TopSpin

Release Letter 4.0.5

User Manual

Version 001

Innovation with Integrity

NMR

Document Number:

P/N: H90088TR4-05

1 Introduction

1.1 For Guidance

About the Release Letter

The Release Letter describes the main aspects of the TopSpin installation with the latest developments. The complete installation is described in the TopSpin 4.0 Installation Guide. This document is electronically available on the TopSpin DVD and at *www.bruker.com*. The detailed information is also available directly in the Help menu of the installed TopSpin program.

The Release Letter provides important information about improvements, deployments and the history of the Bruker software.

Target Audience

The Bruker Software Release Letter, in this case the Release Letter for TopSpin 4.0.5, supports all Bruker users who work with Bruker software products. In order to communicate all improvements as quickly as possible, Bruker routinely provides the Release Letter for all users.

How to get the Release Letter

The Release Letter is only available electronically on the TopSpin DVD, in Acrobat Reader (PDF) format and as html. The Release letter is not available as a hard copy. This allows Bruker to provide an up-to-date version of the Release Letter. The latest version of the Release Letter is also provided on the Bruker Web Server:

http://www.bruker.com/service/information-communication/user-manuals/nmr.html

Please note that a login for the Bruker website is needed to show this document.

Please note furthermore that under macOS the Release Letter will be shown in PDF format.

Release Letter Conventions

The Release Letter utilizes different script types in order to make selected text more transparent and explicable for users. Please note that the Release Letter contains the following conventions:

Bold - commands to be entered from the keyboard or to be clicked on with the mouse

Italic - file names, program messages (e. g. error messages) and web addresses

1.2 Safety Regulations

In order to work safely in laboratories with NMR-spectrometers all users have to follow the safety regulations for magnetic, electrical, cryogenic and chemical safety. For detailed information please refer to the safety instructions in the AVANCE Systems General Safety Considerations Manual (Z31836) provided on the BASH DVD. This manual is available in several different languages.

Introduction

2 TopSpin - Basics

2.1 About TopSpin

TopSpin 4.0.5 is a minor update of TopSpin program package containing many improvements, new and useful features and bug fixes.

TopSpin 4.0.5 has been tested and released only for AVANCE NEO spectrometers.

Older spectrometer types are not supported and TopSpin 4.0.5 cannot be used on them for data acquisition. For continued support of these products please refer to updated versions of TopSpin 3.

2.2 License Requirements

TopSpin 4.0.5 comes as a full program version on DVD and requires a TopSpin 4 license.

Please contact your local Bruker representative for license order and more details. All addresses in detail are listed in *Contact [▸ 47]*.

2.3 TopSpin Program Versions

The TopSpin 4.0.5 DVD contains the following program versions:

- TopSpin 4.0.5
- IconNMR 5.1.4
- NMR Guide 4.4

The following programs are part of the TopSpin 4.0.5 DVD content, but please note that they must be licensed separately in each case:

- AMIX 3.9.15
- Spectra Base 1-1-2

  (Please note that the Spectra Base is only available with AMIX and the different license types (belonging to the pH-value) and the updates must be licensed separately.)
- CMC-se 2.5.5
- CMC-assist 2.11
- InsightMR™ 1.1.3 (for Windows and Linux)
- DynamicsCenter 2.5 (Protein Dynamics)

Please note that for the mac a reduced collection is available.

2.4 Hardware Requirements

2.4.1 PC Hardware

To run TopSpin 4.0.5 a state of the art computer should be used. Bruker recommends and delivers the following PC:

- HP z440, Intel Xeon Quad Core E5-1620v4 / 3.50GHz / 10MB Cache
- Memory: 16GB (2x 8GB) DDR4-2400 ECC, 8x memory slots (2x used)
- Video Card: Graphic adapter: Graphic adapter NVIDIA Quadro K620, 2GB
- Network adapters: 1x Intel I218LM PCIe on Board 10/100/1000 Mbits/s (SPECT),
  1x Intel Ethernet I210AT PCIe GbE 10/100/1000 MBits/s (NET)
- Hard Disc: 2TByte, 3Gb/s, NCQ, SATA, 7200rpm
- Optical Storage: Slim SATA SuperMulti DVD writer
- 3 button mouse or wheel mouse

2.4.2 Apple Computers

- MacBook, iMac or MacMini (state of the art) with Intel CPU
- CPU must be capable of executing 64bit instructions
- Apple mouse or any 3 button or wheel mouse

2.5 Spectrometer Hardware Requirements

TopSpin 4.0.5 runs on any AVANCE NEO spectrometer.

For upgrade possibilities of your spectrometer with TopSpin 4.0.5, please check with your local Bruker office.

2.6 Supported Operating Systems

TopSpin 4.0.5 on spectrometer computers is supported for:

- Windows 10 (64bit)
- Windows 7 (64 bit)
- CentOS 7 (64 bit) (Please note: The minimum required CentOS7 Version is 7.1)

All operating system updates (hot fixes and service packs) at the time TopSpin 4.0.5 was released have been tested and are supported.

TopSpin 4.0.5 on data stations is supported for:

- Windows 10 (64 bit)
- Windows 7 (64 bit)
- CentOS 7 (64 bit) (Please note: The minimum required CentOS7 Version is 7.1)
- Apple macOS X 10.12 or higher

Although not officially supported by Bruker, users reported that TopSpin is also running and is used for data processing on other Linux systems, including Ubuntu-17.10, Ubuntu-16.04, Debian-9, Fedora-27, openSUSE-Leap 42.3 and Linux Mint 18.3. You will find further information in the Bruker Knowledge Base Article #14407.

2.7 Software Requirements

2.7.1 Under Windows

All AVANCE NEO spectrometers do not need any further software or equipment to install TopSpin.

2.7.2 Under Linux

All AVANCE NEO spectrometers do not need any further software or equipment to install TopSpin.

2.7.3 Under macOS

No additional software is required to run TopSpin as data station.

3 TopSpin Installation

3.1 Installation on Windows and Linux

Please note that TopSpin 4.0.5 comes as a full program DVD and, as such, requires a DVD device for installation.

Alternatively, the full TopSpin Installer can be downloaded from this web page:

http://www.bruker.com/service/support-upgrades/software-downloads/nmr.html

Please note: You need a login to access this section. If you haven't registered yet, please register here:

https://www.bruker.com/about-us/register.html

The installation procedure is described in the Installation Guide for Windows, Linux and macOS. This document is available electronically on the TopSpin DVD and on www.bruker.com.

If you have already a previous TopSpin version installed, then install the TopSpin 4.0.5 program in a different directory. This will allow you to utilize and enjoy the new features without affecting your current installation.

3.2 Using a Previous Configuration (TopSpin) on Windows and Linux

TopSpin 4.0.5 usually replaces a previous version of TopSpin and, normally, you want to keep the existing configuration. The installation program automatically detects previous installations of TopSpin, prompts you to select one and then copies its configuration files. If multiple previous installations are found, you can choose which configuration you want to copy to the current installation.

After the installation has finished, you can simply start TopSpin and run **cf**, selecting the copied configuration, and run **expinstall**.

If you have chosen not to copy a previous configuration, you can still do that after the installation has finished with the TopSpin command **nmr_save**. For more information on the command **nmr_save**, enter:

help nmr_save

or refer to the Installation Guide.

3.3 Installation on macOS

Please note, that the Topspin installation on macOS selects the installation folder automatically.

Different versions always use different installation folders. The **expinstall** command is also invoked automatically.

The spectrometer configuration is not copied, because macOS version of TopSpin is always configured as a data station. You may still use the **nmr_save** command to transfer private files (waveforms, pulseprograms) between different TopSpin installations.

4 New Features

4.1 Support of TRX ECL 02

TopSpin 4.0.5 offers full support of TRX ECL 02 boards.

New Features

5 TopSpin Licenses

A license for Bruker software can be ordered from the Bruker website. Just go to

https://www.bruker.com/nmr_license_requests.html

and fill out the request form.

Bruker BioSpin offers the following license types for TopSpin:

license type	contents
Full	Acquisition, Processing, Automation (IconNMR), Plotting, Simulation and NMR-GUIDE
	run of validity: 15 years
Demo	Acquisition, Processing, Automation (IconNMR), Plotting, Simulation and NMR-GUIDE
	run of validity: 3 months
	free of charge
Processing-Only	Processing, Plotting, Simulation and NMR-GUIDE
	run of validity: 15 years
Student and Academia	Processing, Plotting, Simulation and NMR-GUIDE
	run of validity: 15 years
	free of charge

In order to provide students, researchers and teachers with unlimited access to the best tools for off-line NMR processing, Bruker is making their market leading NMR processing software TopSpin available free of charge for all academic users. If you are eligible to use the free license you can download and install the TopSpin software from the Bruker website at the following address:

https://www.bruker.com/service/support-upgrades/software-downloads/nmr.html

On the same web page you can request your free license activation ticket for TopSpin 4.0.5. Or install TopSpin on your system first and start it immediately. The license management dialogue will show up and guide you to the correct web page for requesting a ticket.

TopSpin Licenses

6 History of Changes

6.1 TopSpin 3.5

All changes provided with TopSpin 3.5 are summarized in the release letter of TopSpin 3.5. All release letters for older versions of TopSpin can be found here:

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

Please note: You need a login to access this section. If you haven't registered yet, please register here:

https://www.bruker.com/about-us/register.html

6.2 TopSpin 4.0.1

6.2.1 General

6.2.1.1 New Licensing System: CodeMeter

TopSpin uses the new "CodeMeter" license management. A license for Bruker software can be ordered from the Bruker website. Just go to *https://www.bruker.com/nmr_license_requests.html* and fill out the request form. 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 CodeMeter License Management User Manual.

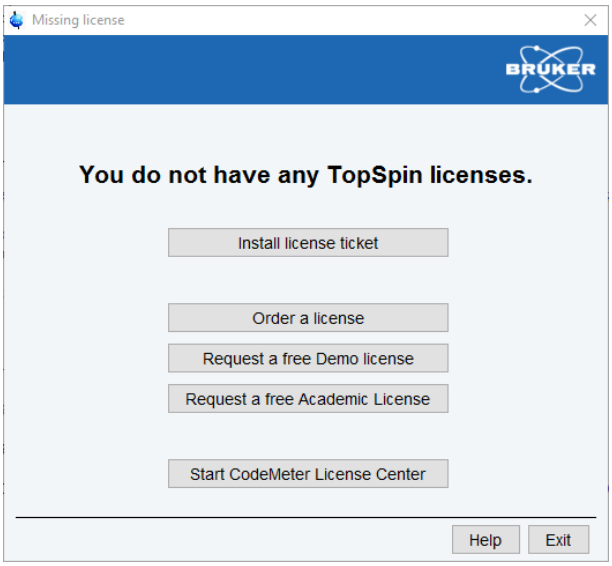
The Linux version of the CodeMeter runtime delivered with TopSpin comes as an RPM package and thus can only be installed on RPM based distributions like Red Hat (CentOS, Fedora) or Suse. If you use a different, not directly supported, distribution (Debian, Ubuntu, …), please download the CodeMeter Runtime here:

https://www.wibu.com/downloads-user-software.html

and follow the given installation details.

6.2.1.2 TopSpin starts without license

TopSpin can start even without a valid license, then informing the user with an interactive dialogue about available licensing options.

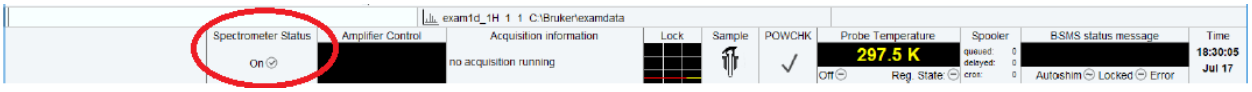


Additional Demo- and Academia-Licenses can be ordered free of charge from the Bruker Website:

https://www.bruker.com/service/support-upgrades/license-requests/nmr-license-requests.html

6.2.1.3 Spectrometer Control

The spectrometer is turned on / off with TopSpin command **pdudisp**.



6.2.1.4 64bit Environment

Topspin 4.0 on Linux is compiled for 64bit environment and needs no 32bit runtime environment anymore.

6.2.1.5 Changes in Software Architecture

Concerning the architecture of the software, the major difference to AVANCE III is that the computer embedded in the spectrometer (AVANCE III: IPSO, AVANCE NEO: EPU) is much more powerful and now hosts all of the software modules used for acquisition as well as the configuration files (i.e. the *conf/instr/spect* folder) of the spectrometer.

The latter is mirrored to a folder *<TSHOME>/conf/instr/remote_spect* on the workstation for the sake of transparency. This means that changing configuration data manually with an external editor will not affect the actual configuration on the spectrometer, but as long as the user interface of TopSpin is used the configuration is synchronized automatically and the changes will take effect as expected.

6.2.1.6 NMRSim integral part of TopSpin

Bruker simulation package NMR-Sim is now an integral part of TopSpin, the corresponding installer option was therefore removed. All NMR-Sim related functions (simulation, pulse program display…) are still available, however NMR-Sim cannot be started as standalone application.

6.2.1.7 Command plot0 temporarily not available

The legacy standalone plot editor as launched by command **plot0** is temporarily not available in this release. A solution is in preparation for a next minor version.

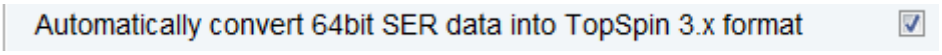
6.2.2 Acquisition

6.2.2.1 Multi-dimensional acquisition (ser-Files) written as 64 bit values

FIDs for multi-dimensional acquisitions (ser-files) are now written as 64 bit values compared to 32bit in older versions of topspin.

As a consequence, it is now not directly possible anymore to process those 64bit ser-files with TopSpin 3.5 or older without converting the data back to 32bit format.

In order to keep compatibility, this conversion is currently automatically performed in TopSpin 4.0 after each acquisition but can be deactivated in the Preferences-menu:



In case you need to optimize acquisition speed or keep GLP-compliance this checkbox should be deactivated.

Even after the acquisition it is always possible to convert ser-files from 64bit to 32bit and back using the au-programs sertoint and sertodouble.

6.2.2.2 cf: combo-box asking for magnet polarity

In **cf**, there is now a combo box that optionally allows to make the polarity of the magnet known to the software. This value is later on used by the BSMS to determine the direction of its shim currents.

6.2.2.3 AQ_mod

The acquisition modes qf, qsim and qseq are obsolete with AVANCE NEO due to the increased performance of the receiver hardware. AQ_mod=DQD can now be used over the whole range of possible sweep widths.

6.2.2.4 What is new in WaveMaker

New parameter (`d1`) allows arbitrary positioning of shaped pulses when constructing complex waveforms, such as composite adiabatic pulses, CHORUS, ABSTRUSE and similar.

Optimized notch pulses often used in bio-molecular NMR experiments, such as SOFAST and BEST type experiments automatically adjust the notch position depending on the flipangle variations.

New arrivals in the WaveMaker shape library – 25 new shapes have been added including five BIP pulses (inversion), e-family pulses (excitation) and Q5sebop (excitation).

6.2.2.5 Command wobbt replaced

The topspin command **wobbt** has been replaced by **wobb thick**.

6.2.2.6 New MAS3-firmware

A new firmware for MAS3 containing significant improvements has been released (available in <*TopspinHome*>*/conf/instr/servtool/mas3*).

6.2.3 Processing

6.2.3.1 2D/nD processing with FnILOOP

Multidimensional AVANCE NEO data sets contain a new acquisition status parameter FnILOOP in each non acquisition dimension. This parameter describes the number of inner loops in this dimension. If one of the FnILOOP status parameters is > 1 the split AU program specified in the pulseprogram must be applied to separate the inner loops.

In contrast to pre AVANCE NEO data sets the acquisition status parameter TD in non acquisition dimensions no longer contains the number of inner loops and therefore is not reduced by the split AU programs.

6.2.4 Automation

6.2.4.1 IconNMR 5.1

User Manager Update Experiment List Tool

- Easily discover and add new experiments contained within this TopSpin release
- Search for experiments in the user's experiment list

General Automation

- Handle Multi-Receive Experiments simply as composite experiments
- Suggest which sample position to use next at login time
- Dedicated SampleCase automation driver
- Improved configuration user interface experience
- Show the sample temperature in the automation window status line (also available in current TopSpin 3.5 Versions)
- Heat individual SampleCase samples as necessary just in time before they are inserted (also available in current TopSpin 3.5 Versions)
- Spreadsheet Import uses flexible column names (also available in current TopSpin 3.5 Versions)

6.2.5 Pulse Programming

6.2.5.1 Command dccorr obsolete

Command **dccorr** is obsolete because the correction is automatically done by the hardware.

6.2.5.2 Command spf obsolete

Command **spf** is no longer needed, because the complete functionality is covered by command **sp**.

6.2.5.3 Command anavpt obsolete

Command **anavpt** is obsolete, because there is no analogue mode anymore.

6.2.5.4 Pulse Program: New RTP Macros

Most of the RTP macros used in the pulse program had to be changed to be in accordance with the architecture of AVANCE NEO, especially those that are used for explicit dwell generation. In rare cases this will cause compilation errors in user-defined pulse programs. Please refer to the Pulse Programming Manual for further details.

6.2.5.5 External Dwell Pulses

The `go` and `adc` statements instruct the digitizer to acquire the desired number of data points with a rate given by the *dwell time*. The dwell pulse (only a short dwell pulse is necessary to acquire a complete scan) is generated by the TRX which is dedicated to the observe channel. This is the meaning of the macro `DWELL_GEN` which evaluates to the statement:

```
aq cpdngs17:f1
```

Please note that DWL_CLK_ON/DWL_CLK_OFF is no longer used.

For further information please look up Pulse Programming Manual section 10.1.8 “External Dwell Pulses”.

6.2.5.6 Parameter DIGMOD

With AVANCE NEO, all incoming FIDs are now digitally filtered, therefore the parameter DIGMOD is now always set to ‘digital’, and the alternative ‘analog’ has become obsolete. Nevertheless, it is of course still possible to acquire single data points explicitly. Please refer to the Pulse Programming Manual for further details.

6.2.5.7 Compile-time variable grpdly

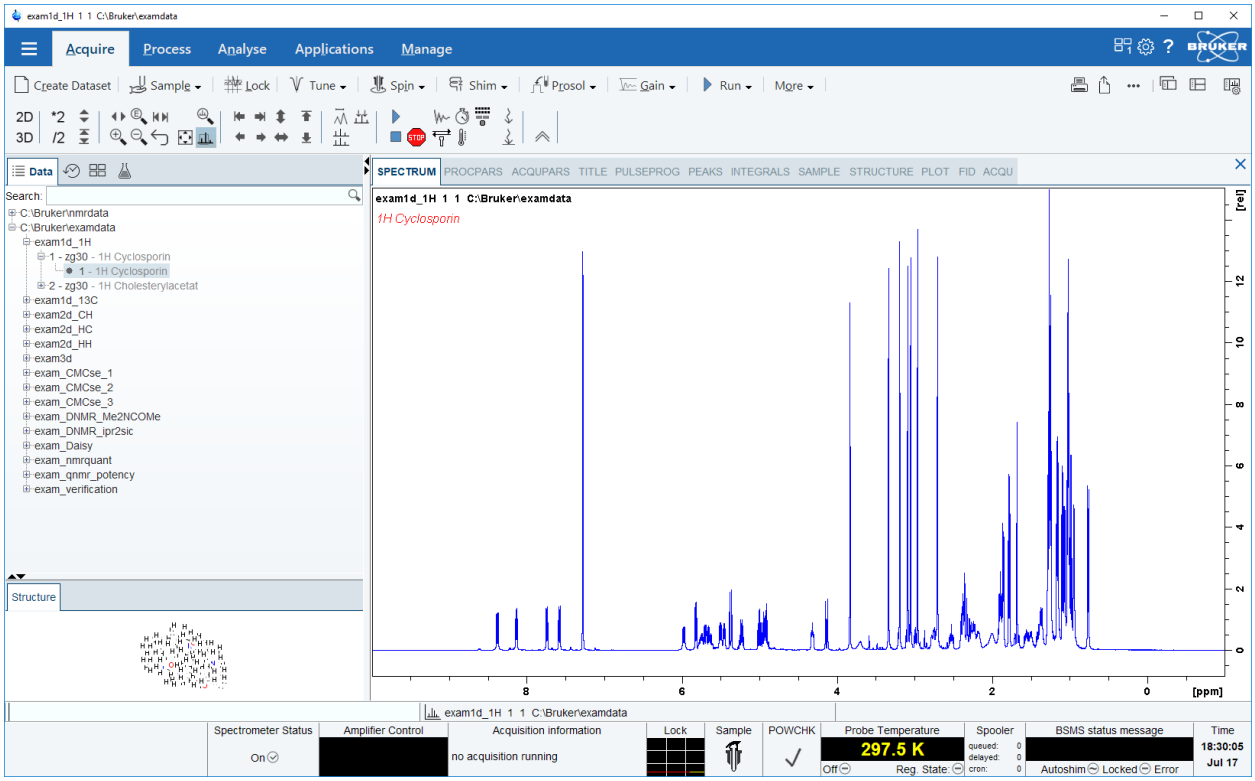
The group delay is available in the pulseprogram as compile-time variable **grpdly**.

It is defined as number of complex points, i.e. a group delay of 78 means that the first 156 points of the FID are affected by the length of the filter pipeline.

For further information please look up the Pulse Programming User Manual.

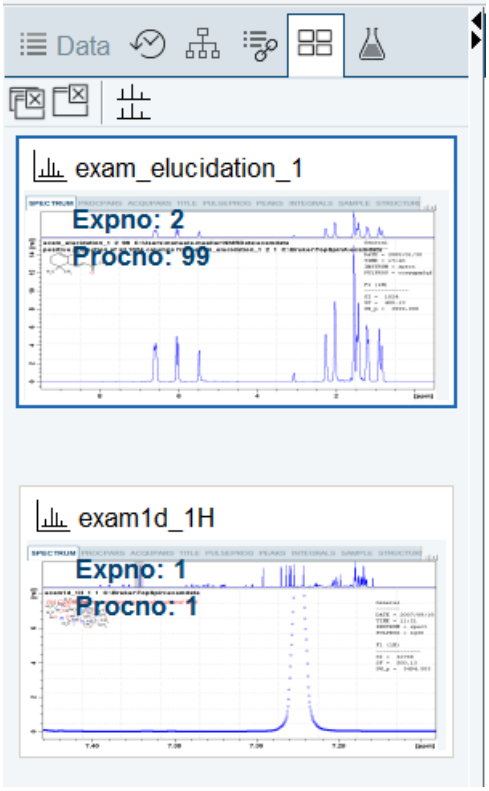
6.2.6 General User Interface

The TopSpin 4 graphical user interface has been modernized and rearranged. A primary goal of this redesign has been to provide the familiar functionality and commands with improved ergonomy and efficiency for daily use. Some adjustments and additions have been made for the AVANCE NEO spectrometer series. Please have a look at the new **Workplace Tour** found in the Help menu (click on the question mark in the top menu bar), and also the following sections.

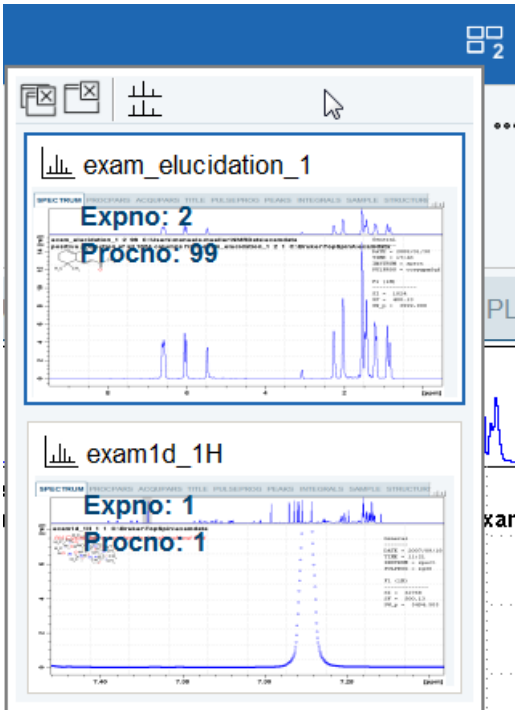


6.2.6.1 Window Switcher - Switch through open Data and Apps

To switch through open datasets use the overview in the Browser Panel or via menu button. Close all or the current Window in the overview. It is also possible to select multiple datasets while pressing CTRL and click datasets in the overview. Close selected window or open it in a multiple display overview.



Window Switcher Browser



Window Switcher Button

6.2.6.2 Quick access to change View Options

Get a quick access to switch the perspective (e.g. full screen), compare open datasets or change spectra view options in the Change View Options menu:

6.2.6.3 Quick access to Publish Options

Share your work from every point in your working routine with your colleagues, send to printer, export in optional data formats or “more” (e.g. copy and paste, send via email or use shared directories):

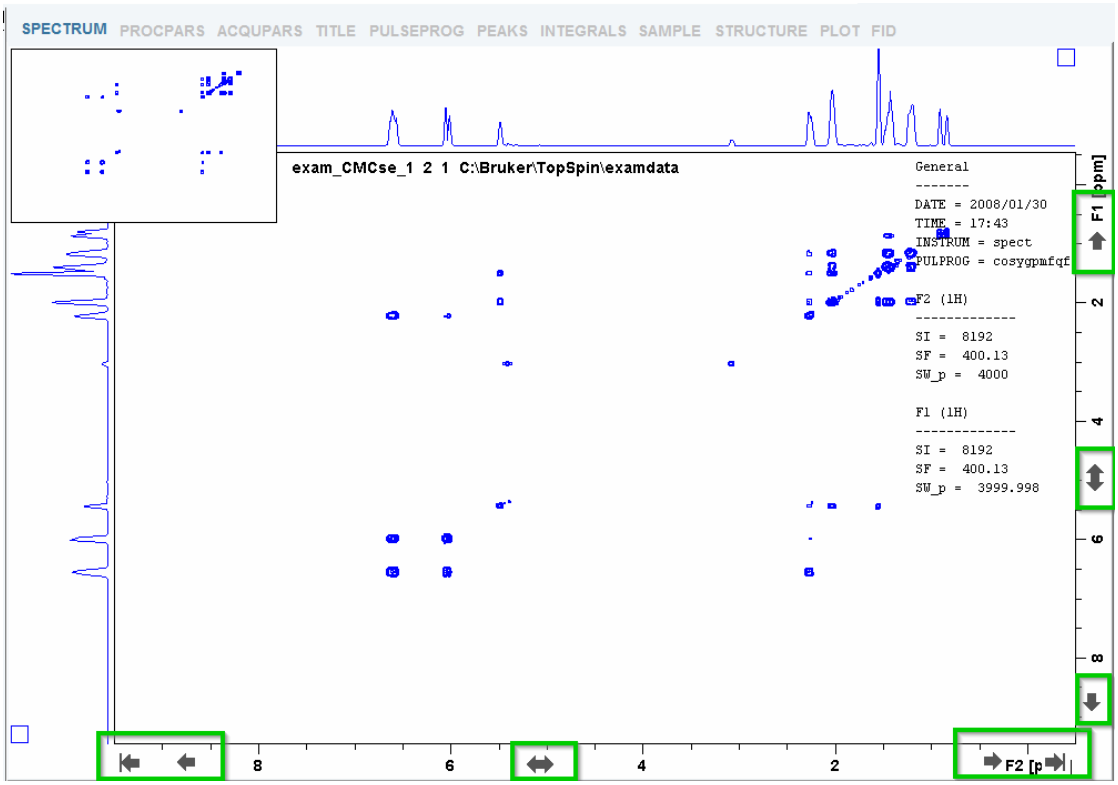
6.2.6.4 Quick Access to Setup Preferences

For all changes in the TopSpin appearance use the global Setup preferences button:

6.2.6.5 New Spectra axes scrolling and shifting behavior

New feature in the spectrum axis allows intuitive scrolling through the spectrum.

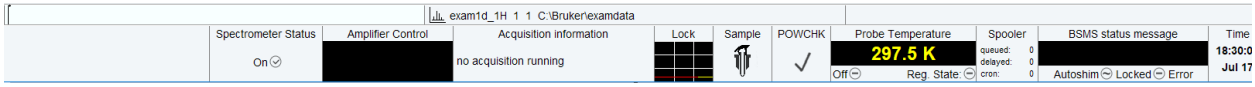
- Single Clicks on the end regions of the axes or a click and dragging the mouse shift through the axes depending on the mouse position (see the following figure).
- Double click in the middle of the spectra axes switch to full axes region.
- Double click in the middle of the spectra itself maximize all axes regions



6.2.6.6 New command line and status acquisition bar features

The line underneath the main TopSpin data window now contains three areas. The left area is the command area where commands can be entered, like **zg**. The middle area contains the dataset information. The right area is the status report area where progress on running commands is being displayed.

The acquisition status bar contains the new Spectrometer Status area to turn the spectrometer on and off. This functionality is also available through the Manage menu or the command **pdudisp**.



6.2.7 GLP Operation

During the installation of TopSpin, the new feature Central Audit File may be selected. This initiates the logging of all TopSpin related actions into one central audit file. This file is always appended to and never overwritten.

6.2.8 Analysis

6.2.8.1 Fragment Based Screening (FBS)

In TopSpin 4.0 we present a novel software tool for interactive analysis of NMR based screening data that is embedded within the software suite from Bruker, which now supports the workflow from data acquisition and processing to data analysis and hit reporting in the field of Fragment Based Lead Discovery (FBLD). The three most popular NMR experiments for fragment screening, Saturation Transfer Difference (STD), waterLOGSY, and relaxation based methods, are automatically identified. Reference 1D ^{1}H spectra of fragments are recognized by unique identifiers of the employed molecules and presented to the user in multi-display mode together with the screening spectra. Hits are visually identified and selected by mouse click on the display. The results are stored in a project file that is automatically loaded on program launch. The tool allows the most flexible implementation in individual laboratory environments with few restrictions with regard to data storage and preparation; for instance, no databases need to be prepared. In addition, automation routines for NMR based screening experiments that are part of the latest Topspin release are presented.

Please note that the FBS demo datasets can be downloaded from Bruker dropbox under the following link: *https://www.dropbox.com/s/v8y8hw3kxolly0m/demo_data_TS35pl7.zip?dl=0*

For further information look up the documentation „Fragment Based Screening Analysis Suite“ reachable with command **help fbs**.

6.3 TopSpin 4.0.2

6.3.1 Bug Fixes

The following topics describe the major fixes which come with TopSpin 4.0.2.

The topics are named by item numbers, referring to the Bruker knowledge base. For detailed information about the different items, please look up the Bruker knowledge base. The Bruker knowledge base can be found on the Bruker Web Server under the following address:

http://www.bruker.com/bkb_access.html?&no_cache=1

Please note: You need a login to access this section. If you haven’t registered yet, please register here:

https://www.bruker.com/about-us/register.html

If you are already connected to the internet and if you have access to the Bruker knowledge base, you can then open the respective item by entering the item number in the appearing window.

• Item # 14287	**rga** fails: No valid RG found after 18 steps
• Item # 14266	Logging in to TopSpin with internal user account 5 times unexpected behavior

• Item # 14257	Error: bad command invoke: must be **bbox, cget,** …
• Item # 14252	**AUDIT** command not working using dataset lists
• Item # 14251	19F routing problems with AVNEO
• Item # 14243	Barcode: Samples beyond row#99 in “Experiment Table” not wasted
• Item # 14233	Pulse programming: incrementing shape lists does not work

6.3.2 New Features

6.3.2.1 General

TopSpin is free for academic use since version 3.5. Academic users can create their personal license ticket after login into the Bruker web pages and activate their installation. When TopSpin has been started with an free Academic license, this is indicated in the title bar of the main application window.

TopSpin informs the user by an information window upon application startup if the currently used license will expire in less than 30 days. This should give the user sufficient time for a renewal before the product license finally expires.

6.3.2.2 Acquisition

In the ‘set’ menu, one can now activate an automatic scaling of the FID by RG and/or NS. The options are “Scale acquired FID according to receiver gain” and “Scale acquired FID according to number of scans”.

Please note that above options may be an issue if you run ERETIC experiments, or if you use data sets with scaled RG in older versions of TopSpin. In these cases automatic scaling must be deactivated.

Independent of the scaling options set in the user interface, you can always run an acquisition without those scaling options by starting zg with the command line parameters “–forceNeverDivideByRg” and/or “–forceNeverDivideByNs”, respectively.

There is also a boolean value in the status acquisition parameters file (acqus) indicating whether the respective option has been used (scaleByRG and scaleByNS).

The new cortab files have a different nomenclature and are not backwards compatible (but old cortab files are forward compatible). Old cortab files are automatically copied into the new format (you have to start ‘cortab’ once to run this procedure) so that they can be used with all versions of TopSpin 4.

Please note that you still can use the old cortab files without problems.

The userA1 – userA5 parameters can be used to hold complete WaveMaker waveform definitions avoiding the need to make changes in the pulse program comments area. In that way automatic pulse shaping can be applied to the sequences in the standard Bruker pulse program library.

New parameter (`d1`) allows arbitrary positioning of shaped pulses when constructing complex waveforms, such as composite adiabatic pulses, CHORUS, ABSTRUSE and similar.

Optimized notch pulses often used in bio-molecular NMR experiments, such as SOFAST and BEST type experiments automatically adjust the notch position depending on the flipangle variations.

New arrivals in the WaveMaker shape library – 25 new shapes have been added including five BIP pulses (inversion), e-family pulses (excitation) and Q5sebop (excitation).

6.3.2.3 Automation

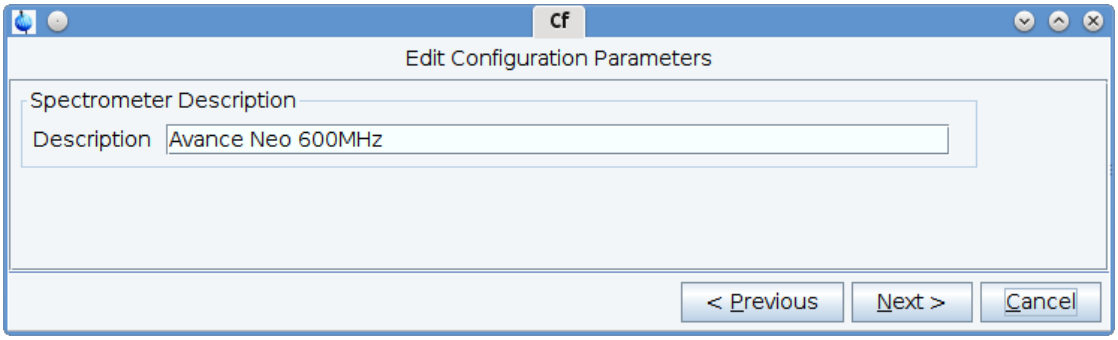
- Option to hide the sref message: “reference peak not found default calibration done” from Preceding Experiments->Remarks
- Assure-SST allows for setting of the Shim routine individually for all SST experiments
- New Dual Receive Composite Experiment Definitions: COSY, HSQC and TOCSY
- New languages available: Chinese, French, Italian, Korean, Portuguese

6.3.2.4 Pulse Programming

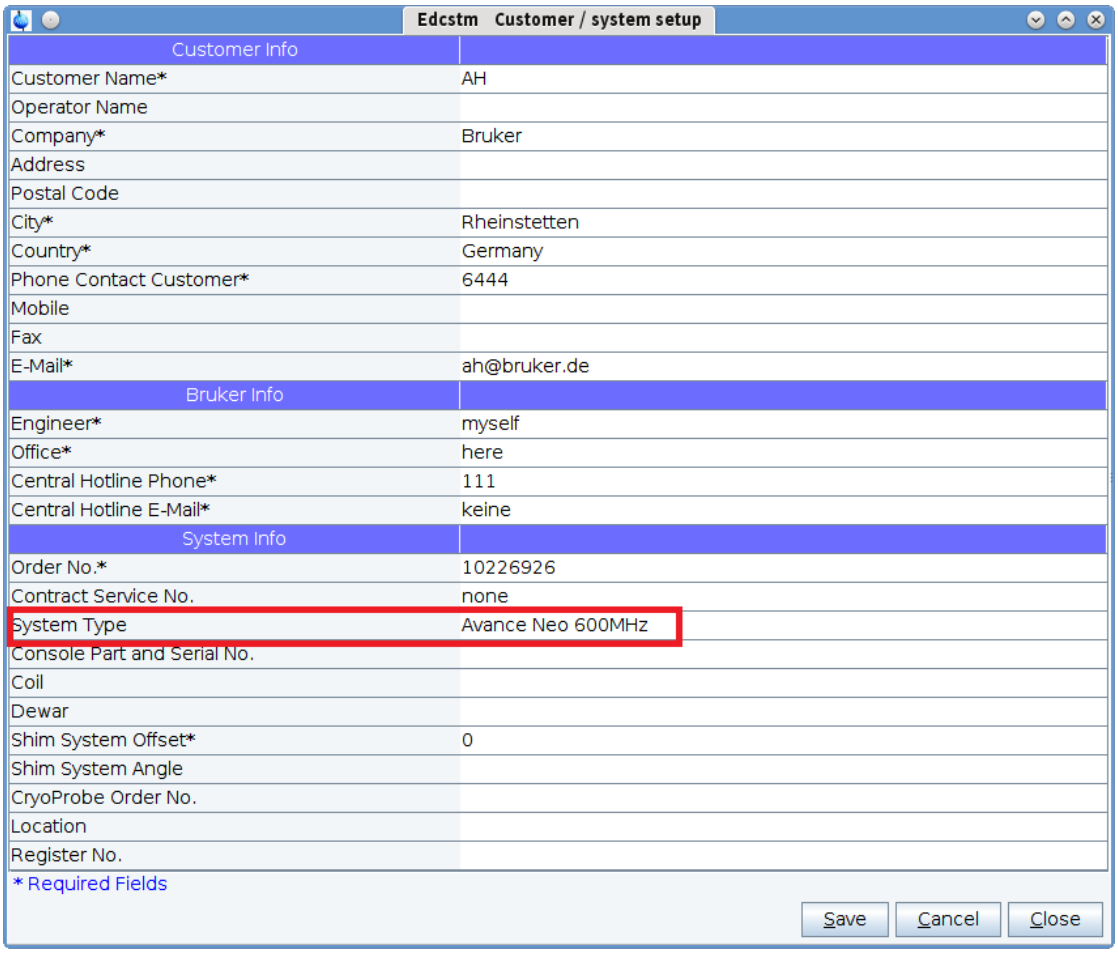
- Bracket operator for lists now working (e.g. powerList[2]:f1)
- Shape lists now available (list<shape>)
- Modification of RG now possible from within the pulse program using a list<receiverGain> Please refer to the Pulse Programming Manual for further details (“Receiver Gain Lists”).

6.3.2.5 General User Interface

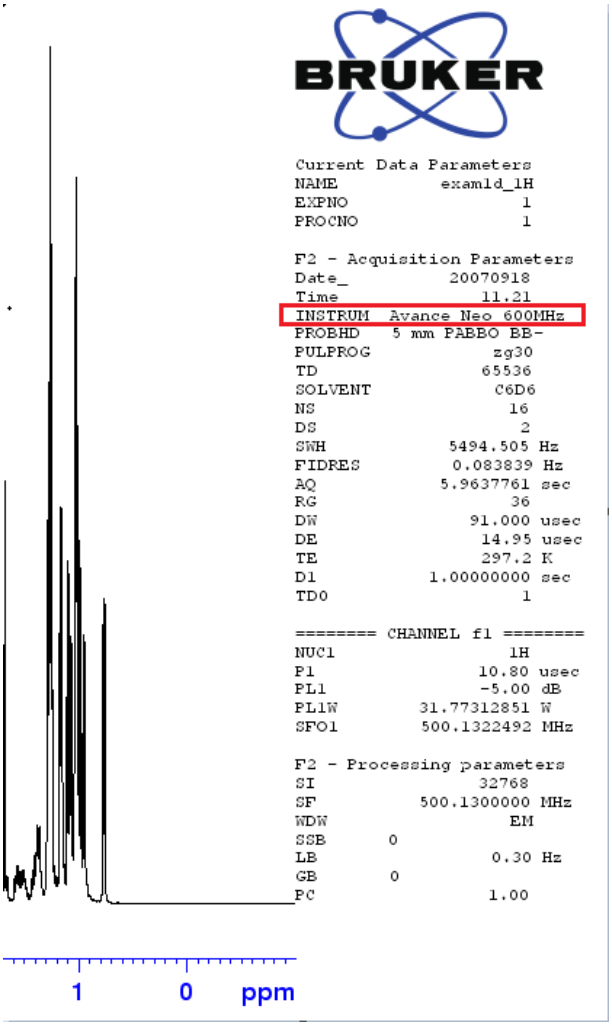
The acquisition status parameter INSTRUM now contains the spectrometer description from cf instead of always "spect". With AVANCE NEO the Spectrometer Description can be edited during **cf**.



Command **edcstm** offers the possibility to edit “System Type”.



The Spectrometer Description is shown in plot legend.



Some flow-bar menus offer a default action when the menu button is clicked directly. This default action is now also shown in the drop-down menu again for convenience and more consistent navigation.

The integrated search functionality in the data browser tab allows to quickly filter for certain data sets. However, the traditional Find dialog had become hidden in the menu system and is now offered again via the 'Find' button directly in the search filter box. The Find dialog now includes the field SPECTYP which relates to the value of this parameter in the data sets searched. Additionally, the keyboard shortcut Ctrl+F can be used to bring up this dialog.

6.3.2.6 GxP Operation

The system administrator can configure more restraints for internal users in order to enhance compliance with GxP regulations:

- Password complexity can be set. An option is available that requires passwords to include at least one character out of each group of characters such as lowercase, uppercase, digit.
- Password aging: It is possible to define that passwords expire after a certain number of days. An expired password needs to be renewed by the user at next occasion when a user authentication is requested by the software. The new password must not be identical to the previous password. It is possible to disable password expiration.

- The default minimum password length is 8 characters when new passwords are set. The minimum password length can be configured. For existing internal users it is sufficient to maintain that condition first when a new password is set.
- Internal accounts can be set to “disabled” or “enabled” instead of being deleted immediately. “Remove” operation proposes to use “Disable” instead.

The command **lockdataset** had been introduced with TopSpin 3.5pl7 for Windows only and is available on command line and from the "Security" flow menu. This functionality is now available for both Windows and Linux environments. Under Linux, execution of **lockdataset** will remove all write permissions from the current dataset including all existing PROCNO directories. It prohibits adding new PROCNO directories since the permission concept of the Unix file system enforces this restriction. The implementation for Windows allows to add new PROCNOs even if the dataset has been locked.

Additionally, a command **unlockdataset** is offered now which allows to take back the lock state. This command requests the user to provide the NMR Administration password in order to authorize the action. The command is not available in the flow menus and can only be entered at the command line. Customers who disallow this functionality in their laboratory's standard operating procedures should remove the AU program 'unlockdataset' from an installation.

6.3.2.7 Plot Editor

The legacy stand-alone plot editor is available again (it was missing in TopSpin 4.0.1) and can be launched with the command 'plot0' for Windows and Linux. Please note the external editor is only provided for convenience and will not contain further developments as found in the integrated Plot tab.

When the Plot tab is selected, data sets can be dragged from the data browser tree to the plot area. Data objects for these data sets are added to the actual layout view then. The dataset portfolio is updated automatically as required. 1D data sets can be added to 1D layouts. This allows to quickly create an overview of several 1D experiments. 1D data sets dragged to 2D layouts will automatically be used as projections of the first 2D object. Dragging 2D datasets to 2D layouts is not supported.

6.3.2.8 AU programming

- The new AU program measureHelev triggers a measurement of the Helium level.
  In addition, the He-log-file can then be copied from EPU to workstation using the AU program getheliumlog.
- AU program bt_calibrate_o1 now working.

6.4 TopSpin 4.0.3

6.4.1 Bug Fixes

The following topics describe the major fixes which come with TopSpin 4.0.3.

The topics are named by item numbers, referring to the Bruker knowledge base. For detailed information about the different items, please look up the Bruker knowledge base. The Bruker knowledge base can be found on the Bruker Web Server under the following address:

http://www.bruker.com/bkb_access.html?&no_cache=1

Please note: You need a login to access this section. If you haven’t registered yet, please register here:

https://www.bruker.com/about-us/register.html

If you are already connected to the internet and if you have access to the Bruker knowledge base, you can then open the respective item by entering the item number in the appearing window.

• Item # 14380	Eretic output is not correct for low concentrated samples
• Item # 14379	Export pf PDF file fails
• Item # 14248	Multiple buffer acquisition doesn't work for some TD values

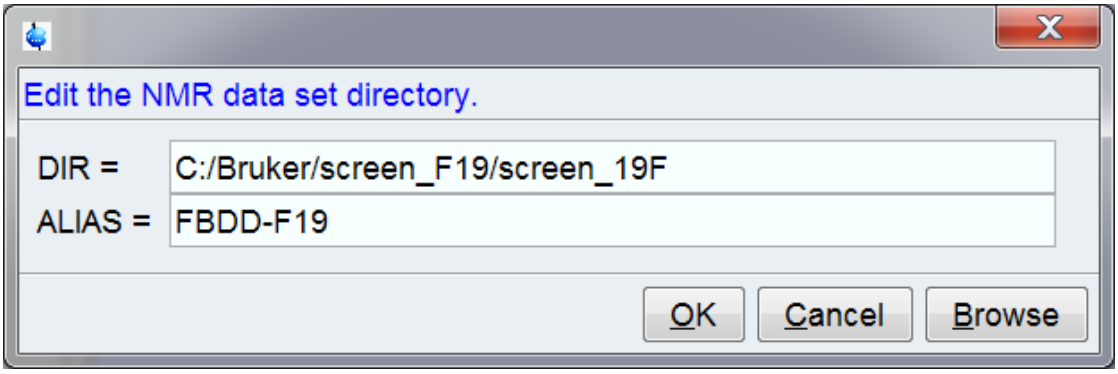
6.4.2 New Features

6.4.2.1 General

6.4.2.2 User Interface

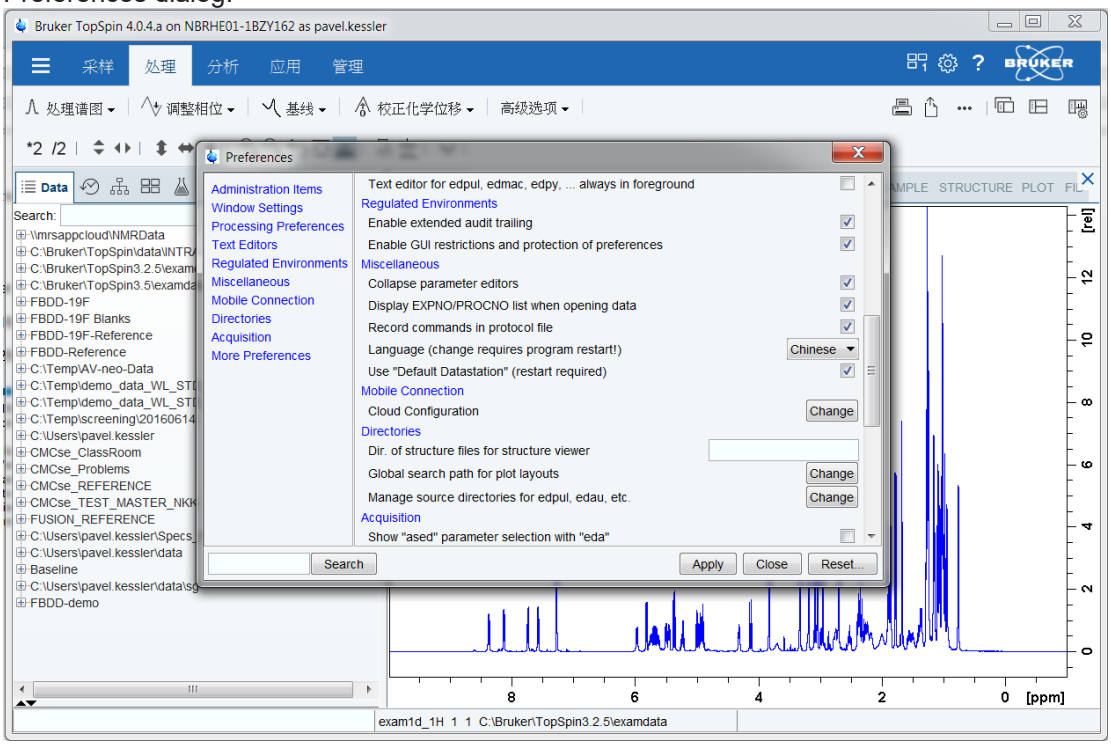
The data directories in the Data Browser can be edited now.

Invoking “**Edit Selected Data Dir**” in the data browser popup menu opens a dialog allowing to modify the data folder and its alias name.



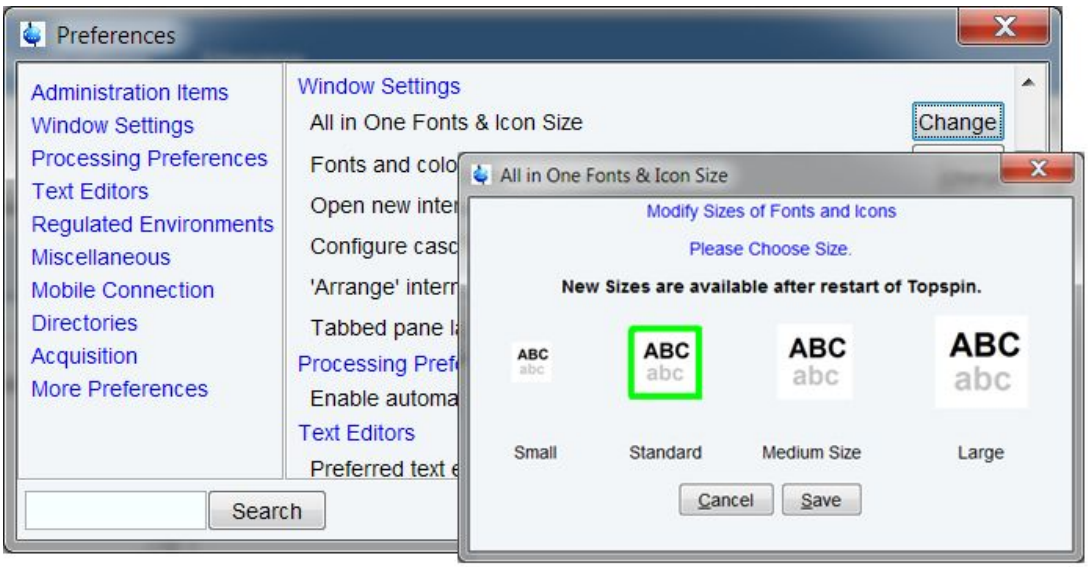
Topspin flow menus are now also available in Chinese translation.

The desired translation (currently English and Chinese) may be selected from the Topspin Preferences dialog.



Applications running on high resolution (4k) displays require often larger fonts and icon.

The TopSpin Prefrences dialog allows to select one of the predefined configurations matching typical screen resolutions.



The dialog offering options for license requests and management can be opened at any time now by choosing **Bruker License** from the Help menu (question mark). Legal information about involved licenses is accessible by the menu entry **3rd party licenses**.

The display of TopSpin's Command History (menu **Manage | Commands**) merges several protocol files into one single track. The included sources can be selected individually now.

6.4.2.3 System Support

6.4.2.4 Acquisition

- The **wvm** command is now available for automation. The ‘quiet’ option, **-q** works in the same way as the auto-setup option, **-a**, except it does not activate the **ased** command making the **wvm** command compliant with the automation requirements and the Icon NMR protocols.
- The **userA1-userA5** parameters can now be used to define waveforms *(sp, gp, cpd)* exactly in the same way as they are defined in the comments section of the pulse programs. This avoids the need for modifying the pulse programs and allows re-definition of shaped pulses for experiments in the standard Bruker pulse program library. The shape definitions are saved with the data (parameter) sets and avoid a potential confusion if the pulse program is changed at a later stage.
- The **userA1-userA5** parameters can also be used to re-define the shape functions. For instance, the *eburp1(450 Hz)* shape can be defined as *userA1(450 Hz)* with the *userA1* parameter set to *eburp1*. A simple change of the *userA1* parameter then allows creating the same shaped pulse or decoupling waveform, but with a different shape. This provides more flexibility to the experiment setup.
- The –b option activates the Bloch simulator and shows the excitation profile of the newly created shape(s). In applications with several shapes the shape number can be specified, e.g. wvm –b 3 (see figure below).

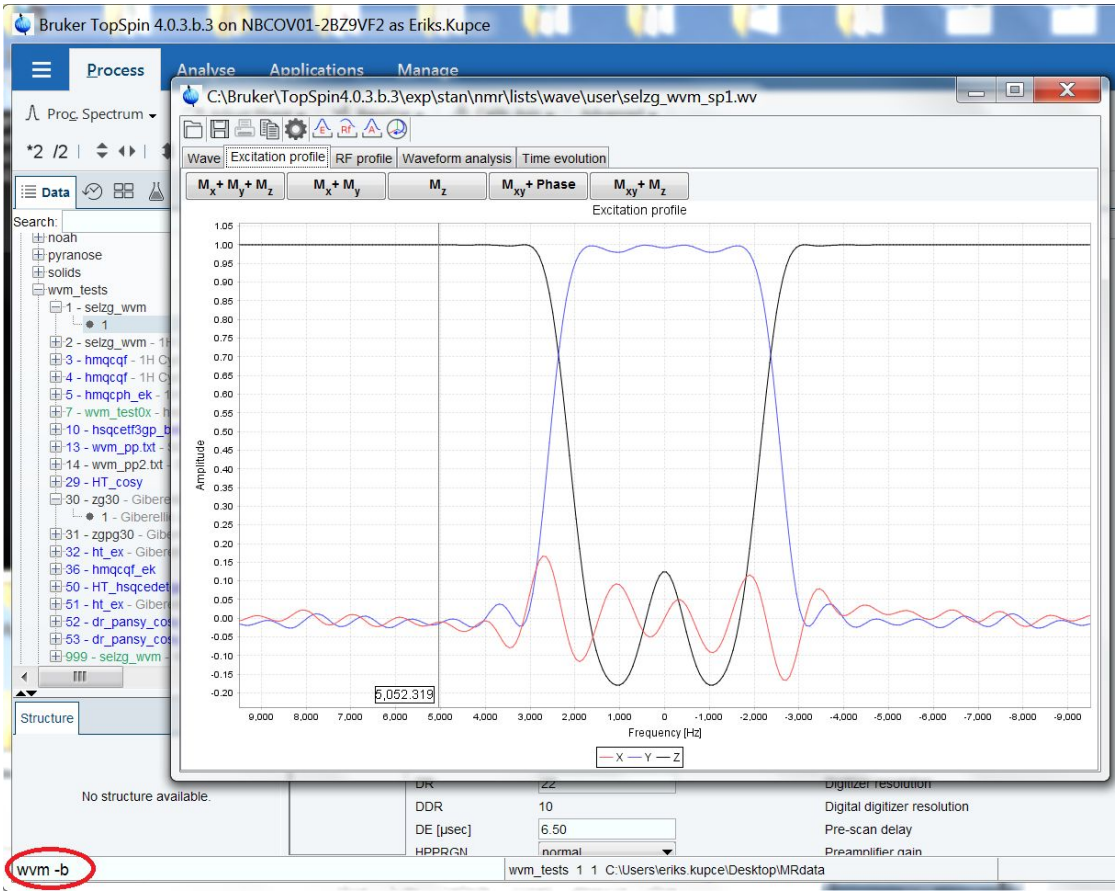


Figure 6.1: The wvm-b option in WaveMaker shows the excitation profile of the shaped pulse(s).

With this latest version of TopSolids you can use the command **topsolids** to open the interface directly from the TopSpin command line.

We introduce a flow bar navigation, which is divided into applications for protein and material (= non-protein) samples. In this context, we re-arranged the “Materials” part of TopSolids into three subdivisions and added new features:

1. “1D Direct Excitation”
2. “1D/2D CP-based Experiments”
3. “1D/2D MQMAS”

Though these new flow bars work independently, optimized parameters are shared between the different modules if needed. Furthermore, for many steps you can decide to optimize parameters on a standard sample first or directly on your sample of interest.

We included the setup of a 2D H-X Hetcor experiment in the “1D/2D CP-based Experiments”. TopSolids automatically checks if the needed cross polarization parameters have been optimized already. If not, it will directly start the optimization, before continuing with the 2D setup.

To avoid offset errors within the automation, the step “Shimming & Referencing” in the “Probe Setup” flow bar is now mandatory for each new TopSolids project.

For security reasons, the import of previous TopSolids Parameter data files (“topsolidsPars.xml”) is allowed if both projects have been create with the same version of TopSolids.

The step “ 13C 90deg Pulse Optimization” in the “Probe Setup” flow bar is up and running again.

New option for **rga** to set a fixed delay: For example, “**rga –setD0=0.02**” sets d0 to 20msec. In this way you could head for the row with maximum intensity in your nD-experiment.

Currently when the sample rotation is active, it stays active when ejecting the sample. This can lead to problems when the next sample is inserted. It can happen that this sample does not fully fall down into the probe because of the still active sample rotation. Now the sample rotation is switched off before the sample is changed.

6.4.2.5 Processing

Parameter SPECTYP specifies the content of the processed data, is used in several application like CMC-se or Fragment Based Screening to identify spectra like HSQC or COSY and Topspin now always updates the status value when the foreground value changed.

Therefore it is not anymore necessary to change the status value as described in the CMC-se or Fragment Based Screening documentation.

The type of the parameter INTSCL changed from float to double (Knowledge Base #Item 14009). So all AU programs evaluating the parameter INTSCL must be changed and supply the address of a double variable as 2nd argument of FETCHPAR / FETCHPARS.

e.g.

float intscl;

FETCHPARS("INTSCL", &intscl)

must be changed to

double intscl;

FETCHPARS("INTSCL", &intscl)

Omitting this adaption will cause runtime errors during execution of the AU program.

6.4.2.6 Automation

- Option to hide the sref message: “reference peak not found default calibration done” from Preceding Experiments->Remarks
- Assure-SST allows for setting of the Shim routine individually for all SST experiments
- New Dual Receive Composite Experiment Definitions: COSY, HSQC and TOCSY
- New languages available: Chinese, French, Italian, Korean, Portuguese

BEST-NMR with Bruker LiquidHandler 215 no more available in TopSpin 4.0.3

6.4.2.7 Pulse Programming

- Bracket operator for lists now working (e.g. powerList[2]:f1)
- Shape lists now available (list<shape>)
- Modification of RG now possible from within the pulse program using a list<receiverGain> Please refer to the Pulse Programming Manual for further details (“Receiver Gain Lists”).

6.4.2.8 GxP Operation

In contrast to previous TopSpin versions, the login dialog does not offer a list of known user IDs in a list for selection. The dialog requires the user to enter both a valid user ID and its corresponding password. In case of invalid input the error message is intentionally unspecific. As a result the login process does not disclose known user IDs, and failed login attempts do not disclose whether a user ID really exists or not. This change had been introduced with TopSpin 4.0.2 already but was not included in the Release Letter.

Topspin maintains a log of startup, shutdown, and internal login/logoff events. This file is protected against unauthorized changes by checksums for every entry. The consistency of the complete log is checked with any new entry made, and inconsistencies logged as a warning message.

The content has been improved to now specifying a “system.user” and “intern.user” for every entry, where “system.user” states the currently used account of the operating system “intern.user” states the TopSpin internal user ID which can be different. If the internal login functionality has not been used, intern.user will be logged as “unknown”.

In case a login attempt has failed e.g. due to unknown user ID or wrong password specified, the entry only uses the entered user ID but not any resolution against existing user IDs. So failed login attempts do not disclose whether a specified user ID really exists or not.

TopSpin data may be viewed using the “-developer” option at TopSpin startup. No license is required for this case.

For the sole review of data sets and audit logs, TopSpin can be started in a review-only mode which does not require an active product license. This is performed by using the command line option “-developer” at start-up:

- On Windows, click on Start, select Bruker NMR Software / Bruker 4.x Utilities / Command Prompt, then enter “*topspin -developer*”
- On Linux / macOS, open a shell, change to the installation directory of this version, then enter “*./topspin -developer*”

6.5 TopSpin 4.0.4

6.5.1 Bug Fixes

The following topics describe the major fixes which come with TopSpin 4.0.4.

The topics are named by item numbers, referring to the Bruker knowledge base. For detailed information about the different items, please look up the Bruker knowledge base. The Bruker knowledge base can be found on the Bruker Web Server under the following address:

http://www.bruker.com/bkb_access.html?&no_cache=1

Please note: You need a login to access this section. If you haven't registered yet, please register here:

https://www.bruker.com/about-us/register.html

If you are already connected to the internet and if you have access to the Bruker knowledge base, you can then open the respective item by entering the item number in the appearing window.

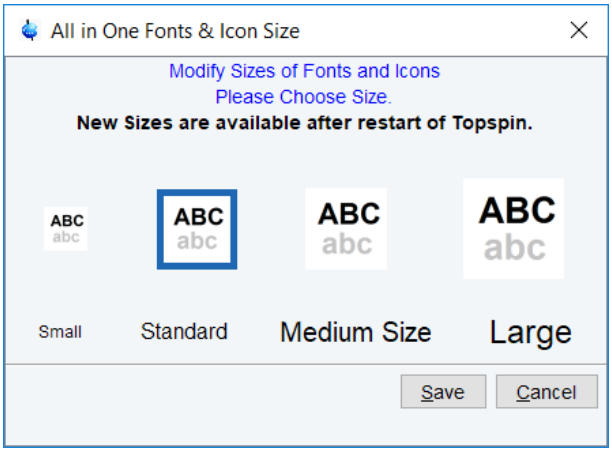
• Item #14460	Barcode Operation: Experiments may be performed on an incorrect sample
• Item #14459	**topshim** fails with THF-H8 solvent
• Item #14458	Sample Express Lite not very suitable for Easy Setup Mode
• Item #14441	proc_1dglp doesn't work with a data path containing a blank character
• Item #14432	Spreadsheet import only increments expno by 1
• Item #14423	INTSCL is wrongly listed as a float in the AU programming manual
• Item #14391	TopShim performs bad after changing from 4.0.1 to 4.0.2 on magnet with inversed polarity
• Item #14388	Emails of zip/jdx files fail if multiple sequential spaces in name
• Item #14383	No/wrong save of the color attributes in plot layouts
• Item #14382	Error messages appear in quick succession - Automation window inoperative
• Item #14378	Automatic spreadsheet import reports fake error
• Item #14373	pulseprogramming: reset:fx:fy does not work as expected
• Item #14371	Print or export to PDF/PS of multiple display output is missing dataset names
• Item #14369	Setting both night mode and start time hangs IconNMR
• Item #14367	**wobb** overwrites fq1list
• Item #14362	Slashes removed from Disk paths
• Item #14356	Spreadsheet import dialog will not open
• Item #14351	Experiment setup using spreadsheets imports always until last line
• Item #14348	Unresponsive Parameters, Analysis and Title popup windows in Experiment List
• Item #14346	Error message containing: AutoSet_Find_CheckAllAveragingCompleted appears
• Item #14345	Automation freezes with hourglass and has to be killed
• Item #14335	Originator item names with : at the end do not work
• Item # 14334	Missing box for path definition of structure file in plot layout

• Item #14325	AssureSST bad window path name error message
• Item #14320	File->Import Configuration does not set various configuration items
• Item #14319	Solvent/Probe dependent lock program settings lost
• Item #14317	Archiving may overwrite previously archived directory
• Item #14316	Invalid command name AutoSet_UpdateHistoryFile - Run crashes when processing switched off
• Item #14297	MWM lockdown mode not recognized
• Item #14295	Wrong user created when using the domain
• Item #14031	Read/Write parameter sets for multi-RX experiments
• Item #14030	Copy multi-RX data sets
• Item # 13601	**edprobe** connection changes might lead to incorrect default routing

6.5.2 New Features

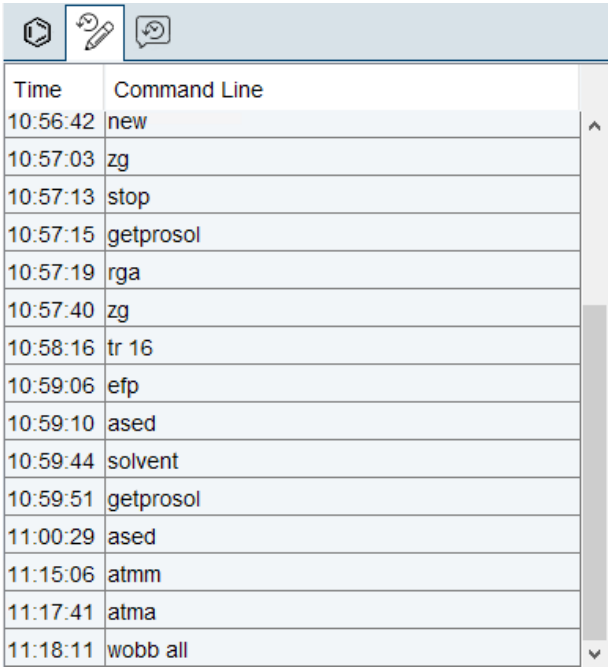
6.5.2.1 User Interface

Sizes of fonts and icons of the TopSpin General User Interface can be modified easily by clicking **Preferences | Windows settings | All in One Fonts & Icon size.** This improves TopSpin's behavior on high resolution displays.



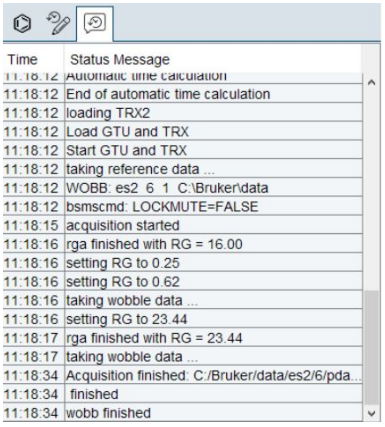
Please note that modified sizes of fonts and icons are available after restart of TopSpin.

The new tab Command Line History, located in the menu bar of the Data Browser window, shows the history of previously entered commands.



Time	Command Line
10:56:42	new
10:57:03	zg
10:57:13	stop
10:57:15	getprosol
10:57:19	rga
10:57:40	zg
10:58:16	tr 16
10:59:06	efp
10:59:10	ased
10:59:44	solvent
10:59:51	getprosol
11:00:29	ased
11:15:06	atmm
11:17:41	atma
11:18:11	wobb all

The new tab Status Message History, located in the menu bar of the Data Browser window, shows the history of TopSpin's status messages.



Time	Status Message
11:18:12	Automatic time calculation
11:18:12	End of automatic time calculation
11:18:12	loading TRX2
11:18:12	Load GTU and TRX
11:18:12	Start GTU and TRX
11:18:12	taking reference data ...
11:18:12	WOBB: es2_6_1_C:\Bruker\data
11:18:12	bsmscmd: LOCKMUTE=FALSE
11:18:15	acquisition started
11:18:16	rga finished with RG = 16.00
11:18:16	setting RG to 0.25
11:18:16	setting RG to 0.62
11:18:16	taking wobble data ...
11:18:16	setting RG to 23.44
11:18:17	rga finished with RG = 23.44
11:18:17	taking wobble data ...
11:18:34	Acquisition finished: C:/Bruker/data/es2/6/pda...
11:18:34	finished
11:18:34	wobb finished

6.5.2.2 Acquisition

The J-compensated adiabatic pulses are now calculated automatically using the following synatx:

`wurst(200 ppm; Jcomp)` – for adiabatic pulses immediately after the 180H pulse

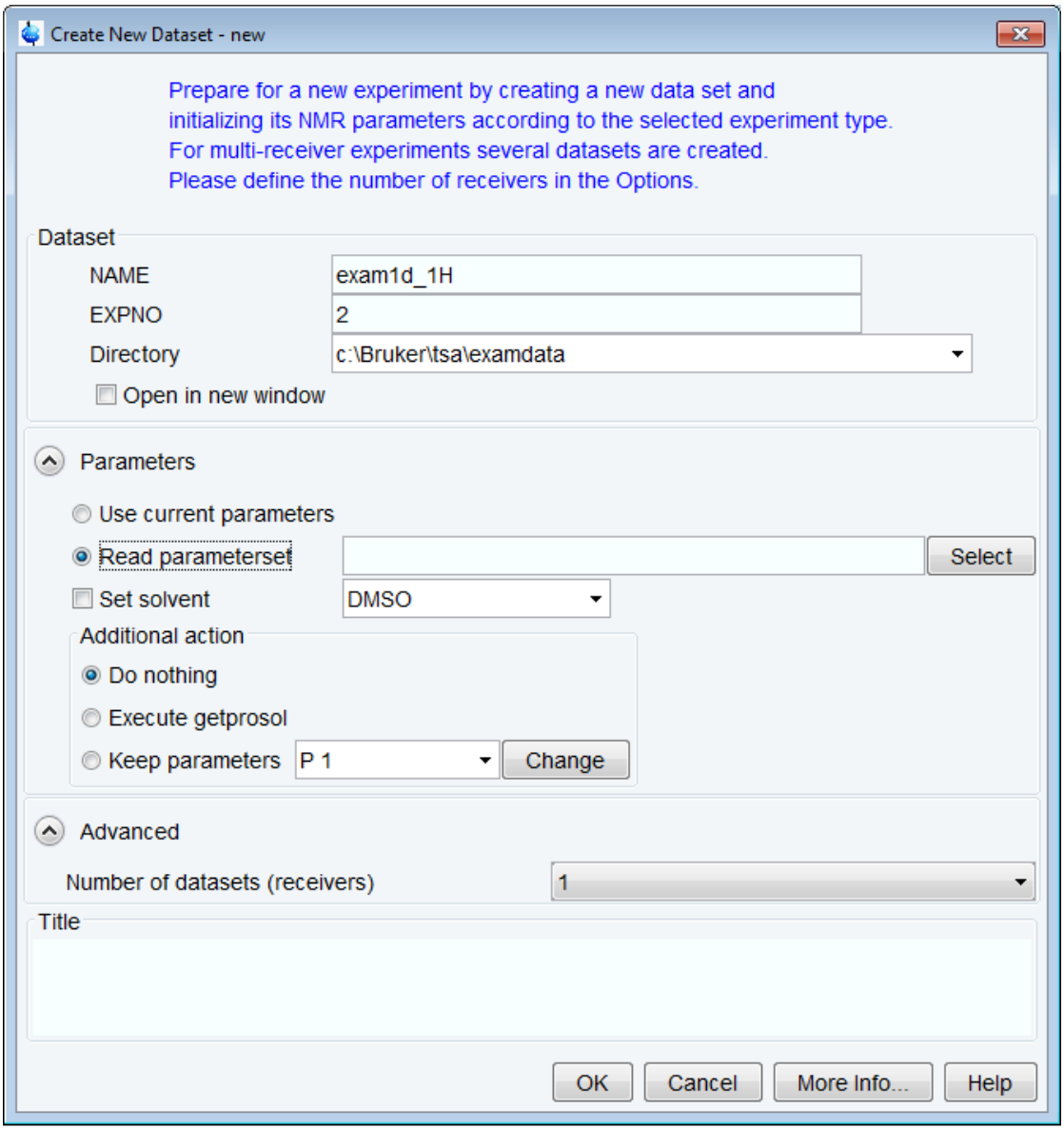
`wurst(200 ppm; L2H, Jcomp)` – for adiabatic pulses immediately before the 180H pulse

Users can define their own J vs CS correlation coefficients using the C2 (A) and C3 (B) constants.

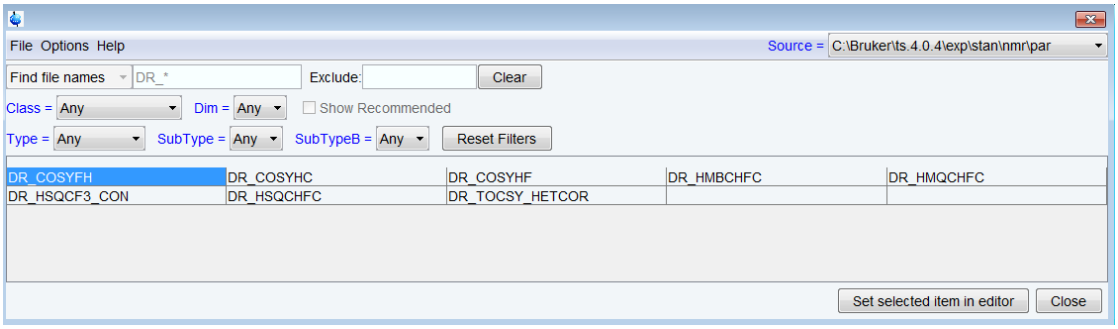
The optimum setting of the J-coupling is calculated provided the following pulse program syntax is used:

`"d2 = 0.5/cnst2" ;JCOMP` – indicates that cnst2 to be adjusted.

The **new/edc** command is now available for Multi-Receiver handling according to the selected experiment type.



The dialog offering the list of all parameter sets can be opened by using the **Select** button.

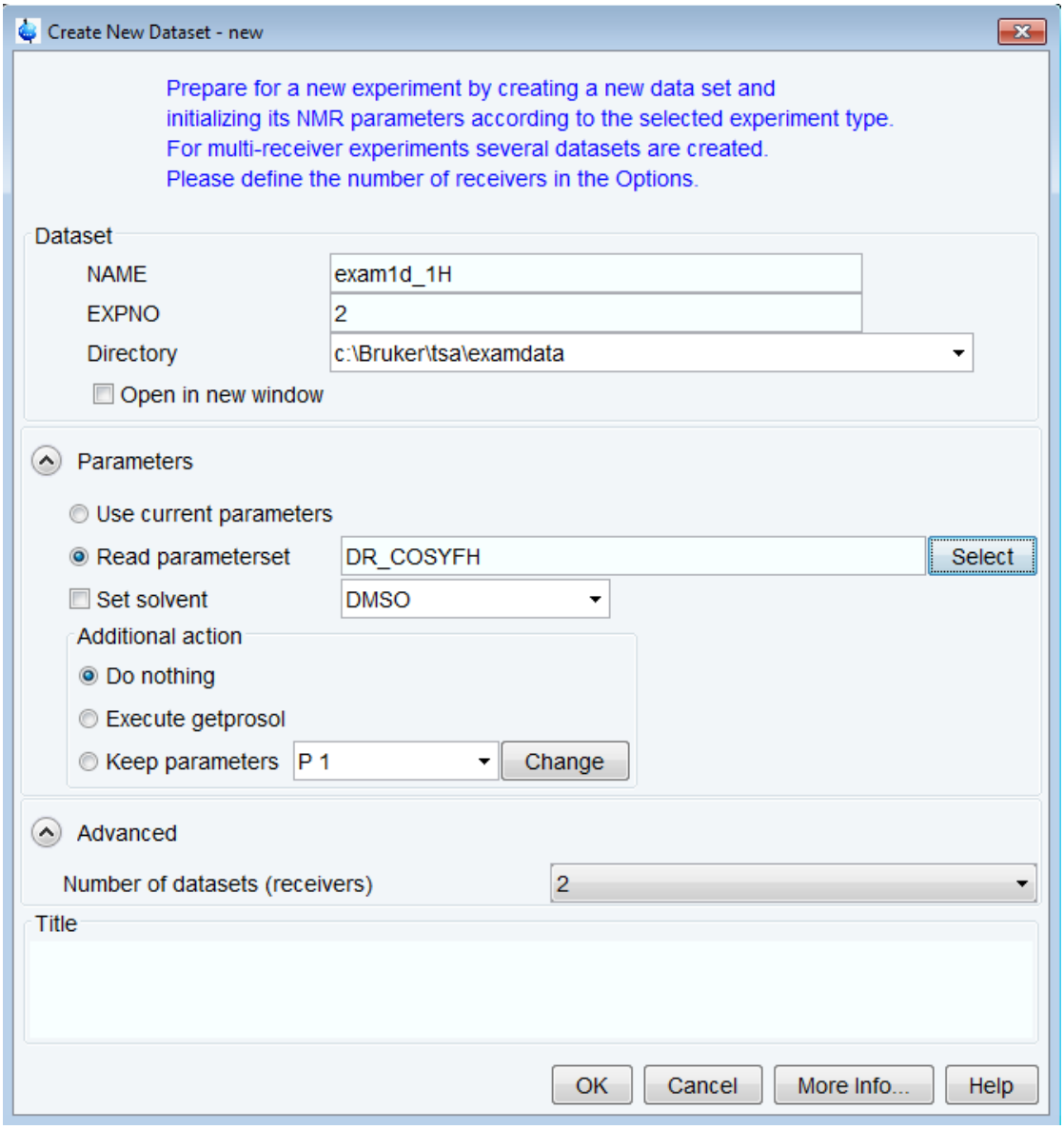


Entering “DR_*” in the **Find file names** field can be used to filter/display the Multiple receiver parameter sets.

Select the desired parameter set and close the dialog by clicking the button **Set selected item in editor**.

Then **edc** dialog reappears. The name of the Multiple receiver parameter sets and the number of datasets (receivers) will be set automatically.

When clicking **OK** the multiple receiver data set will be created, parent with EXPNO=2, child with EXPNO=3.



The commands **rpar** and **wpar** are both supporting multi receiver handling.

The AU program **iexpno** is supporting multi receiver handling too.

In **edprosol** pulse width and pulse power can now be printed for all nuclei at once with **File | Print | 90 deg. Pulses.**

Up to now pulse width and pulse power could only be printed for the selected nuclei.

edprobe: The default values for non-PICS HRMAS-probes have been improved.

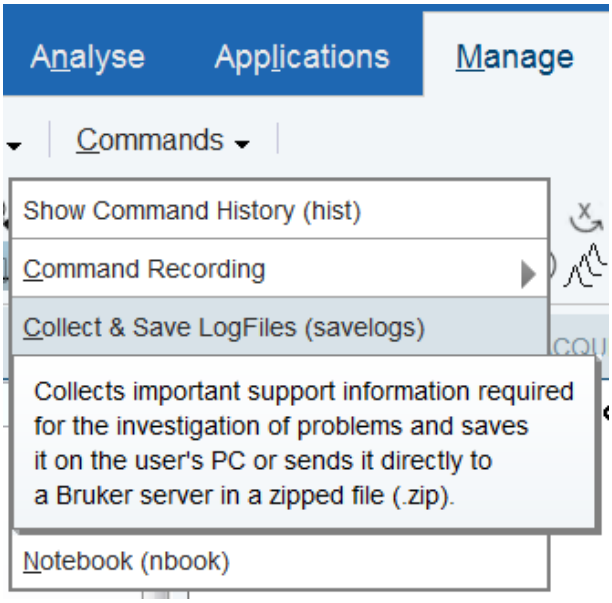
It is now possible to wobble more than one channel simultaneously. The following **wobble** commands are now available:

- **wobb**: standard wobble as before.
- **wobb f<x> f<y>:** simultaneous wobbling of channels F<x> and F<y> in **edasp**. For WBSW the respective array entries are used, i.e. WBSW[0] for channel F1, WBSW[1] for channel F2 etc. If WBSW[x] is 0 then WBSW[0] is used as a fallback.
- **wobb all**: simultaneous wobbling of all channels in **edasp** using the respective WBSW entries.

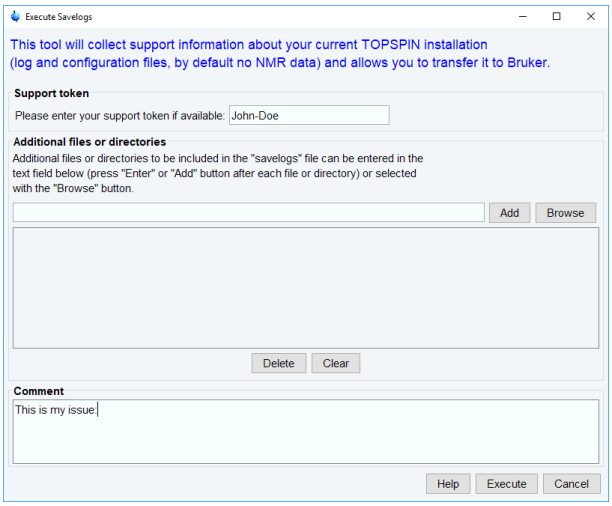
- **wobb wbst 1024 f1 wbsw 4.5 f2 wbsw 60**: simultaneous wobbling of channels f1 and f2 with WBST=1024, and f1 using 4.5MHz and f2 using 60MHz for WBSW

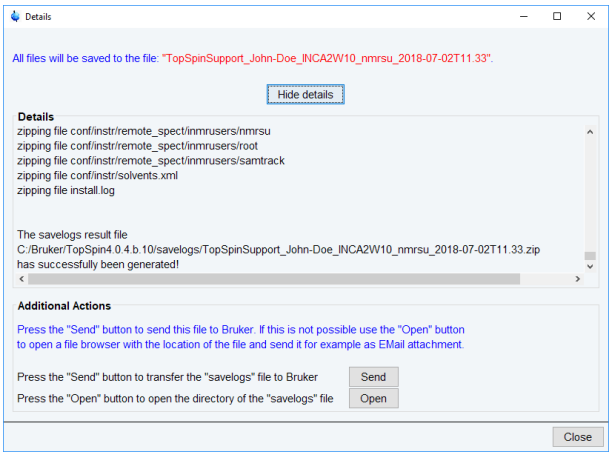
6.5.2.3 Processing

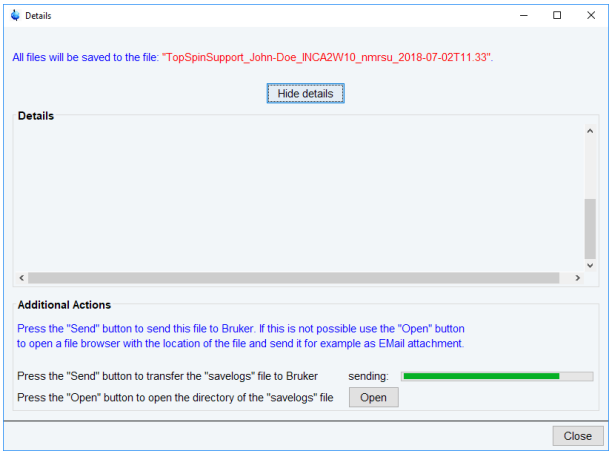
The functionality to "Collect & Save LogFiles (**savelogs**)" has been revised for TopSpin 4.0.4. The command can be started form **Manage | Commands** or by entering **savelogs**.

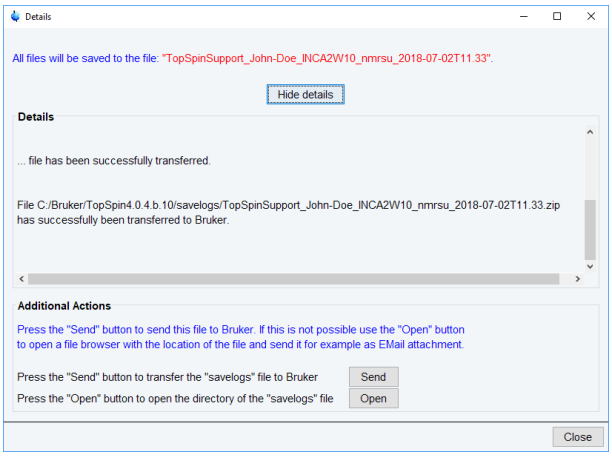


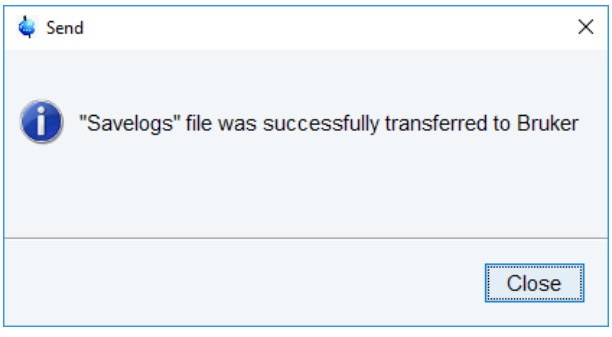
savelogs is mainly used for debugging purposes. This tool will collect support information about the current TopSpin installation (log and configuration files, by default no NMR data) and allows you to transfer it to Bruker. It offers a new "Comments" field to enter a description. Please enter here a description of your issue. If you are already in contact with Bruker, give a reference to a mail or phone call or ticket number.




Details
All files will be saved to the file: "TopSpinSupport_John-Doe_INCA2W10_nmrsu_2018-07-02T11.33".
Hide details
Details
zipping file conf/instr/remote_spect/inmrusers/nmrsu
zipping file conf/instr/remote_spect/inmrusers/root
zipping file conf/instr/remote_spect/inmrusers/samtrack
zipping file conf/instr/solvents.xml
zipping file install.log
The savelogs result file
C:/Bruker/TopSpin4.0.4.b.10/savelogs/TopSpinSupport_John-Doe_INCA2W10_nmrsu_2018-07-02T11.33.zip
has successfully been generated!
Additional Actions
Press the "Send" button to send this file to Bruker. If this is not possible use the "Open" button
to open a file browser with the location of the file and send it for example as EMail attachment.
Press the "Send" button to transfer the "savelogs" file to Bruker
Send
Press the "Open" button to open the directory of the "savelogs" file
Open
Close


Details
All files will be saved to the file: "TopSpinSupport_John-Doe_INCA2W10_nmrsu_2018-07-02T11.33".
Hide details
Details
Additional Actions
Press the "Send" button to send this file to Bruker. If this is not possible use the "Open" button
to open a file browser with the location of the file and send it for example as EMail attachment.
Press the "Send" button to transfer the "savelogs" file to Bruker
sending:
Press the "Open" button to open the directory of the "savelogs" file
Open
Close


Details
All files will be saved to the file: "TopSpinSupport_John-Doe_INCA2W10_nmrsu_2018-07-02T11.33".
Hide details
Details
... file has been successfully transferred.
File C:/Bruker/TopSpin4.0.4.b.10/savelogs/TopSpinSupport_John-Doe_INCA2W10_nmrsu_2018-07-02T11.33.zip
has successfully been transferred to Bruker.
Additional Actions
Press the "Send" button to send this file to Bruker. If this is not possible use the "Open" button
to open a file browser with the location of the file and send it for example as EMail attachment.
Press the "Send" button to transfer the "savelogs" file to Bruker
Send
Press the "Open" button to open the directory of the "savelogs" file
Open
Close


Send
"Savelogs" file was successfully transferred to Bruker
Close

The file transfer process has been changed from ftp to a https secured transfer method.

Please note that usually, you should get the "Support token" from Bruker, if not, please use a descriptive text (e.g. your name and the name of your institution or company).

If issues with spectra are observed, please add the respective NMR data with the "Additional files or directories" option.

6.5.2.4 Automation

- Use sti <holder> in TopSpin to insert current data set in the automation queue at position <holder>
- SmartDriveNMR: Data sets only archived when really completed
- InsightMR: Allow use of Dual-Receive Experiments for experiment iteration
- New language: Spanish (also available in TopSpin 4.0.3)

6.5.2.5 Pulse Programming

- Bracket operator for lists now working (e.g. powerList[2]:f1)
- Shape lists now available (list<shape>)
- Modification of RG now possible from within the pulse program using a list<receiverGain> Please refer to the Pulse Programming Manual for further details (“Receiver Gain Lists”).

Multi-dimensional AV Neo datasets contain the status parameter FnILOOP in each non acquisition dimension which is set according to the inner loop construct in the pulse program to:

```
0: no mc program,
1: no inner loop,
n > 1: number of inner loops.
```

In data acquired with inner-loop pulse programs without mc-syntax all acquisition status parameters `FnILOOP = 0` and the number of inner-loops must be specified when calling the split AU programs.

6.5.2.6 GxP Operation

The updated 21 CFR Part 11 manual contains information about the TopSpin default configuration. In particular, it explains the meanings of the default Bruker users nmr and nmrsu. Also some explanatory text fragments have been corrected and improved.

In TopSpin's login log file, the current operating system user and TopSpin's internal user are logged for startup, shutdown, login, and logoff operations. If no internal user has been used, it is now logged as "intern.user=unused".

In previous versions this has been logged as "intern.user=unknown" which may be misunderstood as indication of a problem when reviewing the login log file e.g. during GxP audits.

A password initially assigned to new accounts expires immediately. This is in order to force any new user to assign a new secret password upon first login.

Some users reported that the execution of command **lockdataset** does not restrict the file permissions as expected for the affected data set. This happens when the data set is located on a network file system (e.g. NFS, Samba, Windows shared folder, NAS instances) instead of the local file system. Please note that the functionality can be ensured for data sets stored on a local file system only. By design, network folders obscure the storage technology behind a shared directory object and may perform mappings of visible permissions to real

permissions on the target system. This mechanism is intransparent for the initiating software application. Therefore **lockdataset** cannot ensure that the intended access restrictions are applied at the remote location correctly.

The functionality of the Central Audit File is currently offered for Windows installations only. An adaption to Linux and macOS environments is work in progress and will be available soon.

6.5.2.7 Analysis

The FBS software for Fragment Based Screening analysis offers new features: spectra color management and mixture browsing from the spectra multiple display. Please note the backward and forward compatibility between this release and the previous releases in TS3 and TS4. A new license is needed to run this software upgrade, please contact us at *fbs@bruker.com*.

The current version is CMC-se 2.5.5. In addition to several bug fixes, an implementation of the data export in **NMReData** format (*www.nmredata.org*) is introduced. This novel format contains assigned molecular structure. The assignment includes 2D correlations such as HMBC or HMBC. CMC-se projects can now be exported to **NMReData** or **NMR Records**. The latter also includes all spectra.

6.5.2.8 AU Programming

Therefore, some new functions were included which can be called from an au-program:

- `int getPeakDimension()`: returns the dimensionality of the considered peak list, returns -1 if the peak list was not read correctly
- `double getPeakFreqHzForDim(unsigned int peakIndex, unsigned int dimIndex)`: returns the frequency of a peak specified by `peakIndex` in Hz for a specific dimension with index `dimIndex` (range from 0 to `getPeakDimension() - 1`), returns -1 if the peak list was not read correctly or one of the indices are out of range
- `double getPeakFreqPPMForDim(unsigned int peakIndex, unsigned int dimIndex)`: the same as `getPeakFreqHzForDim`, but result in PPM
- `int getPeakAddressForDim(unsigned int peakIndex, unsigned int dimIndex)`: returns the address of a peak specified by `peakIndex` for a specific dimension with index `dimIndex` (range from 0 to `getPeakDimension() - 1`), returns -1 if the peak list was not read correctly or one of the indices are out of range

The corresponding old functions for the one-dimensional case (the respective functions without the `ForDim` –extension) are still present, they just call their new counterparts with `dimIndex=0`.

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NMR Hotlines

Contact our NMR service centers.

Bruker BioSpin NMR 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 NMR service center or hotline you wish to contact from our list available at:

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Phone: +49 721-5161-6155

E-mail: *nmr-support@bruker.com*

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