TopSpin

Quick Start Guide

Version 005

Innovation with Integrity

NMR

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P/N: H179023

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1 Introduction

The goal of this manual is to describe the basic steps of working with the TopSpin software package to process NMR data on a data station. This should enable a relatively unexperienced user to install, start, display, process and analyze acquired data independently.

1.1 How to Use this Manual

Please note: The TopSpin icons provide access to many different graphically oriented functionalities. This functionality is also available through commands that one can type into the TopSpin command line or use in automation routines. When the mouse cursor is moved over an icon, further explanatory information about the function of the icon is shown as well as the corresponding command name. For better reading of our manuals, we therefore don't explicitly list or mention these command names in the description of the icons.

2 Installation

In the following chapter, the software installation will be described only for data station. In case of an NMR Spectrometer, used for NMR data acquisition, please refer to the Installation Guide Manual delivered with TopSpin (under **Help | Manuals (docs) | Installation Guides | TopSpin Installation Guide**) or download it from the Bruker website under the following link: *https://www.bruker.com/protected/en/services/user-manuals/nmr/installation.html* (Please note that access to the download section is restricted to customers. Registration for a free customer account is provided directly on the Bruker website.).

There are two main ways to install the TopSpin Software on your computer:

Download from the internet:

If you have access to an internet connection the Topspin up to date version can be directly downloaded from the Bruker website: *https://www.bruker.com/protected/en/services/software-downloads/nmr.html*

If you do not have an account, please register for an account. If you already have an account, please log in to access the download section containing all listed software products.

Using the DVD

Insert the TopSpin DVD and open the DVD drive with your usual system explorer.

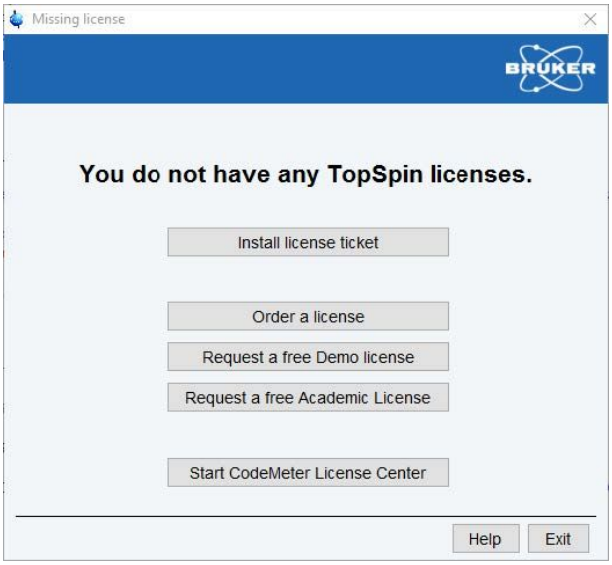
Find and double click the install command (Windows: *install.cmd*, Linux: *install*, Mac OS: *TopSpin<version>.pkg)* and follow the instructions of the Installer.

The Installation Procedure of TopSpin on all operating systems is mainly the same. Nevertheless, there are some small differences that are explained in detail in the Installation Manual delivered with TopSpin (see above).

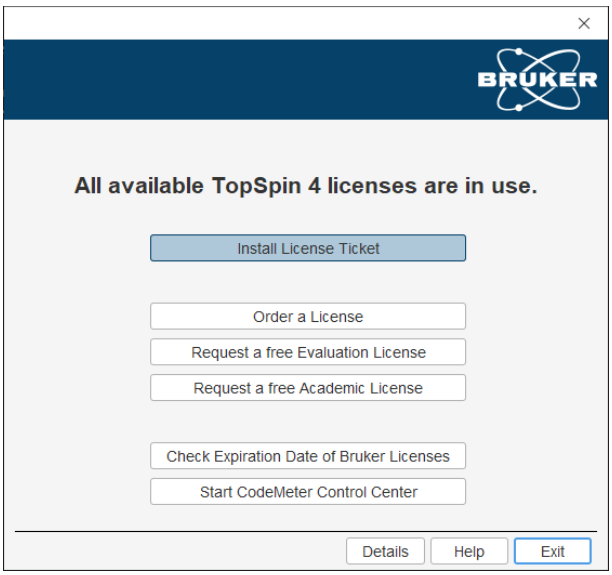
Please note: For all operating systems the administrator password is required when installing TopSpin.

3 First Start and License

Start TopSpin by double clicking the TopSpin desktop Icon ( ). If you already have a TopSpin license, TopSpin will open immediately. If not, a dialog will be opened which guides you through the process of obtaining and installing a TopSpin license (see figure below).



If the number of available licenses is exhausted, the following window will be shown.

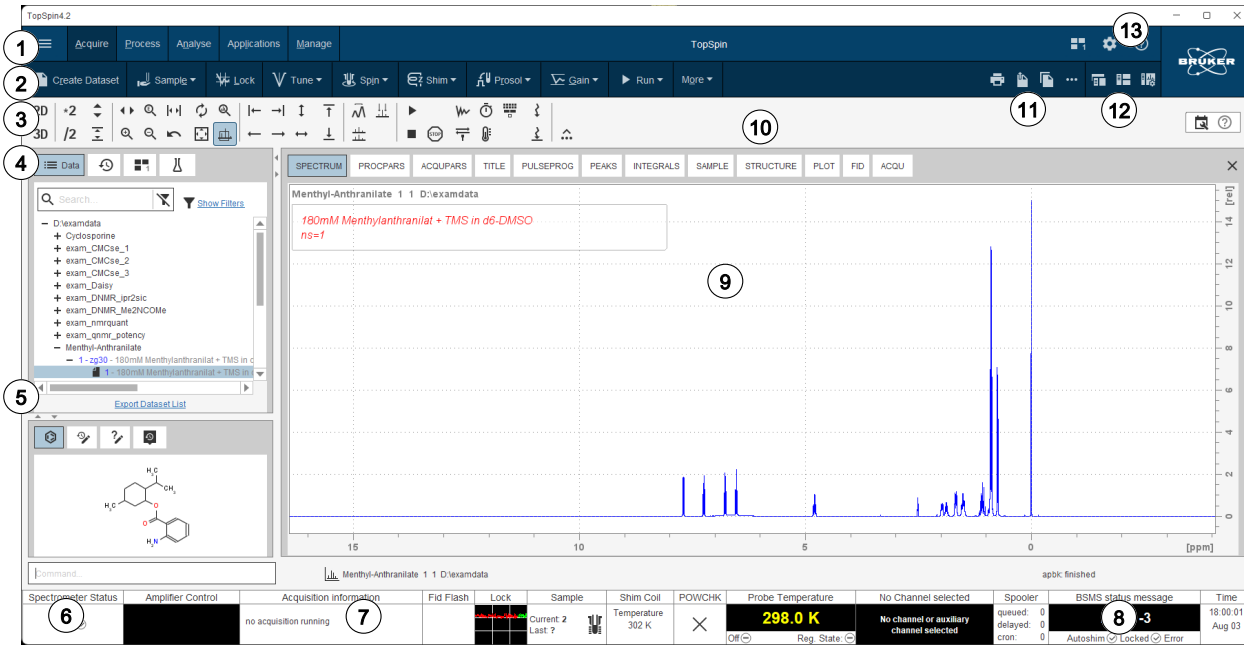


For further information on licenses, please refer to the CodeMeter License Management Manual on the Bruker website: *https://www.bruker.com/protected/en/services/software-downloads/nmr.html*

4 Getting Started

Once the TopSpin license has been activated, TopSpin will start immediately:

4.1 TopSpin Interface - Overview

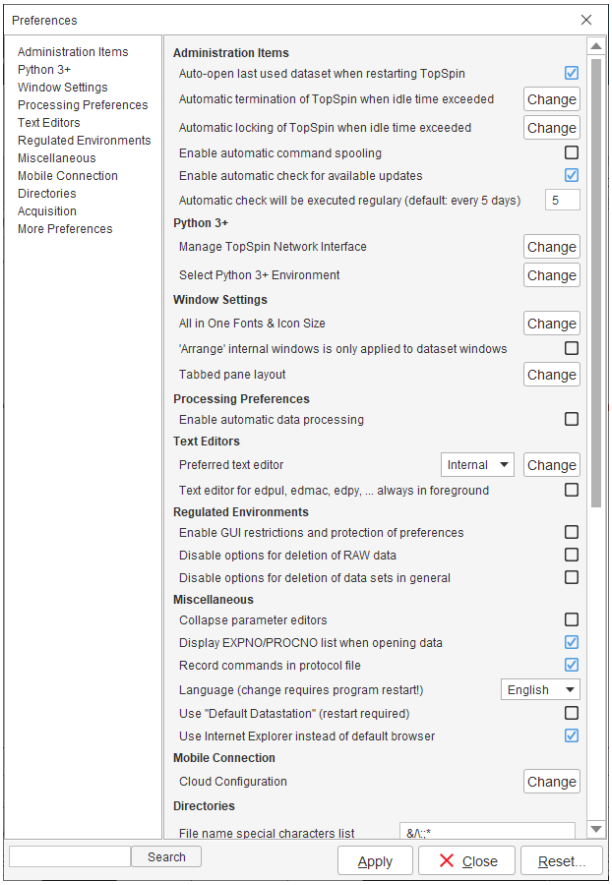


1	Menu Bar	8	Status Display Bar
2	Workflow Button Bar	9	Dataset Window
3	Tool Bar	10	Dataset Window Tabs
4	Browser and Search Window	11	Print, Export, Copy and Publish
5	Structure Window, Command Line History, Status Line History	12	Viewing Options
6	Command Line	13	Window Switcher, Login, Setup Preferences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

4.2 Setup Preferences

TopSpin can in many aspects be tailored to your personal preferences. 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. Please note, that an Administrator password is required, if the **Enable GUI Restriction** option has been activated. If it is set, modifications in the setup preferences are possible only for users who know the NMR administration password

The categories that can be tailored are shown on the left side of the preferences window. Click the category you want to view or change. It will be highlighted, and the corresponding objects will be displayed on the right side of the preferences window. The figure below shows all currently available categories.



4.3 First Start of TopSpin - Load a Dataset

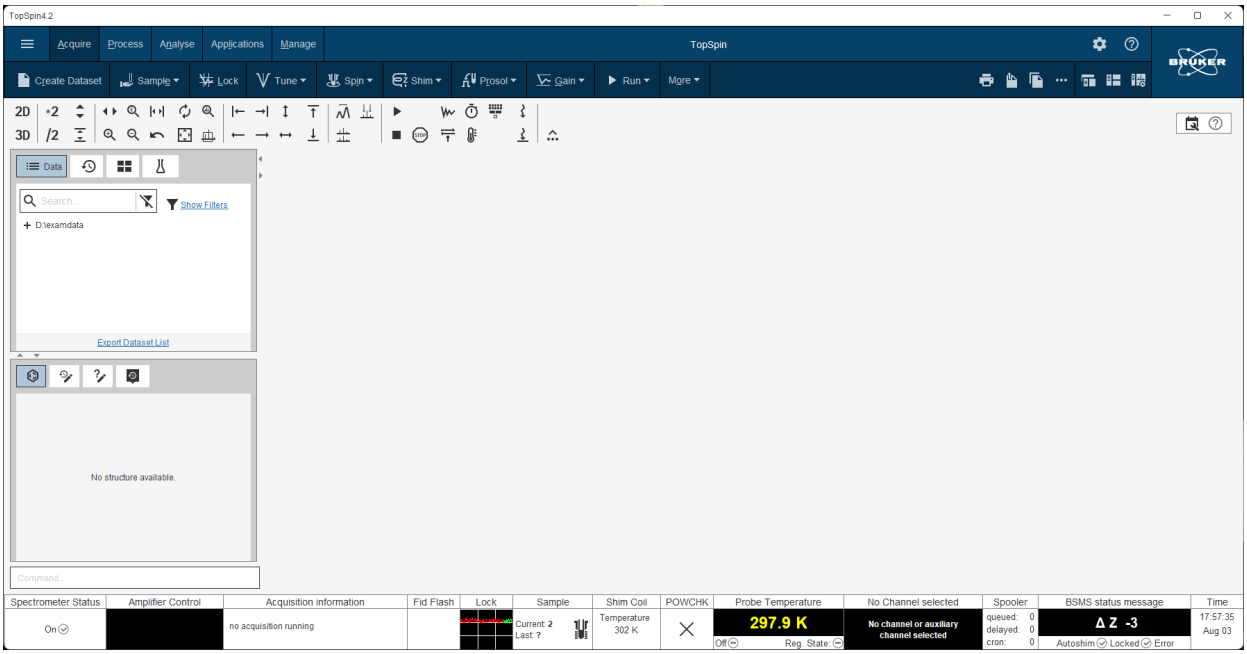


Figure 4.1: TopSpin starting window.

At the starting point of TopSpin no dataset is selected. You first have to select it in the browser (see figure below). Load it in the active window by drag and drop.

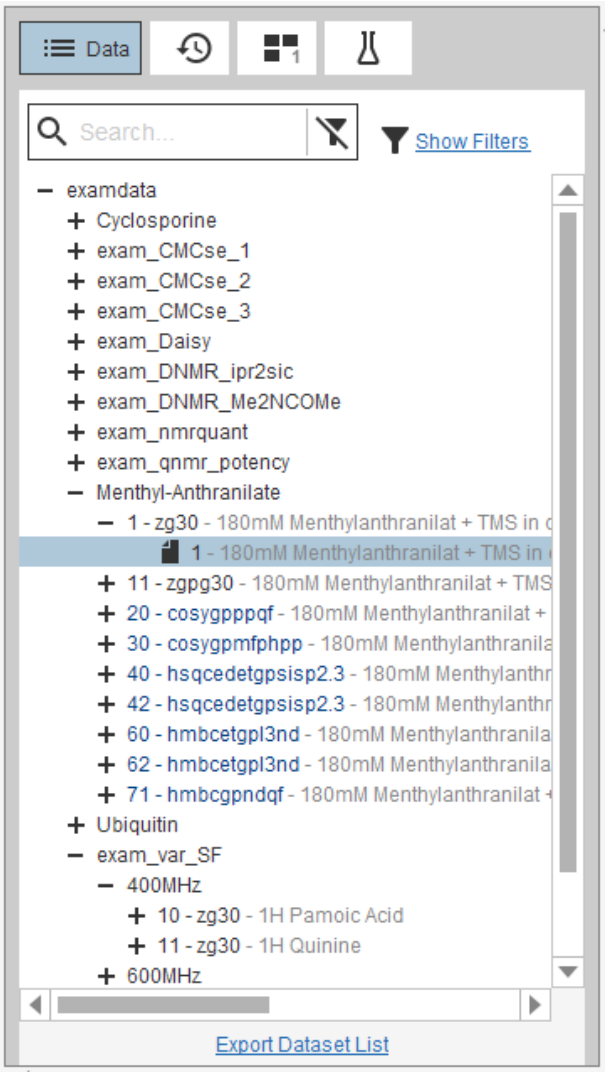


Figure 4.2: Browser window with list of available datasets (spectra+parameters)

Clicking on the plus sign left of a directory or dataset name expands the selection. In the above figure, Menthyl-Anthranilate experiment 1 has been selected. The type of experiment (here **zg30**) and the name of the sample (here **180mM Menthylanthranilate**) are shown.

You can also use the **Search and Filter** functionality to get a list of datasets that match the search criteria (see figure below). This feature is particularly useful for all TopSpin commands or even external applications that will run on a selection of datasets. One example is the **Serial Processing** feature.

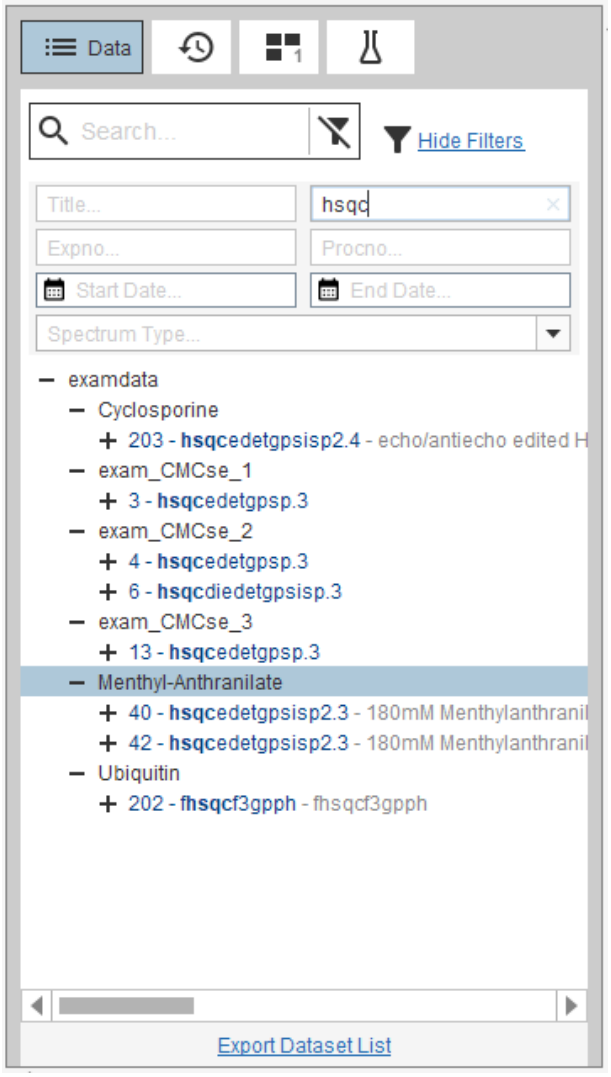


Figure 4.3: List of datasets matching the search and filter criteria (here HSQC).

The above example shows the list of all HSQC experiments of the example datasets delivered with the TopSpin software distribution. This is made possible through a newly implemented database-like mechanism that keeps the information about the available datasets in memory. The content of the database is constantly updated whenever changes anywhere in the top level dataset directory are being made.

You can also load a dataset by drag & drop from an Explorer window (e.g Windows Explorer, Konqueror, Finder etc.).

The figure below shows the TopSpin window with the selected dataset after drag & drop and expansion between 9.5 and -0.5 ppm using the exact zoom function.

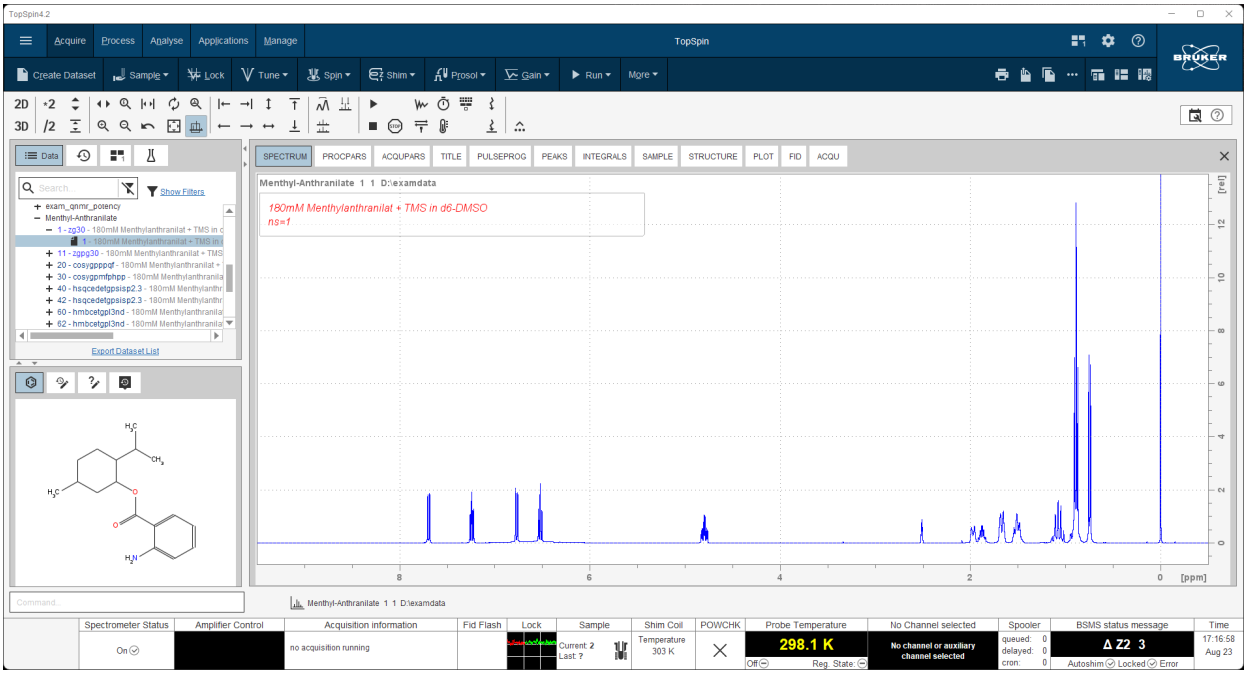


Figure 4.4: TopSpin window showing the selected dataset after drag & drop.

4.4 Basic Processing and Manipulations

The workflow button bar opens the spectrum processing tools.

Figure 4.5: Workflow button bar for spectrum processing.

The toolbar gives access to the most useful tools to manipulate the spectrum.

Please note: offers access to further icons for spectrum manipulation functionalities.

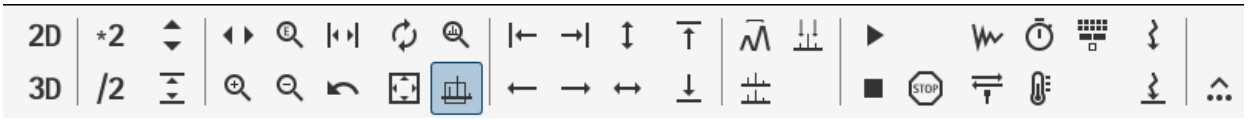
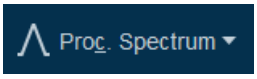


Figure 4.6: Toobar with further icons for spectrum manipulation functionalities.

4.5 Basic Processing

Clicking on the Proc. Spectrum button 

in the workflow button bar (see *Figure 4.5 [▶ 10]*) performs all basic processing steps fully automatically. The steps can be configured through the **proc1d** button in the pulldown menu.

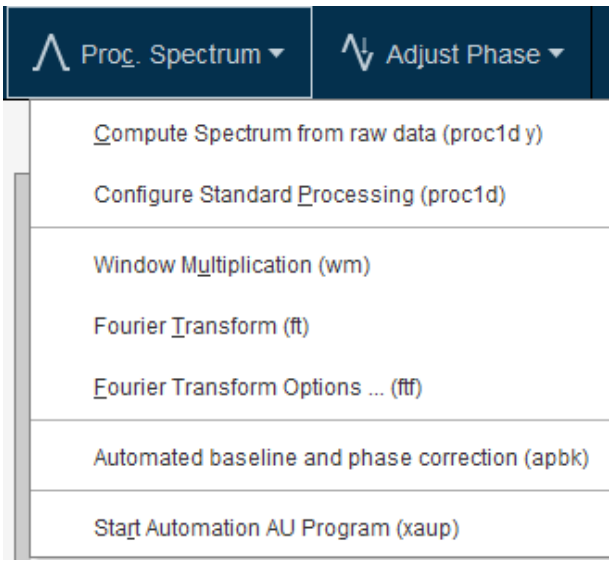


Figure 4.7: Proc. Spectrum pulldown menu.

The screenshot below shows the configuration options for the basic 1D automatic processing.

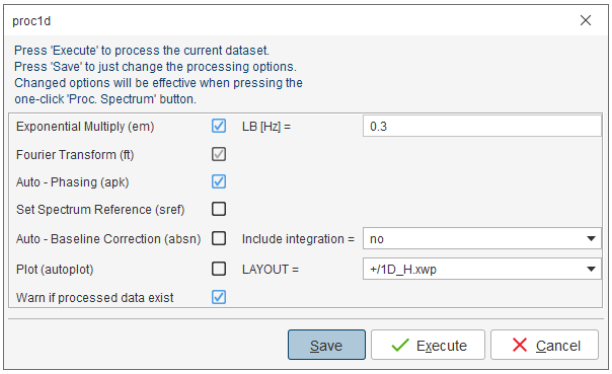


Figure 4.8: Configuration options for the basic 1D automatic processing.

In addition, the Proc. Spectrum pulldown menu gives access to standard spectrum processing operations, like window multiplication, Fourier transform, ft options or start of the automation AU program. A simple click on it will apply the processing parameters contained in the dataset. If the spectrum has already been processed before, you will be asked for an override confirmation.

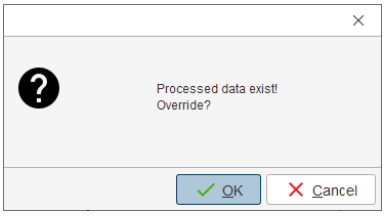
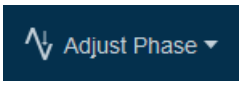


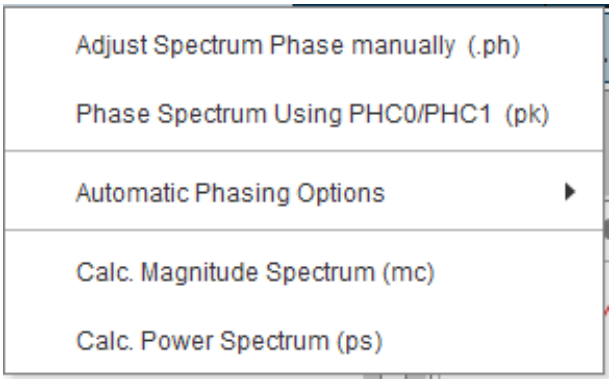
Figure 4.9: Confirmation window before processing of the current dataset.

4.6 Phase Correction

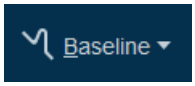
For further improvement of the phase of the spectrum, 

gives access to the interactive phase correction. The dataset window will show icons specific for phasing.

In addition, the Adjust Phase pulldown menu gives access to further phasing operations.

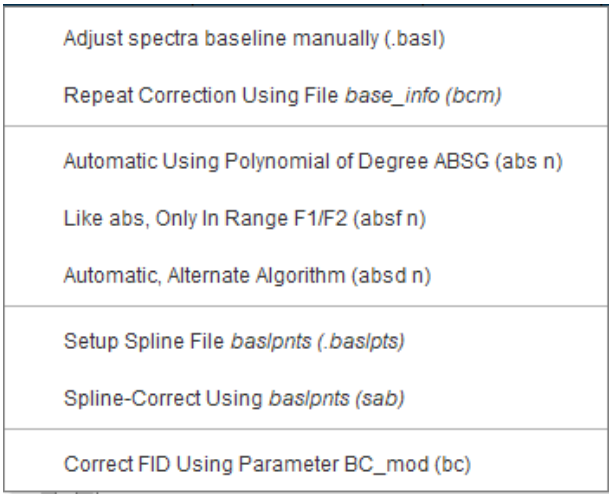


4.7 Baseline Correction

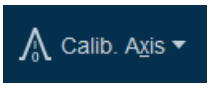
For further improvement of the spectrum baseline, 

leads to the interactive baseline correction. The dataset window will show icons specific for baseline correction.

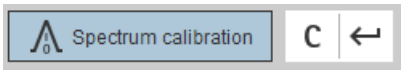
In addition, the Baseline pulldown menu gives access to further baseline correction operations.

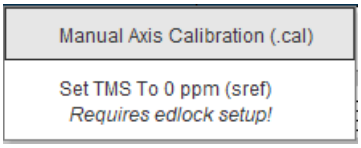


4.8 Axis Calibration

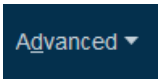


gives access to following pulldown menu with axis calibration options:

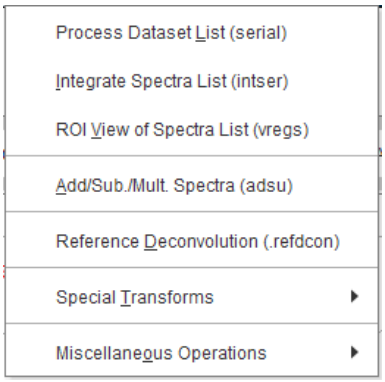




4.9 Advanced Processing Options



gives access to further options through following pulldown menu:



5 Analyse the Spectrum

To enter the Analyse Process, click Analyse, the following workflow appears:

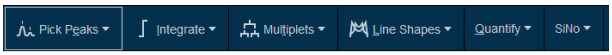
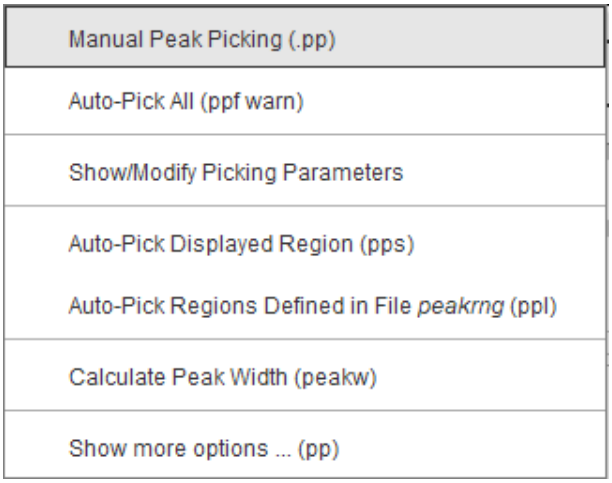


Figure 5.1: Workflow button bar for spectrum analysis.

5.1 Peak Picking

Pick Peaks gives access to the interactive peak picking. The dataset window shows specific icons for peak picking:

In addition, the Pick Peaks pulldown menu gives access to further peak picking operations and options:



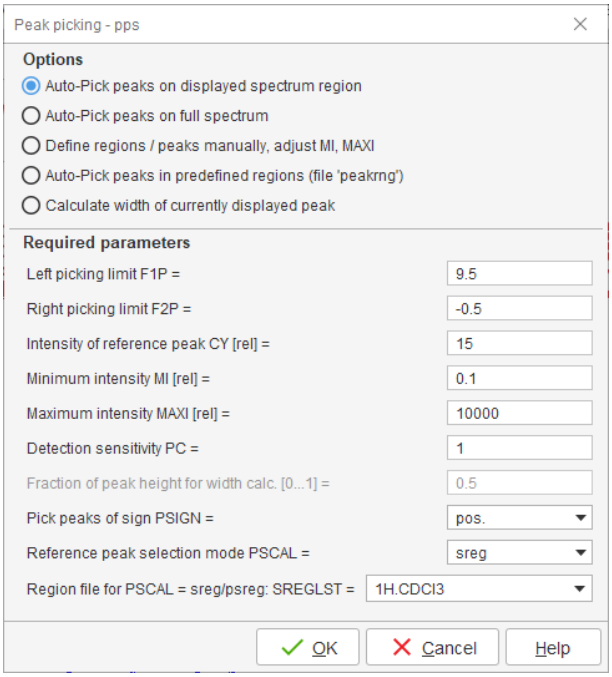
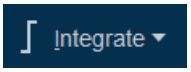


*Figure 5.2: Peak picking pulldown menu and options (command **pp**).*

5.2 Spectrum Integration



button gives access to the integration pulldown menu:

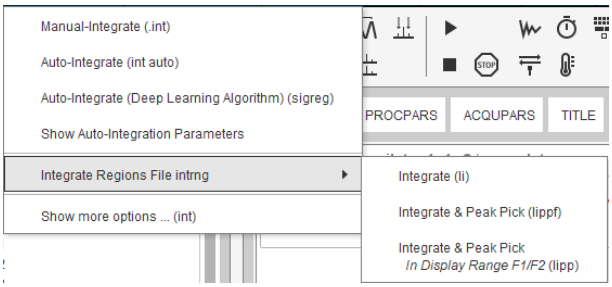


*Figure 5.3: Integration pulldown menu and Integrate Regions File menu (command **intrng**).*

In addition, more options can be obtained through the command **int**:

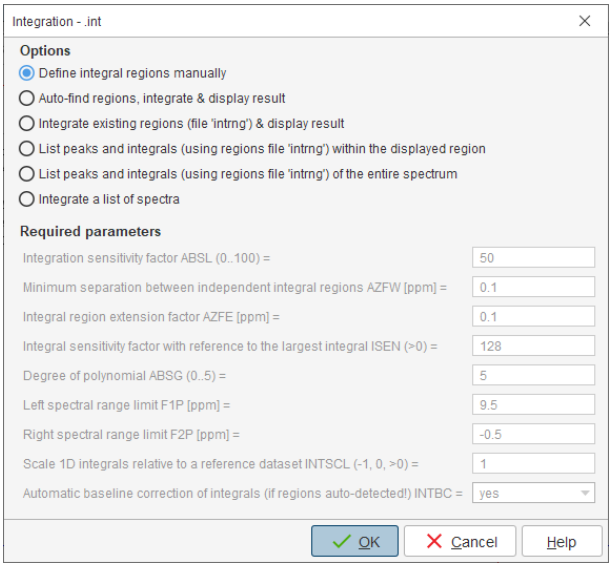
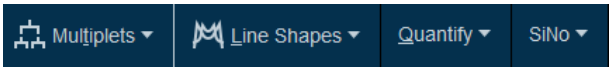


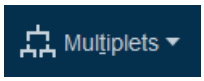
*Figure 5.4: Further options for integration (command **int**).*

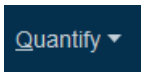
5.3 Further Analysis Options

Further analysis options can be obtained through the corresponding workflow:



Each button gives access to a specific pulldown menu for advanced analysis features.

Please note: For 

and 

operations specific tutorials are available via the pulldown menu.

6 Printing the Spectrum

Printing the spectrum can be done in two different ways:

6.1 Print Screen Directly

Click on the printer icon , located on the upper right part of the TopSpin window, allows direct printing of the spectrum. Details can be obtained as usual by dragging the mouse on the icon. Clicking the button gives access to the print settings:

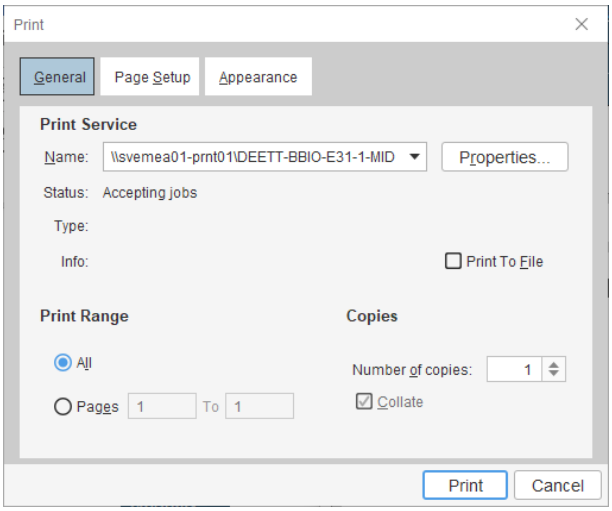


Figure 6.1: Print window.

6.2 Print Spectrum Using Layout (Plot)

To use this TopSpin feature, click the button,

or use the **plot** command in the TopSpin command line. The following TopSpin window appears:

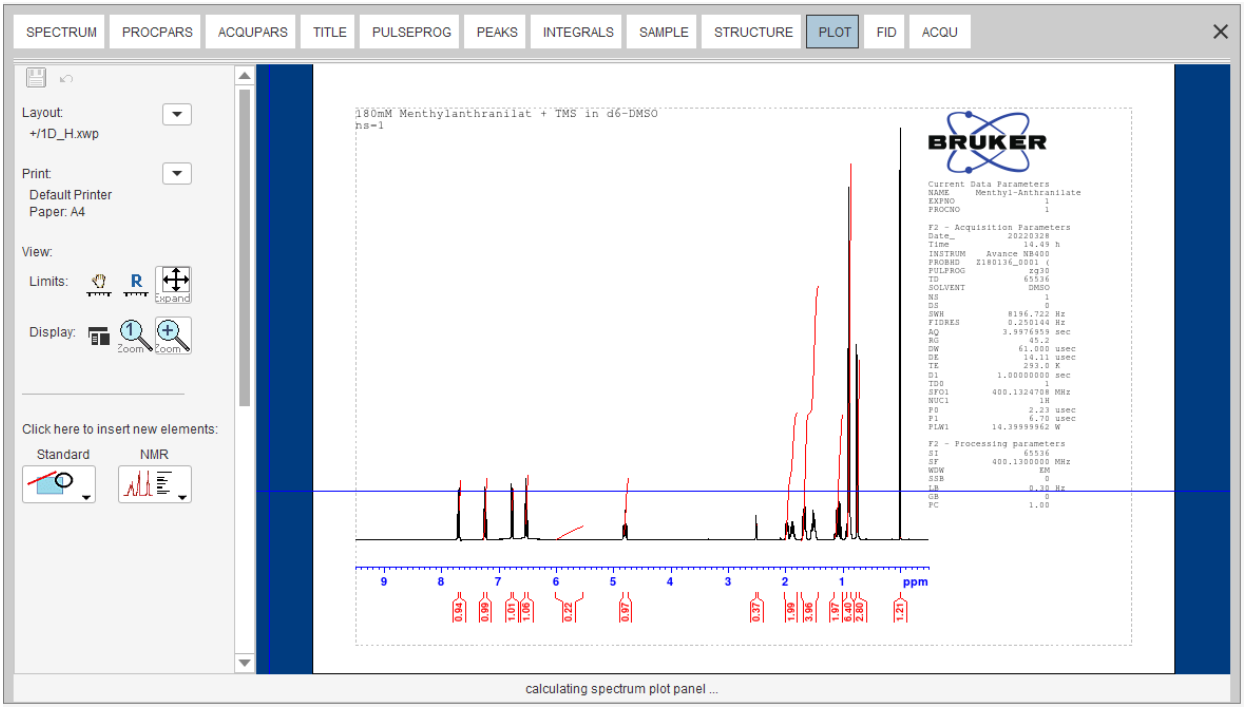


Figure 6.2: Part of TopSpin plot window (with layout).

The left part of the plot window shows the names of the selected layout and printer. They can be changed with the arrow button, as well as other plotting view parameters, like limits or display. New NMR elements (title, parameters, 2D spectrum, etc.) can be inserted.

The right part presents the spectrum like it will be plotted. Changes on the left part will be shown in real time in the layout on the right.

7 Further Documentation

For detailed information please refer to the TopSpin Manual section under | **Manuals (docs)** or visit the Bruker website under *https://www.bruker.com/protected/en/services/user-manuals/nmr.html*. (Please note that a customer account is needed.)

8 Contact

Manufacturer

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Website: *http://www.bruker.com*
WEEE DE43181702

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