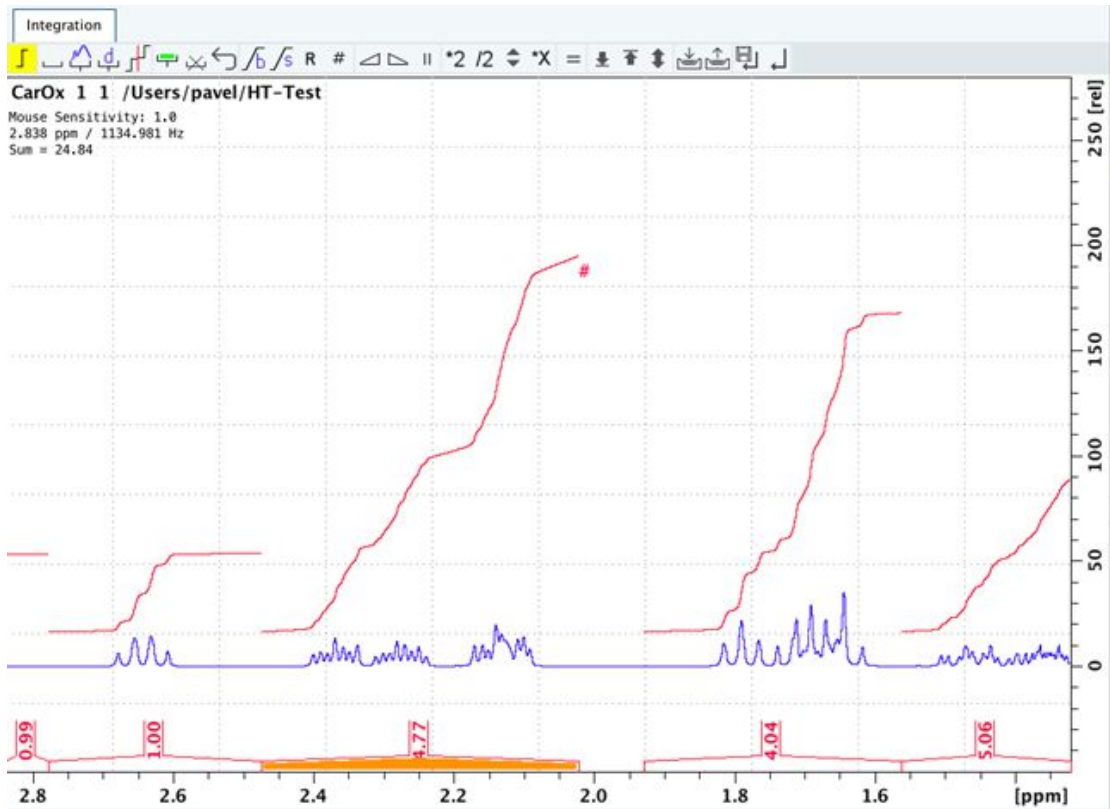
- Select the integral(s) that you want to correct (right-click in the region and choose **Select / Deselect** in the context menu). If no integral is selected, bias correction will work on all integrals.
- Click-hold **Integral bias correction**  and move the mouse until the integral bias is correct.

To perform interactive slope correction:

- Select the integral(s) that you want to correct (right-click in the region and choose **Select / Deselect** in the context menu). If no integral is selected, slope correction will work on all integrals.
- Click-hold the Integral slope correction button  and move the mouse until the integral slope is correct.

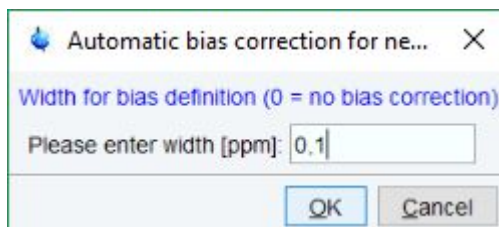
Integrals with a defined slope or bias are marked on the display with “#” at the end of the integral curve.

The button  sets both slope and bias back to zero.






How to Set the Width for Bias Determination

- Click **Width for bias determination** **#** and enter the width in ppm.



How to Change the Mouse Sensitivity

- Click
 -  Increase (double) the mouse sensitivity [**.inc**].
 -  Decrease (halve) the mouse sensitivity [**.dec**].
 -  Reset the mouse sensitivity.

How to Calibrate/Normalize Integrals

Calibrating integrals means setting the value of a reference integral and adjusting all other integrals accordingly.

- Right-click in the reference integral region and in the list, select **Calibrate Current Integral**.

- Enter the desired value for the reference integral and click **OK**.

Normalizing integrals means setting the sum of all integrals and adjusting individual integral values accordingly.

- Right-click in the reference integral region and in the list, select **Normalize Sum of Integrals**.
- Enter the desired sum of all integrals and click **OK**.

Calibrating and normalizing only effects the current dataset. To scale integrals with respect to a reference dataset, choose **lastscale** from the right/click context menu (see below).

How to Scale Integrals with Respect to Different Spectra

Integrals can be scaled with respect to the last spectrum that was integrated interactively:

- Right-click in the reference integral region and in the list, select **Use Lastscale for Calibration**.


As such, you can compare integrals of different spectra.

Note that this only makes sense for spectra which have been acquired under the same experimental conditions. The scaling factor is stored in the file:



```
<tshome>/prog/curdir/<user>/intscale
```

How to Delete Integral Regions from the Display

To delete the selected integral regions:

- Click  to delete selected integral regions from the display.
- Right-click in the integral region and in the list, select **Delete Current Integral**.

To delete all integral regions from the display:


- Click  to select all integral regions.
- Click  to delete them.


Note: Regions are only deleted from the screen and any manipulation of integration regions can be undone with the **Undo** button. Regions which are saved on disk (in the *intrng* file) are not immediately affected. The changes are stored only when a save command or save and return is executed.

How to Scale Selected Integrals

Integral scaling only manipulates selected integrals. However, if no integrals are selected, it works on all integrals.


- Click one of the following buttons:

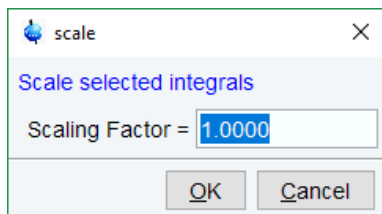
 Scale up selected integrals by a factor of 2.

 Scale down selected integrals by a factor of 2.

 Scale selected integrals up/down smoothly.

To scale up/down integrals by a factor entered via a dialog:

- Click Define scaling factor via dialog .



- Enter a scaling factor, e.g. 2.5.
- Click **OK** to apply this factor.

To scale all selected integrals to the same height:

- Click/Toggle **Autoscale all integrals to the same height** .

The individual scaling factor for each region is displayed above the integral. Clicking this button again rescales all integrals to their original height.

How to Move the Integral Trails Up/Down

To move the integrals (selected and unselected) up or down,

- Click one of the following buttons:



The left edge of the selected integral is put just above the baseline. If no integral is selected, the lowest integral is used.




The right edge of the selected integral is put at 3/4 of the window height. If no integral is selected, the highest integral is used.



Shift all integral trails up/down smoothly.


How to Cut Integral Regions

- Click **Cut integrals into two parts (toggle)**  to activate or deactivate the cutting mode (toggle).
- Move the red cursor line into an integral region to the position where it must be cut and click the left mouse button.
- Repeat the last step for each integral region that must be cut.


In case of overlapping integrals, you must select the integral to be cut before you cut it. Note that if one or more integrals are selected, cutting only works on selected integrals.

With TopSpin 1D Interactive Integration command **cut integral** can be called directly from right-click context menu. Right mouse click on the integral opens a context menu in which cut current integral must be selected.

How to Save Integral Regions

- Click **Save/Export integration regions**  and in the list, select one of the following entries:
 - **Save regions to 'intrng'**: Save the currently displayed integral regions including the slope and bias correction values.
 - **Save Regions to 'reg'**: Save the integral regions to the file reg.
 - **Export integration regions**: Save the integral regions in a new file.
 - **Export Regions To Relaxation Module and .ret**: Used on relaxation data only. Exports the integral regions for T1/T2 relaxation analysis and exits from integration mode.
 - **Save & show list**: Save the currently displayed integral regions including the slope and bias correction values and show the integrals on the screen.

How to Undo the Last Region Operation

- Click **Undo the last region operation** .

How to Return from the Integration Mode with/without Save

To return and save the integrals to the current dataset:

- Click **Return, save regions**  or enter **.sret**.

As such, you will:

- Save the integral regions and corresponding slope and bias corrections to the file *intrng*.
- Save the integral regions, slope and bias corrections and integral values to the file *integrals.txt*. This file is displayed when you click the **Integrals** Tab.
- Leave the integration mode.

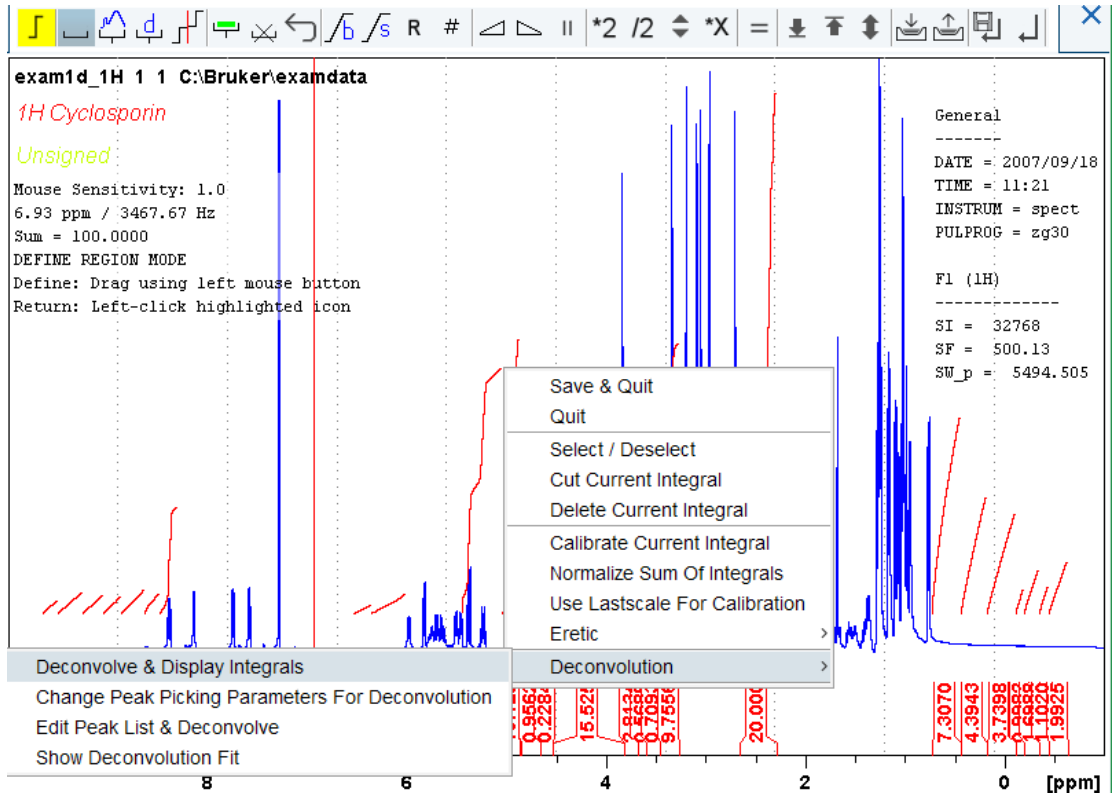
To return without save:

- Click **Return, do NOT save regions**  or enter **.ret**.

How to Deconvolve Overlapping Peaks from Integration Mode

Deconvolution, the line shape tool to interpret complex 1D and 2D spectra with overlapping peaks can be started directly from within integration mode. As described in the Analysis chapter deconvolution calculates theoretical signals with different methods, i. e. Gaussian, Lorentzian or a mixture of these line shapes. The values are stored in the file **dconpeaks.txt** and displayed graphically. For further information please look up the Analysis chapter and the Processing Reference Manual (commands **gdcon**, **ldcon**, **mdcon**, **ppp**, **dconpl** and **dcon**).

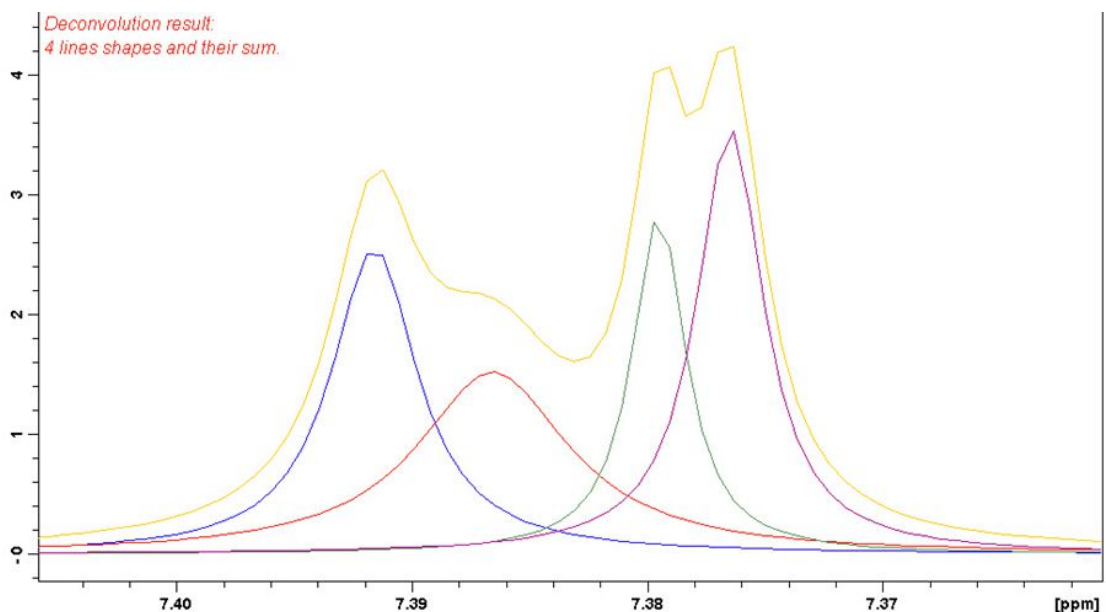
From within the integration mode, after the integration of the respective peak or peak groups, deconvolution can be started by right clicking on the peak. The following window will appear:



Selecting **Deconvolution** offers the following options:

- Deconvolve and display regions.
- Change Peak Picking Parameters for Deconvolution.
- Edit Peak List & Deconvolve.
- Show Deconvolution Fit (graphical display).

With the latter function it is possible to display results after deconvolution graphically:



1D Interactive Manipulation

The integral values of each of the deconvolved signals are available in the integrals tab within the originally defined integral (column Intensity [abs]):

SPECTRUM	PROCPARS	ACQPARS	TITLE	PULSEPROG	PEAKS	INTEGRALS
△ Object	Integral [abs]	Integral [rel]	Peaks	v(F1) [ppm]		
Integral 1	1243141.32	0.5021	0	9.5783		
Integral 2	1956677.80	0.7904	2	9.3781		
Integral 3	1682681.68	0.6797	0	9.1521		
Integral 4	1532414.25	0.6190	1	8.9580		
Integral 5	2189385.79	0.8844	2	8.7466		
Integral 6	1876330.95	0.7579	2	8.5507		
Integral 7	9609294.86	3.8814	0	8.3881		
Integral 8	788677.73	0.3186	1	6.4475		

11.4 1D Interactive Calibration

A 1D spectrum can be calibrated (referenced), automatically, with the command **sref** or, interactively, as described below.

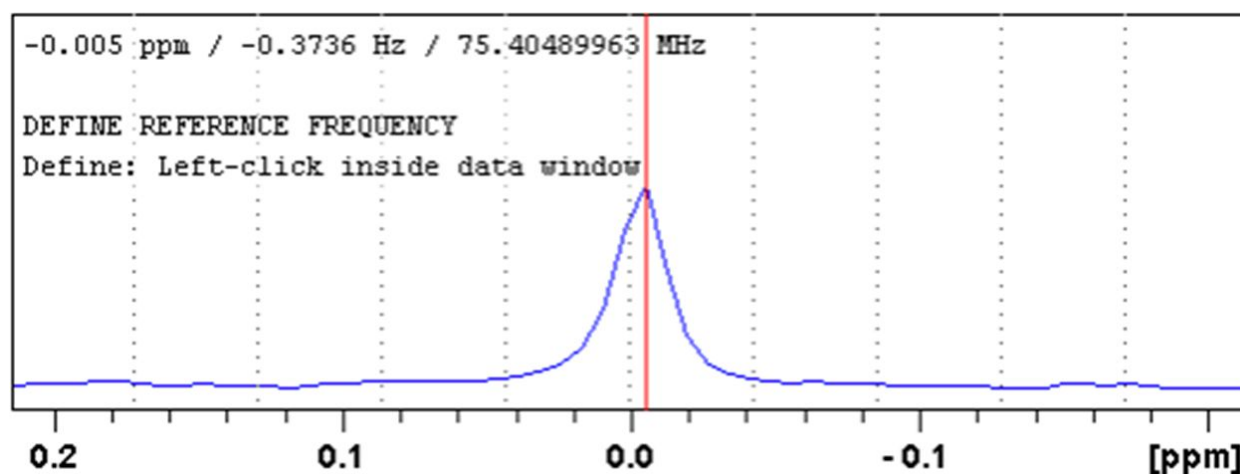
How to Switch to Calibration Mode

- Click **Process | Calib. Axis** or enter **.cal**.

The Tab bar of the active dataset window will be replaced by the Calibration toolbar



The yellow button indicates that the dataset window is in calibration mode.

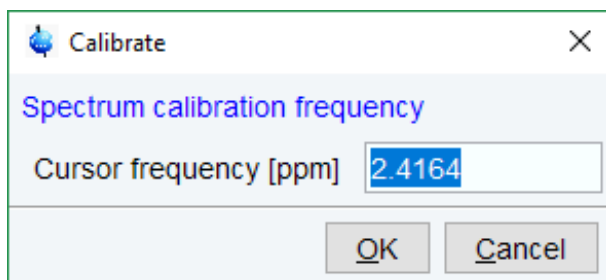


How to Calibrate a Spectrum Interactively

In calibration mode:

- Position the red cursor line at the reference peak.
- Click at that position.

The following dialog box will appear:



Note that the units (Hz or ppm) correspond to the axis units of the display.

- Enter the frequency you want to assign to the reference peak.
- Click **OK**.

The spectrum will be calibrated and re-displayed. TopSpin will automatically leave calibration mode.


11.5 1D Multiple Display

The multiple display mode allows to display multiple superimposed spectra. The spectra will be ppm aligned or Hz aligned, according to the selected axis unit. Each spectrum can be individually shifted and scaled allowing exact alignment of corresponding peaks in different spectra. The number of superimposed spectra is unlimited.

Although multiple display is normally used for spectra with matching nuclei, it allows to superimpose spectra with non-matching nuclei. You will get a warning that the nuclei do not match. Just click **OK** to continue.

How to Switch to Multiple Display Mode and Read Multiple Spectra

One way to superimpose data in multiple display is to read one dataset, switch to multiple display mode and add other datasets:

- Read a 1D dataset.
- Click **Multiple display**  or enter `.md`.

The dataset window will switch to multiple display mode.

Add a dataset as follows:

- Left-click-hold the dataset in the browser and drag it into the dataset window.
or
- Right-click the dataset in the browser and choose **Display** from the context menu.
or
- Enter **re** and specify the additional dataset in the appearing dialog box.

Another way to superimpose data in multiple display is to read multiple datasets simultaneously:

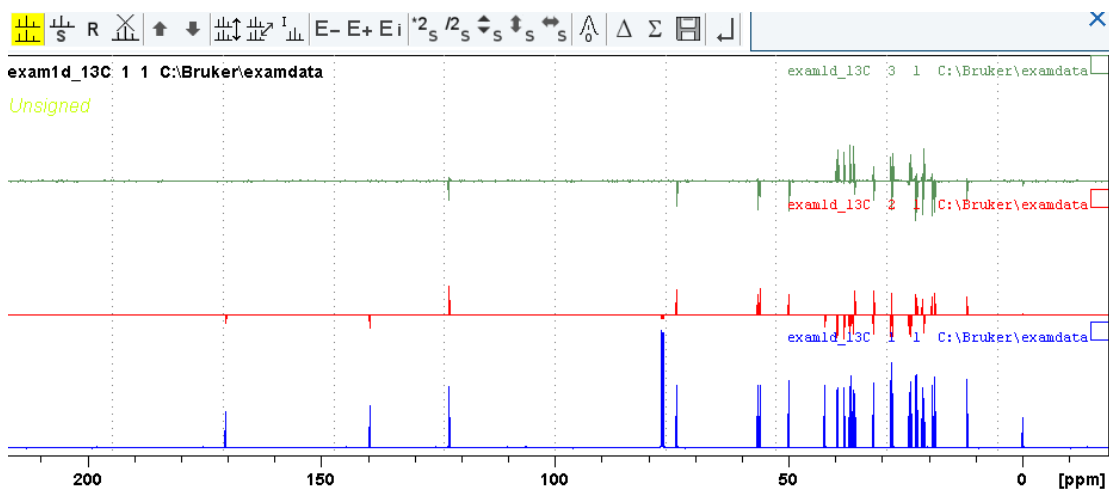
1D Interactive Manipulation

In the browser:

- Hold down the **Ctrl** key and click multiple datasets to select them
or
- Hold down the **Shift** key and click two datasets to select these two and all datasets in between.
- Right-click any of the selected data
 - and in the list, select **Display**. This will show the data in the active dataset window if that is in multiple display mode or, otherwise, show the data in a new window.
or
 - in the list, select **Display in new window**. This will show the data in a new window.

In multiple display mode, the tab bar of the active dataset window is replaced by a toolbar.

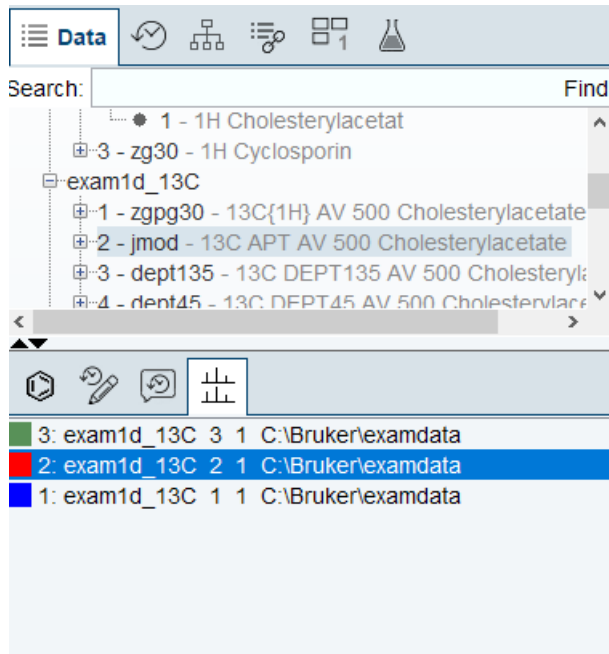
The following figure shows three comparable 1D spectra and the sum of all three.



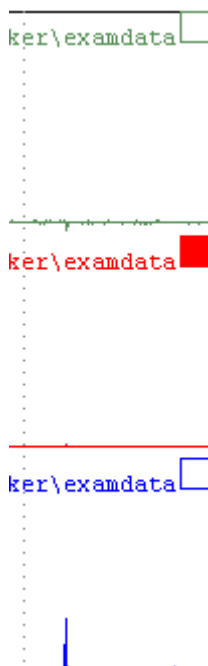
The yellow button indicates that the dataset window is in multiple display mode.

Some buttons will turn gray when they are clicked. If a button is gray, it is active.

Furthermore, the browser is split in two parts:



The additional lower part shows which datasets are displayed in the active dataset window. The selected datasets are highlighted.



How to Work with Multiple Display Command .md

The following arguments of **.md** for controlling datasets from command line, AU-programs or Python programs are available:

Specified dataset names can be shown in the display by command **.md**:

- Enter command and full pathname for a specified dataset in the TopSpin command line:

```
.md <PathToDataset1>\<expno1>\pdata\<procno>  
<PathToDataset2>\<expno2>\pdata\<procno>
```

The command **.md no_load** ignores the datasets stored in the last multiple display session and enters the multiple display.

The command **.md write** writes only the assoc file containing the dataset list for multiple display. Please note that the multiple display module is not started with this command.

- Enter command and full path name of specified dataset in the TopSpin command line:

```
.md write <PathToDataset1>\<expno1>\pdata\<procno>  
<PathToDataset2>\<expno2>\pdata\<procno>
```

Multiple display mode is supported for 1D and 2D spectra. For spectra with a dimension > 2 the selected slice (subplane) is displayed.

How to Select/Deselect Datasets

To select a dataset:

- Click in the corresponding area in the dataset window.

or

- Left-click-hold the dataset in the browser and drag it into the dataset window.

or

- Click the corresponding entry in the lower part of the browser.

In the lower part of the browser, you can:

- Click one dataset to select it.

or

- Hold down the **Ctrl** key and click multiple datasets to select them.

or

- Hold down the **Shift** key and click two datasets to select these two and all datasets in between.

When you select a dataset, the corresponding small square is filled (see the figure above) and its entry in the lower part of the browser is highlighted (see the figure above).

Note that:

No spectrum selected = all spectra selected.

Scale/shift buttons of the dataset window toolbar only work on selected spectra.

To deselect a dataset:

- Select a different dataset.

To deselect all datasets:

- Click  Deselect all datasets.

How to Remove a Dataset from Multiple Display

- Select the dataset(s) you want to remove.

- Click  Remove selected data from the screen.

Note that the data on disk are not affected. Furthermore, the first spectrum cannot be removed from the screen.

How to Display the Sum or Difference Spectra

- Click one of the following buttons (button turns gray):



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



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

How to Save the Sum or Difference Spectra



- Click Save the displayed sum or difference spectrum.
- In the next dialog box, specify the destination procno.

How to Display the Next/Previous Name/Expno

To compare a series of spectra you can interactively increment or decrement the dataset name or expno. A dataset name is incremented according to the IconNMR naming convention of increasing extensions, e.g. name.001, name.002 etc.

- Click one of the following buttons (button turns gray):



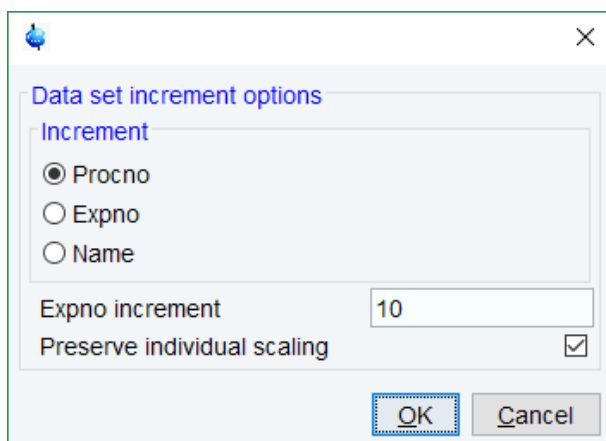
Show the previous name/expno/procno of the last dataset.



Show the next name/expno/procno of the last dataset.



Set the increment options. Clicking this button will open the following dialog:



Here you can choose to increment the procno, expno or name, set the expno increment and switch individual scaling on/off.

How to Toggle between Superimposed and Stacked Display

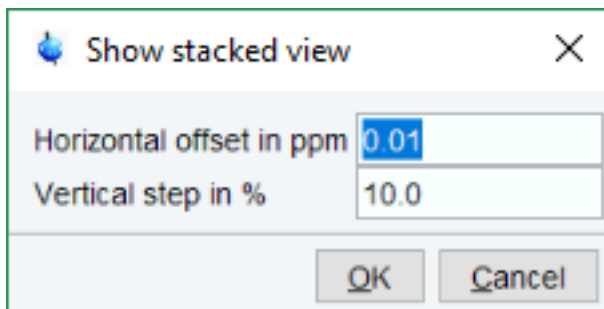
- Click:



Toggle between superimposed and stacked display.






Set the stacked display parameters.



How to Shift and Scale Individual Spectra

To compare the intensity and chemical shift of corresponding peaks, you can shift and scale individual spectra. To do this:

- Display the spectra in multiple display mode as described above.
- Expand the spectra to display the desired region or peak.
- Select one of the spectra (e.g. by clicking it in the lower part of the browser).
- Click-hold  **S** and move the mouse to align the intensities.
- Click-hold  **S** and move the mouse to align the peak positions.

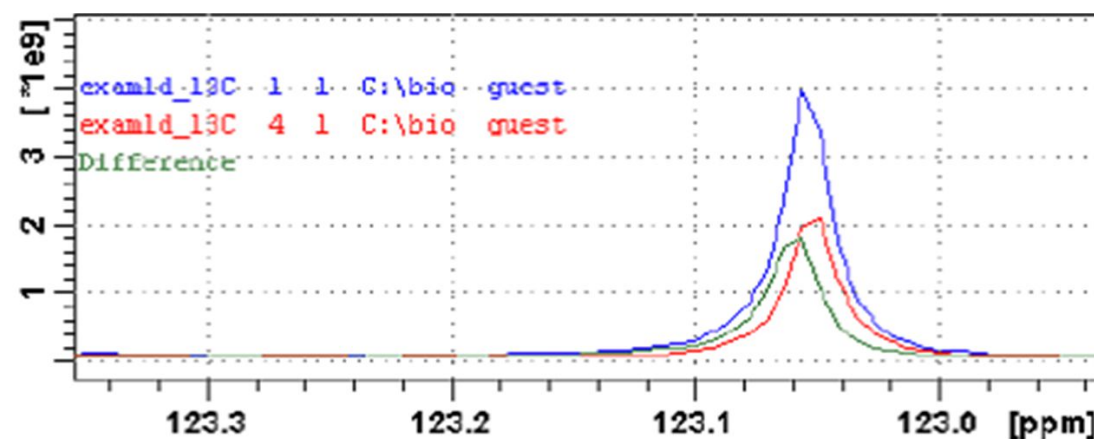
The alignment can be facilitated by activating the difference spectrum  button and minimize that.

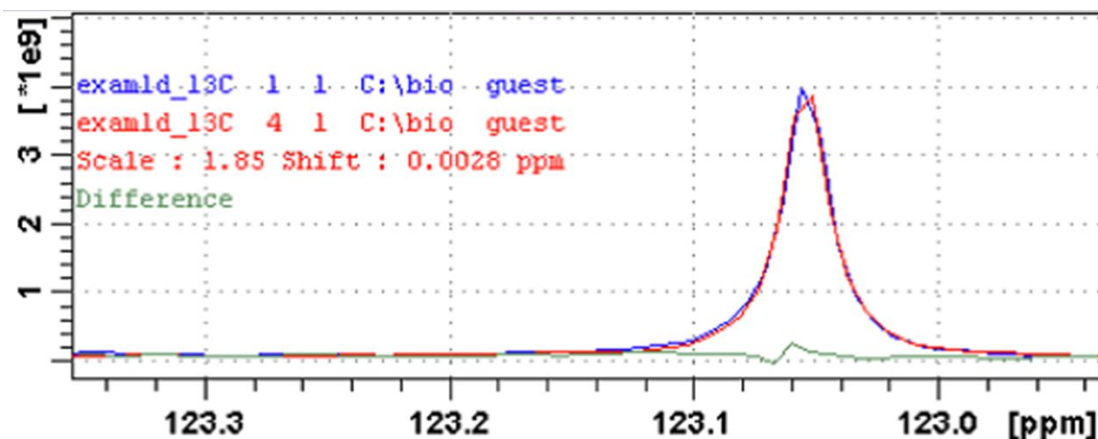
Note that you can also scale the selected spectra up/down with the buttons  and .

 **S** allows to move the selected spectra vertically.

R resets individual scaling and shifting.

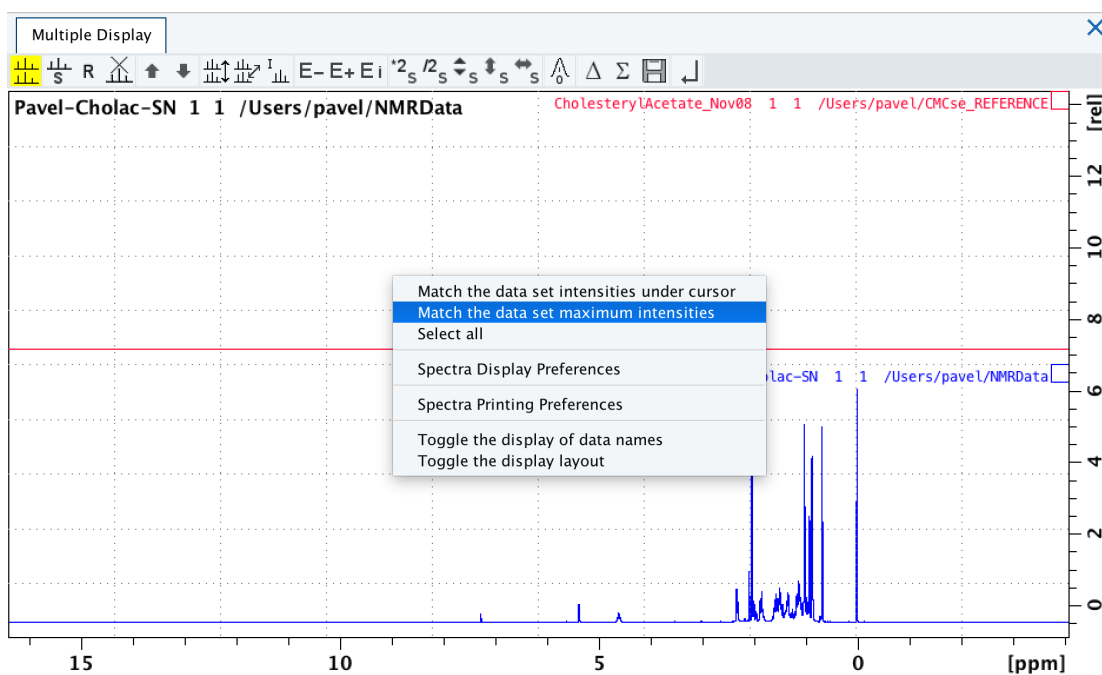
The performed scaling and shifting are displayed in the dataset window:



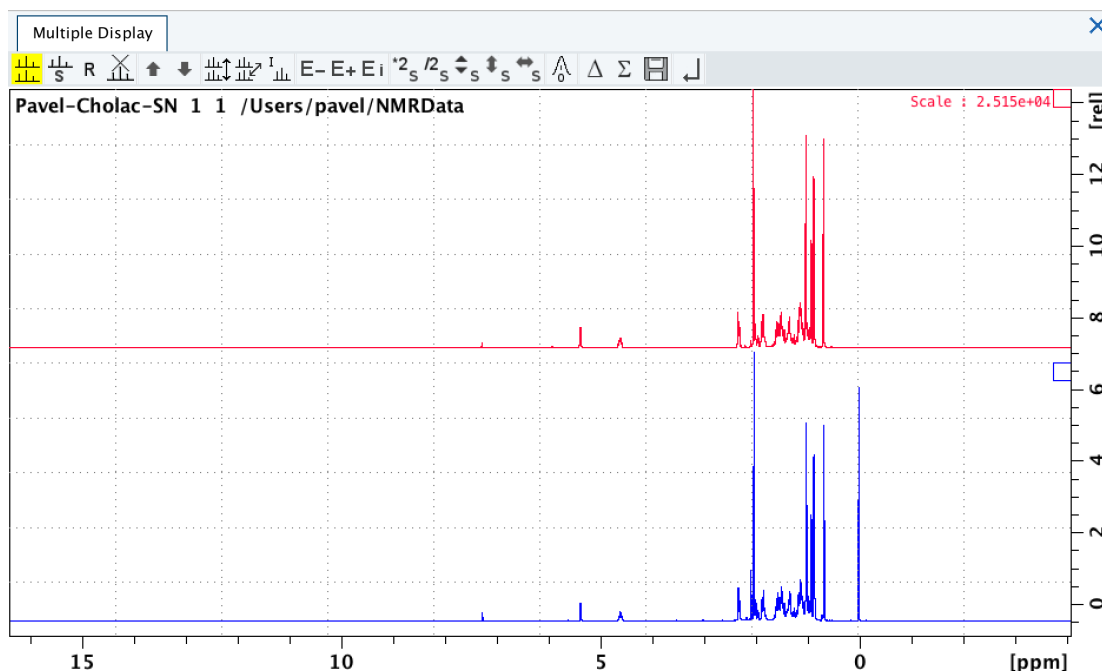


Automated scaling options in multiple display



NMR spectra taken from the same sample on different spectrometer architectures can have very different intensities. To simplify comparison of such spectra, Topspin implements a new scaling option **Match the Dataset maximum intensities**.



The spectra are properly scaled, the required scaling factor is displayed.




How to Move the Selected Spectrum One Place Up/Down

- Click  Move the selected spectrum one place up in the list.
- Click  Move the selected spectrum one place down in the list.

Note that the first spectrum and calculated spectra (sum of difference) cannot be moved up/down.

How to Switch On/Off the Display of Data Paths and Scaling Factors

- Click  Switch on/off display of data paths and scaling factors.

How to Return from Multiple Display Mode

- Click  Return from multiple display mode [.ret].

How to Set the Colors of the 1st, 2nd, .. Dataset

The colors of the different datasets in the multiple display mode can be set in the **User preferences** dialog box. To set, for example, the color of the second spectrum:

- Right-click and in the list, select **Spectra Display Preferences** and click the **Change** button for the item *Color of 2nd 1D spectrum*.

TopSpin allows to set 8 different colors for different spectra in multiple display.

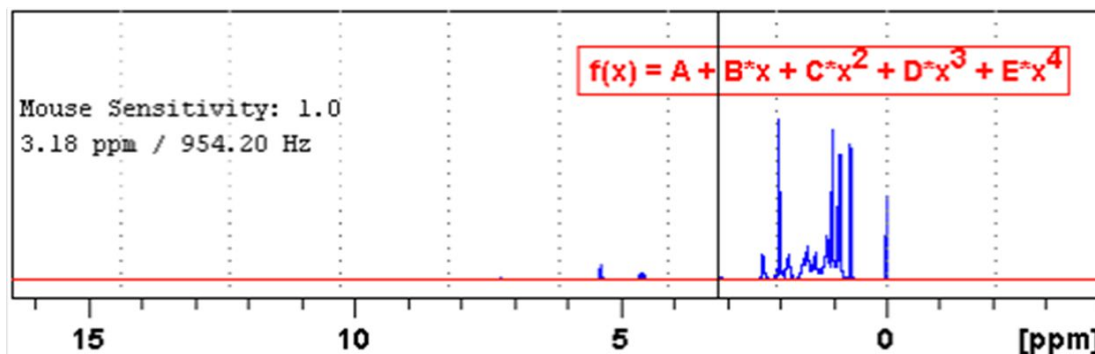
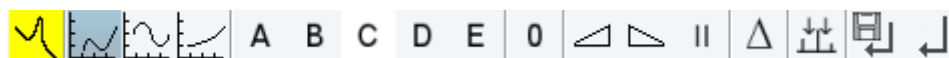
11.6 1D Interactive Baseline Correction


Baseline correction can be performed with commands like **abs** or **absd** or, interactively, as described below.

How to Switch to Baseline Correction Mode

- Click **Process** | **Baseline** or enter **.basl**.

The Tab bar of the active dataset window will be replaced by the baseline toolbar:



The yellow button  indicates that the dataset window is in baseline correction mode. Some buttons will turn gray when they are clicked. If a button is gray, it is active.

How to Perform Polynomial Baseline Correction


- Click  Perform polynomial baseline correction – the button turns gray.

In the dataset window, a red horizontal line will appear as well as the equation that describes the polynomial function:

$$f(x) = A + B*x + C*x^2 + D*x^3 + E*x^4$$

- Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
- Repeat the last step with the buttons **B**, **C**, **D** and **E** until the red line coincides with the entire baseline of the spectrum.

How to Perform Sine Baseline Correction

- Click  Perform sine baseline correction – the button turns gray.

A red horizontal line will appear as well as the equation describing the sine function:

$$f(x) = A + B*\sin(C*x + D)$$

- Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
- Repeat the last step with the buttons **B**, **C** and **D** until the red line coincides with the entire baseline of the spectrum.

How to Perform Exponential Baseline Correction

- Click  Perform exponential baseline correction – the button turns gray.


A red horizontal line will appear as well as the equation describing the exponential function:

$$f(x) = A + B \cdot \exp(C \cdot x)$$

- Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
- Repeat the last step with the buttons **B** and **C** until the red line coincides with the entire baseline of the spectrum.


How to Preview the Baseline Corrected Spectrum

Before performing the baseline correction, you can preview the result by displaying the difference between the uncorrected spectrum and the red correction line.


- Click  Preview corrected spectrum (Display difference) - the button turns gray.

The corrected spectrum will be displayed in red.

If the baseline is correct,

- Click  to save the correction.

If further correction is needed,

- Click  to show the original spectrum and the red correction line.


How to Reset the Baseline Correction Line


- Click  Reset the red correction line to zero.


If the difference spectrum is displayed (the  button is active), clicking the reset button will restore the original spectrum.

How to Change the Mouse Sensitivity

- Click one of the following buttons:

 Increase (double) the mouse sensitivity [**.inc**].

 Decrease (halve) the mouse sensitivity [**.dec**].

 Reset the mouse sensitivity.

How to Save the Baseline Correction and/or Return

To return while saving the baseline correction:

- Click  **Save baseline correction and Return** [**.sret**]

This will perform the following tasks:


- Execute the baseline correction [**bcm**].

- Save the baseline correction values **A**, **B**, **C**, **D** and **E**.
- Leave the baseline correction mode.

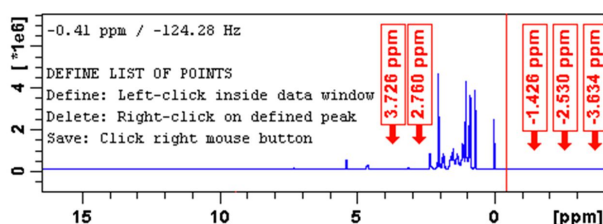
To return while discarding any changes:

- Click  Return, discarding any changes [**.ret**].

How to Perform Cubic Spline Baseline Correction

- Click  Define points for cubic spline baseline correction.

The dataset toolbar is displayed: .




The cursor line in the dataset window turns red. If a list of baseline points already exists, you are prompted to overwrite or append to these points. If you choose **Append**, the labels of the existing points are displayed on the screen. If you choose **Overwrite**, no labels are displayed. Nevertheless, the existing points are only overwritten when you define and save new points.

To define new baseline points:

- Move the cursor line to a baseline point and click at that position.
- Repeat this for at least five baseline points.

The figure above shows a spectrum with five defined baseline points. Note that here the points have been chosen at the right part of the spectrum for display reasons only.

Note that the actual baseline correction is only performed when you click the  button in the spline baseline and interactive baseline mode.

How to Delete Spline Baseline Points from the Screen

To delete one baseline point:

- Right-click the baseline point position in the dataset window.
- In the list, select **Delete Current**.

Quit

Save & Quit

List `baslpnts`

Delete All

Delete Current


Enter Zoom

To delete all baseline points:


- Right-click any position in the dataset window.
- In the list, select **Delete All**.

How to Return from Cubic Spline Baseline Mode with/without Save

To return while saving the baseline points:

- Click  Save baseline points and Return [**.retsab**].

To return while discarding any changes:

- Click  Return, Discarding any changes [**.ret**].

Alternatively, you can right-click in the dataset window and select **Save & Quit** or **Quit**, respectively.

11.7 1D Interactive Peak Picking

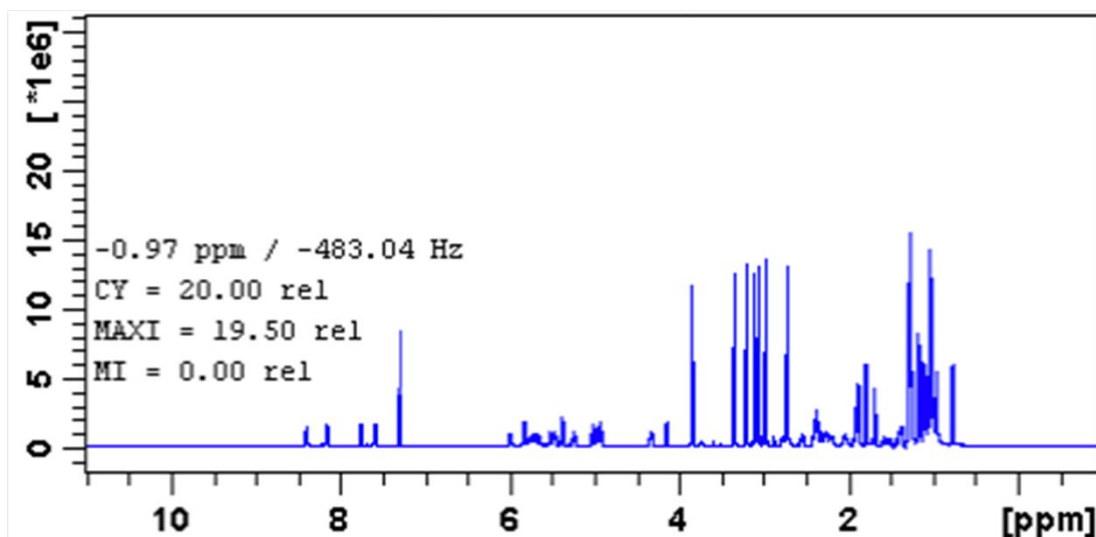
Peak picking can be performed, automatically, with the commands **pps** or, interactively, in the peak picking mode.

How to Switch to Peak Picking Mode

- Click **Analyse | Pick Peaks | Manual Peak Picking** or enter **.pp** on the command line.


The Peak picking toolbar is displayed:





The yellow button indicates that you are in peak picking mode.

Some buttons will turn gray when they are clicked. If a button is gray, it is active.


Note: the  button is automatically activated, i.e. you are in **Define peak picking range** mode

How to Define New Peak Picking Ranges

- Click the upper-left corner of a peak picking range.
- Left-click-hold and drag the mouse to the lower-right corner of the range.
The peak picking range will be marked gray. The minimum and maximum intensity are set and the peaks in the range are picked and displayed.
- Repeat the last 2 steps for each peak picking range to be defined.
- Click the gray button to leave the *Define peak picking range* mode.

Note: the parameters MI and MAXI are set to the lowest minimum and the highest maximum intensity, respectively, of all ranges.

How to Change Peak Picking Ranges

- Click  to change the peak picking ranges. (button turns gray):
- Click on one of the edges of the peak picking range.
The cursor turns into a double-headed arrow.
- Click-hold and drag the peak range edge to its new position.
- Optionally: repeat the last 2 steps for the other edge and for other peak ranges.
- Click the gray button to leave the *Change peak picking range* mode.

How to Pick Peaks in Peak Picking Ranges only


Peaks in a peak range are automatically picked when the range is defined. If peaks have been deleted from a range, they can be picked again as follows:

- Right-click in the data field and in the list select **Pick Peaks On Ranges**.


1D Interactive Manipulation

Alternatively, you can enter **ppl** on the command line. This command can be entered in *Interactive peak picking* mode or in the normal display mode.


How to Delete all Peak Picking Ranges

- In the dataset window toolbar, click .
- or
- Right-click in the data field and in the list, select **Delete All Regions**.

How to Define Peaks Manually

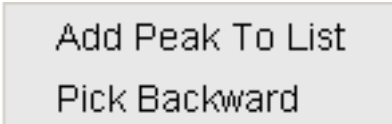
- Click  to define peaks manually. The button turns gray.
A red vertical line will appear in the dataset window.
- Put the red cursor line at the desired peak and click left. The peak label will appear at the top of the dataset window.
- Repeat the last step for each peak to be defined.
- Click the gray button to leave the *Define peaks* mode.

How to Pick Peaks Semi-Automatically

- Click  to define peaks semi-automatically. The button turns gray.
- Move the cursor into the dataset window.
- Put the cursor line near the desired peak.
- Click to pick forward.
- or
- Right-click to pick backward (see the figure below).


A red cursor line will appear at the nearest peak whose intensity is between MI and MAXI.

- Right-click to add the selected peak to the peak list:



Add Peak To List
Pick Backward

The peak label will appear at the top of the dataset window.

- Click  to leave the *Define peaks semi-automatically* mode.

How to Delete Peaks from the Peak List



- Right-click and in the list, select **Delete peak under cursor**.

Save & Quit
 Quit

Add Peak To List
Delete Peak Under Cursor

Pick Peaks On Ranges
 Show Peak List

Set MI
 Set MAXI
 Set PC

- To delete all peaks, click .
- To define a region to delete peaks, click .

How to Return from Peak Picking Mode with/without Save

To return while saving the peak list and peak ranges:


- Click  Save the Peak Region and List and Return [**.sret**].

This will:


Save the peak list to the file *peak.xml* and the peak ranges to the file *peakrng*.

Leave the peak picking mode.

To return while discarding any changes:

- Click  Return, discarding any changes [**.ret**].

How to save Peak Lists and Regions in 1D Interactive Mode

In 1D interactive Peak Picking the  **Save as ...** button opens a window in which two options of saving can be selected:

- **Save Peak Lists and Regions.**
- **Save Peak List for Deconvolution.** The peak list will be saved in a format which is needed for deconvolution).

To save the peak list and start the deconvolution,

- click .

The peak list is saved, and the Deconvolution will be started, after that returning to Peak Picking.

1D Interactive Manipulation

ppp - Peaks found for 'mdcon'

Please adjust Gauss shape percentage(s) as desired

H	#frequency	half width	%gauss/100.
	4308.859	3.52	0.0
	4301.034	6.54	0.0
	4193.761	3.19	0.0
	4184.030	3.02	0.0
	4110.745	5.87	0.0
	4103.500	6.20	0.0
	4087.140	5.87	0.0
	4069.664	2.85	0.0
	4062.391	2.68	0.0
	4020.278	3.19	0.0
	3874.026	2.68	0.0
	3866.258	2.52	0.0
	3839.998	4.19	0.0

Dest.PROCNO

12 2D Interactive Manipulation

The upper toolbar of the 2D menu offers various buttons for interactive manipulation. If you click such a button, the active dataset window will switch to the corresponding mode. An interactive manipulation mode is dataset window specific, i.e. it only applies to the active window.

12.1 2D Interactive Phase Correction

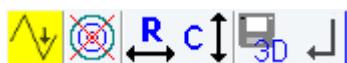
2D spectra can be phase corrected interactively in both the F2 and F1 direction by selecting certain rows and/or columns and phase correct them.

12.1.1 2D Interactive Phase Correction Procedure

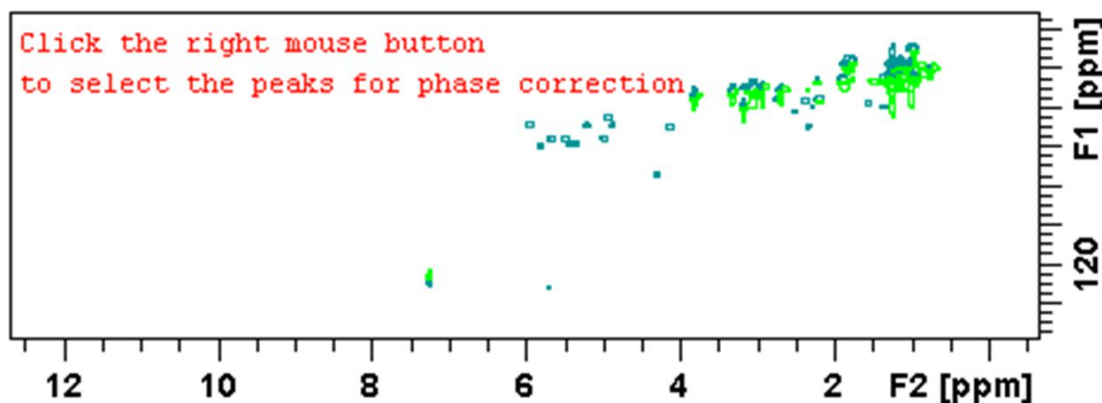
How to Switch to 2D Interactive Phase Correction

- Click **Process | Adjust Phase** or enter **.ph**.

The dataset tab bar of the active dataset window will be replaced by the phase correction toolbar.



The figure below shows an example of an unphased 2D inverse spectrum.



The yellow button indicates that you are in phase correction mode.



Toggle the contour display on/off.



Switch to **phase row** mode to display rows of selected peaks.



Switch to **phase columns** mode to display columns of selected peaks.

2D Interactive Manipulation



Save the phase values to the 3D data from which this 2D was extracted.



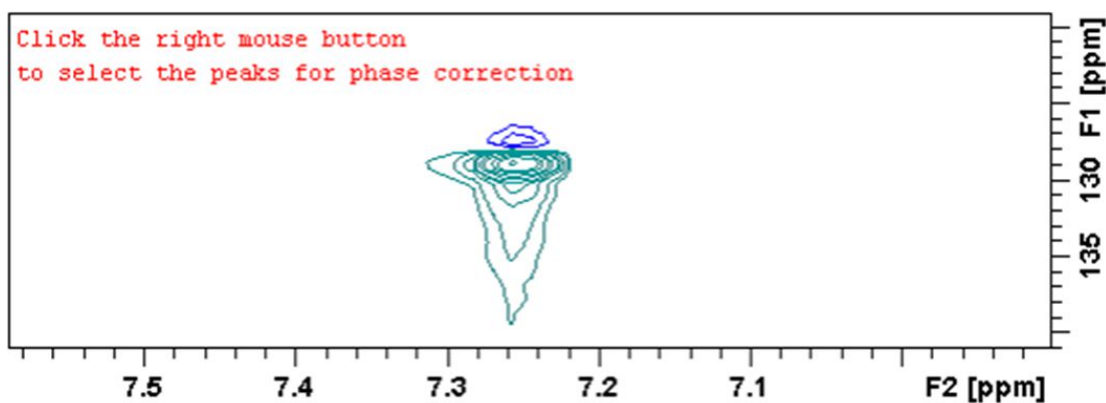
Return.


How to Perform a Typical 2D Interactive Phase Correction

In this example we will perform F1 phase correction (columns) only. Take the following steps:

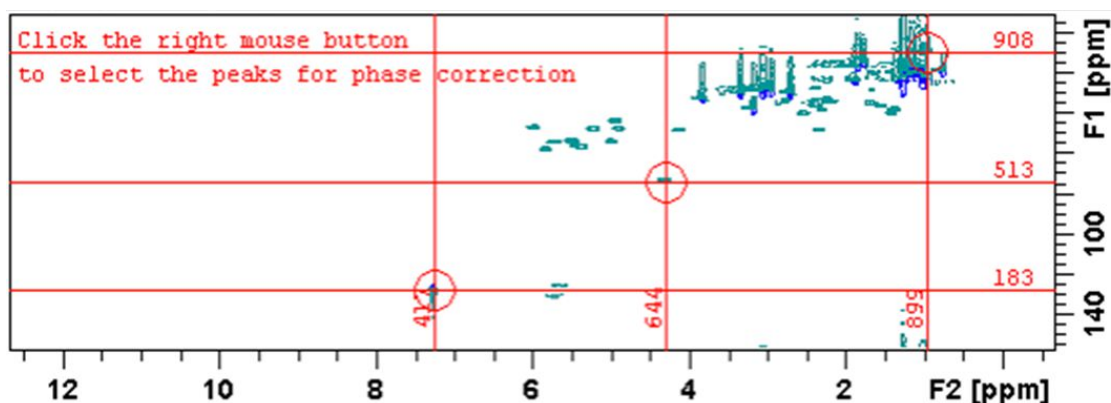
Select two or more peaks in different parts of the spectrum:


- Zoom in on a peak by drawing a box around it. To do that, click-hold the left mouse button and move the mouse.
- Right-click at the peak position and in the list, select **Add**.



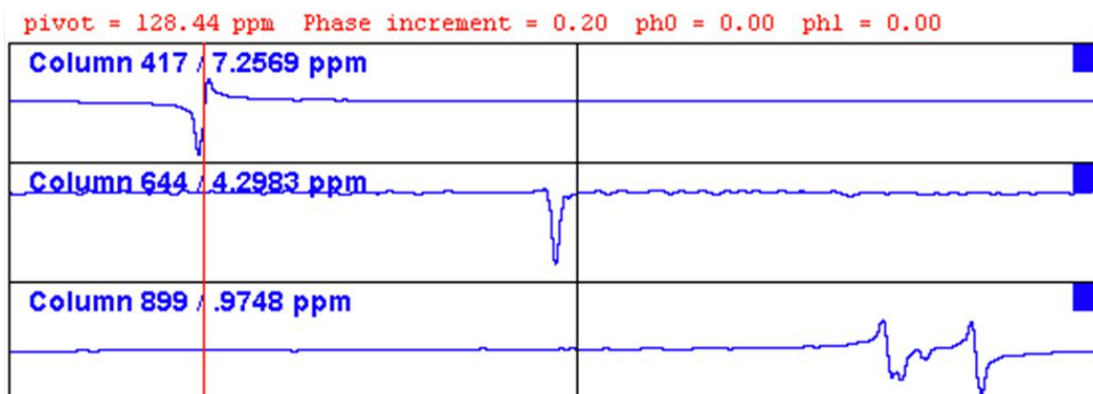
- Click  to display the full spectrum.
- Zoom in on the next peak and add in the same way as the first one.
- Zoom in on the next peak etc.

The following figure shows an example of three selected peaks.



- Click  to phase correct the columns (F1).

A new dataset window called **Phase 2D** will appear displaying the columns of the selected peaks:




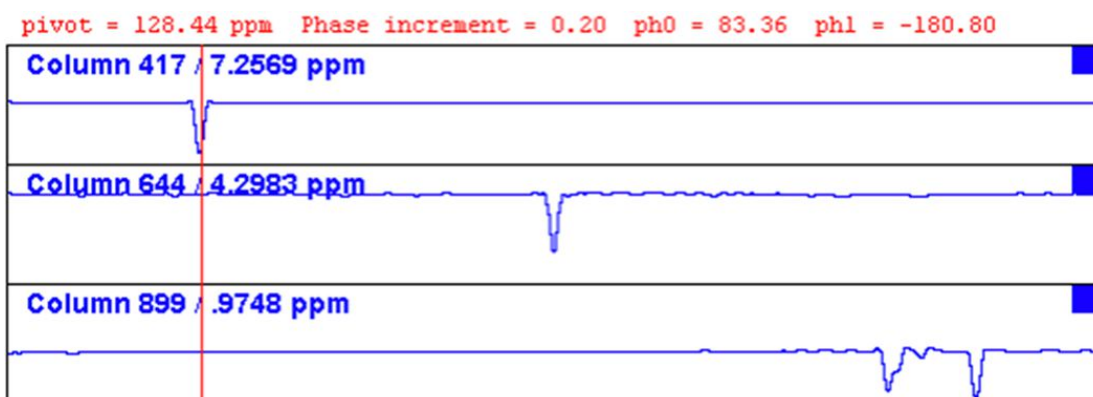
Note that the toolbar and the right-click popup menu offer the full 1D phase correction functions.



By default, all columns are selected as indicated by the filled blue squares ■. The red vertical line indicates the default pivot point in the upper column.

A typical way to perform phase correction is:

- Click-hold **0** for zero order correction and move the mouse until the reference peak of the first column is exactly in absorption mode.
- Click-hold **1** for first order correction and move the mouse until the reference peak in other column is exactly in absorption mode.
- Click  to execute, save and return.



12.1.2 2D Interactive Phase Correction Details

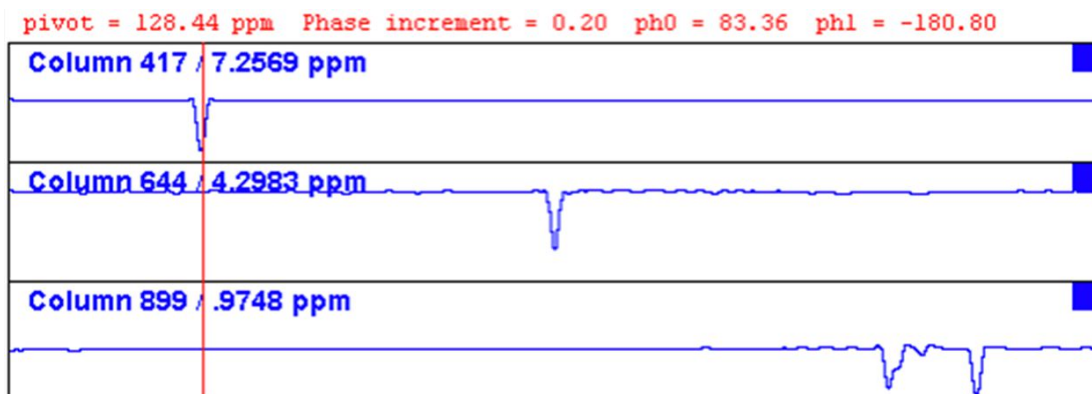
How to Scale or Shift Individual Rows/Columns


To select one row or column:

2D Interactive Manipulation

- Click in the corresponding part of the dataset window.


The selected row/column will be marked with a filled blue square ■ whereas unselected rows/columns will be marked with an unfilled blue square □. Selecting a single row /column allows to shift and scale it separately from the other rows/columns as shown in:



- Click  to select all rows or columns.


How to Perform Smooth Phase Correction

To perform zero order phase correction:

- Click-hold  Zero order phase correction.
- Move the mouse until the reference peak of the first row/column is exactly in absorption mode.
- Release the mouse - button turns gray.




The parameter PHC0 will be set accordingly.

To perform first order phase correction:


- Click-hold  First order phase correction
- Move the mouse until the reference peak of the second and further rows/columns is exactly in absorption mode.
- Release the mouse – the button turns gray.

The parameter PHC1 will be set accordingly.

How to Perform 90, -90 or 180° Zero Order Phase Correction


- Click one of the following buttons:
 -  90° zero order phase correction.
 -  -90° zero order phase correction.
 -  180° zero order phase correction.


How to Reset the Phase to the Original Values

- Click  Reset zero and first order phase.

How to Change the Mouse Sensitivity

- Click one of the following buttons:

 Increase (double) the mouse sensitivity [**.inc**].

 Decrease (halve) the mouse sensitivity [**.dec**].

 Reset the mouse sensitivity to 2.0.

How to Show the Next/Previous Row or Column

To show the next row/column,

- click  **Show next row/column.**

Note that only the selected row/column is increased. If all rows/columns are selected, only the first one is increased.


To show the previous row/column,

- click  **Show previous row/column.**


Note that only the selected row/column is decreased. If all rows/columns are selected, only the first one is decreased.

How to Arrange Rows or Columns


- Click one of the following buttons:

 Arrange rows/columns horizontally.

 Arrange rows/columns vertically.

 Arrange rows/columns vertically in a split window.

How to Return from Multi-1D Phase to 2D Phase Display

- Click  to save, execute and return.

This will perform the following tasks:

1. Execute phase correction.
2. Save the current phase correction values.
3. Leave the multi-1D phase mode.

How to Return from 2D Phase Mode without Save

- Click  Return.

12.2 2D Interactive Integration

TopSpin supports interactive 2D integration.

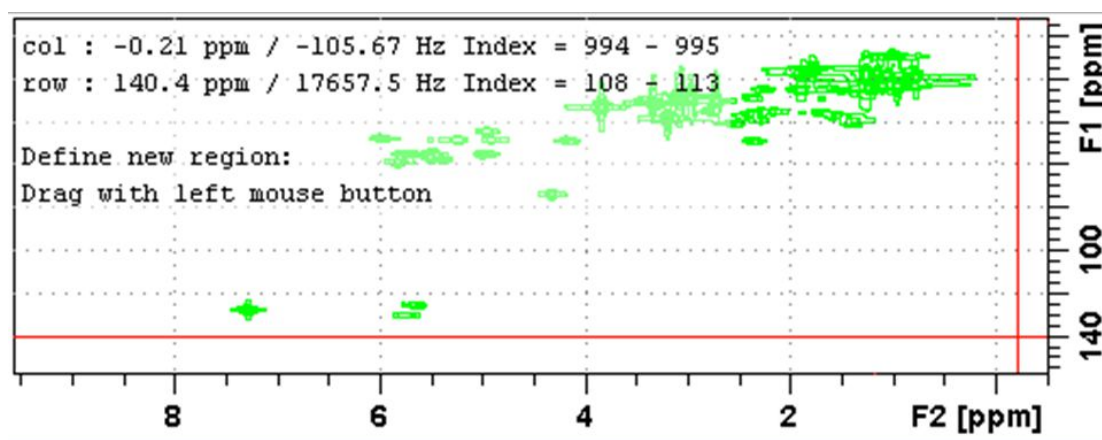
12.2.1 How to Switch to 2D Interactive Integration


- Click **Analyse | Integrate** or enter **.int**.


The active dataset window tabs will be replaced by the Integration toolbar.




The figure below shows an example of a 2D inverse spectrum.



 The yellow button indicates that you are in integration mode.


 "Define integral region" mode (active when gray).


 Move integral region (gray when active).


 Copy a region.

 Delete all integral regions.

 Read/import integral regions.

 Save/Export integral regions.

 Integrate current regions/define reference.

 Save integral regions and return.

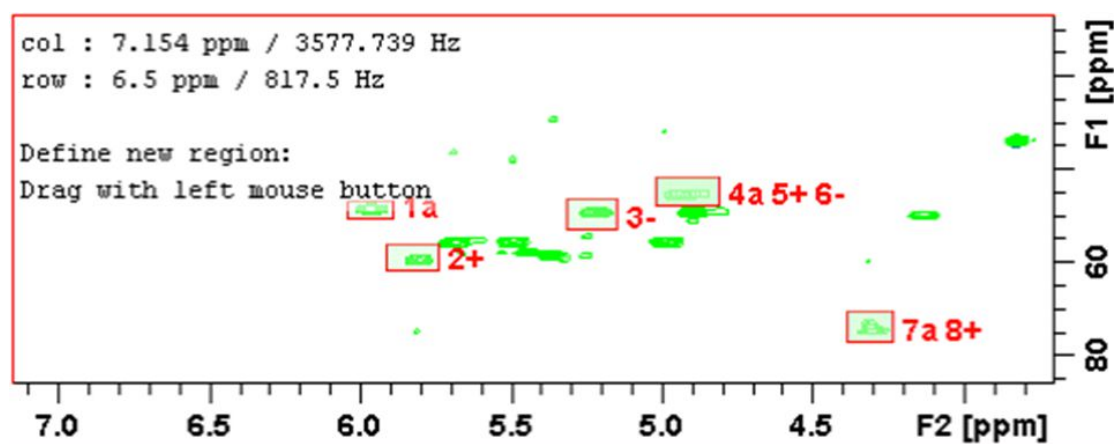
 Return without save.



12.2.2 2D Interactive Integration Procedure

When you switch to 2D integration mode, the "Define integral region" mode is active by default. This means you can immediately start defining the integral regions. To do that:

- Click and hold the left mouse button at any corner of a region to be defined, move the mouse to draw a box around that region and release the mouse.
- Select one of the following options from the appearing popup menu:
 - **Integrate: a**: to add up all intensities in the region.
 - **Integrate: +**: to add up all positive intensities in the region.
 - **Integrate: -**: to add up all negative intensities in the region.
 - **Integrate: a + -**: to add up all intensities in the region and store separate entries for *all*, *positive* and *negative* intensities.
 - **Integrate: a +**: to add up all intensities in the region and store separate entries for *all* and *positive* intensities.
 - **Integrate: a -**: to add up all intensities in the label and store separate entries for *all* and *negative* intensities.
 - **Integrate: + -**: to add up all intensities in the region and store separate entries for *positive* and *negative* intensities.

The integral regions will be displayed along with their storage numbers and modes:




- Click **Integrate current regions**  button and in the list, select **Integrate current regions** to integrate the defined regions.
- Click **Integrate current regions**  button again and in the list, select **List integral values** to display the list of integrals.

The table displays the list of integrals based on the regions defined in the figure above:


#	SI_F1	row1	row2	row1 ppm	row2 ppm	Abs. Int.	Integral	
	SI_F2	col1	col2	col1 ppm	col2 ppm			
1	1024	666	689	50.14583	46.43132	9.2529e+008	882.42	a
	1024	510	522	6.04420	5.89291			

#	SI_F1	row1	row2	row1 ppm	row2 ppm	Abs. Int.	Integral	
	SI_F2	col1	col2	col1 ppm	col2 ppm			
2	1024	597	632	61.28934	55.71759	1.1135e+009	1062	+
	1024	520	533	5.91452	5.74162			
3	1024	652	692	52.46739	45.96701	-3.7699e+007	-35.953	-
	1024	566	579	5.31659	5.15089			
4	1024	683	721	47.35995	41.32388	1.0072e+009	960.57	a
	1024	589	605	5.02122	4.81230			
5	1024	683	721	47.35995	41.32388	1.064e+009	1014.7	+
	1024	589	605	5.02122	4.81230			
6	1024	683	721	47.35995	41.32388	-5.6725e+007	-54.097	-
	1024	589	605	5.02122	4.81230			
7	1024	502	543	76.61168	70.11130	1.2637e+009	1205.2	a
	1024	637	649	4.38726	4.23598			
8	1024	502	543	76.61168	70.11130	1.2911e+009	1231.3	+
	1024	637	649	4.38726	4.23598			


Alternatively, you can define a reference integral and integrate the defined regions of the same or of a different dataset, relative to this integral. For this purpose the  button offers the following menu items:

1. **Integrate current regions rel. to reference:** You will be prompted for the reference integral number and value.
2. **List integral values:** The output list will now show an additional column with the normalized integral values.
3. **Define current dataset as reference:** You will be prompted for the reference integral number and value.
4. **Integrate and use ref. dataset for calibration:** The integral value defined on the reference dataset is used for calibration.


How to Move an Integral region

- Click  - it turns gray.
- Move the mouse into the region to be moved.
- Left-click-hold and move the mouse to move the region.
- Release the mouse at the desired position.


How to Copy an Integral region

- Click  - it turns gray.
- Move the mouse into the region to be copied.
- Click-hold and move the mouse to the desired position.
- Release the mouse to copy the region.


How to Delete all Integral Regions

- Click .
- Click **OK** to confirm deletion.



How to Read/Import Integral Regions

- Click .
 - Click **Read intrng** to read the last stored integral ranges
- or
- Click **Import Integration Regions** to import an exported integral region file (see below)

How to Save/Export Integral Regions

- Click .
 - Click **Save Regions to intrng** to save the regions to the current dataset PROCNO (file *int2drng*)
- or
- Click **Export Integration Regions** to export the integration region file for general usage; i.e. usage with other datasets.

How to Return from 2D Integration mode

- Click  to save the current integral regions and return.
- Click  to return to the 2D integration mode without save.

12.3 2D Multiple Display and Row/Column Handling

2D multiple display shows a 2D spectrum with an arbitrary number of 1D and/or 2D spectra superimposed.

Spectra are ppm aligned or Hz aligned, according to the selected axis unit.


A superimposed 1D spectrum is automatically displayed in the direction of the matching nucleus (for a hetero-nuclear 2D) or in the F2 direction (for a homo-nuclear 2D).

Although multiple display is normally used for spectra with matching nuclei, it allows to superimposed spectra with non-matching nuclei. You will get a warning that the nuclei do not match.

- Click **OK** to continue.

How Switch to Multiple Display mode and Read Multiple Spectra

Switching to multiple display and reading multiple spectra can be done in two different ways:

- Read a 2D dataset and click  to switch to multiple display mode. Then add 1D and/or 2D spectra, e.g. from the browser or with the command **re**.

or

- Select multiple spectra in the browser, right-click one of them and select **Display**.

or

- Enter **.md** in the command line.

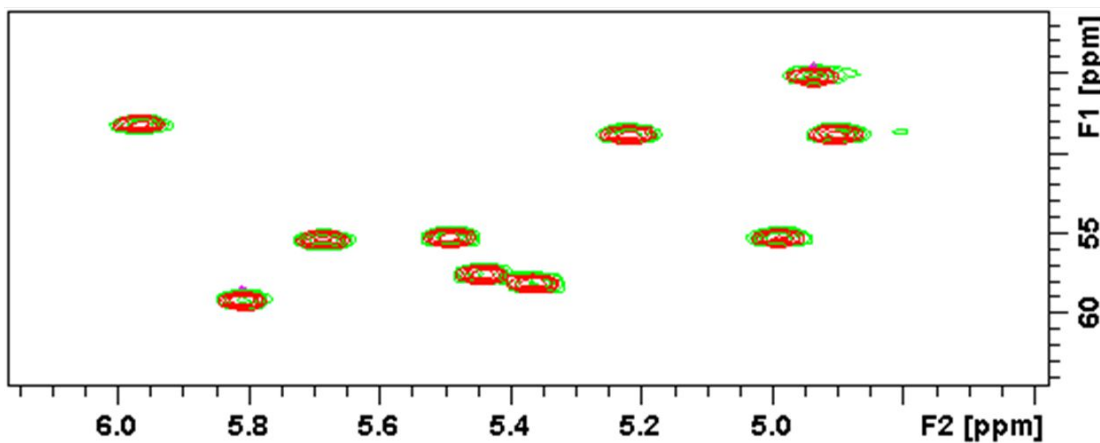
2D Interactive Manipulation

For a more detailed description of reading multiple data in multiple display mode, see chapter [1D Multiple Display \[153\]](#).

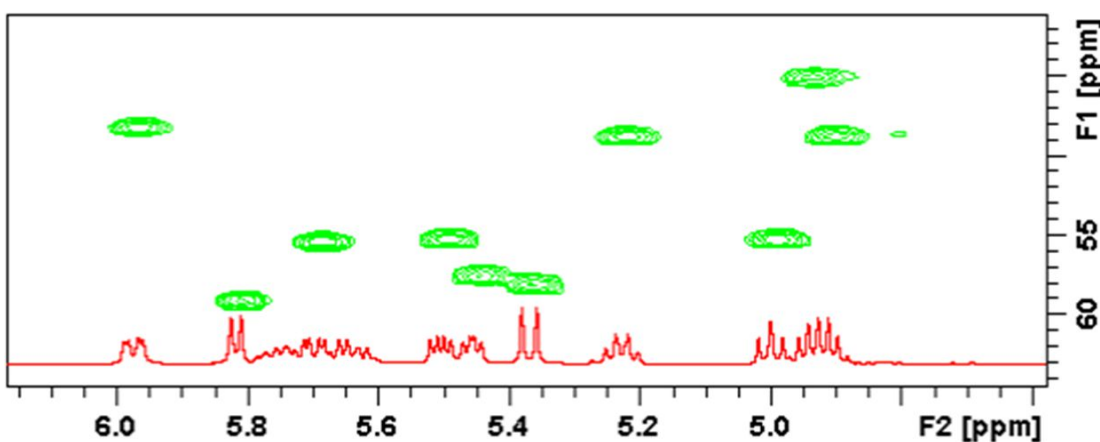
The Multiple display toolbar is displayed:



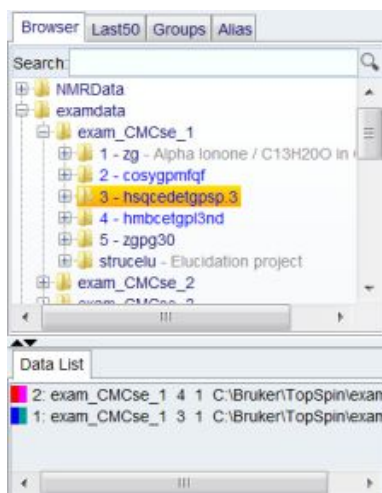
Multiple display with two 2D spectra superimposed:



Multiple display with a 1D spectrum superimposed on a 2D spectrum:




The browser in multiple display lists in the lower Data List part all open datasets (see the figure below):




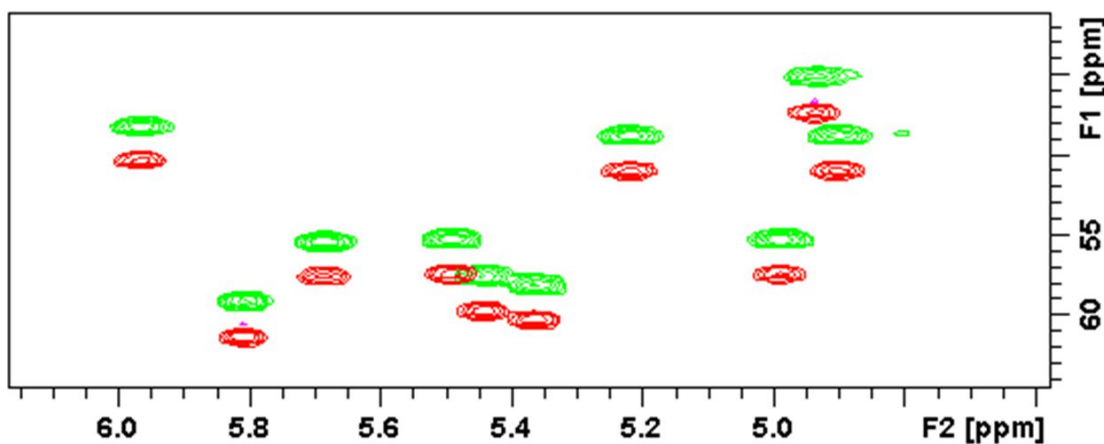
How to Align Multiple 2D Spectra

2D spectra in multiple display can be individually shifted:

- Select one of the spectra in the lower part of the browser.
- Click one of the Shift Buttons in the desired direction up, down or both (e.g. ) hold and move the mouse.

The figure below shows a region of two comparable $^1\text{H}/^{13}\text{C}$ inverse 2D datasets which are shifted relative to each other.

- Click  to reset individual scaling and shifting.



How to Display the Next/Previous Name/Expno

To compare a series of spectra you can interactively increment or decrement the dataset name or expno. A dataset name is incremented according to the IconNMR naming convention of increasing extensions, e.g. name.001, name.002 etc.

- Click one of the following buttons – the button turns gray:

 Show the previous name/expno/procno of the last dataset.

 Show the next name/expno/procno of the last dataset.


E i Set the increment options. Clicking this button will open the following dialog where you can select to increment the procno, expno or name, set the expno increment and switch individual scaling on/off.

How to Scan Rows/Columns

Select desired dataset(s) and click one of the following buttons to activate the scanning modus.

- Deactivation needs a second click on:

 To scan rows in the 2D spectrum.

 To scan columns in the 2D spectrum.

 To scan rows and columns in the 2D spectrum.

Moving the mouse in the data field shows the current row or column in separate. Change the data selection in the Data List to switch between datasets.

To switch the modus quickly:

- right-click and in the list, select **Toggle Rows/Columns**.

To scale up the displayed row/column:

- Click or turn the mouse wheel up.

To scale down the displayed row/column:

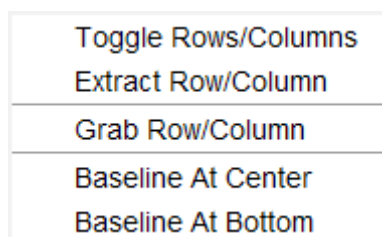
- Click the middle mouse button or turn the mouse wheel down.

How to Grab a Row/Column

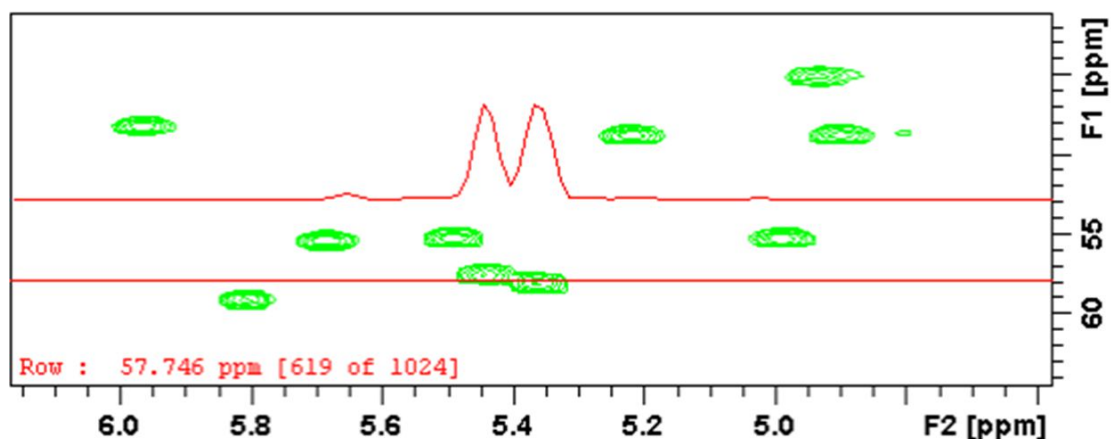
You can grab a row or column, i.e. keep it displayed in the dataset window as follows:

- Scan rows or columns as described above and hold at the desired position.
- Right-click and in the list, select **Grab Row/Column**.

Note that a grabbed row/column appears in the lower part of the browser. It can be selected there and individually scaled or shifted.



The figure shows row 619 with the 1D baseline at the center of the dataset window.



How to Show the Next/Previous Row or Column

To display the next row/column,

- click  **Show next row/column.**

To display the previous row/column,

- click  **Show previous row/column.**

Alternatively, turn the mouse wheel, while pressing the **Shift** key to show the next/previous rows/columns.

How to Move the Selected Dataset Up/Down in the Dataset List

To move the selected dataset up,

- click  **Move the selected dataset up.**

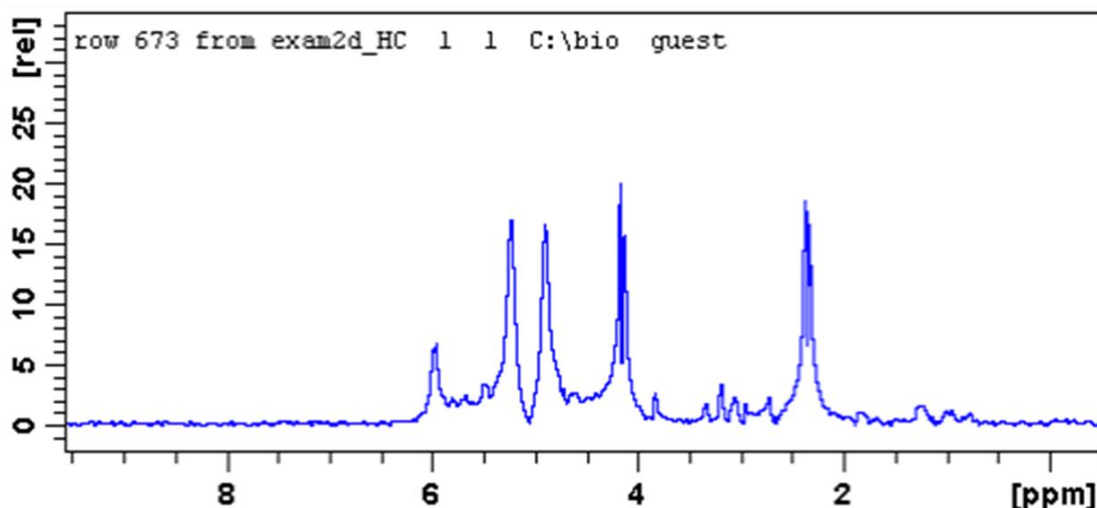
To move the selected dataset down,

- click  **Move the selected dataset down.**


How to Extract a Row/Column

- Scan rows or columns as described above and hold at the desired position.
- Right-click in the dataset window and in the list, select **Extract Row/Column**.
- Specify the row/column number and output procno in the dialog box. Note that the ROW/COLUMN field is initialized with the grabbed row/column or, if no grabbing was done, with the current row/column.
- Click **OK**.

The extracted row or column is stored as a 1D dataset under the specified PROCNO and displayed in a new dataset window. In the upper left part of this, the row number and source 2D dataset is specified:



How to Copy Contour Levels from First to Other Spectra

- Click  Copy contour levels from the first to the other spectra.

Note that the contour levels are only changed on screen, not on disk.

How to Position the Baseline of the Row/Column

To center the baseline:

- Right-click in the dataset window and in the list, select **Baseline At Center**.

To set the baseline at the bottom of the dataset window:

- Right-click in the dataset window and in the list, select **Baseline At Bottom**.




This works both in the scan sub mode or on a grabbed row/column.

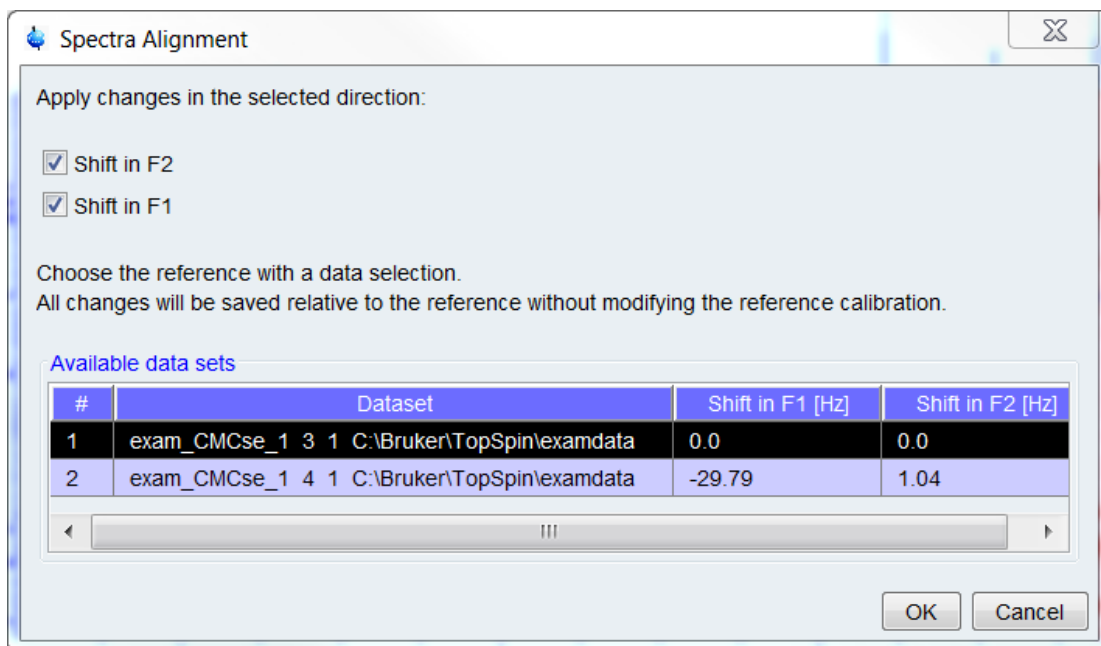
12.3.1 2D Calibration in Multiple Display

How to calibrate data in multiple display

It is possible to align data in a multiple display interactive or in an automated in F1 and F2 direction:

To calibrate data interactively,

- select a spectra and click  or  to align the multiplets.
- Click the calibration button  to display the following window:



The exact shifts are displayed in the dialog. The selection marks the reference data and only the selected direction will be saved. When confirming the dialog, the shifts will be saved in the processing parameter **SR**.

In the automated calibration step the alignment will be determined automatically. Use this feature in one of both ways:

- Click  in the multiple display modus.

Next, the correctly aligned spectra will appear on the screen with a dedicated dialog on the top (see the figure above). The dialog shows the necessary chemical shift relative to the reference. The default reference in the calculation is the first dataset. Change the reference by changing the data selection. With the conformation the current result will be saved in the SR parameter.




Use the command **autocalib** in the command line or in AU programs (for further information read more about the command in the TopSpin Processing Manual - Analysis Commands).


12.4 2D Interactive Calibration

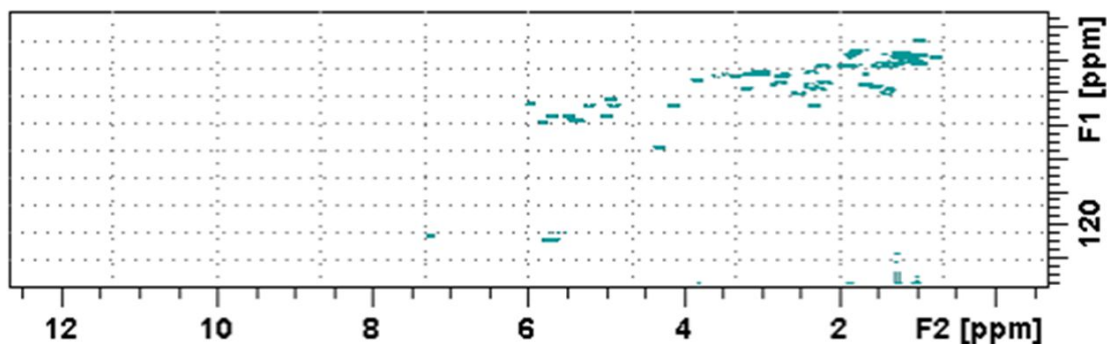
A 2D spectrum can be calibrated, automatically with the command **sref** or, interactively as described below.

How to Switch to 2D Calibration mode

- Click **Process | Calib. Axis** or enter **.cal**.

The tab bar of the active dataset window will be replaced by a toolbar:   

 The yellow button indicates that the dataset window is in calibration mode.



How to Perform a 2D Calibration

In calibration mode:

- Click in the dataset window at the reference peak to display the Calibrate window.


F2[ppm]	F1[ppm]
3.8634	32.8954

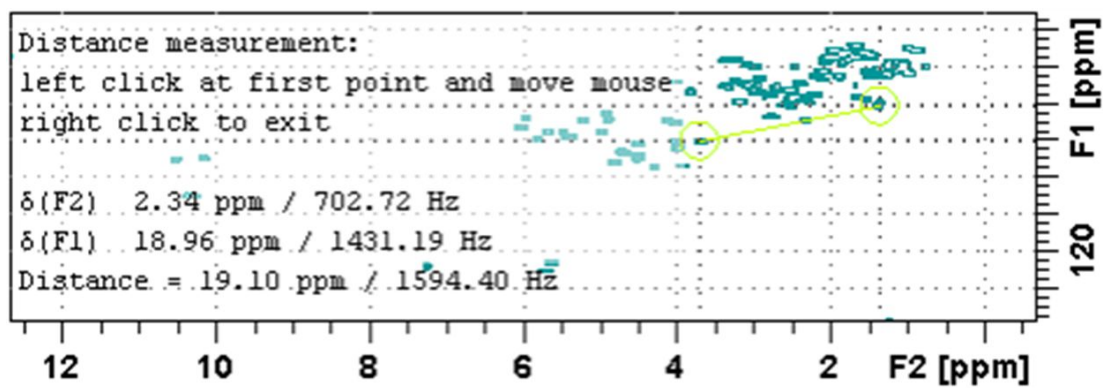
Note that the units for F2 and F1 (Hz or ppm) correspond to the axis units of the display.

- Enter the F2 and F1 frequency you want to assign to the reference peak.
- Click **OK**.

The spectrum will be calibrated and re-displayed.

How to Measure a 2D Chemical Shift Distance

- Click  Chemical shift distance measurement – the button turns gray.
- Click-hold the left mouse button at one peak position and drag the mouse to another peak position.
The distance in ppm, will be displayed.
- Right-click in the dataset window to quit distance mode.



13 Analysis

13.1 Introduction

TopSpin offers various data analysis methods including chemical shift measurement, signal to noise calculation and T1/T2 relaxation analysis as described in this chapter.

Furthermore, it offers the following structure analysis tools:

1. **Multiplet Analysis:** Allows to easily define multiplets and deduce chemical shifts, coupling constants, multiplicities and connections.
2. **Daisy:** Allows to simulate spectra based on chemical shifts and coupling constants.
3. **Solids Line Shape Analysis:** Allows to simulate and fit calculated spectra to various experimental 1D solid NMR spectra.
4. **Jmol:** A 3D Structure Viewer for displaying chemical structures.
5. **D molecule structure editor:** A program for drawing chemical structures, offering many drawing tools.
6. **DNMR (Dynamic NMR) Lineshape Analysis:** A program to simulate temperature dependent NMR spectra, interactively set up and iteratively refine the model parameters to get the best fit of the measured and simulated 1D NMR spectra.


Structure analysis tools can be started from the **Analysis** menu. They are all described in the following manuals:

- Click **Help | Manuals | Analysis and Simulation | Structure Analysis Tools**.

except for Daisy, which is described in the separate manual **Analysis and Simulation | Daisy**.

13.2 Chemical Shift Distance Measurement

How to Measure a Chemical Shift Distance

- Click  **Chemical shift distance measurement** (button turns gray).
- Left-click-hold at one peak position and drag the mouse to another peak position.


The distance in ppm, will be displayed.

- Right-click in the dataset window or move the cursor out of the dataset window to leave distance measurement mode.

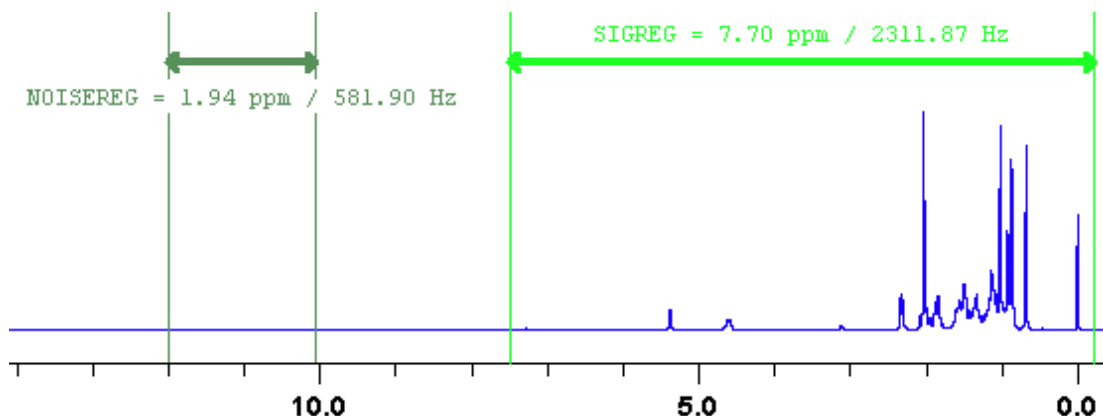
13.3 1D Signal to Noise Calculation

How to Perform Interactive S/N Calculation

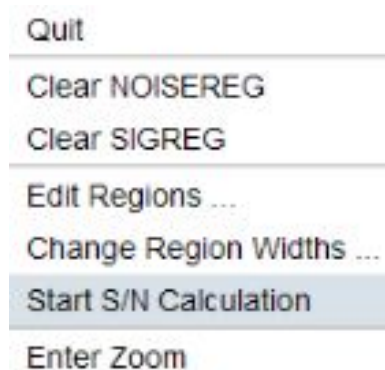
- Click **Analyse | SiNo | Signal/Noise Calculation [.sino]**.

The S/N toolbar is displayed .

The current signal region (parameters SIGF1-SIGF2) and noise region (parameters NOISF1-NOISF2) are displayed.



- Move the mouse into the dataset window.
- Click-hold and drag the mouse from one edge of the *signal* region to the other edge. A horizontal double-headed arrow will indicate the signal region.
- Click-hold and drag the mouse from one edge of the *noise* region to the other edge. A horizontal double-headed arrow will indicate the noise region.
- Right-click any position in the dataset window. In the list, select **Start S/N calculation**.



The other entries allow you to redefine or clear the regions. After the noise calculation has finished, the result will appear on the screen.

How to Delete the Signal Region or Noise Region

To delete the current signal region:

- Right-click in the dataset window and in the list, select **Clear SIGREG**.

To delete the current noise region:

- Right-click in the dataset window and in the list, select **Clear NOISEREG**.

How to Edit the Limits of the Signal Region or Noise Region

- Right-click in the dataset window and in the list, select **Edit regions...**
- Enter new limit values in the appearing dialog box:



- Click **OK**.

The S/N value is automatically recalculated and displayed.

How to Change the Width of the Signal Region or Noise Region

- Right-click in the dataset window and in the list, select **Change region width...**
- Enter new width values in the appearing dialog box:



- Click **OK**.

Note that as you change the width, the right limit is modified correspondingly. The left limit is kept. The S/N value is automatically recalculated and displayed.

13.4 Deconvolution

The Analysis menu of TopSpin offers the possibility of deconvolution. This line shape tool is especially useful to interpret complex spectra in which peaks cannot be defined clearly. Deconvolution calculates theoretical signals with different methods, for example Gaussian, Lorentzian or a mixture of these line shapes. As a result, information of peak position, line width and integrals of deconvolved signals are available. Furthermore, it is possible to display them graphically. With this auxiliary tool peaks of 1D and 2D NMR spectrum can be interpreted more easily. Overlapping peaks may be deconvolved into a sum of such line shapes.

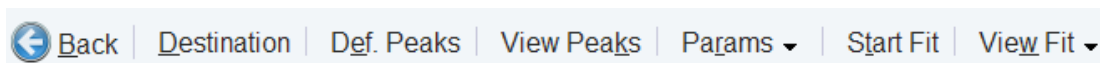
To start deconvolution, expand the spectrum on the display to show the peak or peak group of interest. To activate deconvolution

- click **Analyse | Line Shapes | Fit Lorentz Gauss Functions**.

or

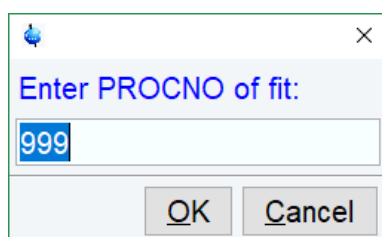
- enter **dcon**

The workflow button bar changes:




- Click **Destination** to define where the result will be stored.

The following dialog box will appear:



- Click **Def. Peaks** to define the peaks to be deconvoluted.

The display changes to peak picking mode. Select the peaks as described in the chapter [1D Interactive Peak Picking \[▶ 164\]](#). When done, click  and in the list, select **Save Peaklist for Deconvolution**.

- Click **View Peaks** to inspect the peak list. Here you can enter individual values for half-width and Lorentz Gauss percentage.
- Click **Params** and in the list, select values for the computation range per line [AZFW] and the integral scaling factor [CY].
- Click **Start Fit** to start the fitting process.

For further information about all deconvolution options and the parameters to be set, please look up the Processing Reference Manual (commands **gdcon**, **ldcon**, **mdcon**, **ppp**, **dconpl** and **dcon**).

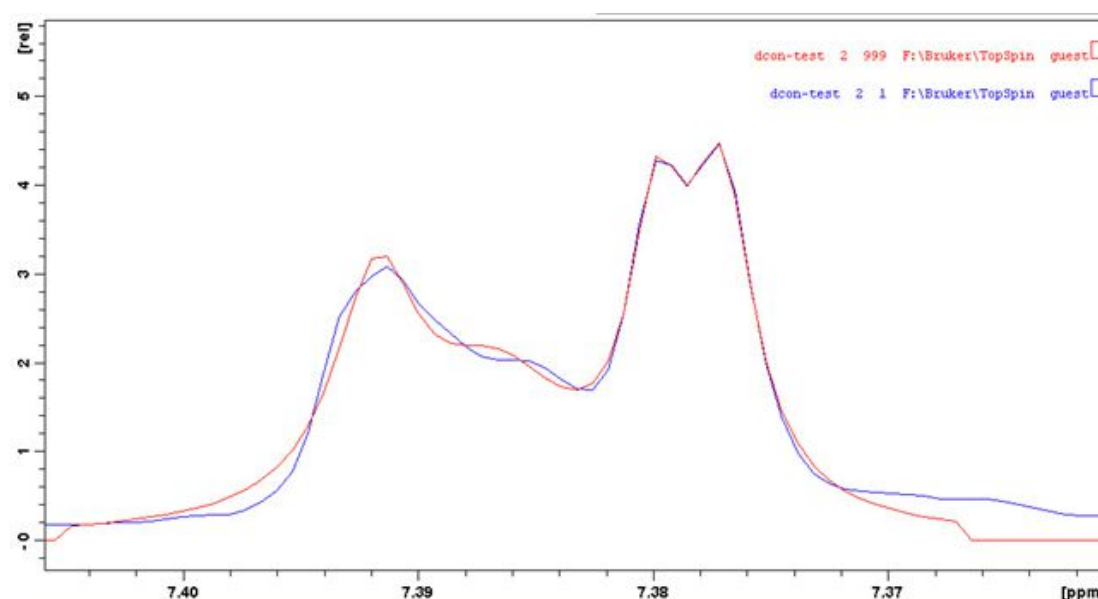
TopSpin shows the deconvolution result, i.e. peak positions, line widths and integrals on the screen and stores it in the file **dconpeaks.txt** within the respective procno of the dataset:

```

1 Data set: F:/Bruker/TopSpin/data/guest/nmr/dcon-test/2/pdata/1/
2
3 Fit type: Lorentzian
4
5 Fit      Frequency      Width      Intensity      Area      %Lor.
6      ppm      Hz      ppm      Hz
7
8 1      7.392  2954.85  0.00438  1.750  2.547  26.064  100.00
9
10 STD:  0.000  0.06  0.00057  0.229  0.242
11
12      7.387  2952.81  0.00789  3.154  1.525  28.119  100.00
13
14 STD:  0.000  0.20  0.00182  0.726  0.148
15
16      7.380  2950.09  0.00271  1.084  2.821  17.879  100.00
17
18 STD:  0.000  0.04  0.00040  0.158  0.224
19
20      7.377  2949.00  0.00344  1.375  3.562  28.633  100.00
21
22 STD:  0.000  0.04  0.00028  0.112  0.196

```

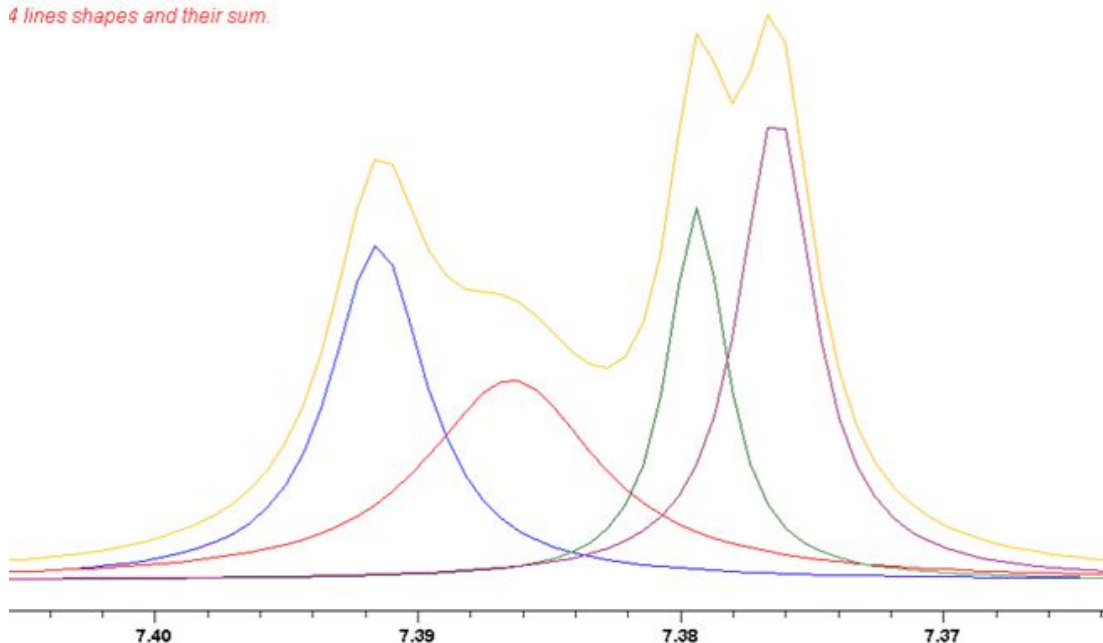
After closing the editor window which shows the deconvolution result, TopSpin switches automatically to multiple display mode to show the original spectrum and the sum of the computed line shapes superimposed:



See also the chapter [1D Multiple Display \[153\]](#) for further multiple display options.

- Click **View Fit** for further display options:
 - **View Fit Overlaid** to switch to multiple display
 - **View Numerical Result** to display the result again
 - **View Fitted Shapes** to display all deconvoluted lines individually

Deconvolution result:
4 lines shapes and their sum.



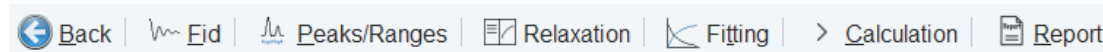
Please note that the results of deconvolution are approximated achievements to interpret complex spectra. These amounts are according to reality if the signal is an ideal Gauss- or Lorentzian shape and if the complete region of the signals is deconvolved.

13.5 Relaxation Analysis

Typically, relaxation data consist of a series of 1D FIDs measured with varying delays and stored as pseudo 2D data. To analyze these data, TopSpin offers an easy to use T1/T2 Relaxation Guide. Relaxation curves of various experiment types with up to six components can be fitted.

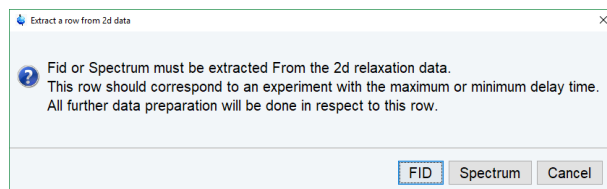
To start the Relaxation Guide click **Applications | Dynamics | T1T2 (t1t2)**.

The T1T2 toolbar is displayed:



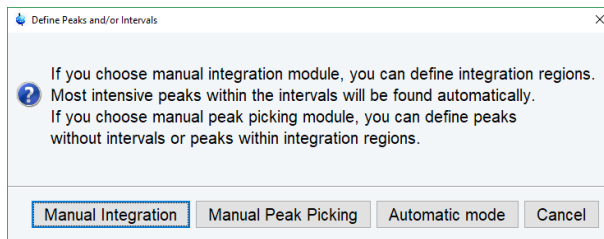
Click the successive icons and follow the instructions on the screen.

- Click **FID** to extract an FID or a spectrum for peak determination.



Note that the latter only works if the pseudo 2D dataset have been processed. If you click FID, the extracted FID is automatically processed. We recommend entering the FID or spectrum number which was measured with the longest delay. It can be found in the *vdlist* file in the EXPNO dataset directory.

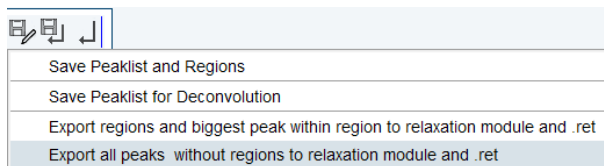
- Click **Peaks/Ranges** to define the peaks or ranges for subsequent T1/T2 calculation.



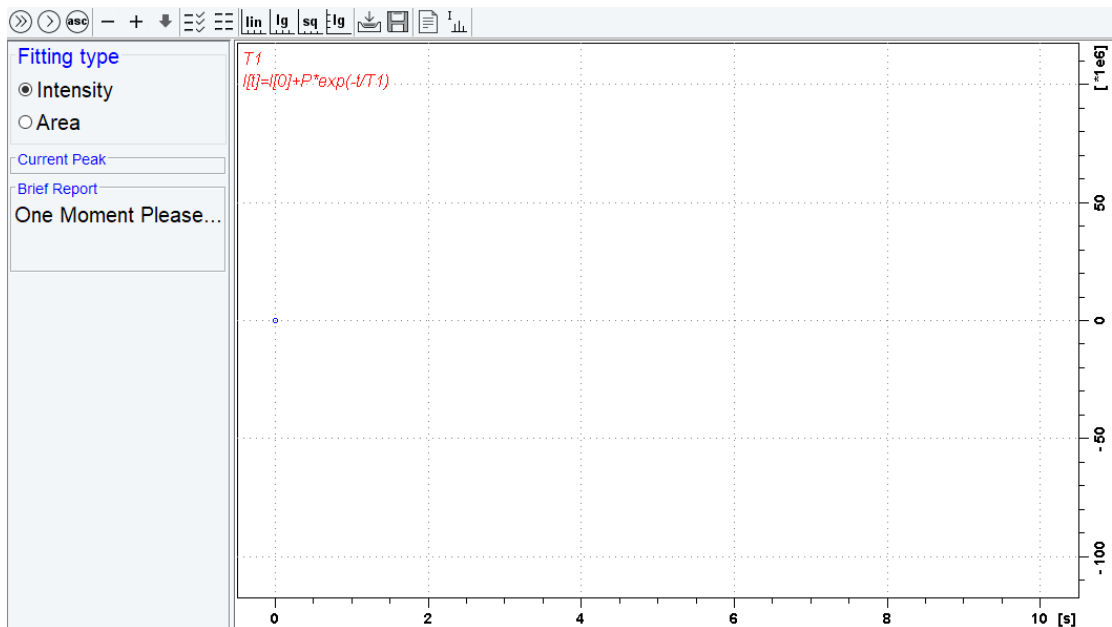
Then you can select between:

- **Manual Integration.** This will switch to Interactive integration mode. The highest peak in each region will be used for relaxation analysis.
- **Manual Peak Picking.** The selected peaks will be used for relaxation analysis.
- **Automatic mode.** Peaks will be picked automatically.

Then click **Save as...** to export regions/peaks to Relaxation Module and quit the interactive mode.



- Click **Relaxation** to switch from the 1D dataset window to relaxation analysis mode.



At the same time the relaxation parameters are displayed and can be set for the fit:

Relaxation parameters
✕

General Parameters

10	FID # for phase determination
1000.0	Left limit for baseline correction
-1000.0	Right limit for baseline correction
5	Number of drift points
1.0E-5	Convergence limit
16	Number of points
1	First slice
1	Slice increment
1.0	Peak sensitivity

Fitting Function

uxnmrt1	▼	Function Type
1		Number of components
vdlist	▼	List file name
0.001		Increment (auto)
pd	▼	to pick data points

Iteration control parameters

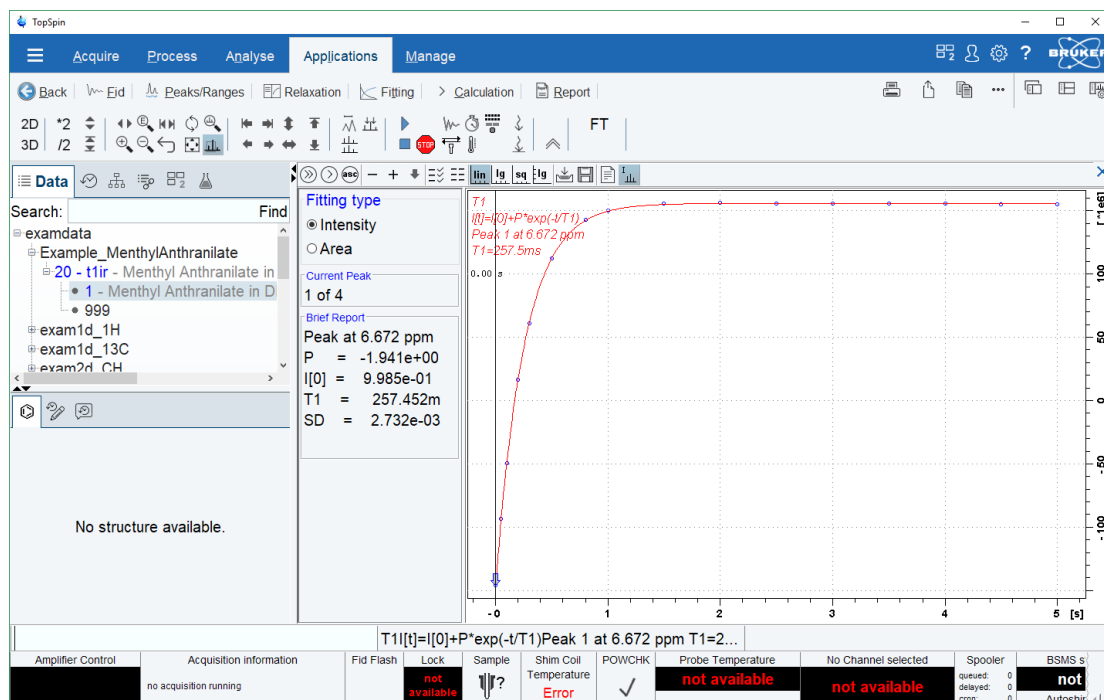
Guesses
Reset

Additional Parameters

10000.0	GAMMA(Hz/G)
10.0	LITDEL(msec)
100.0	BIGDEL(msec)
1.0	GRADIEN(G/cm)





OK
Apply
Cancel

By default, this is one-component, T1-intensity fitting (Function type *uxnmrt1*) for peak 1. If the dataset was already fitted, the previous type of fitting is performed. The fitting curve is displayed in the data section and a *Brief Report* is shown in the parameter section. If this default fitting is appropriate, you can view, interpret and print the results as described below. If not, you can perform the desired fitting as described below.



Perform Fitting and Calculate the Relaxation Time

Depending on the experiment, you can perform the appropriate fitting as follows:

- Select a **Fitting type**: **Intensity** or **Area**. Either every point reflects the intensity of the biggest peak in the defined integral range or the integral itself. Both can be used but, depending on the experiment, one of them usually give a better fitting curve.
- Click **Settings**  to open the parameter dialog box. Select a **Function Type** and set the required parameters (see below).
- Click **OK**.
- Perform fitting and calculate the relaxation time:
 -  Fit the relaxation curve for the current peak.
 -  Fit the relaxation curve for all peaks.
 -  Fit data according to the ASCII file t1ascii.

View and interpret the results as described below.



Function Types and Parameters

The TopSpin relaxation routine offers functions for various relaxation experiments with up to 6 components:

uxnmrt1 for one-component T1 experiments. Set the parameter *List file name* to the list type used during the acquisition. Set **Pick data points** to PD or PD0 (see below). The T1 fitting function is defined by the function:

$$I(t) = I(0) + P \times \exp\left(-\frac{t}{T1}\right)$$



Where I is Intensity or Area according to the Fitting Type. The best fit is calculated by varying $I(0)$, P and $T1$ in an iterative process according to the Levenberg-Marquardt algorithm.

Clicking  and  executes the commands **ct1** (current peak) and **dat1** (all peaks), respectively.


uxnmrt2 for one-component T2 experiments. Set the parameter *List file name* to the list type used during the acquisition. Set **Pick data points** to PD or PD0 (see below). A T2 fitting function is defined by the function:


$$I(t) = P \times \exp\left(\frac{t}{T2}\right)$$



Where I is Intensity or Area according to the Fitting Type. The best fit is calculated by varying P and $T2$ in an iterative process according to the Levenberg-Marquardt algorithm. Clicking

 and  executes the commands **ct2** (current peak) and **dat2** (all peaks), respectively.

invrec, satrec, cpt1rho, expdec, gaussdec, lorgauss linear, varbigdel, varlitdel, vargrad, vardamp: these functions can be used for various experiments with up to 6 components, except for **cpt1rho** and **lorgauss** which allow only 4 and 3 components, respectively. They all use the simplex algorithm and require some parameters to be set:

- Enter the **Number of components**.
- Click the **Settings**  button to set the *Iteration Control parameters*. For each component, the initial guess (G) and step rate (S) can be set. The initial guess for $I[0]$ must be selected such that the sum of all components does not exceed 1. If there is only one component, $I[0]$ is usually set to 1. The step rate is usually set to about one tenth of the initial guess. If the step rate of a variable is set to zero, then this variable is not changed during the iterations.

Note that the initial guesses can also be set with the Guesses  toolbar button.

Clicking  and  executes the commands **simfit** (current peak) and **simfit all** (all peaks), respectively.


The Fitting Function to pick data points can be:










1. **pd** - Pick data points for relaxation analysis (Drift value interpreted).
2. **pd0** - Pick data points for relaxation analysis at constant peak positions (drift value ignored).
3. **pft2** - Pick data points for T2 calculation of 1D raw data.

View the Fitting Results

When the fitting procedure has finished, the fitting curve is displayed in the data section and a *Brief Report* appears in the parameter section. The latter consists of:

1. The calculated relaxation values.
 2. The fitted parameters.
 3. The standard deviation SD.
- For further examination of the result, click one of the following buttons:

 Show the fitting result of the previous peak/area.

-  Show the fitting result of the next peak/area.
-  Switch x-axis to linear scaling.
-  Switch x-axis to logarithmic scaling.
-  Switch x-axis to square root scaling.
-  Switch y-axis to logarithmic scaling. Note that this only works for curves with positive intensities/areas only.
-  Import integrals from dataset ~TEMP.
-  Export integrals to dataset ~TEMP.
-  Toggle button to hide/show information in the curve field, including algorithm, peak number and relaxation value.
-  Show an extended report, including the fitted intensity or area distribution. This consists of the same information as the brief report plus a table with the intensity or area distribution.

Example:

```
Dataset : C:/bio/data/guest/nmr/t1test/1/pdata/1
INTENSITY fit :
I[t]=I[0]+P*exp(-t/T1)
12 points for Peak 1, Cursor Point = 7.221 ppm
Results Comp. 1
```

```
I[0] = 1.215e+000
P = -2.211e+000
T1 = 19.449s
SD = 3.685e-003
tau ppm integral intensity
30.000s 7.221 2.5811e+009 1.9737e+008
10.000s 7.221 -3.2898e+008 -2.9056e+007
8.000s 7.221 -7.8525e+008 -6.4616e+007
5.000s 7.221 -1.6289e+009 -1.3101e+008
...
```

Print, Export or Copy the Fitting Results

To print the fitting curve:

- Click **File | Print**.

To export the fitting curve as a graphics file:

- Click **File** | **Export**.

To copy the fitting curve to the Windows Clipboard:


- Click **Edit** | **Copy**.

14 Printing/Exporting Data

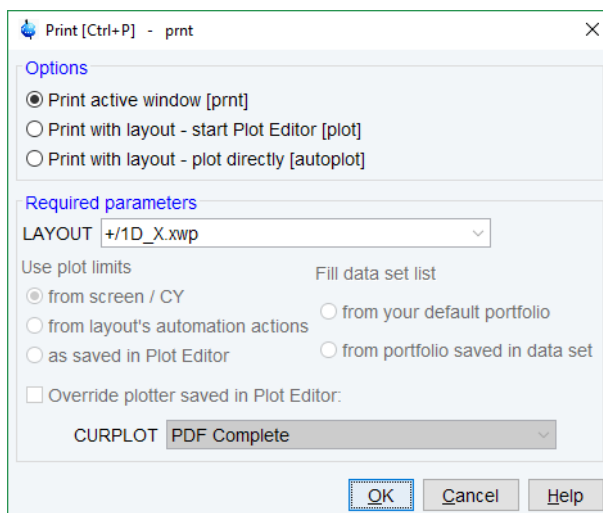
14.1 Printing/Plotting Data

How to Print/Plot from the Menu

The current dataset window can be printed as follows:

- Click the button  in the upper toolbar.
- Or click **File | Print**.
- Or enter **print** or **Ctrl+p**.

All these actions are equivalent; they open the Print dialog box.



In the Print dialog box:

- Select **Print active window [prnt]**.
- Click **OK**.

Before printing starts, the operating system print dialog box will appear. Here you can, for example, select the printer name and the printer properties.

The Print dialog box (see the figure above) contains two further options:

1. **Print with layout - start Plot Editor [Plot]** - If you select this option and click OK, the Plot Editor will be started. This option is equivalent to entering **plot** on the TopSpin command line.
2. **Print with layout - plot directly [autoplot]** - Selecting this option activates the Plot Editor layout list box. Select the desired layout and click to print. Standard layouts are delivered with TopSpin. They use the Windows default printer. User defined layouts use the printer defined in the Plot Editor. On a 1D dataset, only 1D layouts are listed, on a 2D dataset only 2D layouts are listed etc.

For the last two options, the following required Parameters are available:

Use plot limits

1. **From screen/ CY** - The plot limits and maximum intensity are used as they are on the screen (processing parameter F1P, F2P and CY, respectively).
2. **From Plot Editor Reset Actions** - The plot limits and maximum intensity are set according to the Plot Editor Reset Actions (right-click inside the Plot Editor data field and choose **Automation** to set the Reset Actions).
3. **As saved in Plot Editor** - The plot limits and maximum intensity are set in the specified layout

Fill dataset list

1. **From your default portfolio** - The portfolio contains the current TopSpin dataset plus the data from the default Plot Editor portfolio.
2. **From portfolio saved in dataset** - The portfolio contains the current TopSpin dataset plus the data from the portfolio stored in this dataset.

Override Plotter saved in Plot Editor

If enabled, the plotter defined in the Plot Editor layout will be overridden by the plotter defined by the processing parameter CURPLOT.

How to Plot Data from the Processing guide

Printing/plotting data can be done from the Processing guide by clicking the **Plot/Print** button. If **Automatic mode** is checked, the active dataset window will be printed as it appears in the screen. If **Automatic mode** is unchecked, you will get the dialog box as displayed in the figure below.

How to Plot Data with the Plot Editor

The Plot Editor can be started from the Print dialog or from the command line (command **plot**). The Plot Editor allows to create layouts and plot data. The complete functionality is described in the online manual, which can be opened as follows:

- Click **Help | Manuals | Automation and Data Publishing | Data Publishing**

How to Print the Integral list

- Click the **Integrals** tab of the dataset window (see the figure below).
- Enter **print** or **Ctrl+ p** to print.

Object	Integral [abs]	Integral [rel]	Peaks	v(F1) [ppm]
Integral 1	33103793.69	0.0869	0	122.7862
Integral 2	31291180.06	0.0821	0	73.8876
Integral 3	63590972.38	0.1669	0	56.4132
Integral 4	34960372.38	0.0917	0	49.8698
Integral 5	-9588723.88	-0.0252	0	35.9669
Integral 6	5490591.19	0.0144	0	31.7780
Integral 7	-49544582.00	-0.1300	0	28.0115
Integral 8	89129262.75	0.2339	0	22.5767
Integral 9	45133473.81	0.1184	0	21.3345
Integral 10	101099082.88	0.2653	0	19.1714
Integral 11	31159576.38	0.0818	0	12.0719
Integral 12	5532166.88	0.0145	0	0.0504

How to Print the Peak list

- Click the **Peaks** tab of the dataset window (see the figure below).
- Enter **print** or **Ctrl+ p**.

SPECTRUM	PROCPARS	ACQUPARS	TITLE	PULSEPROG	PEAKS
Δ Peak	v(F1) [ppm]	Intensity [abs]			
1	139.6346	439178.44			
2	122.6448	9275534.88			
3	73.9761	9553355.94			
4	56.6876	9518974.19			
5	56.1440	9731787.06			
6	50.0349	11503893.62			

14.2 Exporting Data

How to Copy Data to Other Applications

Under MS Windows, you can easily copy the dataset window contents to other applications. To do that:

- Click **Edit | Copy [copy]**.

This will copy the dataset window contents to the clipboard. After that you can paste the clipboard contents to any Windows application.

On Windows systems the command **Edit | Copy [copy]** saves bmp-format, whereas the command **copy wmf** stores the old wmf-format.

On Linux systems the command **copy** stores png-files into a temporary file. The pathname of this file is copied to clipboard.

Please note:

Some programs, when importing spectra from the clipboard or metafile, do not display the contained information correctly. Particularly when you resize the imported graphics, sections of the text, the spectrum, or the axis sometimes have disappeared. Usually this is only a display problem. When you print the respective page, the representation is correct.

How to Store (Export) a Dataset Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this, TopSpin allows to save the contents of a dataset window in a graphics file of selectable type. Supported formats are .png, .jpg, .jpeg, .bmp, .emf, .wmf and .pdf. To do that:

- Click **File | Export.... [exportfile]**.
- Navigate to the storage folder.
- Enter the destination filename and extension.
- Click **Export**.

The resolution of such a *screen dump* equals the resolution of your screen. When you import a graphics file into another program, you may lose information when resizing the graphics.

How to export projections of peak lists

Certain situations may require that the user wants to store a projection of a peak list (e. g. in order to evaluate an assignment in a 3D by verifying the annotated projected 2D-HSQC peak list on the respective 2D spectrum). Therefore, it is useful and timesaving to use the option "export projections of peak lists".

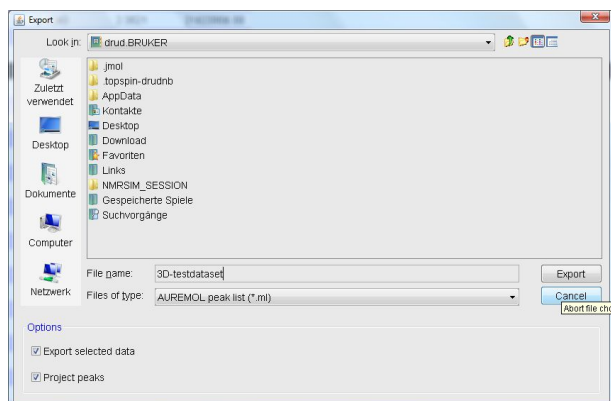
In order to create such a peak list projection, the following steps must be executed:

- Switch to the peaks tab of the dataset from which the peak list projection should be used.
- Select **Export...** from the peak table context menu (right-click).

Printing/Exporting Data

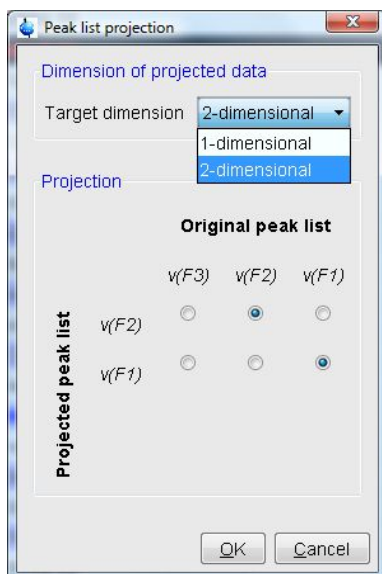
- Select the Project Peaks flag in the options panel of the appearing export dialogue. Please note that the active flag *Project Peak* invokes the export of the entire projections peak list. If separate peaks should be exported, they must be selected in the peak table and the flag *Export selected data* must be set.

Peak	v(F1) [ppm]	Intensity [abs]	
1	139.6346	428178.44	
2	122.6448	9	Show spectrum >
3	73.9761	9	Expand spectrum >
4	56.6876	9	Delete
5	56.1440	9	Edit annotation
6	50.0349	11	Remove >
7	39.7360	-2	Define as reference >
8	39.5236	-11	Annotate peaks >
9	38.1248	-4	Shift peaks...
10	36.9990	-3	Reset intensities >
11	36.5886		Show detailed information...
12	36.1923	-8	Properties...
13	35.8073	7	Copy
14	31.8995	-1	Export...
15	31.8617	9	Import...
16	28.2387	-1	Print...
17	28.0149	8	Print preview...
18	27.7728	-11742427.94	Table properties...



In the dialogue box the file format can be changed according to the required application.

- Define the desired options in the upcoming projections dialogue window (i.e. target dimension and axis mapping).



The exported peak list is now of the specified dimension, where the axis are projected according to the specified axis mapping.

15 Configuration/Automation

15.1 NMR Super User and NMR Administration Password

During TopSpin installation, you are prompted to define:

1. The username for the so called NMR Super user. Under Windows this must be the name of an existing user. Under Linux it can also be a non-existing user, which is then automatically created by the installation program. After the installation, the NMR Super user is the owner of all TopSpin program files. Logging in as this user allows to remove these files, change file permissions etc. The name of the NMRSUPERUSER will be stored in the file:

```
<tshome>/conf/nmrsuperuser
```

2. The NMR Administration password to be used for TopSpin configuration commands. This password can be freely chosen and is not connected to any user. It is asked for by TopSpin commands like **cf**, **expinstall** etc. The encrypted NMR Administration password is stored in the file:

```
<tshome>/conf/nmradminpassword
```

Note that the NMR Super user login password and the NMR Administration password have different purposes and are totally independent. Changing one of them does not affect the other.

How to Change the NMR Administration Password

The NMR Administration password can be changed as follows:

Under Windows

- Login as NMR Super user or Administrator.
- Open a Command Prompt.
- Enter:

```
<tshome>\perl\bin\perl <tshome>\prog\bin\installnmr <NMRSUPERUSER>
```

where <tshome> in the TopSpin installation directory.

- Enter the old password and new password as requested.

Under Linux

- Login as NMR Super user or root.
- Open a Shell.
- Enter:

```
<tshome>/prog/bin/installnmr <NMRSUPERUSER>
```

where <tshome> is the TopSpin installation directory.

- Enter the old password and new password as requested.

If you don't know the old NMR Administration password, you can still define a new one. In that case, you must delete the file:

```
<x>\conf\nmradminpassword
```

before you run the *installnmr* script.

15.2 Configuration

The main configuration steps are performed by the commands **cf** and **expinstall**. They can be started from the:

- Command line

or

- Click **Manage | Spectrometer | Hardware Detection | Configure Hardware (cf)**

or

- Click **Manage | Spectrometer | Experiments/Parameters | Install Standard Experiments (expinstall)**

For more details on **cf** and **expinstall**, please refer to the descriptions of these commands in the TopSpin Installation Guide and in the Acquisition Reference manual.

15.3 Parameter Set Conversion

The command **paracon** changes the basic frequency in parameter sets. This allows to use parameter sets which were created on a spectrometer with a different frequency. It opens the dialog box shown in chapter [Automation \[206\]](#).

Here you can setup a list of available parameter sets. You can select Bruker and/or User defined parameter sets and uses a match string. The matching parameter sets appear in the right part of the dialog box.

- To start the conversion, select one or more parameter sets and click **OK**.

15.4 Automation

How to Install AU Programs

To install AU programs, you have to run the command **expinstall** (see [Configuration \[206\]](#)).

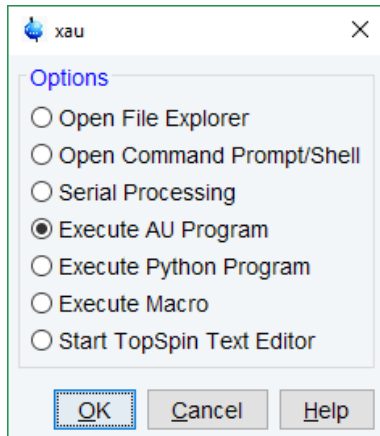
How to Open the AU Program Dialog Box

To get a list of all AU programs,

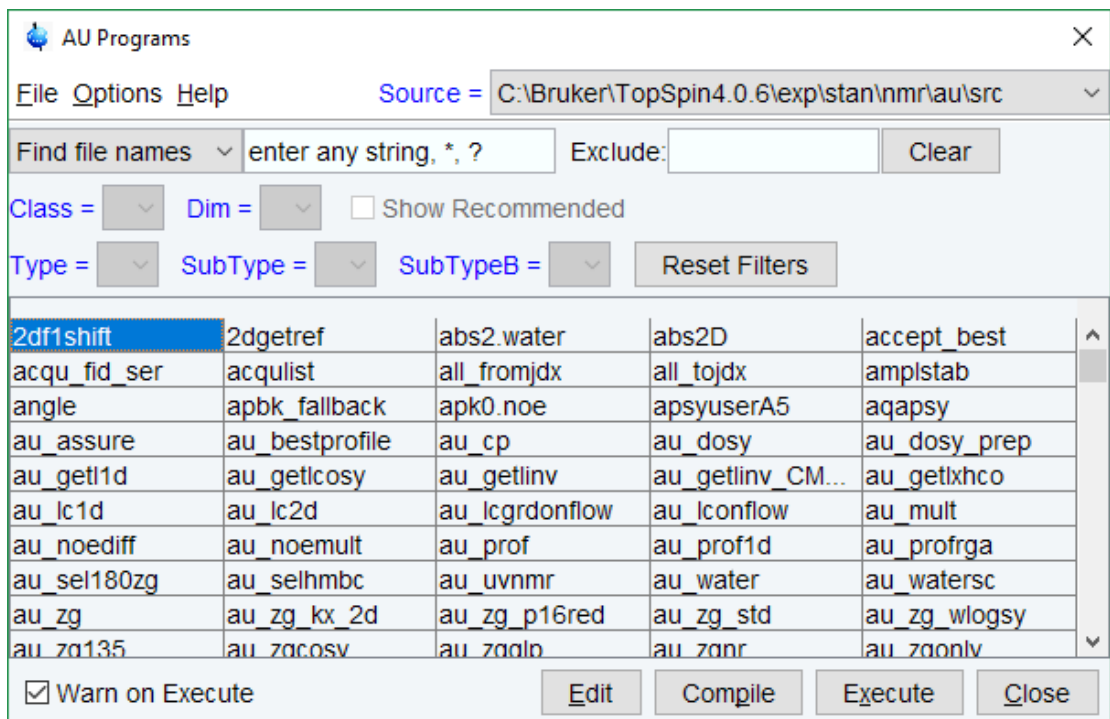
- enter **edau**

or:

- Click **File | Run a Program**
- Select **Execute an AU program** and click **OK**.



The next window displays either the Bruker defined or User defined AU programs as source.



Note that Bruker AU programs are only shown if the command **expinstall** has been executed once, after the installation of TopSpin.

How to Switch to the List of User defined AU Programs

- Click **Setup Preferences | Directories | Manage Source Directories** to open the AU program dialog box.

How to Switch to the List of Bruker defined AU Programs

- Click **Setup Preferences | Directories | Manage Source Directories** in the menu bar to open the AU program dialog box.

How to Define the AU Programs Source Directory

- Click **Setup Preferences | Manage Source Directories** in the AU program dialog box.

- In the field **AU Programs**: Add or modify AU program source directories.

How to Create an AU Program

- Click **File | New** in the AU program dialog box.
- Enter the AU program name in the field New name and click **OK**.
- Enter the AU program lines in the edit field of the appearing dialog box.
- Click **Compile** to compile the AU program.
- Click **File | Save** to store the AU program.
- Click **File | Close** to close the editor.

Alternatively, you can enter **edau <name>** on the command line to create the AU program <name>.

How to Edit an Existing AU Program

- Double-click the AU program name in the AU program dialog box.
- Or
- Click the **Edit** button to edit the highlighted AU program.
 - Modify the AU program according to you wishes.
 - Click **Save** to store the AU program under the name shown in the title bar.
 - You will be prompted to compile the AU program: click **OK**.

Alternatively, you can enter **edau <name>** on the command line to edit the AU program <name>.

How to Execute an AU Program

- Select the AU program in the AU program dialog box.
- Click the **Execute** button.

Alternatively, you can enter **<name>** or **xau <name>** on the command line to execute the AU program <name>.

If the AU program has not been compiled, compilation is automatically performed before the execution starts.

How to Delete an AU Program

- Select the AU program in the AU program dialog box.
- Click **File | Delete** or click the **Delete** button.

How to Show Comments (short descriptions) in the AU Program List

To switch on/off the comments in the AU program list:

- In the AU program dialog box: Click **Options** and select the entry **Comment**.

A comment is a short description of the AU program which is also part of the AU program header.

16 Remote Monitoring

16.1 What is Remote Monitoring

Remote monitoring allows the spectrometer to connect to a server and to send general system information like component temperature, power usage and similar to the server on a regular basis. The amount of data sent may depend on installed software or licenses.



The existing remote magnet monitoring system MICS (Magnet Information and Control System) is not part of it and operation is not affected by it. For more information on MICS refer to the user manual (Z33037) on the BASH DVD.

16.2 How to Enable Remote Monitoring on your AVANCE NEO or FOURIER Spectrometer

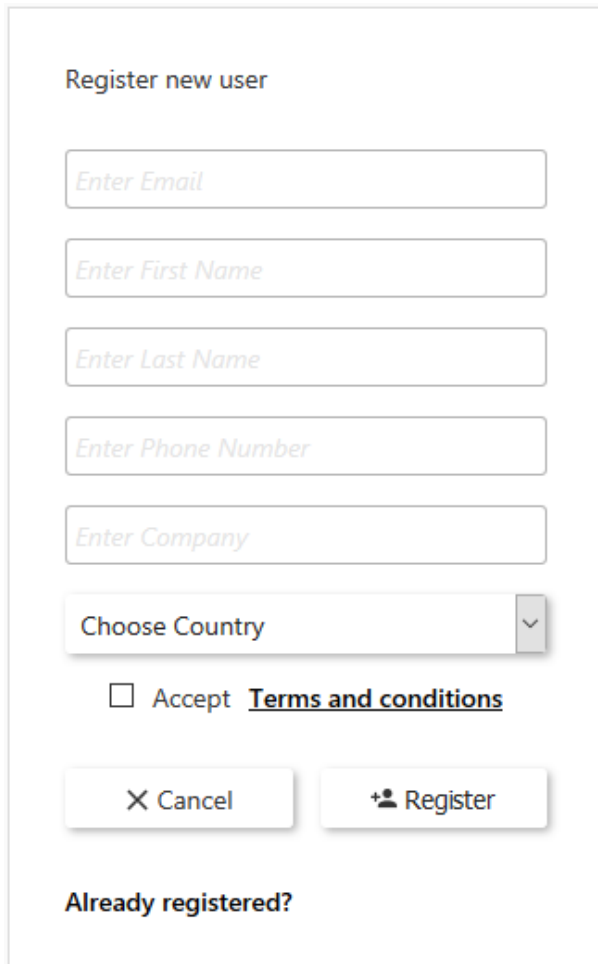
In the TopSpin command line, enter **adiag**. You will be asked for the Administrator password. In the following dialog, please fill in at least the required fields indicated with (*).

Login and Password refers to your user account at the AutoDiagnose web interface. If you do not have an AutoDiagnose account, please click on the button **Register for AutoDiagnose**.

Figure 16.1: Initialisation of Remote Monitoring

This opens up a window in your internet browser that allows you to register at the AutoDiagnose web interface.

Please note that the **system name** is the name that was given to the spectrometer during initialization. It is intended to be an easy identifier for the user to allow for quick referencing. The **Login** required for the Initialisation of Remote Monitoring is the email address.



The registration form is titled "Register new user". It contains the following fields and elements:

- Text input field: "Enter Email"
- Text input field: "Enter First Name"
- Text input field: "Enter Last Name"
- Text input field: "Enter Phone Number"
- Text input field: "Enter Company"
- Dropdown menu: "Choose Country" with a downward arrow icon.
- Checkbox: "Accept [Terms and conditions](#)"
- Buttons: "X Cancel" and "+ Register" (with a user icon)
- Text: "Already registered?"

Figure 16.2: Registration

After registering, you will receive an email with a temporary password. Please login at the AutoDiagnose web interface and change your password.

In the initial dialog, please fill in your password. Click on the link [Accept Terms and Conditions](#) to open the corresponding document. If you agree, select the checkbox.

As soon as all mandatory fields are filled in and you have agreed to the terms and conditions, the button Initialize RM (Remote Monitoring) becomes active. When you click on this button, the spectrometer will start sending health and status information to the cloud platform.

All messages sent to the cloud platform are encrypted. Data for authentication of your spectrometer is stored on the computer within the spectrometer console.



For further information please refer to the AutoDiagnose Software User Manual.

16.3 How to Manage Remote Monitoring

After you have initialized Remote Monitoring, typing **adiag** the TopSpin command line brings up the dialog below. It is protected by the Administrator password. It allows you to check and control whether your spectrometer is connected to AutoDiagnose.

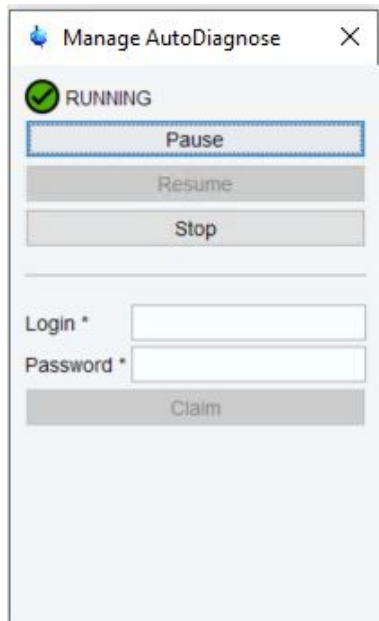


Figure 16.3: Manage AutoDiagnose

Depending on the current state of Remote Monitoring (see further below), one or more actions are possible:

Button	Effect
Pause	Temporary interrupts Remote Monitoring Data for authentication stays stored on the spectrometer
Resume	Continues Remote Monitoring after pausing As data for authentication has been kept, it is not necessary to re-initialize Remote Monitoring.
Stop	Stops Remote Monitoring Stop permanently removes authentication data stored on the spectrometer. If you want to continue Remote Monitoring after stopping it, you have to re-initialize it again. Note: Data acquired during "pause" status are not sent to the web server.



Please note: Stopping the Remote Monitoring will also stop all services of products related to it. There will be no further service and no refund of any kind. To restart the service you have to contact your local Bruker service office.

An icon and a text label show whether your spectrometer is currently connected to the cloud platform and sends health and monitoring data.



Please note that this is not the actual health state of your spectrometer. You can inspect the health state in the Remote Monitoring web interface.

Icon	Text	Remote Monitoring State
	Running	Remote Monitoring is active. This means the spectrometer is sending health and status information.
	Paused	Remote Monitoring has been paused. Data for authentication is still stored on the spectrometer.
	Pending	The authentication of the spectrometer at the cloud platform is not yet complete. In order to complete the authentication, it is required that cf has been executed at least once, and that a connection to the internet is available.
	Unknown	Remote Monitoring is inactive.
	Broken	Remote Monitoring is inactive due to an error, e.g. lost connection to the internet.
	Deactivated	Remote Monitoring is inactive. This state appears directly after click on Stop. It confirms that authentication data has been removed. If you open the adiag dialog later, the state will have switched to Unknown .

16.4 How to Claim a Spectrometer

Consider the case that the user account in the AutoDiagnose web interface, that has been managing your spectrometer, is not accessible any more. You might want to give administrator privileges to another user in the AutoDiagnose web interface, while keeping the complete Remote Monitoring history of your spectrometer. This process is called claiming a spectrometer.



Please distinguish between user accounts & privileges in the AutoDiagnose web interface and on your local system. The AutoDiagnose web interface has its own user management, which is independent from users on your local system. Please refer to the AutoDiagnose web interface help for details.

In order to claim a spectrometer, type in **adiag** at the TopSpin command line to bring up the **Manage AutoDiagnose** dialog. It is protected by the Administrator password. Fill in your Login and Password at the AutoDiagnose web interface and click **Claim**.

The image shows a web interface for logging into the AutoDiagnose system. It features two input fields: the first is labeled 'Login *' and the second is labeled 'Password *'. Below these fields is a button labeled 'Claim'.

Figure 16.4: Login to AutoDiagnose

The result is that this user in the AutoDiagnose web interface will receive administrator privileges.

16.5 Products Using Remote Monitoring

To inspect the health state please login on the Remote Monitoring web interface (<https://autodiagnose.bruker.com>). Most of the products that will use the Remote Monitoring features will be implemented on the server. Access to data will not be within TopSpin and thus all the documentation will be provided there. However, there may be some actions or operations that have to be done on the spectrometer to correct or permit certain actions. These commands are summarized here.

16.5.1 AutoDiagnose

AutoDiagnose uses the setting of remote monitoring to transfer data to the server and to display some of the results. In addition to the connection a licenses and a special sample is needed to use the full functionality, please refer to the AutoCalibrate documentation.



For further information please refer to the AutoDiagnose Software User Manual.

16.5.2 MICS

Please note that MICS is not yet part of this interface. Please refer to Magnet Information and Control System (MICS) User Manual (Z33037) for further information.

17 User Preferences

TopSpin can be tailored to your preference in many respects. This ranges from startup options to spectrum objects, menu settings, remote connections etc. Every standard user can create his own set of preferences.

Please note, that an Administrator password is required, if the **Enable GUI Restriction** options was activated.

To avoid that everyone can access and administer the setup preferences,

- Check **Setup Preferences | Regulated Environments | Enable GUI restrictions and protection of preferences**

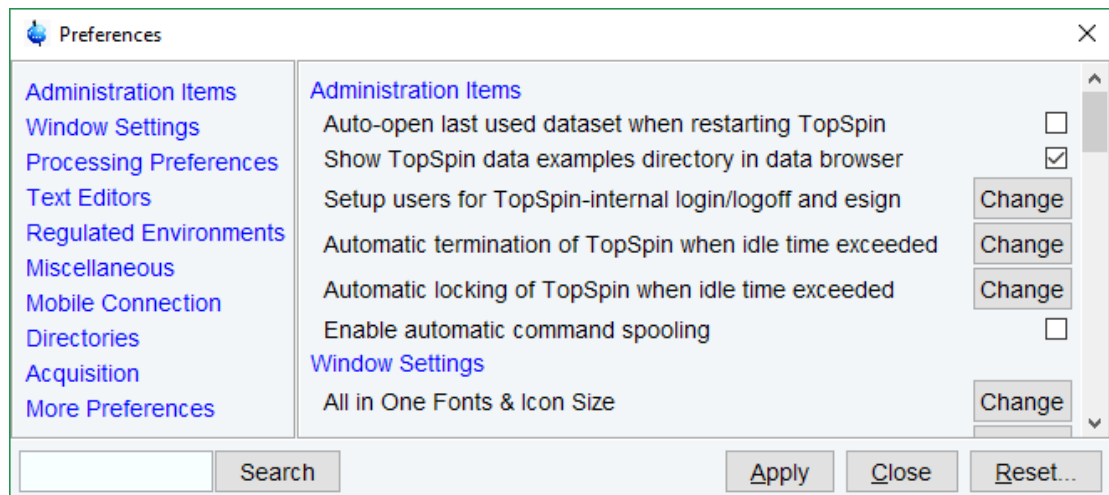
This assures, that modifications in the setup preferences are possible for only the ones who know the NMR administration password.

Read also the chapter [Regulatory Compliance \[247\]](#).

To set user preferences:

- Click **Setup Preferences [set]** .

A dialog box will appear with, at the left side, the categories that can be tailored:



Click the category of which you want to view/change certain objects. It will become highlighted and the corresponding objects will be displayed at the right part of the dialog box.

For example, if you click **Processing References**, the Processing References objects will appear at the top of the dialog box. The rest of this paragraph will describe some examples of setting various user preferences.

17.1 Define User Preferences Location for all Users

User Preferences are, by default, stored in the current user's home directory:

```
<userhome>/topspin-<hostname>
```

During the first TopSpin session, files with default settings are created there. They can then be modified with the **set** command and used in later sessions.

You can, however, also store user preferences at one central location, which are then used by all users. This location can even be a remote drive allowing to use the same preferences on all computers in the network:

- Make a backup copy of the file `<tshome>/javaenv.cmd`.
- Open the file `<tshome>/javaenv.cmd` using a text editor.
- Locate the line "set SYSTEM_PROPS=-DXWINNMRHOME="%XWINNMRHOME%" - DCOMPUTERNAME=%COMPUTE....." near the beginning of the file.
- Append a white space character and then: `-DPROPDIR=<dir>` to the end of this line, where `<dir>` is the definition of the storage directory, consisting of one or more parts (see below).
- Close the editor.

The definition of the storage directory for User Preferences can take three forms:

1. `-DPROPDIR=<mydir>`

Stores the user properties in `<mydir>/prop`.

Example: `-DPROPDIR="/x y z"` (The double quotes are only required if the directory contains white spaces).

2. `-DPROPDIR=<mydir> USER`

Stores the user properties in `<mydir>/<login id>/prop`, where `<login id>` is the id under which the user is logged into the operating system.

Example: `-DPROPDIR="/x y z USER"` (Specify exactly 1 space between the pathname and the string USER).

3. `-DPROPDIR=CURDIR`

Stores the user properties in `<tshome>/prog/curdir/<login id>/prop`, where `<login id>` is the id under which the user logged into the operating system.

Please note that the specified directory must be writable for all TopSpin users.

17.2 Basic Setup Preferences

How to Open the Last Used Dataset on Startup

- Check **Setup Preferences | Administration items | Auto-open last used dataset when restarting TopSpin**.

How to Define the Startup Actions

TopSpin allows to define any commands to be executed automatically after startup:

- Click **Manage | Commands | Setup Commands Executed at TopSpin Start**.

Show Command History (hist)
 Command Recording ▶
 Collect & Save LogFiles (saveLogs)
 Show Currently Active Commands (show)
 Manage Command Queue (spooler)
 Setup Commands Executed at TopSpin Start
 Notebook (nbook)

- Enter the desired startup command(s), in the appearing editor, for example:

```
re exam1d_13C 1 1 c:\\bio guest
efp
apk
abs
```

The above lines would cause TopSpin to display the dataset
C:/bio/data/guest/nmr/exam1d_13C/1/pdata/1
 and execute the command **efp**, **apk** and **abs** on it.

Note that you can use a single forward slash (/) or a double backslash (\\) as path separator.

Note that in TopSpin the file *autostart.mac* is a regular TopSpin macro. In older versions, however, the file *autostart.prop* was used with a different format.

How to Define Auto-Termination after Idle Time

TopSpin can be configured to be terminated after a user specified idle time:

- Click **Setup Preferences | Administration items | Automatic termination of TopSpin when idle time exceeded | Change**.
- Enter the NMR Administration password as requested and enter the number of minutes of allowed idle time.
- Click **OK** to close the dialog, click **OK** to close the Preferences dialog.
- Restart TopSpin to activate the change.

If the user does not execute any commands (from the command line, menu or toolbar buttons), a dialog will appear with an **OK** button (to terminate immediately) and/or **Cancel** button (to continue).

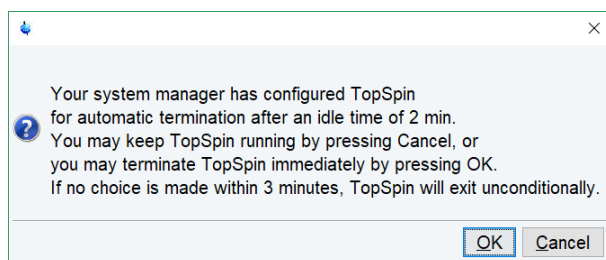
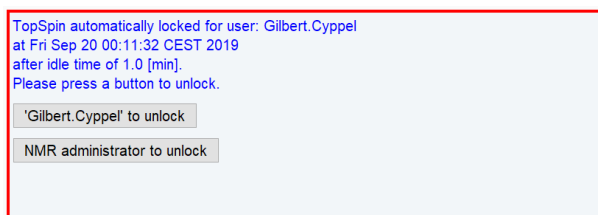
Automatic termination frees the license used by this TopSpin instance for other users. This solves the problem of users leaving TopSpin open and blocking a floating license although they do not currently use it.

How to Define Auto-Locking after Idle Time

TopSpin can be configured to lock the interface after a user specified idle time:

- Click **Setup Preferences | Administration items | Automatic locking of TopSpin when idle time exceeded | Change**.
- Enter the NMR Administration password as requested and enter the number of minutes of allowed idle time.
- Click **OK** to close the dialog, click **OK** to close the Preferences dialog.

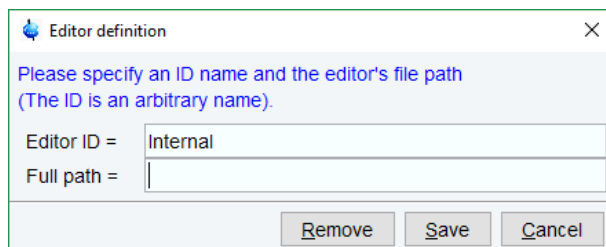
If the user does not execute any commands (from the command line, menu or toolbar buttons), the TopSpin interface will be locked:



How to Change the Preferred Editor

Select your preferred editor as it is used by commands like **edau**, **edpul**, **edcpd** etc.:

- Click **Setup Preferences | Text Editors | Preferred text editor | Change**.
- Enter the desired Editor and its path. For example, for Wordpad:
`C:\Program Files\Windows NT\Accessories\wordpad.exe`



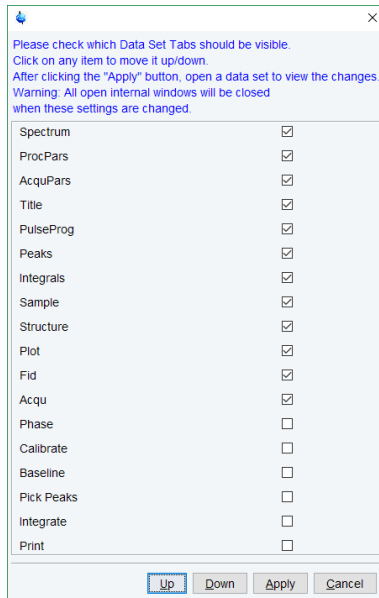
- Click **Save** to save the changes.

If no editor is specified here, the TopSpin internal editor is used. If the file being edited is read-only, the TopSpin internal viewer is used.

How to Configure the Dataset Tab Bar

The default tab bar at the top of the dataset window consists of tabs to switch between various dataset objects like *Spectrum*, *Parameters*, *Title*, etc. You can, however, configure the tab bar to contain tabs for interactive data manipulation like *phase correction*, *integration* etc. These tabs have the same function as the corresponding buttons in the upper tool bar (see chapter [Getting Started \[▶ 29\]](#) and [1D Interactive Manipulation \[▶ 139\]](#)) but are easier to access. You can configure the tab bar as follows:

- Click **Setup Preferences | Windows Settings | Tabbed pane layout | Change**.



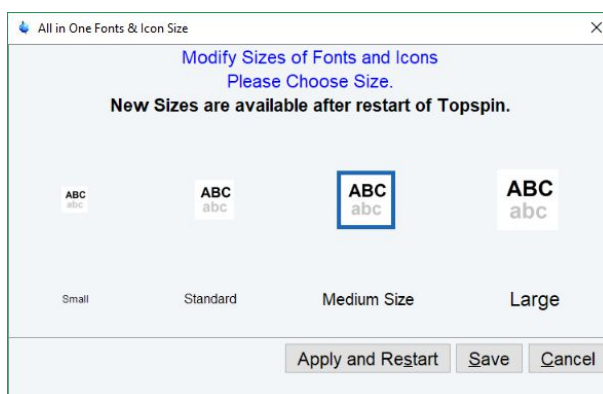
- Check the desired tabs, uncheck the others.
- Click **OK**.

Note that you can change the relative positions of a tab by selecting it and then clicking the **Up** or **Down** button.

17.3 Changing the Sizes of All Fonts and Icons

To improve the usability of Topspin for different screen resolutions, the size of icons and fonts can be changed:

- Click **Setup Preferences | Window Setting | All in One Fonts & Icon Size | Change**

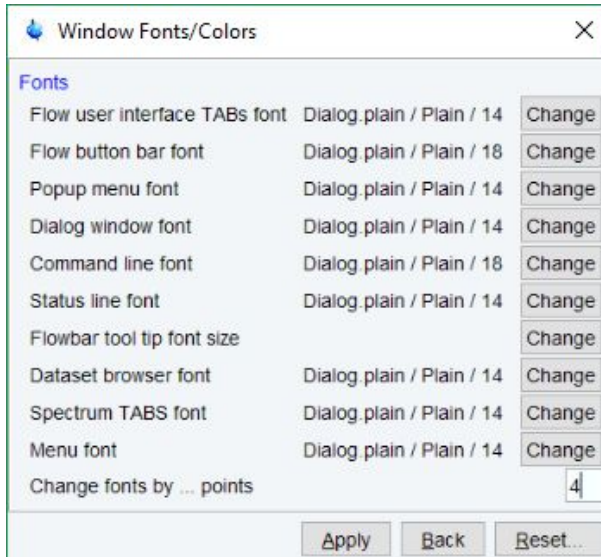


- Select one of the 4 different sizes
- Click **Apply and Restart**

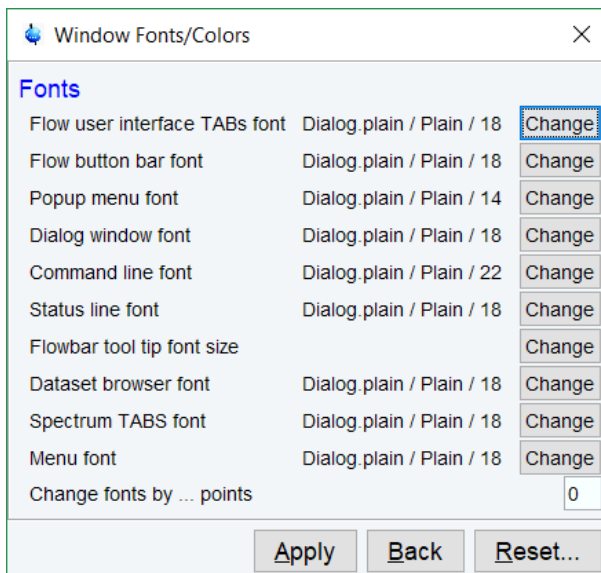
17.4 Changing Individual Fonts

How to Change Individual Fonts of the TopSpin Interface

- Click **Setup Preferences | Windows Settings | Fonts and colors | Change**.
- Set the entry **Change fonts by points**. You can enter a positive or negative number. The following figure shows an example of increasing the font sizes by 4 points.



- Click **Apply**.
- Reopen the Window Fonts/Colors window.



The figure above shows the same part of the Preferences dialog box after the change of fonts. Note that:

1. The value of all font entries has been increased by 4.
2. The font of the dialog box itself is larger.

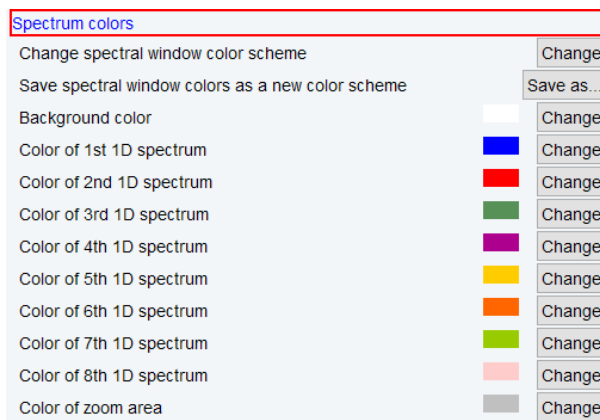
- The change size has been reset to 0.

17.5 Changing Colors

How to Change Colors of Data Objects on the Screen

The color of various objects in a dataset window on the screen, like 1st, 2nd and 3rd spectrum, axis, parameters etc. can be changed. To set these colors:

- Click **Setup Preferences | More Preferences | Spectra Display Preferences | Change**.
- or
- Right-click in the dataset window and in the list, select **Spectra Display Preferences**.



- In the category **Spectrum colors** click **Change** right of the object you want to change.
- Select the desired color in the appearing dialog box and click **OK**.
- Click **Apply**.

How to Change Colors of Data Objects on the Printer

The color of data objects on the printer is independent from the color of the corresponding object on the screen. To set print colors:

- Click **Setup Preferences | More Preferences | Spectra Printing Preferences | Change**.

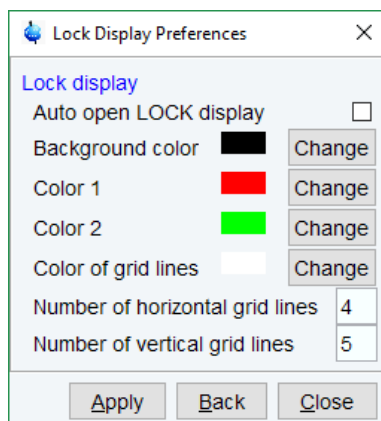


- In the category **Spectrum colors** click **Change** right of the object you want to change.
- Select the desired color in the appearing dialog box and click **OK**.
- Click **Apply**.

How to Change Colors of the Lock Display

The colors of lock display objects can be changed as follows:

- Click **Setup Preferences | More Preferences | Lock Display Preferences | Change**.



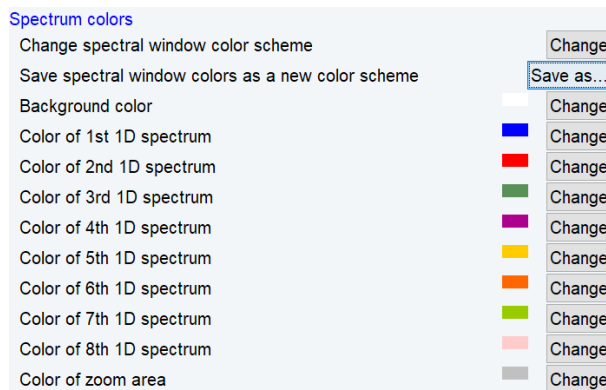
- Select the desired color or number of gridlines in the appearing dialog box and click **Apply**.

How to Create a New Dataset Window Color Scheme

To create a new dataset window color scheme:

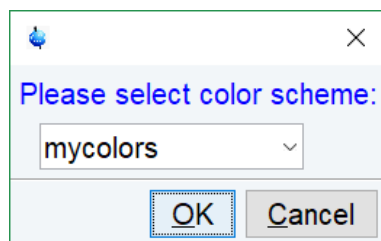
- Click **Setup Preferences | More Preferences | Spectra Display Preferences | Change**.
- or
- Right-click in the dataset window and in the list, select **Spectra Display Preferences | Spectrum colors**.

- In the group *Spectrum colors* change the background color, the color of 1st to 8th 1D spectrum and the zoom area color.
- Click **Apply**.
- Click **Save as ...** right of the option *Save spectral windows colors as a new color scheme*.
- Enter a new name in the appearing dialog box.
- Click **OK**.



How to Read a Different Dataset Window Color Scheme

- Right-click in the dataset window and in the list, select **Spectra Display Preferences | Spectrum colors | Change spectral window color scheme | Change**



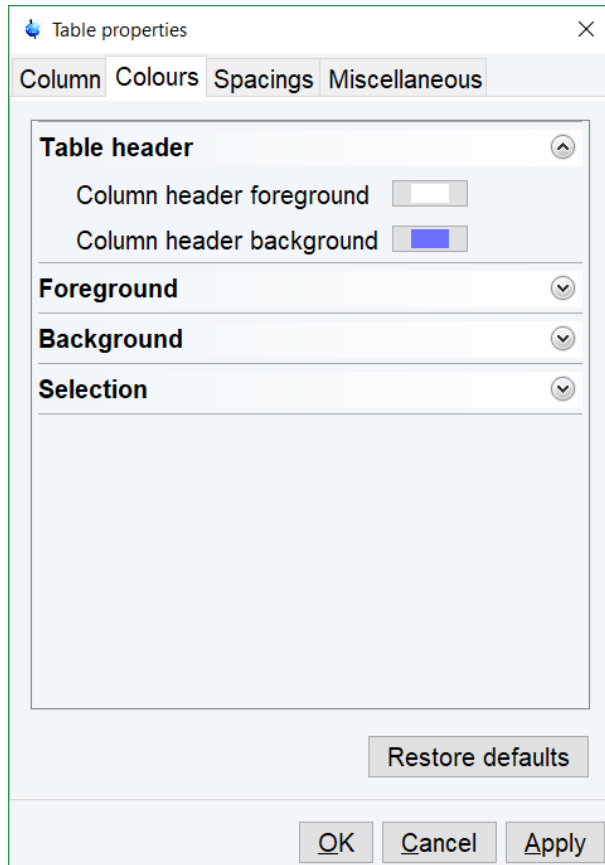
- In the list select the color scheme and click **OK**.

TopSpin is delivered with two colors schemes:

1. *Light* a white background with black axes.
2. *Dark*: a dark blue background with a white axis.

How to Change Peak and Integral Table Color/Spacings

- In the dataset window select the tab PEAKS or INTEGRALS.
- Right-click a Peak or Integral and in the list, select **Table properties...**
- In the Table properties window, in the tabs *Colours* and *Spacings* set the desired colors and spacings.
- Click **OK**.



17.6 Changing Lines

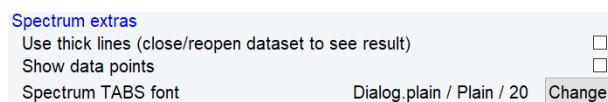
How to Create Thick Lines on the Screen

To create thick (double width) lines for high resolution display or screen dumps:

- Click **Setup Preferences | More Preferences | Spectra Display Preferences | Change**.

or

- Right-click in the dataset window and in the list, select **Spectra Display Preferences**.
- In the group *Spectrum extras* enable the entry **Use thick lines**.
- Click **OK**.



How to Create Thick Lines on the Printer

- Click **Setup Preferences | More Preferences | Spectra printing preferences | Change**
- In the Spectra Printing Preferences window, in the group *Spectrum extras* check **Use thick lines**.
- Click **Apply**.

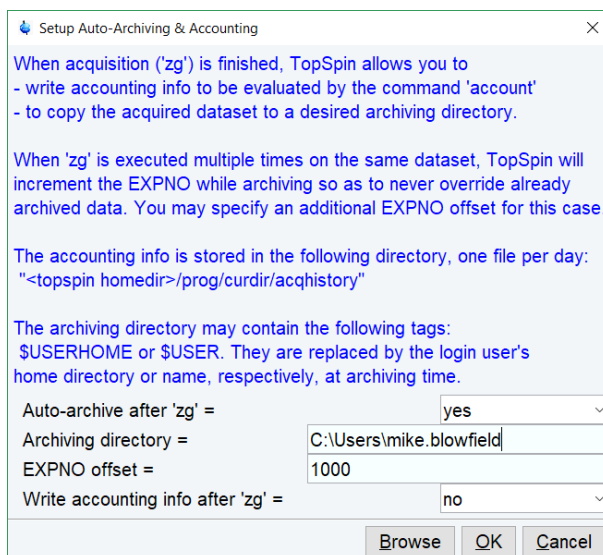


17.7 Auto-Archive and Archive Directory Settings

How to Auto-Archive Existing Expnos

- Click **Setup Preferences | Acquisition | Configure Accounting & Data Archiving after zg' | Change**

Configure archiving as described in the dialog:

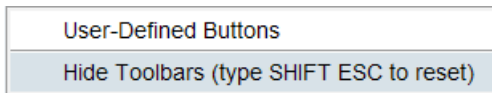


- Click **OK**.

17.8 Disabling/Enabling the Toolbars

How to Hide the Toolbars

- Right-click in an empty area of the toolbar and in the list, select **Hide Toolbars**.

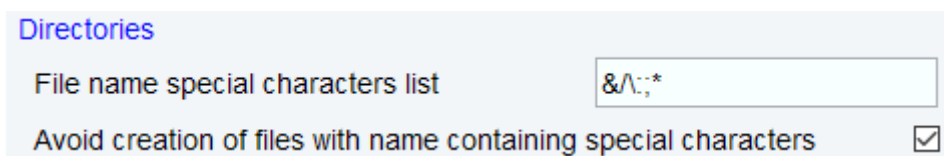


To restore the toolbars:

- Press the keys SHIFT+ESC

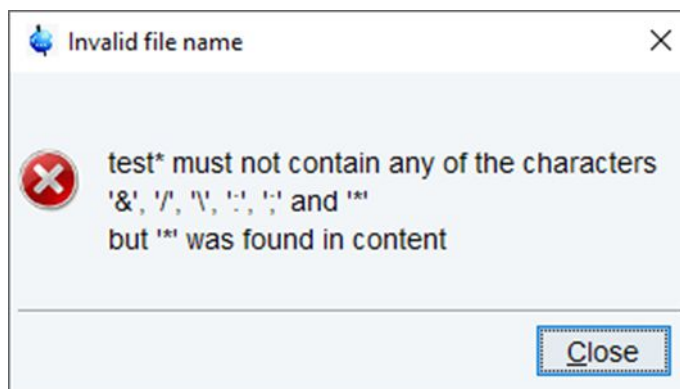
17.9 Restricting the Usage of Special Characters in Filenames

The usage of special characters in filenames used in Topspin may be limited. The default setup avoids creating names, which would harm TopSpin. Go to **Setup | Directories**



This check is applied on any file created in Topspin GUI like parameter sets, lists....

Example: writing a new parameter set **test*** will be declined:



17.10 Defining Source Directory for Programs/Lists etc.

TopSpin allows to define the source directories for pulse programs, AU programs, integral ranges, various lists etc.

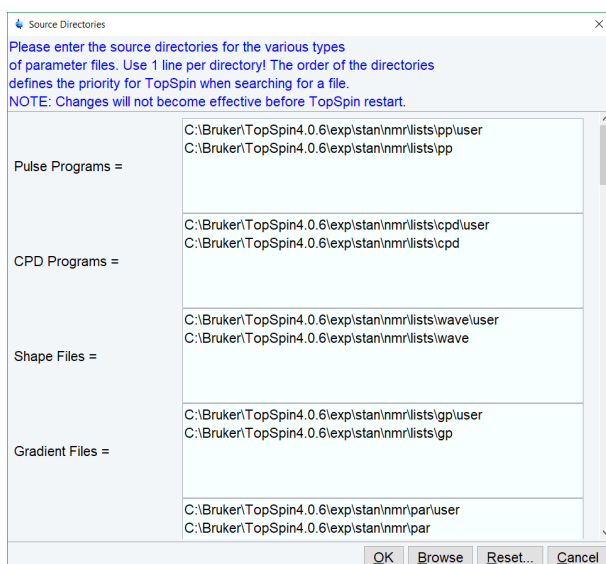
- Click **Setup Preferences | Directories | Manage source directories for edpul, edau etc.| Change**

or

- Open the dialog of any of the items, e.g. with the command **edau**, **edlist** or **edmisc**.
- Click **Options | Source**.



A dialog displays a list of items with the current source directories:



By default, two source directories are present, one for user defined items and one for Bruker items. This list can be modified or extended with your preferred source directories, e.g.:

*C:\my-pulse-programs\
C:\ts21\exp\stan\nmr\lists\pp\user
C:\ts21\exp\stan\nmr\lists\pp*

You can do this for each item separately. Items will be searched for in the order of the directories specified.

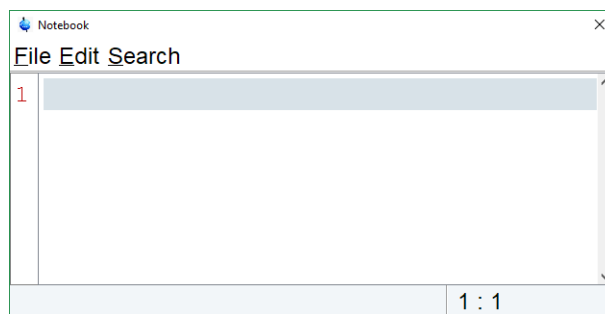
18 User Extensions

TopSpin offers various ways to extend the standard commands, buttons, programs etc.

18.1 User Notebook

You can create your own user specific notebook with the command:

- **Click Manage | Commands | Notebook [nbook]**



This can be used to store and retrieve any personal notes, information etc.

18.2 Macros

A macro contains a sequence of TopSpin commands. It can be created with the command **edmac**. A simple macro for processing and plotting the current dataset is:

```
em
ft
apk
sref
autoplot
```

All entries in a macro file must be written in lower case letters.

In TopSpin a macro may contain Python commands. Any line in a macro that starts with:

```
py>
```

Executes a Python command. An example of such a macro is:

```
re exam1d_13C 1 1 C:\bio guest
efp
py>NEWWIN() # open new window
re exam1d_1H 1 1 C:\bio guest
efp
py>x = INPUT_DIALOG()
py>if x == None: EXIT()
py>y = 2* int(x[0])
```

```
py>MSG("done: y=" + str(y))
```

Note that commands like `NEWWIN()`, `INPUT_DIALOG()`, `MSG()` and `EXIT()` are Bruker defined whereas `"x="` and `"if"` are original Python commands.

Once created, a macro can be executed by entering its name on the command line.

18.3 AU Programs

An AU program may contain TopSpin commands, AU macros and C-language statements. It can be created with the command `edau`. A simple AU program which performs the `efp` command on a series of dataset expnos is:

```
#include <lib/util.h>
int first, max;
char string[80];
first = expno;
GETINT ("Enter first expno to process : ",first)
max = 10;
GETINT ("Enter number of expnos : ",max)
WPAR("tmpmefp","proc")
expno =first;
TIMES(max)
RPAR("tmpmefp","proc")
EFP
IEXPNO
END
DEXPNO
DELPAR("tmpmefp")
QUITMSG("--- multiefp finished ---")
```

Note that TopSpin commands like `EFP` and `RPAR` and AU macros like `IEXPNO` are written in upper case letters whereas C-language statements like `"max = 10;"` are written in lowercase letters. Once created, an AU program can be executed by entering its name on the command line.

For more information on writing AU programs:

- Click [Help | Manuals | Programming Manuals | AU programming](#)

18.4 Python Programs

A Python program may contain TopSpin commands, User Interface functions and Graphic functions. It is created with the command `edpy`.

The Python program below reads a region of the real part of a spectrum and the corresponding region of the imaginary part and displays both. The simplest form of `DISPLAY_DATALIST` is used.

```
from TopCmds import *
import math
region = [80, 72] # define region in ppm
```

```
# open testdata, don't display
testdata = ["exam1d_13C", "1", "1", "c:/Bruker/topspin", "guest"]
RE(testdata, "n")
# read real and imaginary points of the region
reals = GETPROCdata(region[0], region[1])
imags = GETPROCdata(region[0], region[1], dataconst.PROCdata_IMAG)
if reals == None or imags == None: EXIT()
# set up list of data to be displayed and respective axis info list
dataList = [reals, imags]# display the data in the list
DISPLAY_DATALIST(dataList)
```

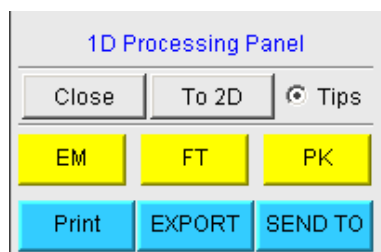
For more information on writing Python program:

- Click [Help](#) | [Manuals](#) | [Programming Manuals](#) | [Python programming](#)

18.5 Button Panels

A button panel is a window with user-defined buttons for executing TopSpin commands, AU programs, Python programs or macros. It appears as an integral part of the active dataset window and acts on that Bruker delivers a few standard button panels like **bnmr** and **bnmrse1**. To create your own button panels, you can modify one this or write one from scratch.

In this description we will create a very simple button panel with some 1D processing commands and print/export buttons:



To write this button panel, take the following steps:

- Open the Windows Explorer and navigate to the subdirectory:
userdefined
Of the user's properties directory (To locate this, enter **hist** and look for the entry "User properties directory=").
- Create a text file with the name:
cmdpanel_<name>.prop
Where <name> is the name of the button panel.
- Enter the button definitions including *Panel title*, *Colors*, *Toggle buttons*, *op buttons*, *Panel layout*, *Panel buttons* and *Tooltips*.
- Save the file under a name:
cmdpanel_<xxx>.prop
where <xxx> is the actual name of your command panel.
Make sure the extension of the file is *.prop* and not *.txt*, *.prop.txt* or anything else.

- Enter **bpan <xxx>** on the command line to open the button panel.

Example for a small button panel for 1D processing:

```
# Color definitions used in this file (RGB)
BLUE1=51$ 204$ 255YELLOW1=255$ 255$ 0GREEN1=84$ 196$ 20
# Title definition
TITLE=1D Processing PanelTITLE_COLOR=0$ 0$ 255
# Toggle button definition
TOGGLE_BUTTON=To 2D
TOGGLE_CMD=bpan bproc2d
TOGGLE_TIP=Switch to 2D processing
# Top row button definition
TOP_BUTTONS=EM$ $FT$ $PK$ $TOP_COLORS=YELLOW1$ YELLOW1$ YELLOW1
TOP_CMDS=em$ ft$ pk
TOP_TIPS=Exponential multiplication $\Fourier transform$\Phase
correction
# Panel button definitions
# LAYOUT format: rows columns hgap vgapPAN_LAYOUT=1$ 3$ 8$ 8
PAN_BUTTONS=Print$ $ EXPORT$ $SEND TO$ $
PAN_COLORS=BLUE1$ BLUE1$ BLUE1
PAN_CMDS=prnt$ exportfile$ smail
PAN_TIPS=Print the spectrum<br>\
as it appears on the screen$\
Export the dataset<br>\to png, jpg, bmp etc.$\Send the dataset by
email
```

Enter **bpan exam** to display a panel with 75 buttons: 5 rows and 15 columns. The corresponding panel file is called *cmdpanel_exam.prop*, which resides in the directory:

<tshome>/classes/prop/English

In the same directory, you can find the files *cmdpanel_bnmr.prop* and *cmdpanel_bnmrsel.prop*, which are used to display the *bnmr* and *bnmrsel* panel described above.

The texts displayed on the buttons can be graphically adjusted in various ways, because the text may optionally be specified in html format. In the example above, the PAN_BUTTONS property has no html tags. Therefore, the texts are displayed in black using the default *TopSpin Dialog window font* as specified in the User Preferences (command **set**). If you replace the text `Print` by the following:

```
<html><font size=10><font color=\"00BF00\">Print<br>Now</font></html>
```

Then the new text "Print Now" is displayed in green (the color to be specified in RGB hex code), with 10 points font size. Also, "Now" is display below "Print" due to the html `
` (= break line) tag.

Note that:

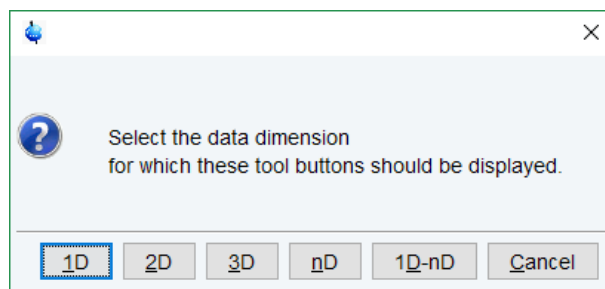
1. The **Close** button and **Tips** switch are automatically created. You don't need to specify them.
2. The TOGGLE button is typically, but not necessarily, used to call another button panel. In this example it calls the panel **bproc2d**. If TOGGLE_BUTTON is specified without a value, i.e. the entry is "TOGGLE_BUTTON=" instead of "TOGGLE_BUTTON=action text", the corresponding button is not shown in the panel.
3. Items must be separated with the "\$" character, button items with "\$ \$"
4. A "\" followed by "end of line" continues an item on the next line.
5. Tooltips may use html tags for text formatting.
6. Commands may be specified as single commands like "em" or as composite commands like "em\nft\npk". Note that in the latter case, the commands must be separated by "\n".
7. When the **bpan <name>** command comes up with an error message, carefully check the syntax of your cmdpanel file. A common mistake is to specify the button items incorrectly. With the keyword PAN_LAYOUT you define the number of rows and columns, and the number of items will become rows*cols. All specifications such as PAN_BUTTONS, PAN_COLORS, etc. must have this number of members, otherwise you will result in a Topspin error. Please insert the "\$" separator to make sure the item count is correct.

18.6 Adding User Defined Buttons to the Toolbars

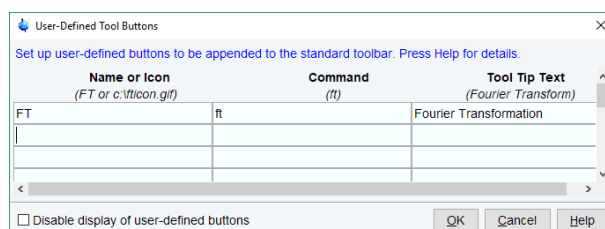
The upper and lower toolbar at the top of the TopSpin window can be extended with user defined buttons. They can be assigned to any TopSpin command, macro, AU program or Python program.

To create a user defined button

- Right-click in an empty area of the upper or lower workflow toolbar.
- In the list, select **User-Defined Buttons**.
- Select the data dimension, where the button will be displayed, in the example **1D**.



- In the next window enter
 - the button text or the graphic file and pathname
 - the command to be executed
 - the tool tip text.



For an icon label, you must store the icon image file in one of the following directories:

1. `<user-home>/topspin-<hostname>/prop/user` defined (only available for this user).
2. `<tshome>/classes/prop` (available for any user).
3. Any directory (the full pathname must be specified in the icon label field).

The formats `.gif`, `.jpg`, `.jpeg` and `.png`, are supported. Standard TopSpin icons have a size of 16 * 16 pixels. If your own icons have a different size, they are automatically rescaled and displayed at the standard size.

In the example above, a button **FT** is created with a separator, which only appears for 1D datasets, and executes the command **ft**.

How do I Remove or Disable a User Defined Toolbar Button?

- Right-click in an empty area of the upper or lower workflow toolbar.
- In the list, select **User-Defined Buttons**.
- Select the data dimension
- Select a line and click Disable Display of user-defined buttons or delete the entries

18.7 Adding User Defined Guides

TopSpin offers several guides like the Acquisition Guide (command **aqguide**), the Processing Guide (command **prguide**) and the T1/T2 Guide (command **t1guide**). You can set up your own guides, which can be adaptations of Bruker guides or new written ones. In order to do that, you must edit the file `toolbar_user.prop` and `cmdtab_user.prop` in the directory:

```
<user properties directory>/userdefined/
```

To identify this directory, enter the command **hist** in TopSpin.

The file `toolbar_user.prop` contains the guide definition. If the file does not exist, it must be created. Here is an example of a user modified T1/T2 guide.

```
MyT1T2Toolbar=\
NM=t1fid_40.gif, NM2=$Extract fid, TIP=$Do rser,
CMD=_t1_fid, END=,\
NM=t1spec_40.gif, NM2=$Transform, TIP=$Do ef+apk,
CMD=_t1_spec, END=,\
NM=t1ranges_40.gif, NM2=$Ranges, TIP=$Enter integ. mode,
CMD=_t1_ranges, END=,\
NM=t1screen_40.gif, NM2=$Relax. Window, TIP=$Enter Relax mode,
CMD=_t1_relax, END=,\NM=-, END=,\
NM=myicon.gif, NM2=$Fit Methods, TIP=$Select fit funcs.,
CMD=_t1_func, END=,\
NM=c:/myicons/myicon1.gif, NM2=$Start, TIP=$ct1,ct2, simfit,
CMD=_t1_start, END=,\
NM=c:/myicons/myicon2.gif, NM2=$Show Report, TIP=$report,
CMD=_t1_report, END=,\
NM=t1print_40.gif, NM2=$Print it, TIP=$print,
```

```
CMD=_t1_export, END=
```

Notes to this guide definition:

1. The original Bruker guides are defined in the file *toolbar.prop* in the directory `<tshome>/classes/prop`. The corresponding commands are defined in *cmdtab_main.prop* in the same directory.
2. The bold lines in the example above are user-modified lines.
3. `NM=t1fid_40.gif`: a Bruker defined icon with a size of 40x40 pixels.
4. `NM=myicon.gif`: a user-defined icon, which must be located in the user properties directory (Caution: not in its subdirectory `userdefined`).
5. `NM=C:/myicons/myicon1.gif`: a user-defined icon located `C:/myicons`. Using the absolute pathname allows you to store icons in an arbitrary directory.
6. `NM=` Indicates the start of the second icon column.
7. `NM2=` The text to appear underneath of the icon. The \$ sign is mandatory.
8. `CMD=` The command to be executed when the icon is clicked. This can be a regular TopSpin command, a macro or an AU or Python program.
9. `TIP=` The tooltip to be displayed when the cursor is held over the icon. Note that the \$ sign is mandatory.

Before you can start a user defined guide, you must edit the file *cmdtab_user.prop* and define the corresponding command in the file, for example:

```
myt1guide=EM=J, MC=N, CL=tutor.TutStarter,
ME=startTutorial,AR=MyT1T2Toolbar;My T1 T2 Tutorial=
```

Here:

1. "MyT1T2Toolbar" is the toolbar identifier as it is used in the file *toolbar_user.prop*.
2. "My T1 T2 Tutorial" is the title as it appears at the top of the guide.

If your guide is a Bruker modified guide, you can also redefine the original Bruker command, i.e. specify *t1guide* instead of *myt1guide*. Note that the original Bruker guide is then no longer accessible.

If you want to access a user defined guide from the TopSpin toolbar, you must create a new toolbar button. To do that, right-click in an empty area of the toolbar and define a button in the appearing dialog.

19 Commands and Function Keys

19.1 Command Line Usage

How to Put the Focus in the Command Line.

In order to enter a command on the command line, the focus must be there. Note that, for example, selecting a dataset from the browser, puts the focus in the browser. To put the focus on the command line:

- Click **Esc**

or

- Click inside the command line.

How to Retrieve Previously Entered Commands

All commands that have been entered on the command line since TopSpin was started are stored and can be retrieved. To do that:

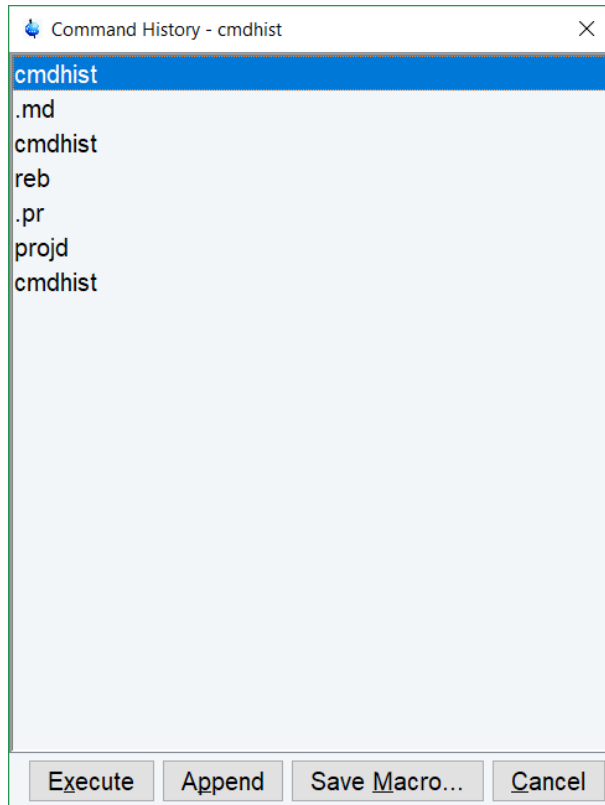
- Click ↑ (**Up-Arrow**) .

By hitting this key repeatedly, you can go back as far as you want in retrieving previously entered commands. After that you can go forward to more recently entered commands as follows:

- Click ↓ (**Down-Arrow**) .

How to Change Previously Entered Commands

- Click ← (**Left-Arrow**) or → (**Right-Arrow**) to move the cursor.
- Add characters or click **Backspace** to remove characters.
- Mark characters and use **Backspace** or **Delete** to delete them, **Ctrl+ c** to copy them, or **Ctrl + v** to paste them.



In combination with the arrow-up/down keys, you can edit previously entered commands.

How to Enter a Series of Commands

To execute a series of commands on a dataset, enter the commands on the command line separated by semicolons, e.g.:

em;ft;apk

To use a series regularly, store it in a macro as follows:

- Right-click in the command line and select **Save as macro**.

19.2 Command Line History

TopSpin allows to easily view and reuse all commands, which were previously entered on the command line. To open a command history window, select the **Command Line History** tab.

Time	Command Line
13:43:41	abs
13:43:44	.1d
13:43:51	efp
13:43:53	pp
13:44:13	re 3
13:44:17	xfb
13:44:21	.md

The executed command may be relaunched using a double click. Other options are available from a popup menu.

<input type="checkbox"/>	Execute selected command(s)
<input type="checkbox"/>	Edit selected command (F2), press F3 to leave edit mode
<input type="checkbox"/>	Delete selected command(s)
<input type="checkbox"/>	Save selected command(s) as macro
<input checked="" type="checkbox"/>	Remove duplicates

Only the last executed instance for each command in the table is shown, if **Remove duplicates** is selected.

19.3 Command Line Help

TopSpin commands that match the command line input are displayed on the fly when the **Command Help** tab is selected.

Command	Description
xf2	Process data, including FT, in F2 (2D)
xf2m	Calculate magnitude spectrum in F2 (2D)
xf2p	Phase correction in F2 (2D)
xf2ps	Calculate power spectrum in F2 (2D)

xf2

The corresponding command description is also included. The commands listed can be executed directly with a double click in the command column. A double click in the Description column opens the corresponding help page. Additional functions are available in the corresponding pop-up menu.

19.4 Starting TopSpin Commands from a Command Prompt

TopSpin commands can be executed outside of the TopSpin interface, from a Windows Command Prompt or Linux Shell.

Under Windows

1. Open a Windows Command Prompt.
2. Enter a TopSpin command in the following format:
`<tshome>\proglbin\sendgui <topspincommand>`, where `<tshome>` is the TopSpin installation directory.

Examples:

`C:\ts2.1\proglbin\sendgui ft` executes a 1D Fourier transform.

`C:\ts2.1\proglbin\sendgui re exam1d_1H 1 1 C:/bio joe` reads the dataset `C:/bio/joe/nmr/exam1d_1H/1/pdata/1`.

Under Linux

1. Open a Linux Shell.
2. Enter a TopSpin command in the following format:
`<tshome>\proglbin\scripts\sendgui <topspincommand>`, where `<tshome>` is the TopSpin installation directory.
or
`sendgui <topspincommand>`, if the TopSpin home directory is in the users search path.

Examples:

`C:\ts2.1\proglbin\scripts\sendgui ft` executes a 1D Fourier transform.

`sendgui re exam1d_1H 1 1 C:/bio joe` reads the dataset `C:/bio/joe/nmr/exam1d_1H/1/pdata/1`.

Note that commands are executed on the currently active TopSpin dataset window.

19.5 Function Keys and Control Keys

For several TopSpin commands or tasks, you can use a control key or function key short cut.

Note, that some of the keys are available only on a QWERTY keyboard. On an AZERTY keyboard use **Suppr** instead of **Delete**, **Fin** instead of **End**...

Focus anywhere in TopSpin

Esc	Put the focus in the command line.
Shift + Esc	Display menu bar and toolbars (if hidden).
F2	Put the focus in the browser.
F1	Search for string in command help or NMR Guide [help].

F6	Select the next window in the data area.
Alt + F4	Terminate TopSpin [exit].
Ctrl + d	Switch the browser on/off.
Ctrl + o	Open dataset [open].
Ctrl + f	Find data [find].
Ctrl + n	New dataset [new].
Ctrl + p	Print current data [print].
Ctrl + s	Save current data [sav].
Ctrl w	Close active window [close].
Ctrl c	Copy a text that you selected/highlighted in an error box, dialog box, pulse program, title etc., to the clipboard.
Ctrl + v	Paste text from the clipboard into any editable field.

Focus in the command line

Ctrl+ Backspace	Kill current input.
Ctrl+ Delete	Kill current input.
UpArrow	Select previous command (if available).
DownArrow	Select next command (if available).

Focus in the "striped" tables (e.g. edsolv, ednuc, peaks, integrals, cortab etc.)

Ctrl + C	Copy the currently selected table rows to the system's clipboard as a CSV-formatted table.
Home	The table package assumes that data will always be represented by complete rows rather than individual cells. This makes a re-binding of [Home] necessary, to enforce the behavior of jumping to the first row.
End	The table package assumes that data will always be represented by complete rows rather than individual cells. This makes a re-binding of [End] necessary, to enforce the behavior of jumping to the last row.
Shift + Home	The table package assumes that data will always be represented by complete rows rather than individual cells. This makes a re-binding of [Shift + Home] necessary, to enforce the behavior of selecting all rows starting from the current anchor to the first row.
Shift + End	The table package assumes that data will always be represented by complete rows rather than individual cells. This makes a re-binding of [Shift + End] necessary, to enforce the behavior of selecting all rows starting from the current anchor to the last row.
Ctrl + Numpad +	Auto-resizes all columns such that the data fits optimally.
Ctrl + Shift + X	Opens the export dialog.
Ctrl + Shift + I	Opens the import dialog.
Ctrl + Shift + P	opens the table properties dialog.

Commands and Function Keys

Ctrl + Shift + V	Opens the print preview.
-------------------------	--------------------------

Focus in the peak table

Delete	Deletes the current selection of peaks.
Enter	Zooms the spectrum pane in the current MDI window such that all selected objects are visible.
Ctrl + e	Starts the annotation editor of the currently anchored peak. See the example in the next figure.
Ctrl + Shift + R	Opens the Axis Rotation window.
Ctrl + Shift + S	Opens the Shift peaks window.
Ctrl + Shift + D	Opens the Detailed peak picking information window for the current selected peaks.
Ctrl + Shift + A	Opens the Annotate by reference window. Before, a reference peak must be defined: right-click and in the list, select Define as reference .

Peak	v(F1) [ppm]	Intensity [abs]	Annotation
10	2.3210	51725.44	
11	2.2948	52362.75	Example
12	2.1757	202825.38	

Focus in the browser

UpArrow	Select previous dataset.
DownArrow	Select next dataset
Enter	dir/user/name/expno selected: expand node or collapse node, depending on the current state.
Enter	procno selected: display this dataset.
Ctrl+Enter	name/expno selected: display this dataset.
Enter	multiple procnos selected: show in multiple display
Delete	one or more name/expno/procno nodes selected: delete these datasets.

Focus anywhere in TopSpin

Scaling Data	
Alt+ PageUp	Scale up the data by a factor of 2 [*2].
Alt+ PageDown	Scale down the data by a factor 2 [/2].
Ctrl+ Alt+ PageUp	Scale up by a factor of 2, in all dataset windows.
Ctrl+ Alt+ PageDown	Scale down by a factor of 2, in all dataset windows.
Alt+ Enter	Perform a vertical reset.
Ctrl+ Alt+ Enter	Perform a vertical reset in all dataset windows.
Zooming data	

Alt+ Plus Click the + plus sign on the standard keyboard, not on the numeric keypad.	Zoom in [.zi].
Alt+ Minus Click the - minus sign on the standard keyboard, not on the numeric keypad.	Zoom out [.zo].
Ctrl+ Alt+ Plus	Zoom in, in all dataset windows.
Ctrl+ Alt+ Minus	Zoom out, in all dataset windows.
Shifting Data	
Alt+ UpArrow	Shift spectrum up [.su].
Alt+ DownArrow	Shift spectrum down [.sd].
Alt+ LeftArrow	Shift spectrum to the left [.sl].
Alt+ RightArrow	Shift spectrum to the right [.sr].
Ctrl+ Alt+ UpArrow	Shift spectrum up, in all dataset windows.
Ctrl+ Alt+ DownArrow	Shift spectrum down, in all dataset windows.
Ctrl+ Alt+ LeftArrow	Shift spectrum to the left, in all dataset windows.
Ctrl+ Alt+ RightArrow	Shift spectrum to the right, in all dataset windows.

Focus in a table (e.g. peaks, integrals, nuclei, solvents)

delete	Delete the selected entries.
home	Select the first entry.
end	Select the last entry.
Shift+ Home	Select the current and first entry and all in between.
Shift+ End	Select the current and last entry and all in between.
DownArrow	Select next entry.
UpArrow	Select previous entry.
Ctrl+ a	Select all entries.
Ctrl+ c	Copy the selected entries to the clipboard.
Ctrl+ z	Undo last action.
Ctrl+ y	Redo last undo action.

Focus in a plot editor

F1	Opens the help window.
F5	Refresh.
Ctrl+F6	Display next layout.
ctrl+ Shift+ F6	Display previous layout.
Ctrl+ tab	Display next layout.
delete	Delete the selected objects.

Ctrl+ a	Select all objects.
Ctrl+ i	Open TopSpin Interface.
Ctrl+ c	Copy the selected object from the Clipboard.
Ctrl+ l	Lower the selected object.
Ctrl+ s	Save the current layout.
Ctrl+ p	Print the current layout.
Ctrl+ q	Close the Plot Editor window (Linux only).
Ctrl+ r	Raise the selected object.
Ctrl+ t	Reset X and Y scaling of all marked objects.
Ctrl+ v	Paste the object from the Clipboard.
Ctrl+ w	Open the attributes dialog window.
Ctrl+ x	Cut the selected object and place it on the Clipboard.
Ctrl+ z	Undo the last action.

Note that the function of function keys can be changed as described in chapter [User Defined Functions Keys \[▶ 245\]](#).

19.6 Help for Individual Commands, Command Index

To get help for an individual command, for example **ft**:

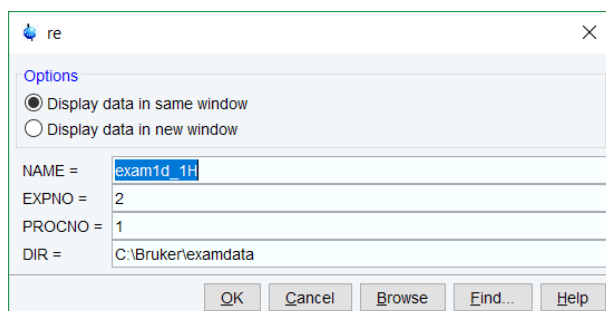
- Enter **ft?**

or

- Enter **help ft**

In both cases, the HTML page with a description of the command will be opened.

Note that some commands open a dialog box with a **Help** button. Clicking this button will show the same description as using the **help** command. For example, entering **re** and clicking the **Help** button in the appearing dialog box opens the same HTML file as entering **help re** or **re?**



How to Use the Command Index

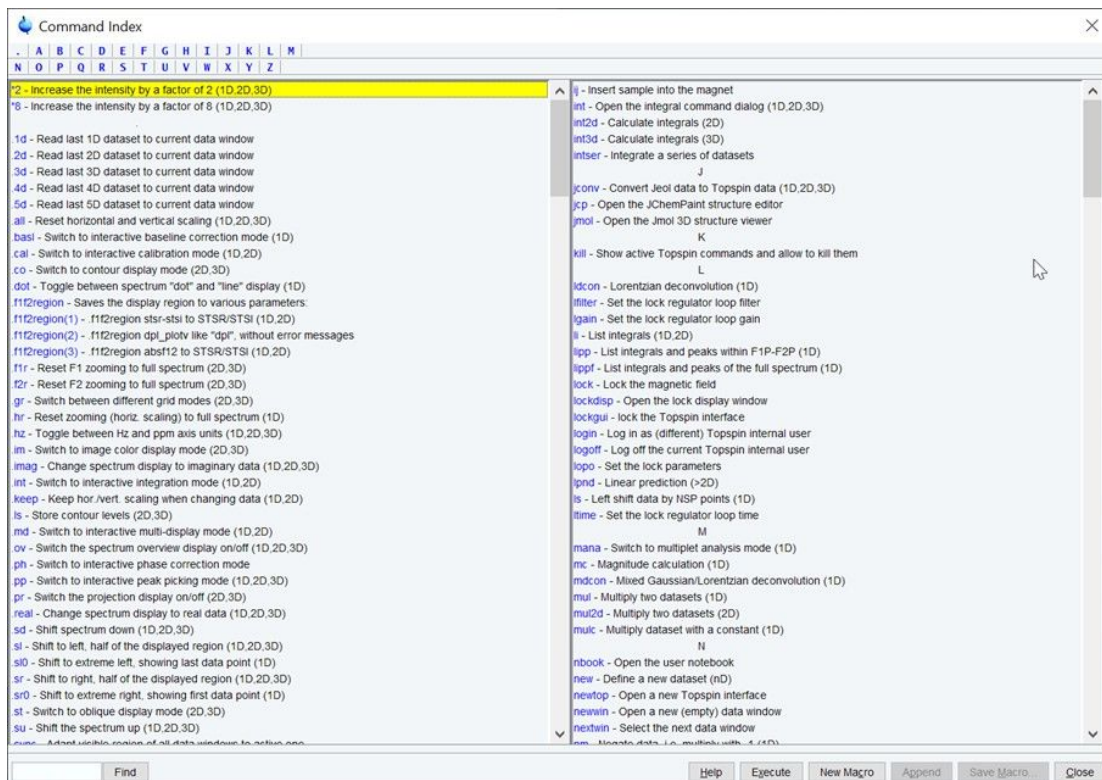
To open the TopSpin command index:

- Enter **cmdindex**.

or

Click **Help | Commands**

From there you can search for and click any command and jump to the corresponding help page.



19.7 User Defined Functions Keys

The default assignment of functions keys is described in chapter [Function Keys and Control Keys \[240\]](#) and in the document *TopSpin Control and Function Keys*.

Click [Help](#) | [Manuals](#) | [General](#) | [Control & Function Keys](#).

Assign own commands to functions keys. Example:

1. Open the file *cmdtab_user.prop*, located in the subdirectory *userdefined* of the user properties directory (to locate this directory, enter **hist** and look for the entry "User properties directory="). The file *cmdtab_user.prop* is initially empty and can be filled with your own command definitions.
2. Insert e.g. the following lines into the file:
`_f3=$em_f3ctrl=$ft_f3alt=$pk_f5=$halt_f5ctrl=$reb_f5alt=$popt`
3. Restart TopSpin.

Strike the **F3** key and the command **em** will be executed. In the same way, **Ctrl+ F3**, **Alt+ F3**, **F5**, **Ctrl+ F5** and **Alt + F5** will execute the commands **ft**, **pk**, **halt**, **reb** and **popt**, respectively. You can assign any command, macro, AU program or Python program to any function keys. Only the keys **Alt+ F4**, **F6**, **Ctrl + F6**, and **Alt + F6** are currently fixed. Their function cannot be changed.

19.8 How to Open Multiple TopSpin Interfaces

TopSpin allows to open multiple User Interfaces. This is, for example, useful to run an acquisition in one interface and process data in another. To open an addition interface, enter the command **newtop** on the command line. To open yet another interface, enter **newtop** in

the first or in the second interface. The display in each interface is completely independent from the others. As such, you can display different datasets or different aspects of the same dataset, e.g. raw/processed, regions, scaling etc. When the dataset is (re)processed in one interface, its display is automatically updated in all TopSpin interfaces.

The command **exit** closes the current TopSpin interface. Interfaces that were opened from this interface remain open. Entering **exit** in the last open TopSpin interface, finishes the entire TopSpin session. The position and geometry of each TopSpin interface is saved and restored after restart.

20 Regulatory Compliance

TopSpin complies with the FDA 21 CFR Part 11 regulations. Please read the document, accessible under **Help | Manuals | Good Laboratory Practice | 21 CFR Part 11 compliance**.

For user instructions please read the GxP Regulatory Compliance User Manual, accessible under **Help | Manuals | Good Laboratory Practice | GxP Regulatory Compliance**.

21 Troubleshooting

21.1 General Tips and Tricks

On a spectrometer, make sure the commands **cf** and **expinstall** have been executed once after installing TopSpin. **cf** must be executed again if your hardware configuration has changed. Sometimes, executing **cf** is useful in case of acquisition problems.

On a data station, a default configuration is automatically done during the installation. No configuration commands are required. Only if you want to use AU programs, you must run **expinstall** once.

21.2 History, Log Files, Spooler Reports, Stack Trace

If you have a problem with TopSpin and want to contact Bruker, it is useful to have as much information as possible available. If TopSpin is still running, you can view log files with the commands **hist** and **ptrace**. If TopSpin hangs, you can create a stack trace by hitting **Ctrl+V** (Linux) or **Ctrl+Break/Pause** (Windows) in the TopSpin startup window.

21.2.1 Topspin Command Log

By default, the history (protocol) feature is switched on. This means all TopSpin commands will be protocolled and can be examined by entering **hist** on the command line.

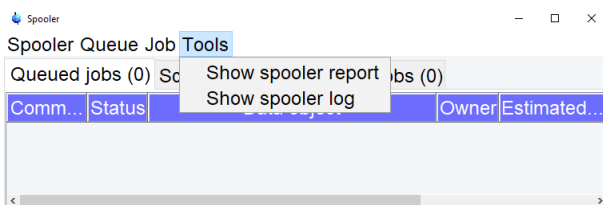
If, for some reason, history is switched off, you can switch it on as follows:

- Click **Setup Preferences | Miscellaneous**.
- Check the entry **Record commands in protocol file**.
- Click **Apply** and **Close**.

21.2.2 Topspin Spooler Report

TopSpin reports all queued, delayed and cron jobs in the so-called spooler report file. The spooler report stores all jobs since TopSpin installation and can become very large. Therefore, it should be cleaned from time to time. To do that:

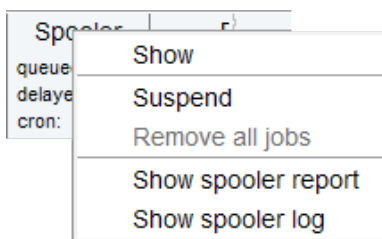
- Enter the command **spooler**.
- Click **Tools | Show spooler report**.



- Mark the entries to be deleted.
- Right-click in the dialog and choose **Delete**.
- Close the Spooler report.

Note that the spooler report can also be opened from Spooler field (if enabled) in the Acquisition Status Bar.

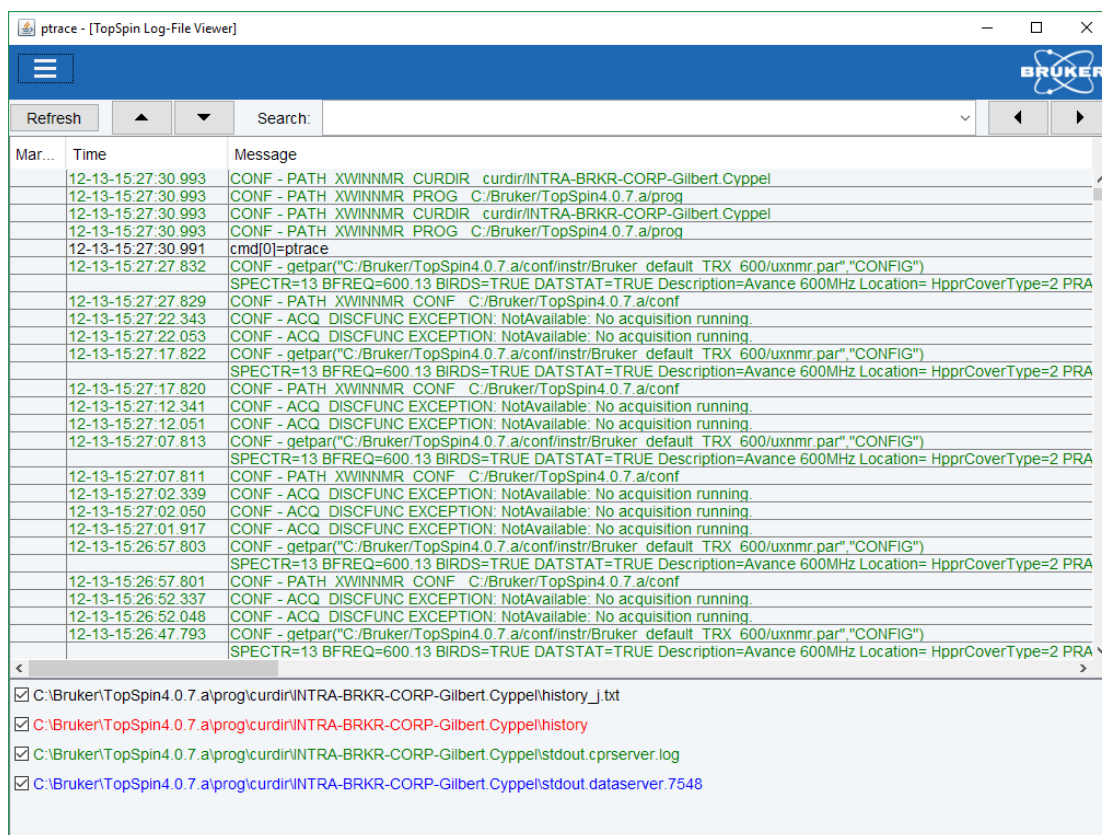
- Right-click the current dataset bar and toggle the Acquisition Status Bar **ON**.



- Right-click **Spooler** and select **Show spooler report**.

21.2.3 Topspin Command, Data Server and Network Log

A full protocol including not only TopSpin commands but also data server and network traffic is displayed by the command **ptrace**. This opens the following dialog window:



Here TopSpin log messages from various log files are displayed time sorted.

Messages from different log files are shown in different colors. The color assignment and location of the files is shown in the lower part of the dialog window.

ptrace supports the following functions:

Search keywords

To search the displayed log files for a certain keyword, just enter it in the text bar at the top of the window and hit **Enter**.

Anchor specific entries


To anchor an entry:

- Double-click in the first column of the entry.

The entry is marked with an **X**. Now you can use the < > buttons at the upper right of the window to go to the previous or next entry, respectively.

Add log files

By default, the *procol.txt*, *history* and *data server* log files are shown. To include additional log files to the **ptrace** list:

- In the ptrace [TopSpin Log-File Viewer] window, click **File | Add** , specify the file and click **Open**.

Note that most log files are stored in the directory:

`<tshome>/prog/curdir/<user>`

Save the log messages

To save log messages in a text file:

- Click **File | Save** and specify the output text file.

21.2.4 Create a Stack Trace

If TopSpin hangs it can be useful to send Bruker a stack trace about a possible cause. You can create a stack trace as follows.

- Move the cursor into the TopSpin startup window.
- Under Windows: hit **Ctrl+Break/Pause**, under Linux: hit **Ctrl+** (Control backslash). On a notebook enter **CTRL+Fn+Insert/Pause**.
- Copy the appearing text into a text file.

21.2.5 Store Complete Log with savelogs

To write a complete set of TopSpin log files, click **Manage | Commands | Collect & Save Logfiles** or enter **savelogs** on the command line.

If TopSpin has hung up or has crashed **savelogs** can be executed as follows.

Under Windows:

- Click the **Bruker Utilities<topspin version>** icon on your desktop. An Explorer will be opened.
- Double-click **Miscellaneous**.
- Execute the script **savelogs**.

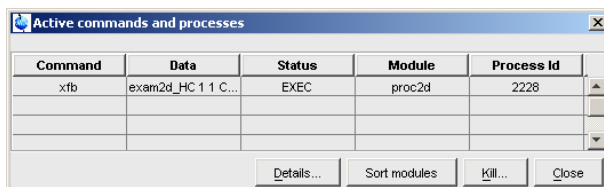
Under Linux:

- Open a shell.
- Type **savelogs**

For detailed information about saving all possible log files and about the upload to the Bruker file server please refer to the Processing Commands and Parameters Manual.

21.3 How to Show or Kill TopSpin Processes

To show the currently running TopSpin processes, click **Manage | Commands | Show Currently Active Commands** or enter the command **show** or **kill** on the command line. A list of processes displays the process command, dataset etc.



The figure above shows a list with one process (command **xfb**). To kill a process, select it in the list and click the button **Kill...**

The commands **show all** or **kill all** work like **show** and **kill**, except that they also show TopSpin system processes. Note that killing such processes may kill TopSpin.

21.4 What to do if TopSpin Hangs

If, for some reason, TopSpin hangs, please do the following.

Under Linux:

- Open a Shell.
- Enter `<tshome>/prog/bin/script/killtopspin`, where `<tshome>` is the TopSpin installation directory.

Under Windows:

- Click **Start | Programs | Bruker NMR Software | Bruker <version> Utilities**

The file explorer opens with a path, e.g. `C:\Bruker\TopSpin<version>\prog\bin\utilities`

- Open the sub-directory **Miscellaneous** and double-click **killtopspin**.

Normally, this kills all TopSpin processes including *cpr*, *cprserver*, *dataserver* and *java*.

21.5 How to Restart the TopSpin User Interface during Acquisition

If TopSpin hangs up during a data acquisition, you can restart the user interface without disturbing the acquisition. To do that:

- Open the file: `<tshome>/prog/curdir/<user>/history` where `<tshome>` is the TopSpin home directory and `<user>` is the user who started TopSpin. Look for the term 'Java Virtual Machine' and check its PID.
- Open the Task Manager (Windows) or System Monitor (Linux).
- Stop the Java(w).exe process with the PID found in the history file.
- Open a Windows Command Prompt or Linux Shell.
- Go to the TopSpin Installation directory.
- Enter **topspin -client**.

22 Contact

Manufacturer

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E-Mail: nmr-support@bruker.com

<http://www.bruker.com>

WEEE DE43181702

Bruker BioSpin Hotlines

Contact our Bruker BioSpin service centers.

Bruker BioSpin provides dedicated hotlines and service centers, so that our specialists can respond as quickly as possible to all your service requests, applications questions, software or technical needs.

Please select the service center or hotline you wish to contact from our list available at:

<https://www.bruker.com/service/information-communication/helpdesk.html>

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Part No: H9469SA4