

TopSpin

- Release Letter 4.1.4
User Manual
Version 010



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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 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 4.1.4, 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.

2 TopSpin - Basics

2.1 About TopSpin

TopSpin 4.1.4 is an update of TopSpin program package containing many improvements, new and useful features and bug fixes.



TopSpin 4.1.4 has been tested and released for AVANCE NEO, AvanceCore and Fourier 80 spectrometers.

Older spectrometer types are not supported and TopSpin 4.1.4 cannot be used on them for data acquisition. For continued support of these products please refer to updated versions of TopSpin 3.



Important notice for operation with AvanceCore:

Please note that not all functions and additional products which are described in the TopSpin 4.1.4 documentation are available for AvanceCore spectrometers. The AvanceCore is a streamlined spectrometer with reduced functionality. Not all parts of the TopSpin 4.1.4 documentation are applicable to the operation of an AvanceCore.



Important notice for operation with Fourier:

Once the system has been upgraded to TopSpin 4.1.4, you **MUST NOT** use any former version of TopSpin, since this could potentially lead to a status of the system's shim boards in which they do not operate properly and can not be reset without a service visit.

Therefore, do not change back to an older TopSpin version!

2.2 License Requirements

The operation of TopSpin 4.1.4 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 \[109\]](#).

2.3 TopSpin Program Versions

TopSpin 4.1.4 includes several additional products.

The following products are part of TopSpin and are included in the TopSpin license:

- IconNMR
- TopSolids
- bioTop
- NMR-Sim
- NMRGuide

The following products are part of TopSpin but require additional licenses:

- AutoCalibrate
- Assure-SST
- SmartDriveNMR
- CMC-q
- CMC-se
- CMC-assist
- PotencyMR
- FBS

The following products must be installed individually and require additional licenses:

- AMIX 4.0.2
- 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.)
- InsightMR™ 2.0.0 (for Windows and Linux)
- DynamicsCenter 2.8 (Protein Dynamics)

2.4 Hardware Requirements

2.4.1 PC Hardware

To run TopSpin 4.1.4 a state of the art computer should be used. Bruker recommends and delivers the following PC:

- HP Z4 G4 Workstation with
 - Intel Xeon W21233.6GHz, 4C CPU
 - 16GB DDR4-2666MHz (2x8GB) RAM
 - NVIDIA Quadro P400with 2GB dedicated RAM
 - 256 GB PCIe SSD Disk
 - 2TB 7200 RPM SATA HDDo2 x RJ45 1GB Ethernet (integrated)
 - HP 9.5mm Slim DVD Writer
 - USB US keyboard and USB mouse
 - China Regulatory CCC Compliance Mark
- Ethernet cable 5m
- Power cords: CH, EU/ SCHUKO and US

The Fourier 80 spectrometer is delivered as default with the following workstation:

- HP MS-Windows PC Mini
- Workstation to be placed between screen and screen base
- HP monitor with touchscreen (23"); screen resolution at least 1920 x 1080 at 60 Hz
- At least Windows 10, Intel® Core™ i7 Processor, 16 GB SDRAM; 256 GB SSD

2.4.2 Apple Computers

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

2.5 Spectrometer Hardware Requirements

TopSpin 4.1.4 runs on any AVANCE NEO, AvanceCore and Fourier 80 spectrometer.

For upgrade possibilities of your spectrometer with TopSpin 4.1.4, please check with your local Bruker office.

2.6 Supported Operating Systems

The end-of-support date for the Linux variant CentOS 7 is communicated for June 30, 2024. CentOS 8 and up do not appear as suitable successors due to changes in their support model. Bruker therefore is evaluating potential candidates. The final decision is scheduled for mid of 2022, and introduction of the new Linux variant in 2023.

Spectrometer Control

TopSpin 4.1.4 on spectrometer computers is supported for:

- Windows 10 (64bit)
- 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 4.1.4 was released have been tested and are supported.



Please note: the Fourier 80 has only been tested on Windows 10 (64 bit).

Processing Workstation

TopSpin 4.1.4 on data stations is supported for:

- Windows 10 (64 bit)
- CentOS 7 (64 bit) (Please note: The minimum required CentOS7 Version is 7.1)
- Apple macOS X 10.14 or higher

Although not officially supported by Bruker, TopSpin is also running on Windows 7 and several 64-bit Linux distributions.



Additional important details considering the macOS may be found in the section [Installation on macOS](#) [▶ 19].

2.7 Information about Java Technology

Several parts of TopSpin use Java technology, namely the AdoptOpenJDK (Adoptium) LTS distribution which is officially supported at least until end of 2026 including bug fixes, in particular addressing potential security vulnerabilities. This distribution is not affected by the introduction of commercial support models as such have been announced by the company Oracle.

TopSpin does not offer public services that are available over an external network. This significantly reduces the risk of the NMR instrument to be affected by potential security vulnerabilities. However, Bruker carefully monitors potential security vulnerabilities. Recently, the known Log4j issue CVE-2021-44228 was discovered. TopSpin 4.1.4 contains the latest version of the Log4j library, in which the problem has already been fixed.

Please note that the used Java environment is embedded in the TopSpin installation and so does not use any other Java environments installed elsewhere on the operating system.

2.8 Supported Browsers for License Activation

Several different browsers can be used for the CodeMeter license activation, but sometimes we have seen problems with certain versions of browsers. If you encounter a problem, it's a good idea to simply try another browser or browser version.

3 TopSpin Installation

3.1 Installation on Windows and Linux

TopSpin is distributed as a full program. The installation media are available as USB stick (Bruker part number H183244), and for download 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 installation media and on www.bruker.com.

If you have already a previous TopSpin version installed, then install the TopSpin 4.1.4 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 4.1.4 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.

Please note: On some installations this automatic execution might not run correctly (e.g. Bruker pulse programs or plot layouts were not installed). In such case, restart TopSpin and please wait five minutes after TopSpin has started. Then enter the command "expinstall" manually at TopSpin's command line. It is completely sufficient to have it run once after installation.

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.

The latest version of CodeMeter runtime is available for download here: <https://www.wibu.com/support/user/user-software.html>

3.3.1 Configure macOS Disc Access

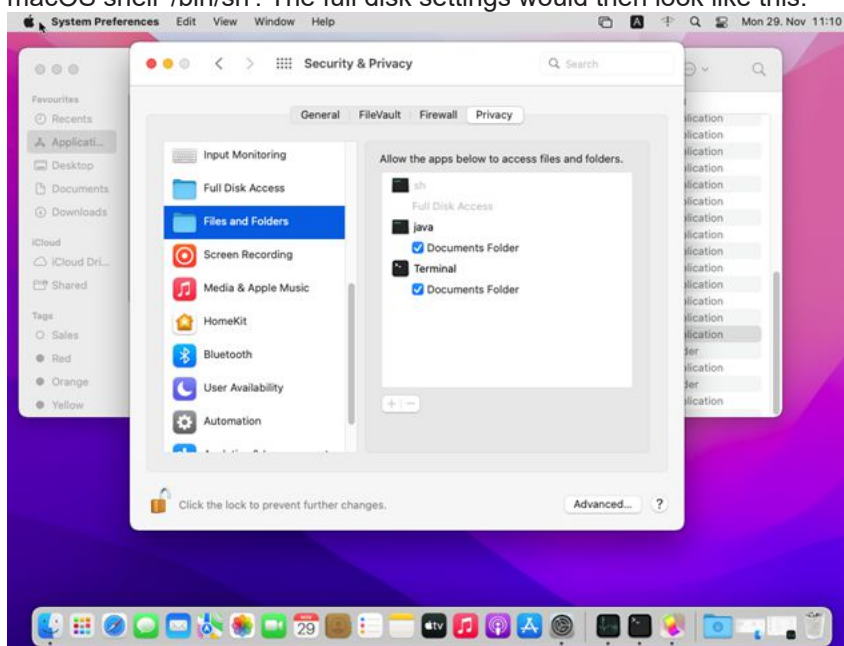
NMR spectra are stored on the Mac in the same way as on any other computer.

With macOS version 10.15 "Catalina", some security restrictions have been introduced. Apps now have to ask permission to access certain parts of the file system. Unfortunately, Apple's implementation is not well documented and does not take all possible software architectures into account.

This can affect the functionality of TopSpin. Viewing and processing example data stored in the TopSpin installation folder works as expected. However, viewing and processing data in other folders such as "Home" or "Documents" may fail.

There are two possible workarounds.

- Open the Terminal application (found in the `/Application/Utilities/` directory) and launch TopSpin from the command line (e.g. `./opt/topspin4.1.3/topspin`). For some folders, macOS requires confirmation that the software (Terminal, or Java) can access the disk. You need to confirm such request. This approach does not require administrator privileges but would not grant access to some special folders. For example, the Documents or Downloads folder cannot be accessed from TopSpin.
- Full file system access and thus full TopSpin functionality can be configured as follows: Use the "Preferences/Security and Privacy" dialog and grant full disk access to the macOS shell `'/bin/sh'`. The full disk settings would then look like this:



From now on, TopSpin will be able to access the data on your disk, even if you start TopSpin from the macOS Launchpad and do not use the command line. This option requires administrator privileges.

This is valid for all TopSpin versions.

3.3.2 AU Programs and macOS

The macOS release 11.0.1 "Big Sur" introduced several low-level changes, which affect the compilation of AU programs in TopSpin. In order to be able to compile and link AU programs, an installation of Apple's Xcode or Xcode command line tools is now required.

When installing TopSpin on macOS, the installer will offer a choice to install the required tools. As an alternative solution, the Xcode command line tools may also be installed from the App store at a later time. Please consider, that the download of the Xcode requires significant data volume (typically several GB).

3.4 CodeMeter Security Updates

For the CodeMeter Runtime, security advisories are published in regular intervals on the website of the manufacturer:

<https://www.wibu.com/support/security-advisories.html>

We recommend to check these notes and if necessary to update the CodeMeter Runtime accordingly.

The respective download page is located here:

<https://www.wibu.com/support/user/user-software.html>

Under Linux, in case of an update, additional RPM packages may have to be updated or installed to resolve possible software dependencies.

3.5 Spectrometer Configuration

Each TopSpin release includes also latest firmware releases for any hardware supported by TopSpin. During the spectrometer configuration procedure (command **cf**) the firmware versions found in the spectrometer are verified and automatically upgraded to their newest release where appropriate. This approach is mandatory in order to achieve a consistent installation which corresponds to spectrometer configurations the TopSpin release has been validated with.

Firmware upgrades cannot be rolled back by end users. It also should not be required to do so since newer firmware versions are backwards compatible to previous TopSpin releases whenever possible. Nevertheless, connecting a new TopSpin release to your spectrometer even once for testing purposes may apply changes to the firmware status.

Under certain circumstances this may be an undesired result. Please contact Bruker NMR Support for assistance if you would like to return to older TopSpin versions and see the need to roll back also the firmware upgrades.

Please note that such firmware packages come as part of the TopSpin installation package. Firmware packages are never downloaded via internet connections during software operation.

3.6 GxP Package

Since TopSpin 4.1.1, Bruker offers a special GxP package that comes as a separate TopSpin package with two different components.

1. The TopSpin Server component that contains the central audit trail and user management software tools.
2. The TopSpin Client component that contains the actual TopSpin version specifically for the GxP environment. Amongst many other features, data deletion is restricted to certain user roles.

Please contact your local Bruker office for more information.

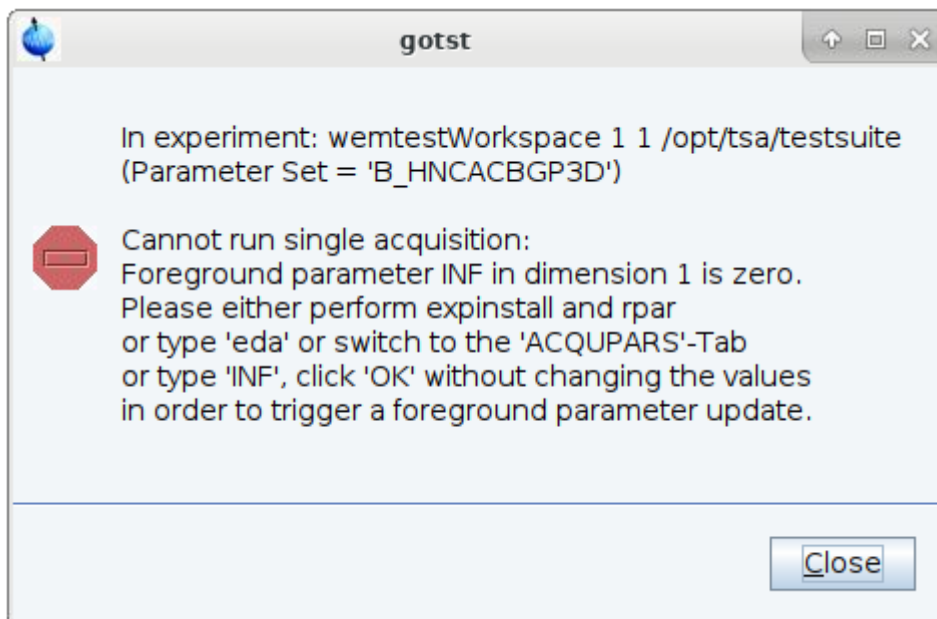
4 Bug Fixes

4.1 Bug Fixes in TopSpin

The following topics describe the major fixes which come with TopSpin:

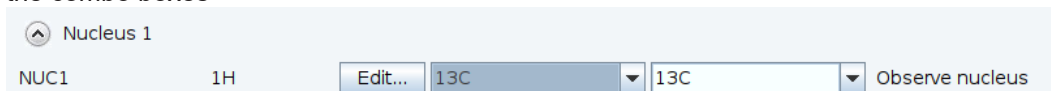
- **SKB-264:** masdisp and MAS/3 website are not synchronized correctly (LT-MAS <> flush mode)
- **SKB-279:** wrong OFFSET or SR for 3D experiments after expinstall/paracon
- **SKB-289:** Duplication of standard parameter sets should require administrator password.
- **SKB293:** Audit check failure on freshly acquired dataset.
- **SKB-301:** Activated TopSpin auto lock screen in TopSpinGxP requires administration privileges to unlock TopSpin.
- **SKB-307:** LIFTMODE not available for BSMS configurations without SPB or SPB-E.
- **SKB-311:** Start of atma may lead to several java exceptions.
- **TOPS-2509:** In the pulse program relations, certain mathematical formulas were not evaluated according to the applicable rules, i.e. a formula "a/b*c" was evaluated as "a/(b*c)" and not as "(a/b)*c".
This has been corrected now, but unfortunately has the obvious implication that existing pulse programs may now yield unexpected results.
Therefore, an error message is now thrown if an ambiguous pulse program expression like "a/b*c" without braces is detected, and the user is asked to set the braces accordingly in order to clarify how the formula should be evaluated.
We apologize for the inconvenience.
- **TOPS-2637:** When TDav is set greater than 1, any whole (multi-dimensional) experiment should be repeated TDav times.
Acquisition-wise this worked correctly but while the experiment was running the size of the raw data files on the workstation were decreased to zero again after the first repetition has been completed.
This became obvious to the user via a broken FID display and error messages about inconsistent file sizes from intermediate processing steps while the actual acquisition was still working normally.
When the whole experiment with all TDav repetitions was finished, also the final data on the workstation were consistent.
Corrected the behavior in such a way that the data on the workstation is always consistent and thus also allows intermediate processing while the acquisition is still running for TDav > 1.
- **TOPS-2846:** The plot editor now shows proper line breaks in the text when instructed by the layout.
- **TOPS-2881: edprosol:** The edsolv list is empty
- **TOPS-2932:** Improved consistency of acquisition parameter INF.
When INF has been changed within the TopSpin user interface, the actual foreground value in the file acqu was not updated consistently. This has been improved, foreground INF in file acqu is now synchronized with the user interface.
Also the acqu / acqu files the user interface and the pulse program variable inf<dimension> did not use the same rounding of INF. This has been improved, acqu / acqu files, the user interface and the pulse program variable inf<dimension> now use the same correct rounding in steps of 12.5 ns.
In addition, if the foreground value of INF in the acqu file is zero, the acquisition module calculated it on the fly and wrote it back into the acqu file, which is not desired in terms of data integrity. This has been corrected which means that an acquisition requires that a

nonzero INF has been passed as foreground parameter. If this is not the case, the acquisition will abort with the following error:



So you just need to access the parameter INF from the GUI in order to trigger a parameter update on disk but you don't need to modify any foreground parameters. In all Bruker default parameter sets the correct foreground INF is maintained by **expinstall**, but in user defined parameter sets foreground INF might have to be updated in such a way.

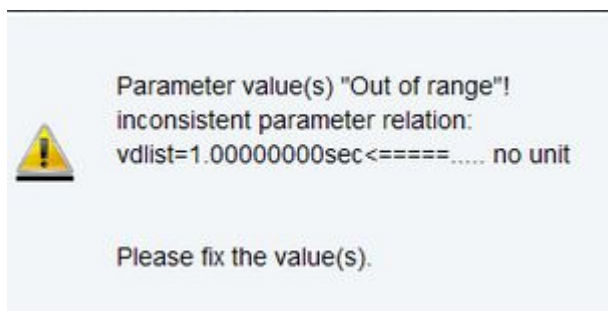
- **TOPS-2957:** **eda** shows parameters as file name
- **TOPS-2980:** When changing the observe nucleus in a multi-dimensional experiment via the combo boxes



The corresponding parameters O1, O1P, SFO1, SWH, INF and AQ were changed accordingly in the user interface but in case of SWH and INF those changes were not forwarded to the respective foreground parameter files (acqu in case of INF and higher dimensional acqu<dimension> in case of SWH).

This has been corrected, the values of INF and SW in the foreground files and the user interface are kept in sync after a change of the observe nucleus.

- **TOPS-2997:** Fixed a problem that after rebooting the spectrometer via topspin the "Spectrometer is running" message is displayed too early while some shims are not yet ramped up by the ELCB.
Please note that this also requires installation of the latest ELCB firmware 210921 which is part of the topspin distribution.
- **TOPS-3028:** When defining a delay list in the pulse program with the special name "vdlist" which is actually the lower case version of the reserved TopSpin list tag VDLIST, e.g.: define list<delay> vdlist=<\$VDLIST> the list was not correctly displayed in ased and when modifying the list via the user interface after ased has been run before, an error occurred:



This has been corrected, also a list with name “vclist” will be handled correctly by the user interface.

- **TOPS-3071:** Some special rather simple manifest blocks in a pulse program like:
`manifest_append 42 manifest_end`
caused precompilation errors.
This has been corrected, any kind of string between the tokens `manifest_append` and `manifest_end` will be accepted now.
- **TOPS-3133 + SKB-280:** Fixed a bug that Hystar can't be used together with ICON-NMR.
- **TOPS-3166:** Peak Picking now works correctly when the dataset name contains ampersand (&) or single quote (') characters.
- **TOPS-3229:** `cf` hangs if no ethernet connection to Bruker exists.
- **TOPS-3237:** Fixed a bug that the commands **wobb high** and **wobb low** have the inverse functionality, i.e. **wobb high** wobbles the nucleus with the lowest frequency and vice versa.
- **TOPS-3246:** The search range of the interactive O1 calibration routine `o1calib` can be specified as additional command line parameter, but was erroneously ignored in former versions of topspin. This is fixed now.
- **TOPS-3252 + SKB-293:** Fixed a bug that **gs** and **ii** modify some files in the dataset leading to inconsistencies when checking the audit file integrity.

See also

- [Installation on macOS \[▶ 19\]](#)

4.2 Bug Fixes in IconNMR

Issues corrected since IconNMR 5.2.3 / TopSpin 4.1.4:

- Composite Experiment Manager – “Save to Users” inoperable
- Temperature not adjusted on subsequent experiments when “First sample” is already inserted
- Projection References can be set incorrectly when Composites are added via IconWeb.

5 New Features

5.1 General

5.1.1 New Version of the Python Interface

Upgraded example files and minor bug fixes are included. The license required for the TopSpin Python API is now included in the free TopSpin license for academia.

5.1.2 LabScape ProCare

TopSpin is now able to connect to a LabScape ProCare installation, which tracks the maintenance status of the instrument.

The maintenance status is visible in the TopSpin User Interface and a reminder to plan a maintenance will occasionally be displayed when acquiring data while the system's maintenance is overdue.

For further information please refer to the LabScape ProCare User Manual.

5.1.3 SmartDrive NMR

- It is now possible to extend the experiment list available in SmartDriveNMR to any common 1 or 2 dimensional parameterset.
- Already extend by Bruker with appropriate settings concerning all common Bruker probeheads are these parametersets:
 - CMC_COSY
 - CMC_TOCSY
 - CMC_NOESY
 - CMC_C13DEPTQ135
 - CMC_F19 and CMC_F19CPD
- The sequence in which the experiments are handled can now be edited by the user.
- The desired Signal-to-Noise ratio for each experiment is now available as a user input.
- Non uniform sampling (NUS) within SmartDriveNMR is now utilized using the Python script TAnD.py and the AU macros ta_acqu and ta_proc . This allows to broaden the field of application for NUS to any multidimensional experiment.
- Functionality of SmartDriveNMR prior to this TopSpin release can be achieved by using the setting "STANDARD PORTFOLIO".

5.1.4 CMC-assist

The signal regions in 1D ¹H spectra without solvent suppression are now being determined with the help of the TopSpin command **sigreg**. Compared to the previous way to determine the regions this leads to an improvement concerning their symmetry relative to the signal.

5.1.5 Default Browser for Windows

Currently IE is used as browser for Windows. This can be changed to the system default browser in the Miscellaneous section of TopSpin preferences.

5.1.6 Improved Preamplifier Hardware Protection

Topspin includes an improved preamplifier hardware protection if frequency selective power limits are provided by the preamplifier.

5.2 General User Interface (GUI) / GxP Version

Two slightly different TopSpin interfaces are installed depending on whether the standard or the GxP version of TopSpin is installed. Please see the respective TopSpin manuals for more details.

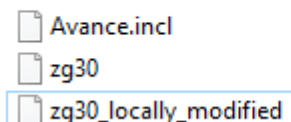
5.3 Acquisition

5.3.1 Datasets Contain a Copy of All Input Files

When an acquisition is run with **zg** or **go**, all used input (pulse programs, shapes, ...) are copied into a new subfolder *lists* in the dataset. There are subfolders *pp*, *wave*, ... equivalent to the structure in `<tshome>/exp/stan/nmr/lists`.

At acquisition start, TopSpin in a first step searches all required input files in the global source directories (as before). If a file is not found there, starting with TopSpin 4.1.4 also the *lists* subfolder in the dataset is searched in a second step.

```
SYSTEM (C:) > Bruker > examdata > NewListHandlingExample > 1 > lists > pp
```



This makes it possible to use individual input files within a single dataset, e.g. special shapes or pulse programs.

Furthermore, as datasets are now self-contained, it is easy to transfer them to other computers including all relevant files e.g. using the **tozip** command.

The command **zg repeat** runs an acquisition using only input files from the *lists* subfolder in the dataset. In other words, there is no lookup in the global source directories. This makes it easy to repeat an experiment, even if files in global source directories have changed in the meantime.

Earlier versions of TopSpin renamed list files when storing them in the dataset (e.g. as *spsnam1*) to avoid name collisions. With the new subfolder hierarchy, this is not necessary anymore, so that now the original filename is kept.

5.3.2 Enter Magnet ID During **cf**

With TopSpin $\geq 4.1.4$, the magnet ID (BZH-number or HSN-number) and the cryostat ID are entered during **cf** (from there, values are automatically copied into **edcstm** and cannot be changed in **edcstm** anymore. It is necessary pay attention to the number format: Enter the number exactly as written on the magnet label (the magnet ID must contain a “” and the

cryostat ID must contain “-” (see example below)). Failing to do so prevents the BIS-file from being downloaded and will cause an **autodiagnose** error (**autodiagnose** is mandatory for AvanceCore), which leads to an email alert towards the AvanceCore service team.

5.3.3 Expinstall Improvements

Expinstall steps were shortened to skip the “items to install” section, all items will be installed. User AU programs will not be recompiled.

5.3.4 Expanded Arrays in Acquisition and Processing Parameters

The USERA and USERP arrays in the acquisition (respectively processing) parameters have been increased from five to ten.

5.3.5 Acquisition Parameter Editor

Obsolete parameters DECIM, DWOV and DDR were removed from the acquisition parameter editor.

5.3.6 New ELCB Firmware

A new ELCB-firmware is provided which determines more accurately when the spectrometer is actually ready (i.e. including the complete ramp-up of the shims) after a system reboot.

5.3.7 LT-MAS

Support for all LT-MAS cabinets.

5.4 Automation

Changes in IconNMR 5.2.4 / New Features:

- InsightMR Supported on F80
- InsightMR now possible with Dynamics Center and/or Mnova
- F80 CTC Automation Robot supported
- Use SampleTrack Experiment Orders without Barcode Hardware (Enable Interactive & Easy Mode)
- SmartDrive allows much more flexible choice of possible experiments using Experiment 'Portfolios'
- SampleCase MAS integration active

5.5 Documentation

Updated documentation under Help | Manuals (docs) available for:

- Acquisition Commands and Parameters – User Manual
- Processing Commands and Parameters – User Manual
- NMR Pulse Programming for AVANCE NEO and Fourier 80
- AU Programming – User Manual
- NMR Sim – Experiment Simulator – User Manual
- TopSpin User Guide – User Manual
- Python Programming in TopSpin – User Manual
- SmartDrive NMR – User Manual

New documentation under Help | Manuals (docs) available for:

- GxP – Regulatory Compliance – User Manual

6 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.

The software can also be purchased directly from the Bruker WebShop:

<https://bruker-labscape.store/collections/mr-software-1>

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, NMR Guide CMC Classroom edition, TopSpin Python interface
	run of validity: 3 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. 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.

If you have any questions or problems regarding licenses, please use the web form here to directly contact the license team at Bruker:

<https://www.bruker.com/protected/en/services/software-downloads/nmr/nmr-license-questions.html>

6.1 License Expiry

TopSpin will issue a notice about expiring licenses 30 days prior to the actual expiry. The notice will be repeated again two weeks before the expiry and then again one week before the expiry. Please contact your local Bruker office if you have any questions, in particular also regarding your options and quotes for license renewals.

7 History of Changes

7.1 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>

7.2 TopSpin 4.0.1

7.2.1 General

7.2.1.1 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>

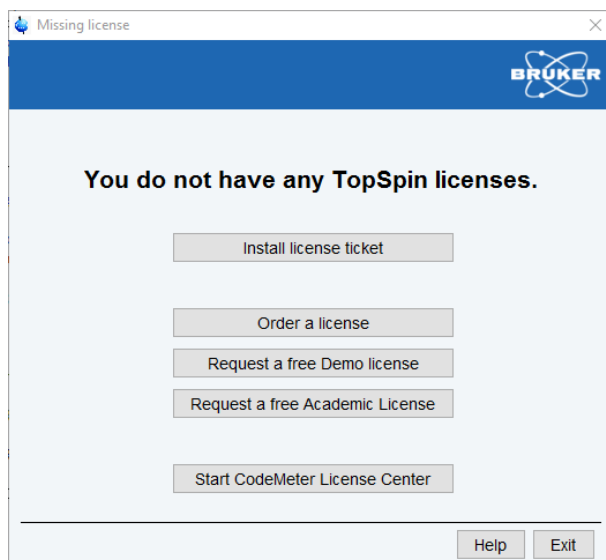
For further Information please look up the CodeMeter License Management User Manual.

7.2.1.1.1 CodeMeter Installation on Linux and macOS

- 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/support/user/downloads-user-software.html> and follow the given installation details.
- CM runtime for diverse **macOS** versions are available on the same site.

7.2.1.2 TopSpin starts without license

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

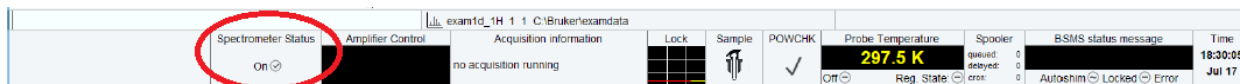


Additional Demo- and Academia-Licenses can be ordered free of charge from the Bruker Website:

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

7.2.1.3 Spectrometer Control

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



7.2.1.4 64bit Environment

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

7.2.1.5 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.

7.2.1.6 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.

7.2.1.7 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.

7.2.2 Acquisition

7.2.2.1 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:

Automatically convert 64bit SER data into TopSpin 3.x format

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.

7.2.2.2 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.

7.2.2.3 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.

7.2.2.4 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).

7.2.2.5 Command wobbt replaced

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

7.2.2.6 New MAS3-firmware

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

7.2.3 Processing

7.2.3.1 2D/nD processing with FnLOOP

Multidimensional AVANCE NEO data sets contain a new acquisition status parameter FnLOOP in each non acquisition dimension. This parameter describes the number of inner loops in this dimension. If one of the FnLOOP 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.

7.2.4 Automation

7.2.4.1 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)

7.2.5 Pulse Programming

7.2.5.1 Command dccorr obsolete

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

7.2.5.2 Command `spf` obsolete

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

7.2.5.3 Command `anavpt` obsolete

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

7.2.5.4 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.

7.2.5.5 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”.

7.2.5.6 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.

7.2.5.7 Compile-time variable `grpdy`

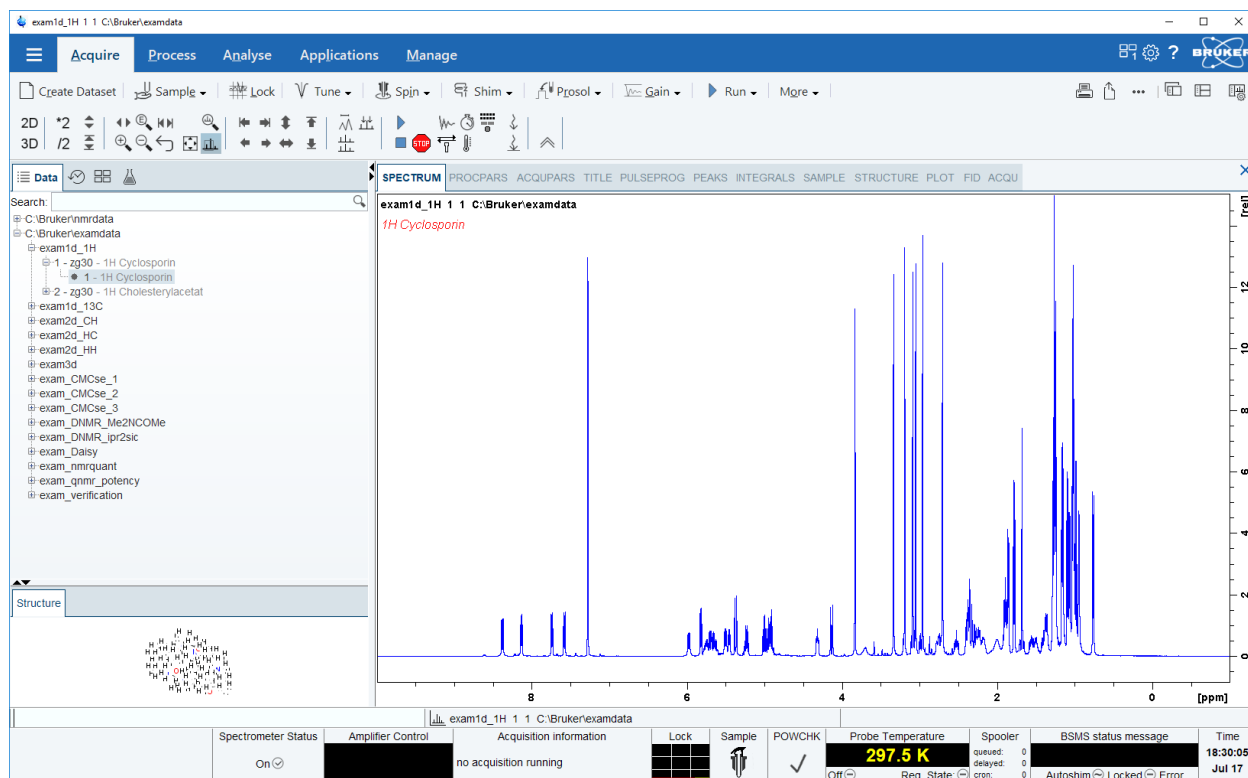
The group delay is available in the pulseprogram as compile-time variable `grpdy`.

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.

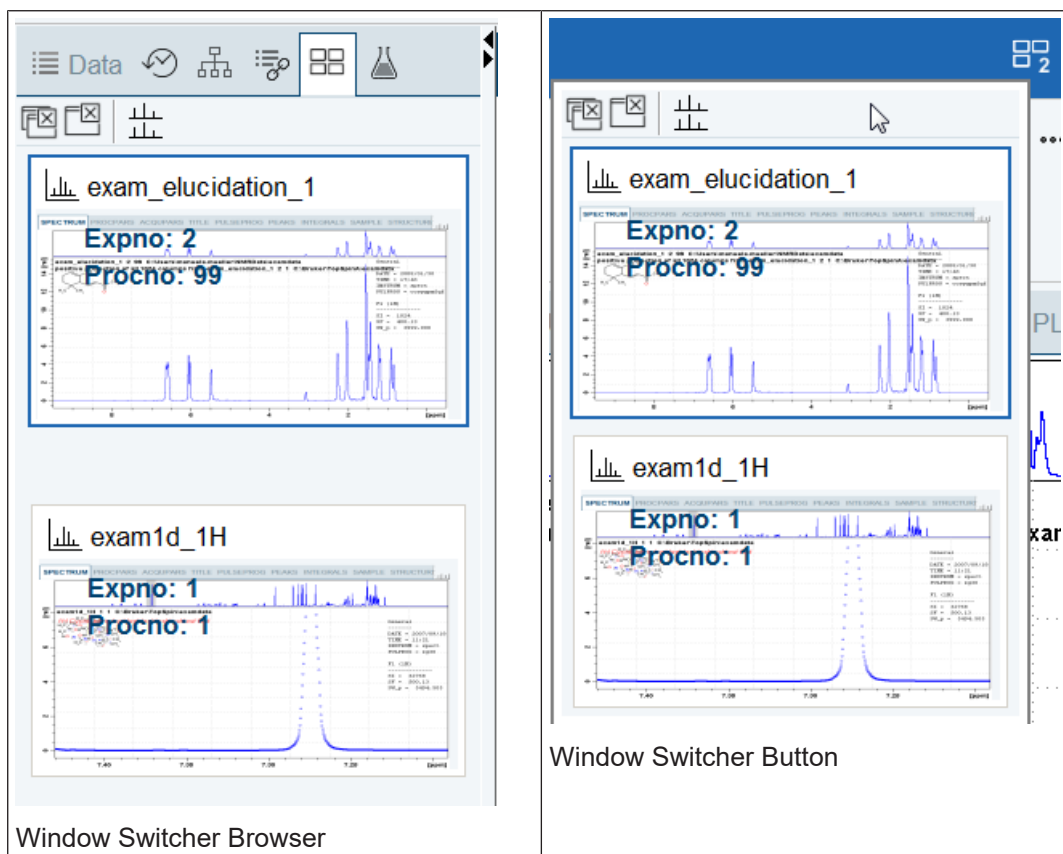
7.2.6 General User Interface

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 ergonomics 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.



7.2.6.1 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.



7.2.6.2 Quick access to change View Options

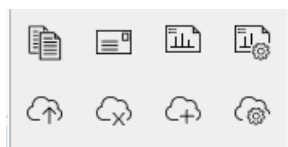
Get a quick access to switch the perspective (e.g. full screen), compare open datasets or change spectra view options in the Change View Options menu:



7.2.6.3 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):



7.2.6.4 Quick Access to Setup Preferences

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

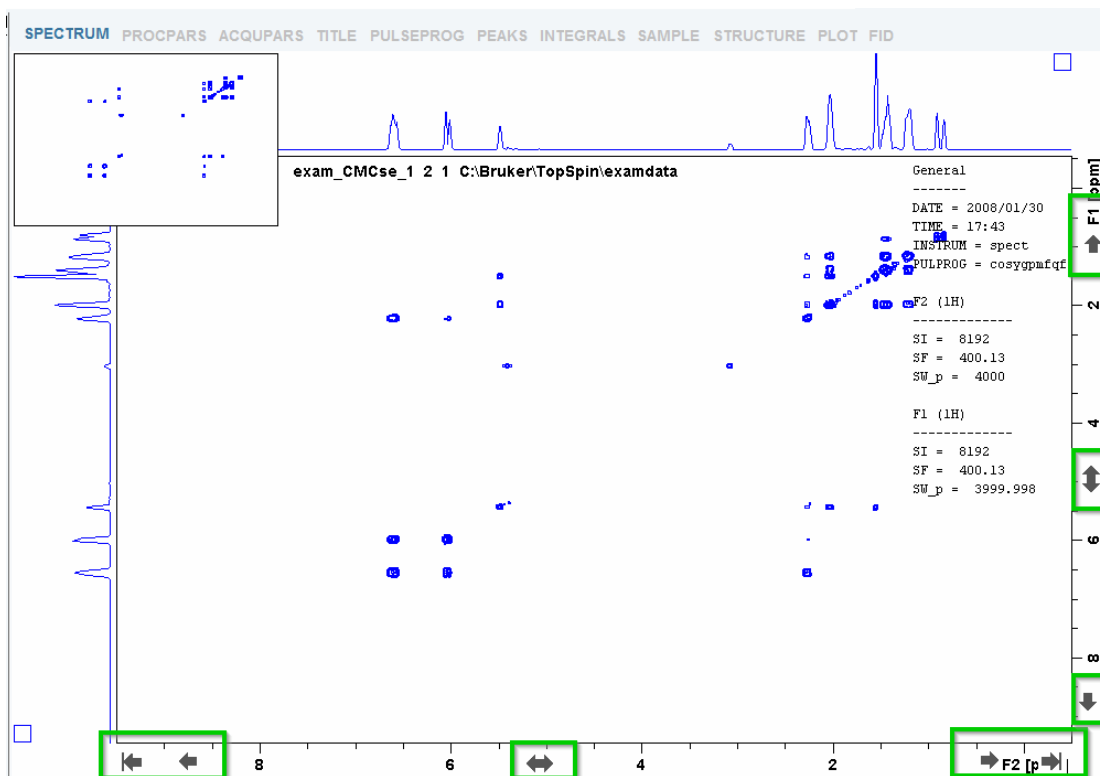


7.2.6.5 New Spectra axes scrolling and shifting behavior



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



7.2.6.6 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**.

exam1d_1H 1 1 C:\Bruker\examdata									
Spectrometer Status	Amplifier Control	Acquisition information	Lock	Sample	POWCHK	Probe Temperature	Spoiler	BSMS status message	Time
On ☺	██████████	no acquisition running	██████████	🔒	✓	297.5 K	queued: 0 delayed: 0 cron: 0	Autoshim ☺ Locked ☹ Error	18:30:0 Jul 17

7.2.7 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.

7.2.8 Analysis

7.2.8.1 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 ¹H 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**.

7.3 TopSpin 4.0.2

7.3.1 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

7.3.2 New Features

7.3.2.1 General

7.3.2.1.1 Academic License

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.

7.3.2.1.2 License expiration warning

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.

7.3.2.2 Acquisition

7.3.2.2.1 New options to scale the FID by RG and/or NS

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 (acqu) indicating whether the respective option has been used (scaleByRG and scaleByNS).

7.3.2.2.2 New cortab procedure

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.

7.3.2.2.3 What is new in WaveMaker

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 Q5sebob (excitation).

7.3.2.3 Automation

7.3.2.3.1 New in IconNMR

- 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

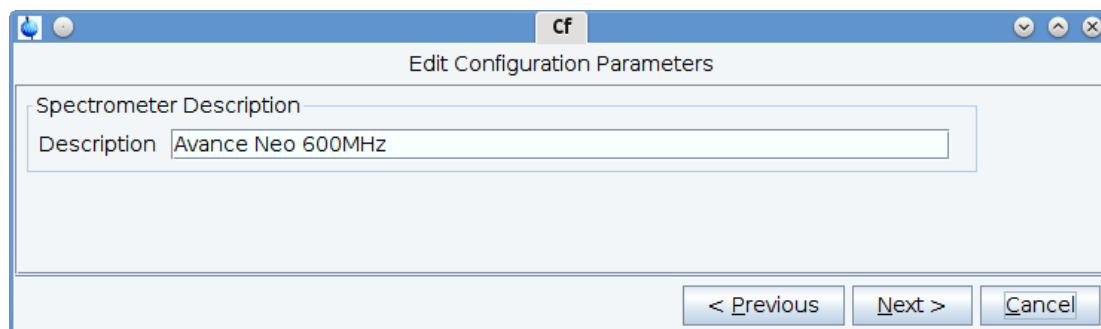
7.3.2.4 Pulse Programming

- 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”).

7.3.2.5 General User Interface

7.3.2.5.1 Parameter INSTRUM contains spectrometer description

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”.

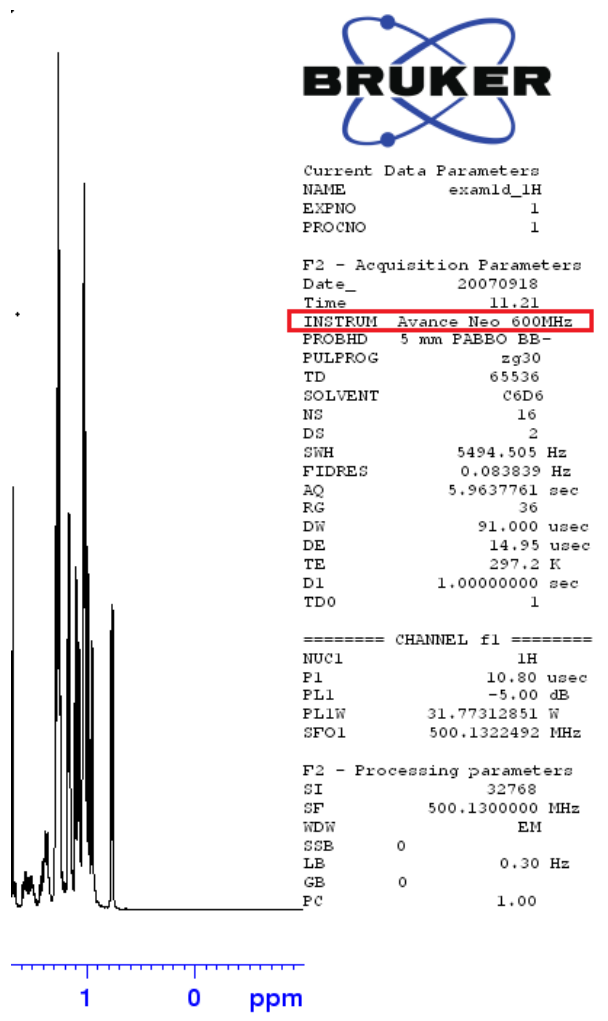
History of Changes

Customer Info	
Customer Name*	AH
Operator Name	
Company*	Bruker
Address	
Postal Code	
City*	Rheinstetten
Country*	Germany
Phone Contact Customer*	6444
Mobile	
Fax	
E-Mail*	ah@bruker.de
Bruker Info	
Engineer*	myself
Office*	here
Central Hotline Phone*	111
Central Hotline E-Mail*	keine
System Info	
Order No.*	10226926
Contract Service No.	none
System Type	Avance Neo 600MHz
Console Part and Serial No.	
Coil	
Dewar	
Shim System Offset*	0
Shim System Angle	
CryoProbe Order No.	
Location	
Register No.	

* Required Fields

Save Cancel Close

The Spectrometer Description is shown in plot legend.



7.3.2.5.2 CU/5 now fully supported in TopSpin User Interface

7.3.2.5.3 Default action in flow menus

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.

7.3.2.5.4 "Find" functionality

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.

7.3.2.6 GxP Operation

7.3.2.6.1 Restraints for internal users

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.

7.3.2.6.2 Improvements for "lockdataset" functionality

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.

7.3.2.7 Plot Editor

7.3.2.7.1 "plot0" available in TopSpin 4

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.

7.3.2.7.2 Drag and drop data sets to Plot Editor

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.

7.3.2.8 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.

7.4 TopSpin 4.0.3

7.4.1 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

7.4.2 New Features

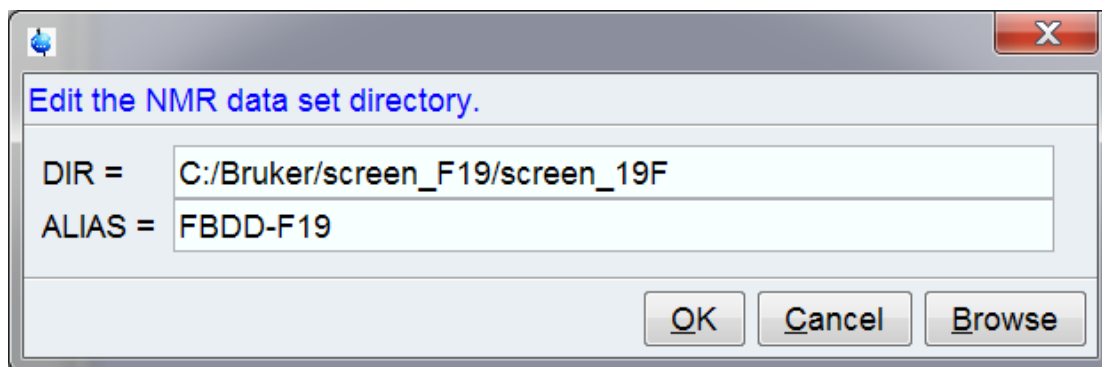
7.4.2.1 General

7.4.2.2 User Interface

7.4.2.2.1 Data Browser

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

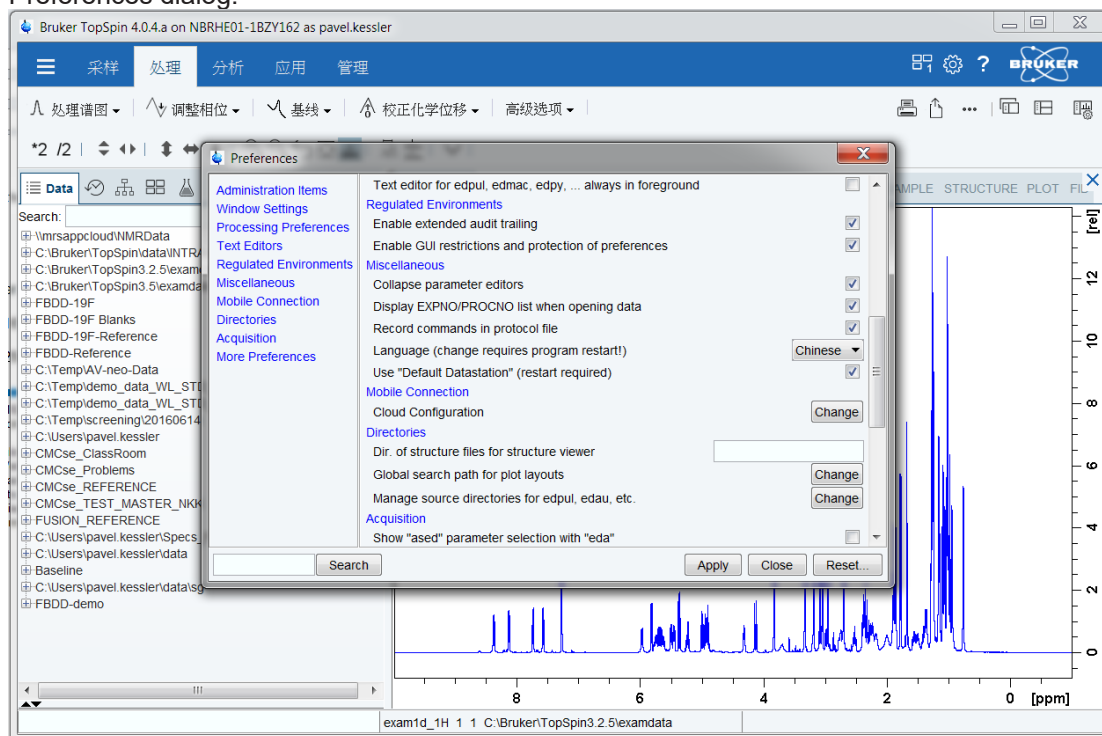
Invoking "**Edit Selected Data Dir**" in the data browser popup menu opens a dialog allowing to modify the data folder and its alias name.



7.4.2.2.2 TopSpin Internationalization

Topspin flow menus are now also available in Chinese translation.

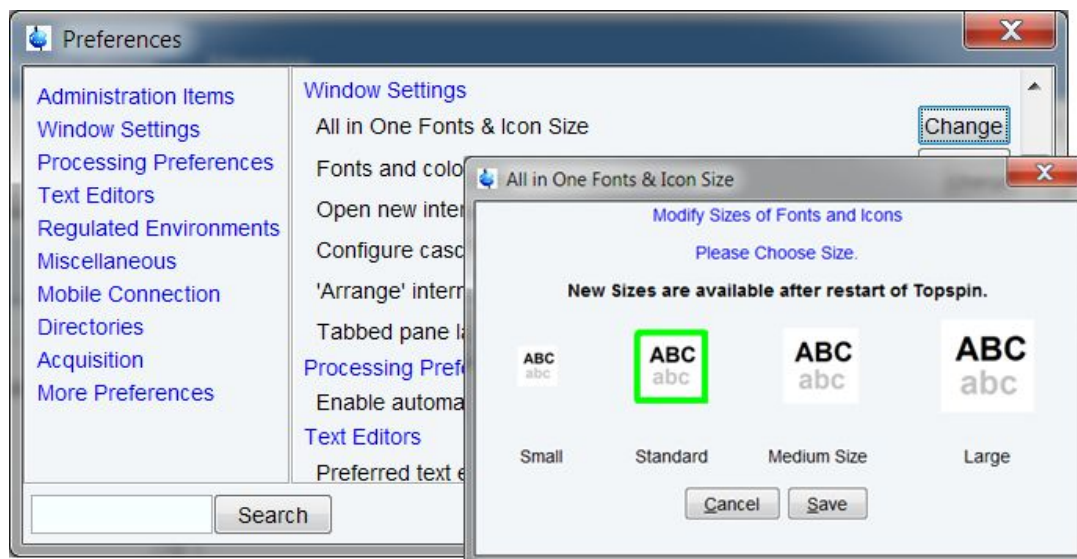
The desired translation (currently English and Chinese) may be selected from the Topspin Preferences dialog.



7.4.2.2.3 TopSpin on High Resolution Screens

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

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



7.4.2.2.4 License information and management

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**.

7.4.2.2.5 Command History configurable

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.

7.4.2.3 System Support

7.4.2.4 Acquisition

7.4.2.4.1 What is new in WaveMaker

- 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).

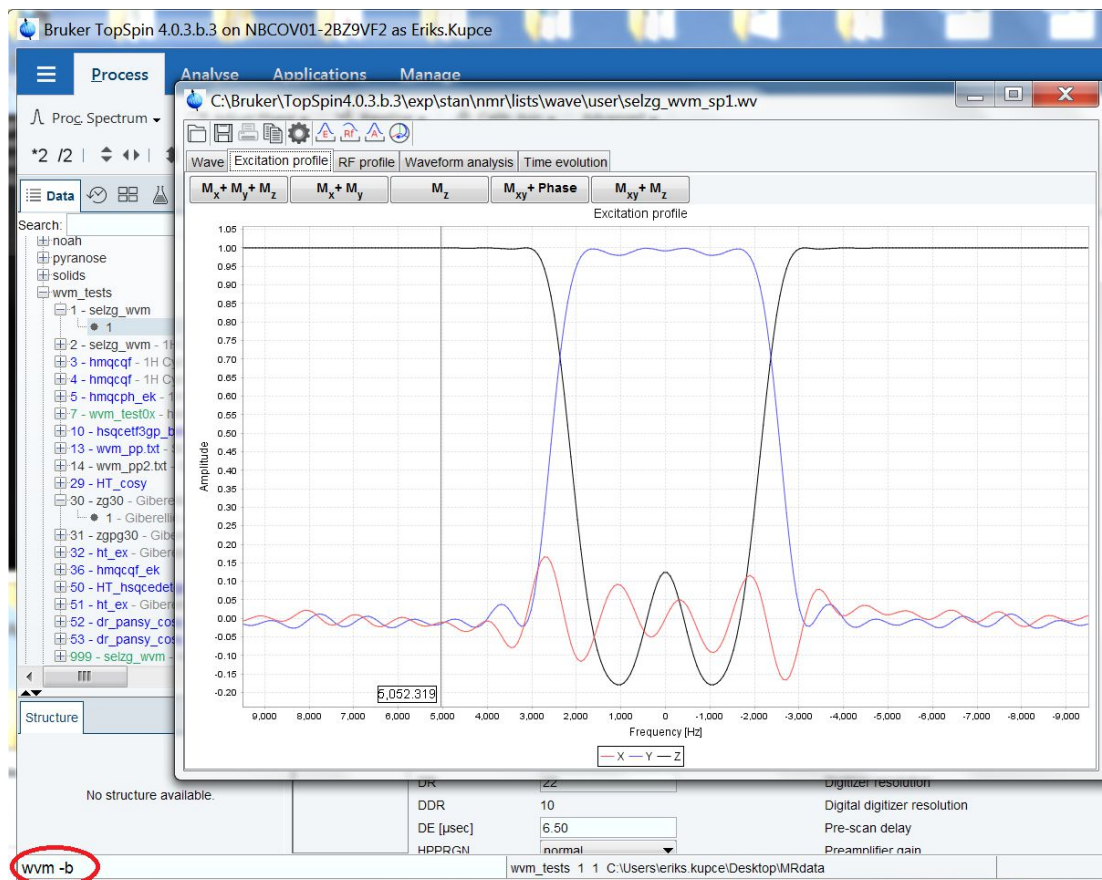


Figure 7.1: The `wvm-b` option in WaveMaker shows the excitation profile of the shaped pulse(s).

7.4.2.4.2 TopSolids 2.1

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:

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

7.4.2.4.3 rga -setD0

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.

7.4.2.4.4 Switch off Sample Rotation during sample exchange with ej and sx command

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.

7.4.2.5 Processing

7.4.2.5.1 Handling of parameter SPECTYP changed

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.

7.4.2.5.2 Parameter INTSCL changed from float to double

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.

7.4.2.6 Automation

7.4.2.6.1 New in IconNMR

- 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

7.4.2.6.2 BEST-NMR with Bruker LiquidHandler 215 no more available

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

7.4.2.7 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”).

7.4.2.8 GxP Operation

7.4.2.8.1 Changes to login dialog

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.

7.4.2.8.2 Improvements to login protocol file

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.

7.4.2.8.3 Review of data sets and audit does not require TopSpin license

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”

7.5 TopSpin 4.0.4

7.5.1 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:

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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

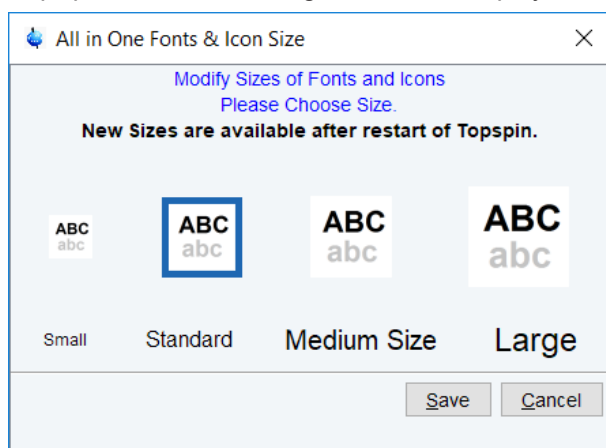
• Item #14335	Originator item names with : at the end do not work
• Item # 14334	Missing box for path definition of structure file in plot layout
• Item #14325	AssureSST bad window path name error message
• Item #14320	File->Import Configuration does not set various configuration items
• Item #14319	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

7.5.2 New Features

7.5.2.1 User Interface

7.5.2.1.1 Improved behavior on high resolution displays

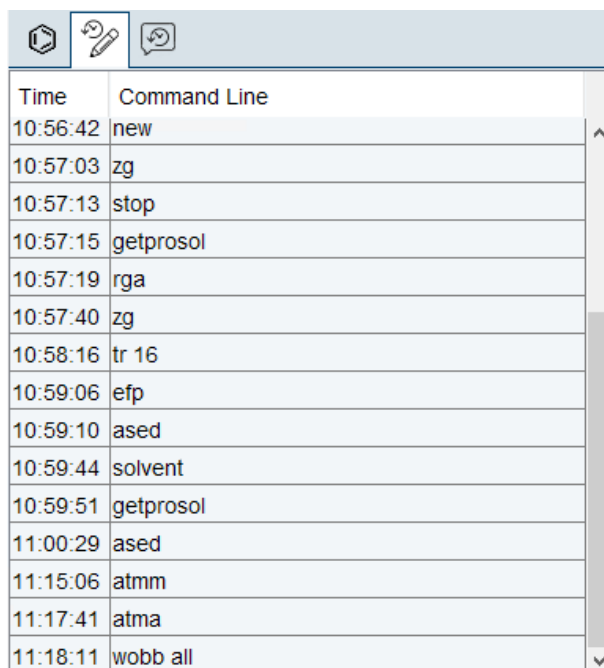
Sizes of fonts and icons of the TopSpin General User Interface can be modified easily by clicking **Preferences | Windows settings | All in One Fonts & Icon size**. This improves TopSpin's behavior on high resolution displays.



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

7.5.2.1.2 Cmd History Panel

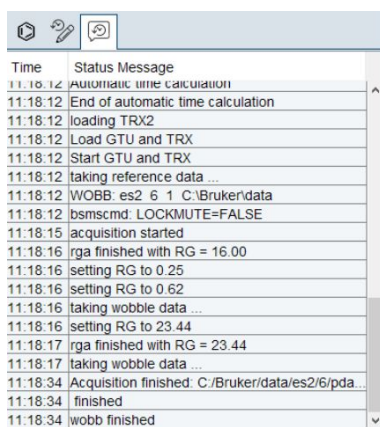
The new tab Command Line History, located in the menu bar of the Data Browser window, shows the history of previously entered commands.



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

7.5.2.1.3 Status Message History

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

7.5.2.2 Acquisition

7.5.2.2.1 What is new in WaveMaker

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

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.
```

7.5.2.2.2 Multi-Receiver Handling

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

Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

Dataset

NAME: exam1d_1H
EXPNO: 2
Directory: c:\Bruker\tsalexamdata
 Open in new window

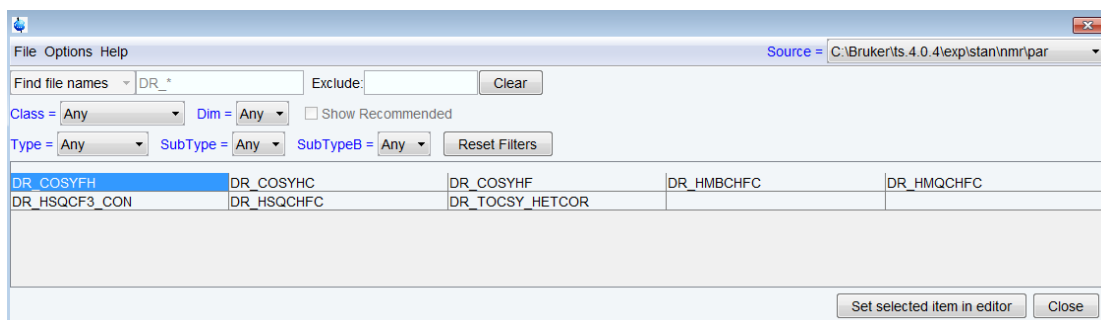
Parameters

Use current parameters
 Read parameter set
 Set solvent: DMSO
Additional action
 Do nothing
 Execute getprosol
 Keep parameters: P 1

Advanced

Number of datasets (receivers): 1
Title:

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

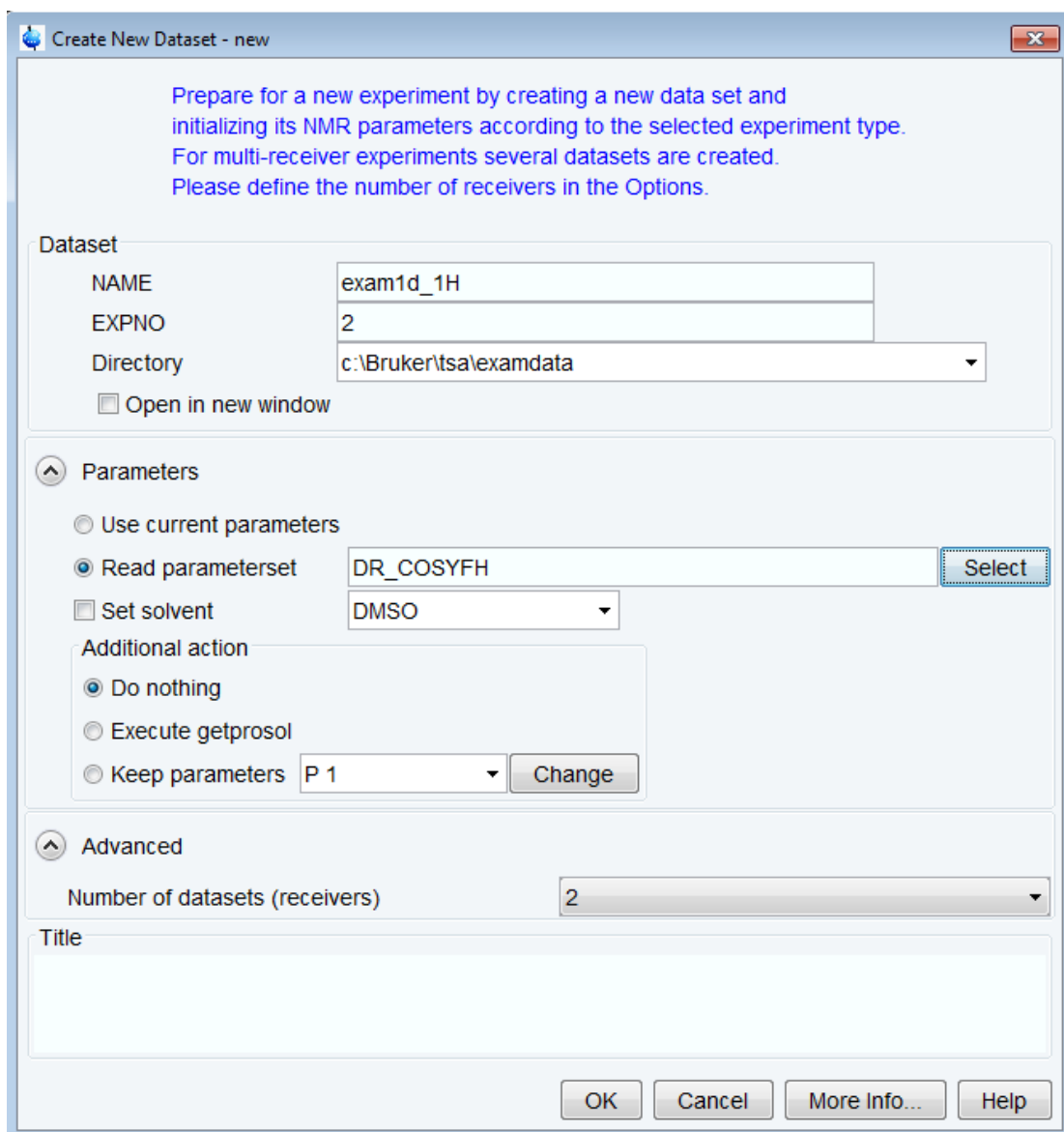


Entering “DR_*” in the **Find file names** field can be used to filter/display the Multiple receiver parameter sets.

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.

7.5.2.2.3 Simplified Print Function in edprosol

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.

7.5.2.2.4 Improved configuration of non-PICS HRMAS-probes

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

7.5.2.2.5 Multi-Wobb in Acquisition

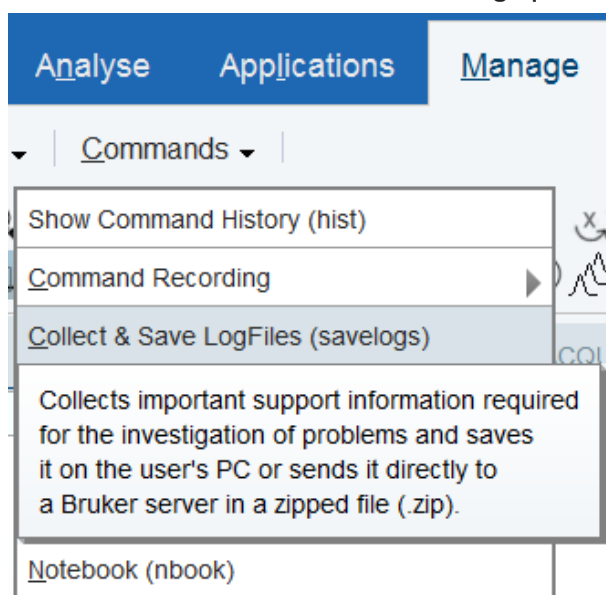
It is now possible to wobble more than one channel simultaneously. The following **wobble** commands are now available:

- **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

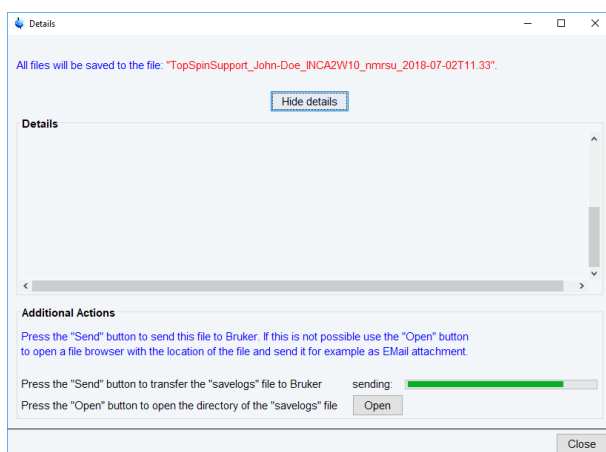
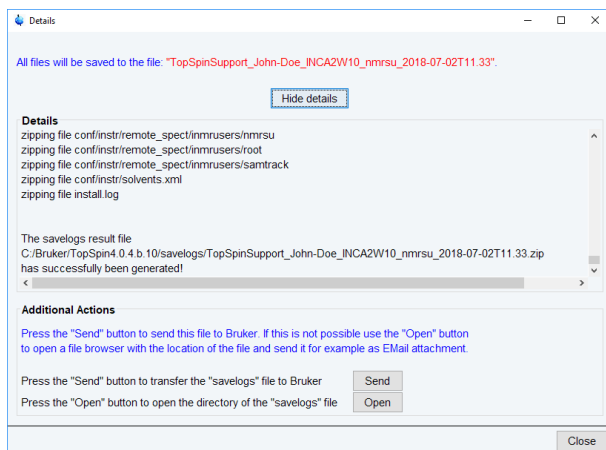
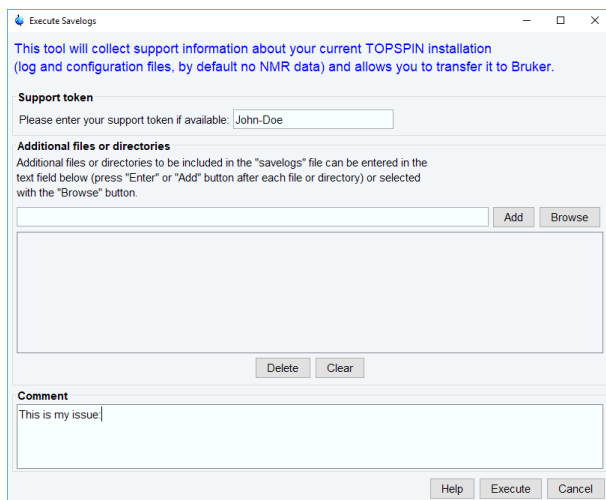
7.5.2.3 Processing

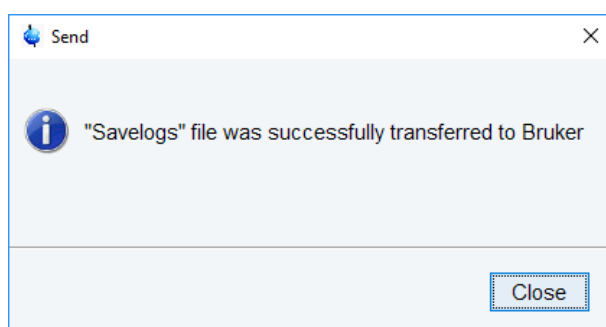
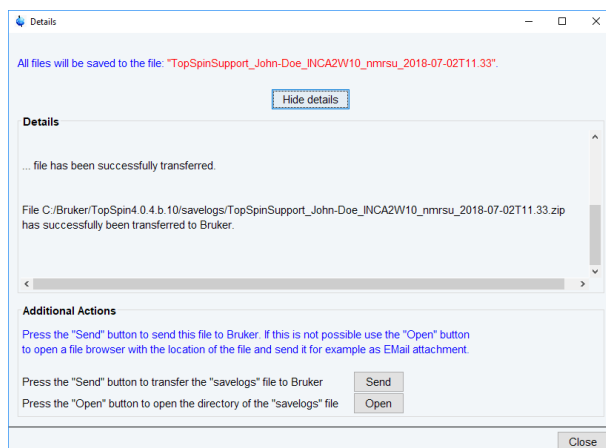
7.5.2.3.1 Revision of savelogs

The functionality to "Collect & Save LogFiles (**savelogs**)" has been revised for TopSpin 4.0.4. The command can be started from **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.





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.

7.5.2.4 Automation

7.5.2.4.1 Icon NMR

- 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)

7.5.2.5 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").

7.5.2.5.1 Write FnILOOP depending on mc Existence

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.

7.5.2.6 GxP Operation

7.5.2.6.1 Updated version of the 21 CFR Part 11 User Manual

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 `nmsu`. Also some explanatory text fragments have been corrected and improved.

7.5.2.6.2 Use 'unused' instead of 'unknown' in TopSpin's Login Protocol

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.

7.5.2.6.3 Initial Password for Internal User expires immediately

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.

7.5.2.6.4 Functionality of 'lockdataset' on Remote File Systems Limited

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.

7.5.2.6.5 Central Audit File Available on Windows Installations

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.

7.5.2.7 Analysis

7.5.2.7.1 Fragment Based Screening (FBS)

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.

7.5.2.7.2 Structure Elucidation

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.

7.5.2.8 AU Programming

7.5.2.8.1 Reading peaklists from inside an au-program now works in arbitrary (up to 8) dimensions

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`.

7.6 TopSpin 4.0.5

7.6.1 New Features

7.6.1.1 Support of TRX2

TopSpin 4.0.5 offers full support of TRX2 boards.

7.7 TopSpin 4.0.6

7.7.1 Bug Fixes

7.7.1.1 Bug Fixes in TopSpin

The following topics describe the major fixes which come with TopSpin 4.0.6.

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 #14495	Wrong DIGMOD and DSPFIRM combination in PROTON parameter sets
• Item #14477	TopSpin crashes exiting multiplet analysis mode
• Item #14363	AU program to reduce T1 noise in 2D spectra
• Item # 14235	User defined prosol pulseassign files not found
• Item # 14518	Data processed with nusft incorrectly scaled
• Item #14532	Wrong display of atom isotope numbers
• Item #14531	Repeated switching to Plot tab makes plot editor unusable

7.7.1.2 Bug Fixes in IconNMR

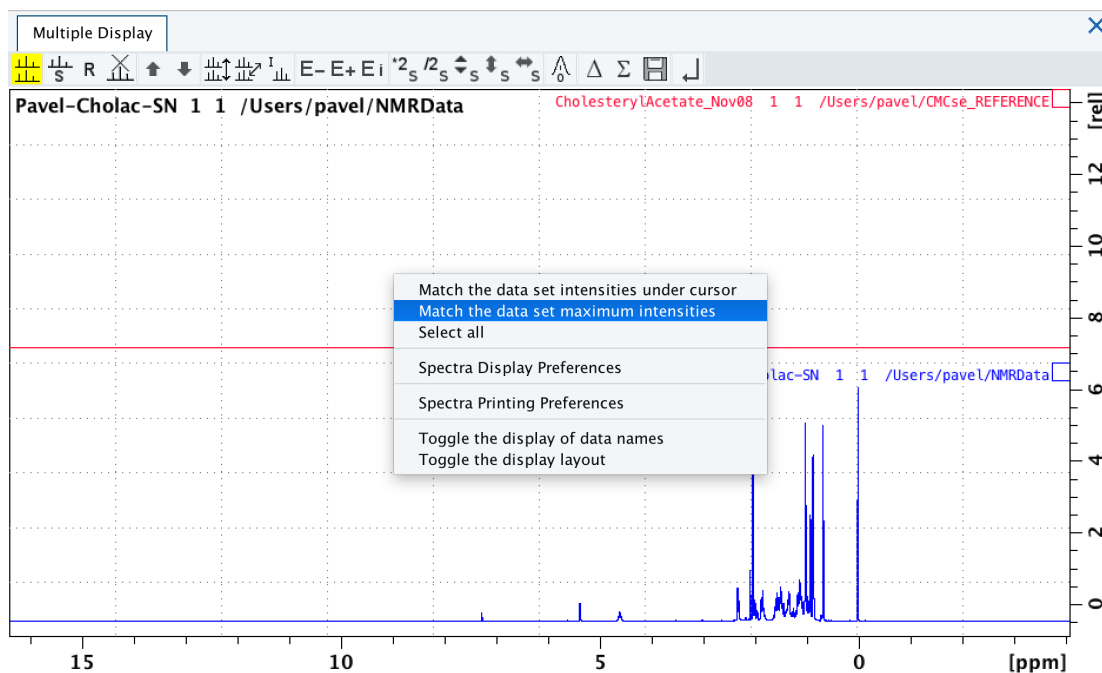
• Item # 14510	Long night time experiments hang – error message appears
• Item # 14497	IconWeb Web Server Settings 'Make Certificate' button broken
• Item # 14494	Automation will not start - Jump to next sample active
• Item # 14491	Skip Identify User Feature not activating Non-Supervisor lockdown in TopSpin
• Item # 14489	MS Runtime libraries missing in IconNMR Installation
• Item # 14442	Archiving directory permissions too restrictive

7.7.2 New Features

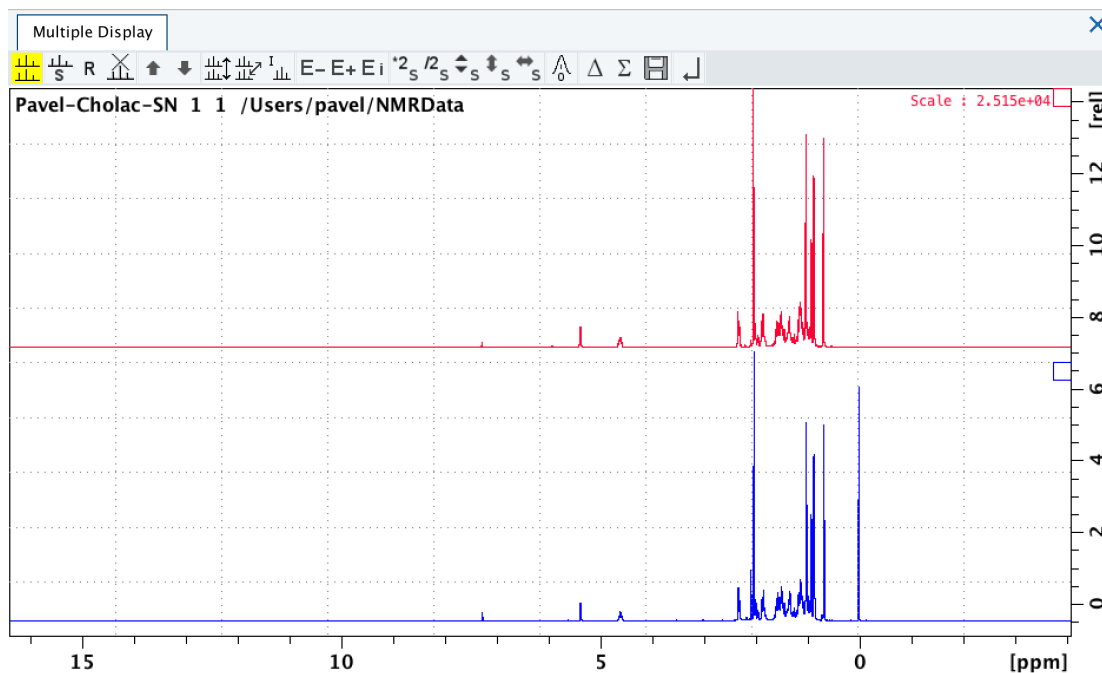
7.7.2.1 General User Interface

7.7.2.1.1 New 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**.

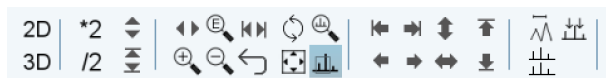



The spectra are properly scaled, the required scaling factor is displayed.



7.7.2.1.2 Data View Synchronization

The command **.sync** is now available also in Topspin toolbars.



Clicking the synchronization button  adjusts the visible part of all spectra so, that they match the displayed region of active (selected) dataset.

7.7.2.2 Acquisition

7.7.2.2.1 Interactive Magic Angle Adjustment Supports Additional Parameter

The interactive magic angle adjustment (**gs mas**) now supports an optional additional parameter (**mc** or **pk**) which allows to choose between a magnitude spectrum (**mc**) and a phase corrected spectrum (**pk**).

7.7.2.2.2 Command edlist Supports Gradient Files

The **edlist** command supports the Gradient Files: **edlist <gp>**

gp entry appears in the **edlist** dialog in the menu **Options | Manage Source Directories | Gradient Files**.

The gradient files can be found in the directory:

```
<tshome>/exp/stan/nmr/lists/gp
```

7.7.2.3 Processing

7.7.2.3.1 New processing command apbk

A new algorithm for baseline and phase correction has been developed.

The command **apbk** provides both phase and baseline correction. The current implementation has been designed and tested for ¹³C, ¹⁹F and ³¹P spectra.

Support for other nuclei will follow in subsequent software releases.

The comparison of the traditional processing and the **apbk** command shows the advantages of the new algorithm.

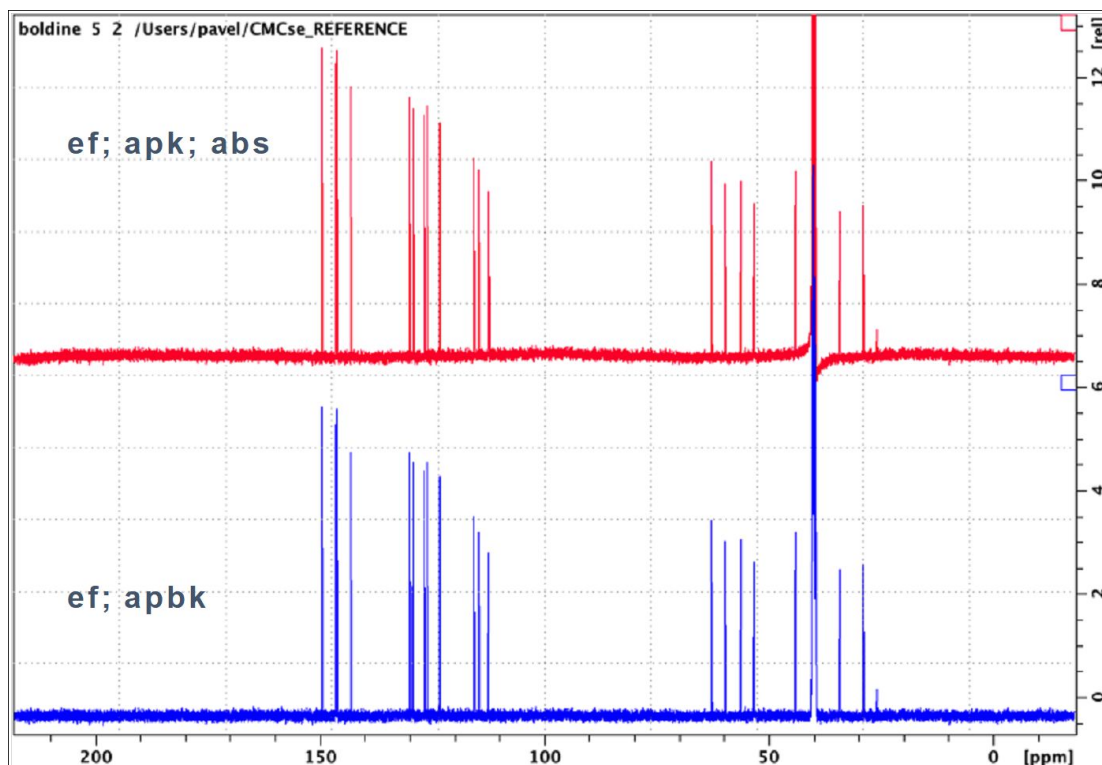


Figure 7.2: Comparison of traditional processing and the apbk command.

7.7.2.4 Automation

7.7.2.4.1 IconNMR 5.1.6 New/Updated Features

AutoCalibrate (New – Requires additional license)

AutoCalibrate calibrates the 1H p90 pulse length, temperature calibration and 3D shims.

The calibration is performed on a single optimized sample containing the molecule sucrose in 90% / 10% H₂O / D₂O with DSS (2mM) as the chemical shift reference.

As well as those parameters listed above, AutoCalibrate also performs integral integrity/ concentration calibration, ensuring the entire system is running optimally.

- Fully automated, runs at off-peak hours with minimum inconvenience
- Dedicated sample from Bruker to maintain instrument performance
- AutoCalibrate requires a license as well as the AutoCalibrate Test Sample.

Smart DriveNMR (Update - Requires additional license)

- simplified set-up using operation modes
- providing structural information is now optional
- structure verification in automation is no longer mandatory
- improved acquisition and processing of 1D ¹³C

- acquisition of 2Ds is performed with NUS in a fail-safe way
- additional license needed

PotencyMR (Update - Requires additional license)

- Analyte's integral is now defined using methods
- **Peak snapping** feature - improving automatic analysis
- Structure Verification is now optional
- Option to eject/reinsert the sample – **Repeats**
- Integration using factors of half width in CMC-assist

CMC-q (Update)

- improved set-up dialog
- support for generation of sd-files
- automatic selection of experiment numbers possible
- position information available in batch table view

Automation Features (New)

- Reworking of Automation window, streamlining Analysis integration
- TopSpin command: **sti <holder>** - Send any data set to Automation for measurement on any sample
- Allow [] in Data Set Names
- Option to not remove existing permissions (Windows Access Control Lists) from Data directories after processing
- Option to allow for re-shimming of the sample after repeated ATMA optimization

Security

- Option to not list available users at the login window: **Configuration | Options | General**

7.7.2.5 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").
- The obsolete pulseassign folder in <tshome>/conf/instr/remote_spect/prosol has been removed.

Pulseassign files are exclusively located in <tshome>/exp/stan/nmr/lists/prosol/pulseassign

7.7.2.6 GxP Operation

7.7.2.6.1 User friendly Dataset Audit Report

New command **auditreport** displays the audit entries recording the data set history in readable form.

The report includes a consistency statement that validates the integrity of the dataset.

auditreport is available either from the command line, or from the security menu in Topspin (**Manage | Security | Audit**).

Audit Trail Report



Dataset Name: A2 2 1 /Users/pavel/CMCse_REFERENCE
 User: pavel
 Date: 2018-09-26 14:09:21.0610 +0200

Consistency Check:

Acquired Data Audit Log

File Checksum: (hash MD5)
) da c7 a8 f6 5c 64 68 56 b8 86 46 e6 a4 c4 2c d4

	WHEN	WHO	WHERE	WHAT	Explanation
1	2008-11-28 10:09:44.831 -0500	nmrsu	AVIII400	created by zg , started at 2008-11-28 02:21:37.940 -0500. , POWCHK enabled, PULCHK disabled.	
2	2008-11-28 10:09:45.972 -0500	nmrsu	AVIII400	user comment: , ICON-NMR User ID: SELU	

Processed Data Audit Log

File Checksum: (hash MD5) fe 40 08 d3 37 2f 43 af 6e 73 95 7a 5a 22 44 2a

	WHEN	WHO	WHERE	WHAT	Explanation
1	2008-11-28 10:09:44.831 -0500	nmrsu	AVIII400	created by zg, started at 2008-11-28 02:21:37.940 -0500, POWCHK enabled, PULCHK disabled	Perform an acquisition overwriting possible existing data
2	2008-11-28 10:09:45.972 -0500	nmrsu	AVIII400	user comment:, ICON-NMR User ID: SELU	
3	2018-09-10 11:24:52.557 +0200	pavel	pavels- mbp.intra.brkr.corp	Start of raw data processing, ef LB = 1.5 FT_mod = 6 PKNL = 1 SI = 128K	Exponential window mult. + Fourier Transform (1D)
4	2018-09-10 11:25:04.178 +0200	pavel	pavels- mbp.intra.brkr.corp	apk	Automatic phase correction (1D)
5	2018-09-10 11:25:05.355 +0200	pavel	pavels- mbp.intra.brkr.corp	abs ABSG = 5	Automatic baseline correction with integration (1D)

Figure 7.3: Dataset Audit Report (**auditreport**)

7.7.2.6.2 Multiple Subsequent Electronic Signatures Displayed in Plot

The electronic signature which has been applied to a data set can be included in a data plot as part of the parameter object. This used to recognize the last applied, valid signature. If multiple signatures have applied subsequently they now will be all shown.

Please note that electronic signatures are only valid if they are contiguously following and are the last entries in the processing audit file.

7.7.2.6.3 Electronic Signature Function also available for System User Account

Users can apply the electronic signature function also with their current login account of operating system in order to easily perform signing without being forced to setup a TopSpin-internal user account first. When not logged with an 'internal user account', entering the command **esign** will ask for entering the password for the currently logged-in system account, then open up the **esign** dialog.

In this mode the field 'meaning' is preset with a default value **Review** and is editable. An arbitrary meaning for this signature then can be entered. With internal logins enabled, the available entries for 'meaning' would be defined by the dialog for internal user administration and not be editable when signing. So in both operating modes the requirements of the 21CFRpart11 document are fulfilled.

This functionality is available for Windows and Linux operating systems.

7.7.2.6.4 Internal User Management allows Reset of User Password

If a TopSpin user has forgotten the password of the associated internal user account, the password can be reset by the NMR Administrator. The **uadmin** dialog offers a button **Reset Password** which asks for entering a new one-time password for the selected user. When this user performs a log on the next time with the one-time password the system enforces the user to update the password immediately.

7.7.2.6.5 Data Deletion recorded also in Central Audit Trail

Central audit trails independently records the date and time of operator entries and actions that create, modify, or delete electronic records.

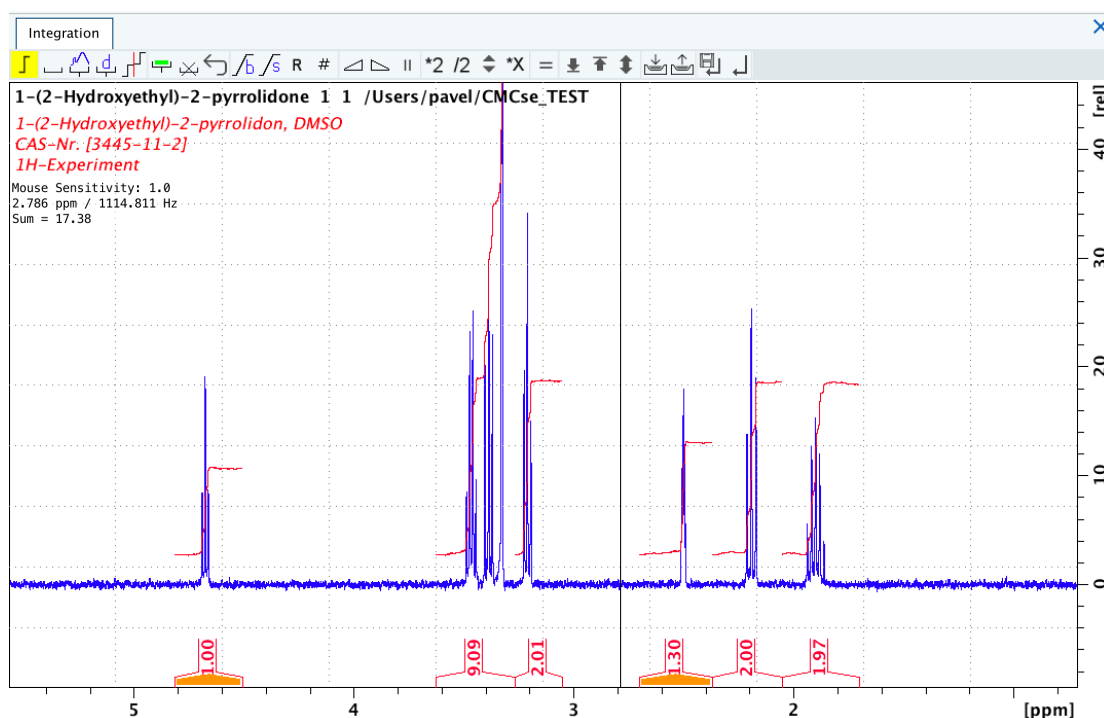
7.7.2.7 Analysis

7.7.2.7.1 Improvement in Interactive Integration Module

The selection of integrals has been simplified.

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. Any manipulation of integration regions (including deletion) can be undone with the **Undo** button.



7.7.2.8 AU Programming

7.7.2.8.1 New AU program t1noisereduction

The new AU program t1noisereduction is useful for removing T1 noise from any 2D spectrum.

7.7.2.9 Documentation

New documentation under **Help | Manuals (docs)** available for:

- AutoCalibrate
- AssureSST
- PotencyMR

Updated documentation under **Help | Manuals (docs)** available for:

- Acquisition Commands & Parameters
- Processing Commands & Parameters
- Advanced NMR Experiments
- CMC-assist
- SmartDriveNMR
- CMC-q
- APSY
- CodeMeter License Management
- EULA – End User License Agreement
- Pulse Programming
- biotope
- PotencyMR Quick Start Guide
- ShapeTool

7.8 TopSpin 4.0.7

7.8.1 Bug Fixes

7.8.1.1 Bug Fixes in TopSpin

The following topics describe the major fixes which come with TopSpin 4.0.7. The topics are named by item numbers, referring to the Bruker-internal knowledge base system. For detailed information about the different items, please contact Bruker NMR support.

Item# 14636	Electronic signature not applied to 2D audita.txt
Item # 14628	Non logical parameter settings in CMCse_INAD parameter set
Item # 14610	H2BC may not work if NUS is enabled
Item # 14562	Wavemaker fails on PPs stored in non-default user dir
Item #14561	Wavemaker fails to locate user CPD sequence
Item #14566	Experiment selector creates NOAH2_SB wrongly

Item # 14582	Error message in ased due to cnst30 calculation
Item # 14465	Wavemaker fails to locate user pulse sequence
Item # 14419	Creation of 1D stacked plot not possible without predefined layout

- Central audit log file can be removed involuntarily without first changing the file access rights.
- Errors fixed which caused incomplete default routing in **edasp** involving selective and non-selective connectors for 19F.
- Errors fixed in **edtune** regarding finding an existing 'Probe tune file', creating a new one, and synchronizing the changes with the EPU.

7.8.1.2 Bug Fixes in IconNMR

Item #14646	Barcodes are never found
Item # 14642	AutoCalibrate skips the next day when running late night
Item # 14641	AutoCalibrate runs at unexpected times
Item # 14634	User Manager: can't read "exp_comment": no such variable
Item # 14625	User Specific Originator Items not being used
Item # 14624	MAS III - Failed rotation halts automation
Item # 14623	Send to icon (STI) data path handling changed
Item # 14622	AssureNMR: Error message: unknown antype ->AN_ASSURE<-
Item # 14618	Default experiment not set
Item # 14605	AssureSST runs with Analysis/Quantification on
Item # 14604	Error when adding an experiment in PotencyMR
Item # 14600	Problems with printing and mailing of SmartDrive reports
Item # 14594	Various problems creating Composite Experiments in External Setup
Item # 14593	User Manager doesn't show full Composite Experiment Name
Item # 14591	Easy Setup Mode: AutoSampler Position Window opens in background
Item # 14590	Exit from Automation still possible if mwm not in use
Item # 14588	Analysis/Quantification activated unnecessarily
Item # 14583	Pause removing sample from magnet hangs
Item # 14576	IconNMR user group not captured in accounting files
Item # 14568	UserManager: Users may not be deleted
Item # 14565	CMC-q experiments run in wrong mode
Item # 14559	SmartDrive message: Job with id <ID> cannot be found
Item # 14539	Automation window crashes immediately on opening

7.8.2 New Features

7.8.2.1 General

7.8.2.1.1 Update of CodeMeter Runtime

On macOS-based computers, the new CodeMeter Runtime version 6.80 is installed which includes support for macOS 10.15. Linux and Windows configurations have been successfully validated for continued use of version 6.40.

7.8.2.2 General User Interface

7.8.2.2.1 Two New Plot Layouts available

Two new plot layouts have been added to the Bruker plot layout library: *2ppm-5stack.xwp* and *2ppm-5stack-1.xwp*.

2ppm-5stack.xwp: plots 5 expansions of 2 ppm each from the current spectrum (from 0 to 10 ppm) in a stacked plot-like appearance. No integrals or peak picking results are shown. The global scaling option is used for each expansion, so that the expansions are comparable with a plot of the whole spectrum.

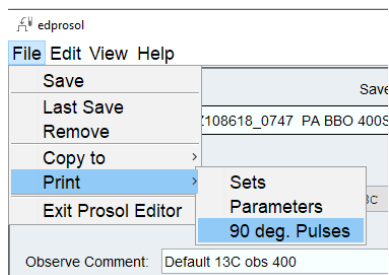
2ppm-5stack-1.xwp: plots 5 expansions of 2 ppm each from the current spectrum (from 0 to 10 ppm) in a stacked plot-like appearance. No integrals or peak picking results are shown. The scaling is done to the height of the biggest peak in the expansion and respecting solvent regions.

Both layouts can be used as an example for similar types of plots, but with different region limits and/or number of expansions.

7.8.2.3 Acquisition

7.8.2.3.1 edprosol: Simplified Print Function

edprosol offers a simplified print function for 90 deg. pulses, which is available from the menu bar **File | Print | 90 deg. Pulses** in the **edprosol** window:



This function prints out the selected probe, the solvent, all hard 90 degree pulses and the power levels for all nuclei.


```

Preview of Prosol Parameter List
File Edit Search
1 | Prosol 90 deg. Pulses
2 | -----
3 | Screen dump date: Dec 14, 2018 10:18:53 AM
4 |
5 | Probe: Z108160_0059 CP TCI 600S3 H-C/N-D-01.7 Z
6 | Solvent: generic
7 |
8 |
9 | *** Saved Observe Pulse Parameters:
10 | Comment: Default 1H obs 600
11 | Nucleus: 1H
12 |
13 |      Nucleus   Pulse Width[μs]   Att. Lvl. [dB]
14 |           1H           0.02           70.00
15 |           2H           57.90          -16.79
16 |           13C          0.02           70.00
17 |
18 |
19 | *** Saved Decouple Pulse Parameters:
20 | Comment: Default 1H dec 600
21 | Nucleus: 1H
22 |
23 |      Nucleus   Pulse Width[μs]   Att. Lvl. [dB]
24 |           1H           0.02           70.00
25 |           2H           57.90          -16.79
26 |           13C          0.02           70.00
27 |

```

7.8.2.3.2 What is New in WaveMaker

The maximum number of steps for shaped pulses on AVANCE NEO systems is increased to 1e6. The `cw()` and `cw_d()` functions for multi-frequency pre-saturation and multi-selective decoupling applications added to the WaveMaker shape library.

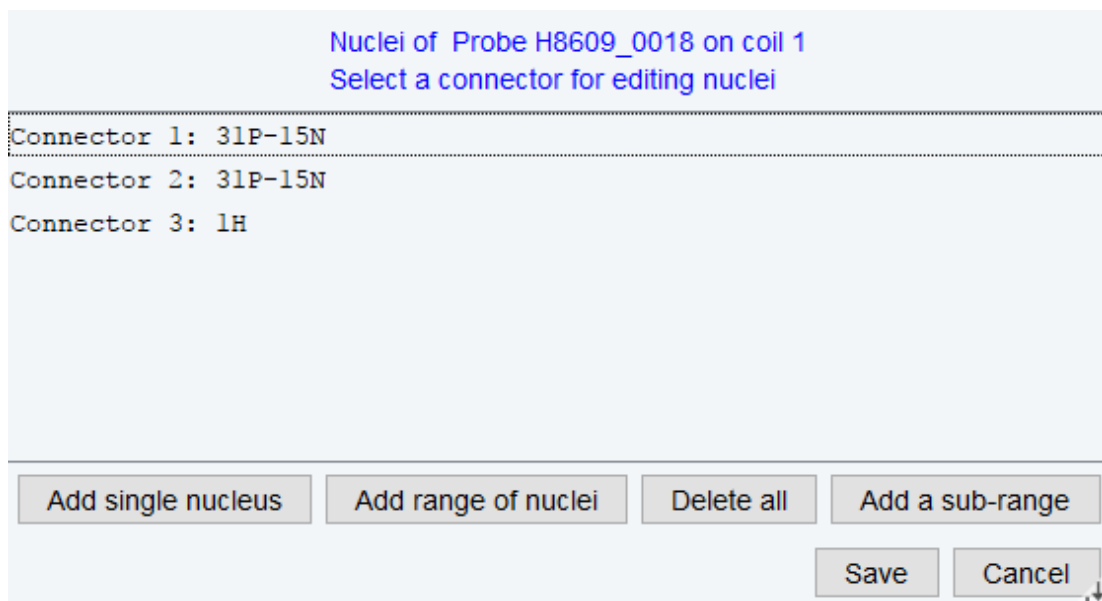
Updated WaveMaker manual pages include:

- examples of easy setup of bi-level decoupling, section 3.4;
- examples of multiple (solvent) peak suppression in automation, section 3.21;
- applications adiabatic pulses in fluorine-19 NMR, section 3.9.

The WaveMaker User Manual can be found under **Help | Manuals (docs) | Acquisition – Application Manuals**.

7.8.2.3.3 edprobe: Option to define subrange frequencies

Added option to define subrange frequencies for broadband coils.



7.8.2.3.4 Changes in prosol Synchronized to the Workstation

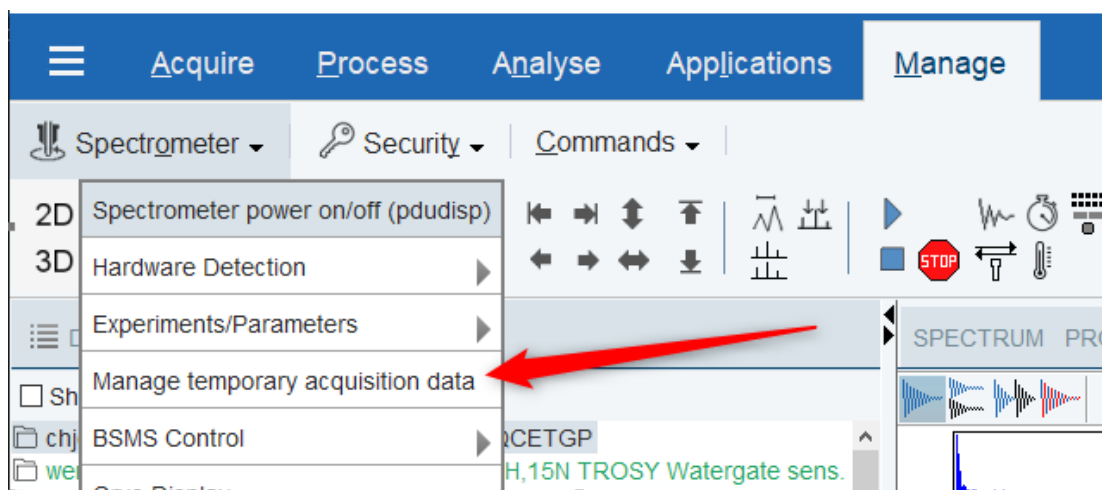
Changes made in **prosol** will automatically be synchronized from the EPU to the workstation when exiting **prosol**.

7.8.2.3.5 NUS Acquisition Scheme Respecting TDMAX

NUS acquisition scheme now respects pulseprogram feature TDMAX.

7.8.2.3.6 Data Storage on EPU

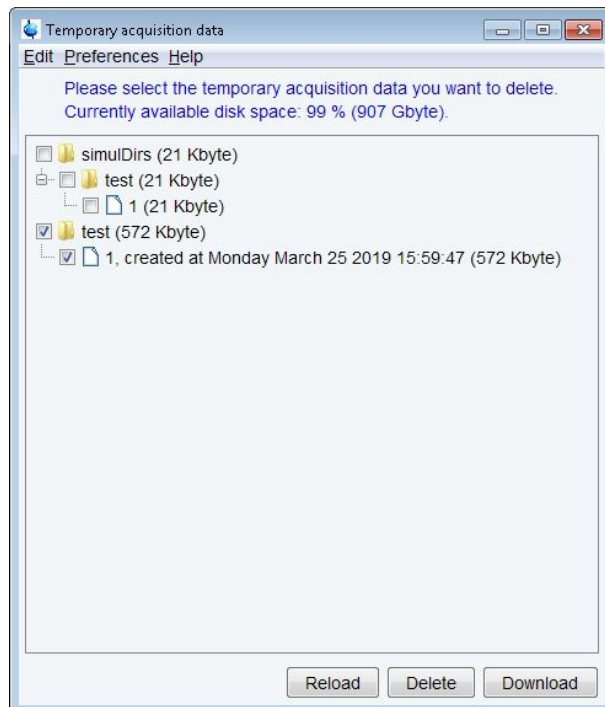
On an AVANCE NEO spectrometer, by default all data stored temporarily on the EPU during an acquisition are deleted after completion of the experiment. This automatic deletion routine can be modified by clicking **Manage | Spectrometer | Manage temporary acquisition data** (or entering the command **deletetmpfiles**).



With TopSpin 4.0.7, the capabilities of this **Temporary acquisition data** - dialogue were extended and slightly changed.

Changes:

The file tree in the main window displays only the data of those experiment numbers which were created by the same user which currently uses TopSpin:



Any temporary acquisition data of other users are not shown, i.e. also cannot be modified by the current user.

The dialog appearing via the menu **Preferences | Edit temporary acquisition data preferences** was slightly reorganized:

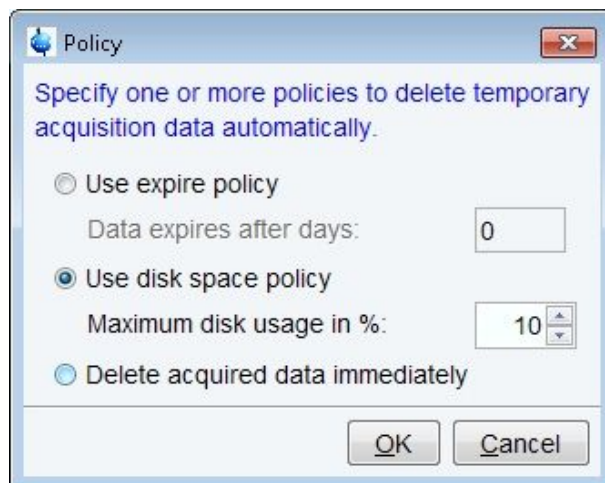


Figure 7.4:

It is not possible anymore to define an expire policy and a disk space policy at the same time, the user has to choose between those options.

The default setting is **Delete acquired data immediately**.

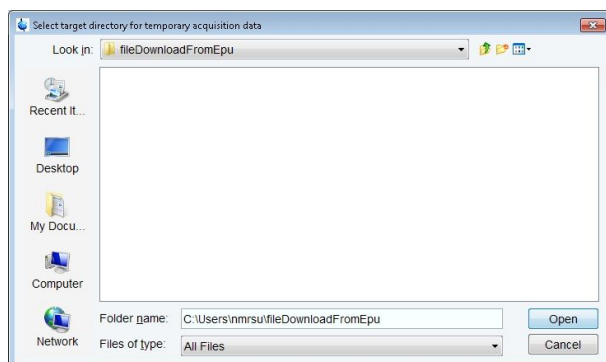
The functionalities of the **Reload-** and the **Delete-**Button in the main window basically remain unchanged except for the user restrictions for the data displayed, as mentioned above.

New:

With TopSpin 4.0.7, the main window of the **Temporary acquisition data** - dialogue now shows an additional **Download-**Button.

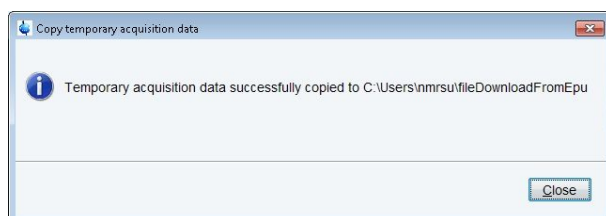
Via this button, the user can copy the experiment directories which were selected in the file tree from the EPU into an arbitrary directory on the workstation.

Clicking **Download** opens a common file dialogue (shown below for a Windows - workstation) where the user can choose or create a target directory on the workstation:



Clicking **Cancel** aborts the copy process.

Clicking **Open** starts the copy process and yields a message in case of success:



Notice: Data copied from EPU to workstation are still present on the EPU afterwards. They have to be explicitly deleted by either clicking the **Delete** - button or by changing the deletion policy.

7.8.2.3.7 wobb: Nucleus Name shown on Hppr Cover Module Display

wobb now shows nucleus name on Hppr Cover Module display.

7.8.2.3.8 New FnMode QF(no-frequency) available

FnMode QF(no-frequency) indicates non-spectroscopic dimensions (pseudo-dimensions). Processing in this dimension will issue a warning.

7.8.2.3.9 New Acquisition Status Parameter UUID

Status Parameter UUID is a status acquisition parameter holding a unique identifier for each acquired data (fid, ser files).

The identifier is written in the **universally unique identifier** format:

```
##$UUID= <edaf27e8-40f9-11e9-bb21-001395173487>
```

The value of the UUID parameter is generated when the data acquisition has finished and also recorded in the dataset audit trail. Duplicating a data set (**wrpa** command) preserves the original value. This allows to identify copies of the original data.

7.8.2.3.10 Using two different gradient systems

In some special configurations your spectrometer can be equipped with two different kinds of gradient amplifiers:

- The internal GAB in the BSMS common to most spectrometers
- An additional imaging gradient system (BGA, GREAT)

In most of such cases, there are also two different probes available, one which should be used together with the GAB and another one which should be used together with the imaging system.

Once the assignment of a specific probe to a certain type of gradient amplifier system and the preemphasis settings for that probe have been saved, the acquisition (and in particular also **topshim**) will always take those saved settings and choose the gradient system according to the currently installed probe, as specified in **edprobe**.

Choosing a different gradient system for a specific probe can be accomplished as follows (applies also for the rare case of using the same probe with two different gradient systems):

- If you need your current preemphasis settings for future work, make a backup before: enter **setpre** and click on **write to epu** and close the **setpre** window
- Enter **setpre -select** and choose the desired system by clicking on it
- Then the usual **setpre** window pops up
- Perform all relevant settings there
- Click on **save as default**, otherwise these changes will have no effect
- Remember that this overrides all your previous settings for the default configuration

The respective parameters formerly used in **edskon** (GRADCHAN, GRADPRE) have no effect anymore.

7.8.2.4 Processing

7.8.2.4.1 3D Processing command **tf3** no longer supports option **p**

3D processing command **tf3** no longer supports option **p**. This option is no longer required, because disc capacity is large enough to store output data locally.

7.8.2.5 Automation

7.8.2.5.1 General Automation Features

- MAS III handling improved - Non-rotating samples are skipped
- Domain Users are displayed much faster
- Preceding experiment "failed" experiment colors now configurable - see Fail Safe/Error handling

7.8.2.5.2 SST - qPQ Performance Qualification Test

This new addition to the standard suite of System Suitability Tests (SST) is designed to enable users to perform a process qualification test, specifically for application to quantitative NMR (qNMR) analyses. The test utilises samples that are available from Merck KGaA, Darmstadt, Germany (which operates as MilliporeSigma in the U.S. and Canada), and consists of a binary mixture of two well-known Certified Reference Materials (CRM).

The samples are manufactured to current best practices and concentrations as well as the calculated uncertainty values that are given on the sample certificates are entered into the dialog screen together with sample lot number, sample position number and shim program.

The results of the test are added to standard test report.

7.8.2.6 Pulse Programming

7.8.2.6.1 cphd Pulseprogram Statement

The cpdhd pulseprogram statement is now correctly working.

7.8.2.6.2 Assignment of nbl in the Pulse Program possible

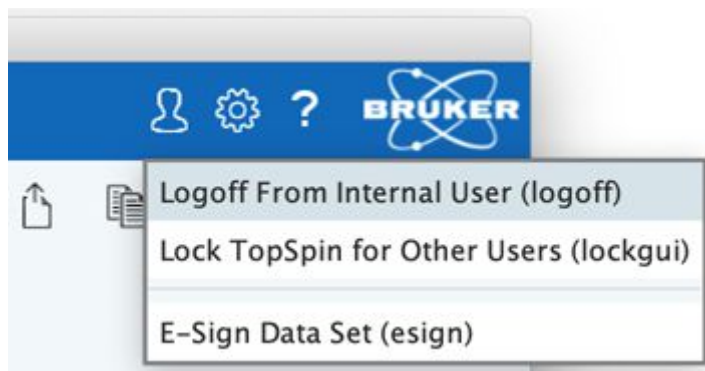
The parameter nbl is used to acquire FIDs in multiple acquisition memory blocks. Some experiments only work correctly when nbl is set to a specific value depending on other acquisition parameters.

So far, it was necessary to do that manually. Now, nbl can be assigned in the pulse program before the ze statement, e.g. "nbl=td1".

7.8.2.7 GxP Operation

7.8.2.7.1 Improved Usage of TopSpin Internal User Accounts

New **Internal User** icon in the TopSpin toolbar simplifies access to frequently used functions like locking of TopSpin GUI and signing of data sets.



7.8.2.7.2 Enhancements to Central Audit File

The capability to maintain a Central Audit File is available also for Linux and macOS installations. The related option in the installation routine is now enabled by default.

The storage location of the Central Audit File has moved from the Topspin installation to a central, operating system dependent location:

- macOS: */Library/Logs/Bruker/TopSpin/Audit/CentralAudit.log*
- Linux: */var/opt/Bruker/TopSpin/Audit/CentralAudit.log*
- Windows: *C:/ProgramData/Bruker/TopSpin/Audit/CentralAudit.log*

This means, there exists only one Central Audit File on a computer, and all TopSpin installations share the same file for storage.

7.8.2.7.3 Example Layout for Inclusion of Information Parts

A new plot layout is delivered as part of the layout collection which demonstrates various aspects of including meta information in layouts that may be of interest in regulated environments. The layout is based on a 1D layout and comes with the name "1D_H+gxp_info.xwp". Some explanatory texts are included which should be removed before use in production context.

The "NMRTText" object can be used to include content of external files in the data set, like e.g. the audit log (*auditp.txt*), or information from the **Sample** tab (which is held in file *sample.prop*).

For 'Parameter' objects, the option "Use custom definition" can be set. The content of the object is freely defined then, and the following special tokens are available:

- <DISK>, <NAME>, <EXPNO>, <PROCNO> items will be replaced by the respective elements of the data set identification
- <CREATIONDATE> replaced by time/date stamp for the time of plot creation, i.e. printing, or PDF generation
- <TOPSPINVERSION> indicates which Topspin version creates the plot
- <\$VARIABLE> includes the current value of a system environment variable (see specific examples in the layout)
- <PARAMNAME> includes the current value of a single data set parameter, e.g. <SF> includes the spectrometer frequency
- Any other text is reproduced without further change

7.8.2.7.4 Extended Audit Trail Report Information

The PDF-based „Audit Trail Report“ (command **auditreport**) includes information about creation of the report. This has been supplemented by an entry about the TopSpin version which has generated the document.

Entries in the column “Explanation” have been reviewed in order to be more precise and sensitive to found command options.

7.8.2.8 Documentation

Updated documentation under **Help | Manuals (docs)** available for:

- NUS Parameters
- SmartDriveNMR
- Acquisition Commands & Parameters
- Processing Commands & Parameters
- CodeMeter License Management
- Pulse Programming
- AssureSST – System Suitability Test
- WaveMaker
- Software License Agreement

7.9 TopSpin 4.0.8

7.9.1 Bug Fixes

7.9.1.1 Bug Fixes in TopSpin

The following topics describe the major fixes which come with TopSpin:

- nmrsim crashes when TD>64k is used
- Simulation of experiments using frequency shifted shaped pulses may fail
- installnmr deletes `<TSHOME>\prog\logfiles\login.txt`
- Sola: Command not implemented fit1d_savecsv
- Pulse programs with "spoffX=Y" break plotting
- AU programs don't run on macOS
- Receiver phase correction fails in Cortab for MRI systems

7.9.1.2 Bug Fixes in IconNMR

SKB-12	Title-Parameters Windows do not open after some time
SKB-36	ICONNMR automation intermittently hangs with a remarkloc error message
SKB-22	Barcode Use (SampleXpress) Experiments measured on incorrect sample
SKB-15	Archiving not functional
BKB Item #14666	AssureSST Report contains 1H qNMR FailPass Line

Please note, a version specific knowledgebase containing minor patches and other items is online and continuously updated.

Direct Access is available when the Instrument is on the net, or where IconNMR is running on a networked system with Internet access.

Use the **Help | About** menu entry and click on **Knowledgebase** where available.

7.9.2 New Features

7.9.2.1 General

7.9.2.1.1 Support of Fourier 80 Spectrometers

TopSpin 4.0.8 now supports the new Fourier 80 benchtop spectrometer. Great care has been taken to make the Fourier 80 fully compatible with TopSpin. Therefore, there are only minor differences between the handling of a Fourier 80 and an AVANCE NEO spectrometer. The main differences relate to the Lock and Shim procedures. Please refer to the Fourier User Manual.

7.9.2.2 Acquisition

7.9.2.2.1 64bit double number used as a default for any NMR data

With TopSpin 4.0.8 64bit double number format is used for the storage of acquired multidimensional data (SER file). As TopSpin 3 (starting with 3.6.2) is now also able to process nD-data from NEO experiments, the automatic conversion of the acquired data into Topspin3.x format is by default not enabled anymore.

If necessary, the conversion to the 32-bit integer is still possible: Select the checkbox **Automatically convert 64bit SER data into TopSpin 3.x format in the Preferences | Acquisition** tab.

7.9.2.2.2 Parameter FILCOR can be defined individually

The parameter FILCOR has been moved from the **edscon**-parameters to **edprosol** so that it can now be defined individually for each probe.

It can be edited in **edprosol** and is automatically copied to the acquisition parameters via **getprosol**.

7.9.2.2.3 FILCOR Parameter Moved

The probe dependent FILCOR parameter has been moved from the 'scon' to the 'prosol' menu. It is now part of the prosol tables and the acqu file, and is read automatically by **getprosol**.

7.9.2.2.4 edlock: Lock Powers Optimization

edlock: lock powers can now automatically be optimized for an installed probe. Please refer to the edlock/edsolv manual for further information.

7.9.2.3 Processing

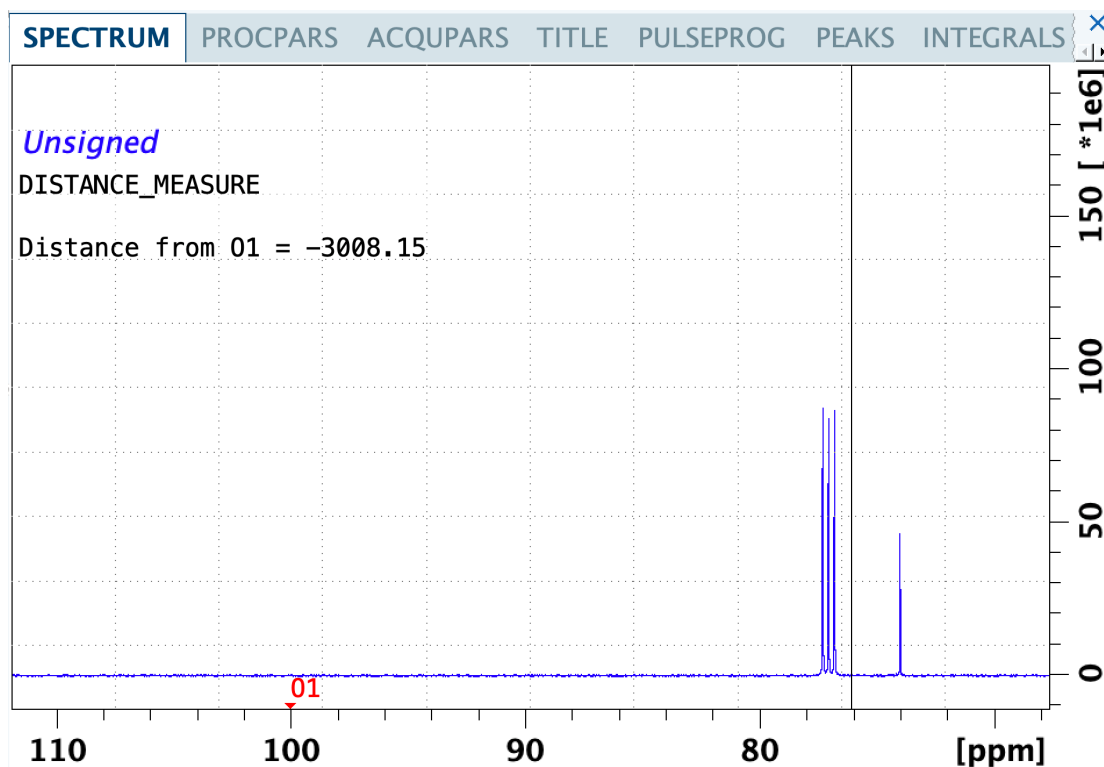
7.9.2.3.1 sref with Peak Position

It is now possible to call the processing command **sref** with a desired peak position in ppm as parameter.

- So if, for example, a spectrum has a peak at 4.2 ppm, typing **sref 4.1** would perform the following steps:
- Look if a peak exists in a certain solvent specific range (search width specified in edsolv) around 4.1 ppm
- If the peak was found, the whole spectrum will be shifted such that the peak finally appears at 4.1 ppm
- If the peak was not found, an error message will be displayed and the default calibration will be done

7.9.2.3.2 Display of Cursor Position Relative to O1

The distance measurement tool (**.dist**) shows the position of the O1 frequency on the spectrum. Additionally, the distance between cursor and O1 is shown.



7.9.2.4 Automation

- Domain Groups: (Windows) Only display users from particular ActiveDirectory Groups in the User Manager. See Options | Resource File Settings | Domain
- Enable/Disable Users – Use the Enable/Disable buttons in the User Manager to revoke particular measurement rights temporarily
- Configuration option to block empty passwords. See Options| General| Security
- “ICON-NMR User” also saved to data set audit trail processing file
- One click/Automatic logout complete Lock down of Automation and TopSpin. See Options | Resource File Settings | Automation
- TopSpin’s lockdataset AU program available as a setting under Umask User Manager options
- User Files no longer created automatically on start-up (apart from the very first user)
- Windows: Parent data set directories paths which are to be generated should now inherit the permission of their parents
- Restrict Disk units to sub directories of supplied disk paths. See Options| Resource File Settings| Automation
- IconWeb Server TLS 1.3 support
- Create partial .xml Configuration Export files which may be loaded only replacing their partial content
- PotencyMR now provides four parameter sets for experiments with 90deg or 30deg excitation pules with or without 13C decoupling.
 - P_PROTON
 - P_PROTON30

- P_PROTON_IG
- P_PROTON30_IG

Please refer to the manual for further details.

7.9.2.5 Analysis

7.9.2.5.1 CMC-se 2.7

CMC-se 2.7 is the latest version of Bruker structure elucidation Plug-In. It includes several bug fixes and following new features:

- NMRData implementation.
- NMRData (www.nmredata.org) is a format for the publishing of NMR signal assignment for small molecules.

CMC-se assignment of NMR signals to atoms in a elucidated structure may be exported in NMRData format. NMRData may imported into CMC-se project.

- HOESY spectra were added to the list of supported datasets (display only).
- List of possible charged atom states was updated (e.g. perboric acid).

7.9.2.6 Pulse Programming

7.9.2.6.1 New Pulse Program Statement 'scaleByNs'

The new pulse program statement 'scaleByNs' is used to force scaling of acquired FIDs by the applied number of scans. Please refer to the Pulse Programming Manual for more details.

7.9.2.6.2 Definition of Minimum Required TopSpin Version in a Pulse Program

With TopSpin 4.0.8 it is possible to specify a minimum required TopSpin version in any pulse program.

This is useful if the pulse program uses a new feature which is only supported with a certain TopSpin version but not with older versions.

The pulse program syntax is as follows: `require TopSpin <majorNumber>.<minorNumber>.<patchLevel>`

The version specification needs those three numbers and the text TopSpin in front of it, otherwise a compiler error will occur.

For example, if the current release version is required for a pulse program, the syntax would be: `require TopSpin 4.0.8.`

If the currently running software version does not meet the requirement specified in the pulse program, the acquisition will not start with an error message stating that the currently used Software is too old.

Of course in TopSpin versions older than 4.0.8, such a version requirement will abort with a compiler error because this syntax is only supported with 4.0.8. But even this would then protect the pulse program from being executed with older versions.

7.9.2.6.3 Original Pulse Program Copied to Data Directory

With TopSpin 4.0.8 the original pulse program (parameter PULPROG) will be copied into the `<data set>/<expno>` directory as "pulseprogram".

Note that in earlier versions the file “pulseprogram” had a different meaning – it used to be the the modified pulse program, where the command `mc` was expanded according to the `FnMODE` parameter.

To resolve this conflict, the `mc` – expanded version of the pulse program now will have the new name “pulseprogram.precomp”.

7.9.2.6.4 Commands for Delay Lists Handling

Please note that the following old commands for handling delay lists (**vd** and **ivd**) and pulse lists (**vp** and **ivp**) have been described as deprecated in the documentation for quite some years now.

These commands will not be supported anymore in the future versions of Topspin. Topspin 4.0.8 is the last version supporting **vd** and **vp** in pulse programs.

If necessary, please adjust your pulse programs accordingly using the modern and more flexible syntax for user defined delay and pulse lists (**define list<delay>** and **define list<pulse>**).

7.9.2.7 AU Programming

7.9.2.7.1 AU Prgram measureHelev

The AU-program `measureHelev` can now accept a ‘-quiet’ parameter in order to run without displaying any messages on the screen.

7.9.2.8 GxP Operation

7.9.2.8.1 Example Layout for Inclusion of Information Parts

A new plot layout is delivered as part of the layout collection which demonstrates various aspects of including meta information in layouts that may be of interest in regulated environments. The layout is based on a 1D layout and comes with the name “1D_H+gxp_info.xwp”. Some explanatory texts are included which should be removed before use in production context.

The “NMRTxt” object can be used to include content of external files in the data set, like e.g. the audit log (*auditp.txt*), or information from the **Sample** tab (which is held in file *sample.prop*).

For ‘Parameter’ objects , the option “Use custom definition” can be set. The content of the object is freely defined then, and the following special tokens are available:

- `<DISK>`, `<NAME>`, `<EXPNO>`, `<PROCNO>` items will be replaced by the respective elements of the data set identification
- `<CREATIONDATE>` replaced by time/date stamp for the time of plot creation, i.e. printing, or PDF generation
- `<TOPSPINVERSION>` indicates which Topspin version creates the plot
- `<$VARIABLE>` includes the current value of a system environment variable (see specific examples in the layout)

- <PARAMNAME> includes the current value of a single data set parameter, e.g. <SF> includes the spectrometer frequency
- Any other text is reproduced without further change

7.9.2.8.2 Report for central audit trail (CAT)

A report for central audit trail (CAT) is available in pdf format. With command **catreport** or via menu **Manage | Security | Review Central Audit Trail** a search dialog opens:

Figure 7.5: Central Audit Trail File Viewer Search Dialog

The report may be filtered hierarchically by date (WHEN), user (WHO), dataset name (WHERE), keyword (WHAT) and/or file (FILE).

Clicking **Create report** creates a pdf report of central audit trail:

Central Audit Trail (CAT) Report

User: John Smith
 Date: 2019-08-22 11:50:33.0700 +0200
 Report created by: TopSpin 4.0.8
 CAT file data read: 100.0 %
 Audit records found: 901
 Audit records listed: 1

Search terms:
 WHEN (date from): 2019-08-22
 WHEN (date to): 2019-08-22

#	WHO	WHERE	PROCESS	VERSION	FILE	ENTRY	WHEN	WHAT	Explanation
1	INTRA-BRKR-CORP\JohnSmith	JohnsPC	ctserver	TopSpin 4.0.8	C:/Bruker/TopSpin4.0.8/conf/audit_cf.txt	1	2019-08-22 10:34:38.917 +0200	Created by 'cf'.	

Aug 22, 2019 (11:50:36 GMT+2) 1 of 1

Figure 7.6: Central Audit Trail File Viewer Report in pdf



If the number of found records exceeds that number it is recommended to narrow the filter criteria. In any case the header section of the report indicates whether all found records have been listed.

7.9.2.8.3 Command unlockdataset Removed

The **unlockdataset** command introduced in Topspin 4.0.2 is no longer available. It has been removed for reasons of GxP compliance.

7.9.2.9 Documentation

New documentation under **Help | Manuals (docs)** available for:

- Auto Calibrate Quick Start Guide

Updated documentation under **Help | Manuals (docs)** available for:

- Acquisition Commands & Parameters
- Processing Commands & Parameters
- 21 CFR Part 11 Compliance
- Pulse Programming
- User Manual
- Structure Elucidation with CMC-se
- Edlock/Edsolv Guide – User Manual
- PotencyMR User Manual
- PotencyMR Quick Start Guide

7.10 TopSpin 4.0.9

7.10.1 Bug Fixes

- HTML setup file now displays status of experiment correctly

7.10.1.1 Bug Fixes in TopSpin

The following topics describe the major fixes which come with TopSpin:

- nmrsim crashes when TD>64k is used
- Simulation of experiments using frequency shifted shaped pulses may fail
- installnmr deletes `<TSHOME>\prog\logfiles\login.txt`
- Sola: Command not implemented fit1d_savecsv
- Pulse programs with "spoffX=Y" break plotting
- AU programs don't run on macOS
- Receiver phase correction fails in Cortab for MRI systems

7.10.1.2 Bug Fixes in IconNMR

- HTML setup file now displays status of experiment correctly.
- Error while setting the Instrument Idle Temperature corrected.

Please note, a version specific knowledgebase containing minor patches and other items is online and continuously updated.

Direct Access is available when the Instrument is on the net, or where IconNMR is running on a networked system with Internet access.

Use the **Help | About** menu entry and click on **Knowledgebase** where available.

7.10.2 New Features

7.10.2.1 General

7.10.2.1.1 AutoDiagnose

Topspin 4.0.9 introduces an early adopter version of AutoDiagnose. AutoDiagnose supervises vital spectrometer functions and reports the spectrometer performance helping the user in keeping the system at the best by means of a user friendly graphical interface remotely accessible. For more info please refer to TopSpin User Manual chapter 16.

7.10.2.1.2 Improved Drag & Drop Functionality

The opening of NMR data sets using Drag & Drop has been improved.

Dataset Drag & Drop from external sources, like Windows Explorer, now behaves exactly the same way as Drag & Drop from Topspin internal browser.

Drag & Drop from external sources now offers a new feature: 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:

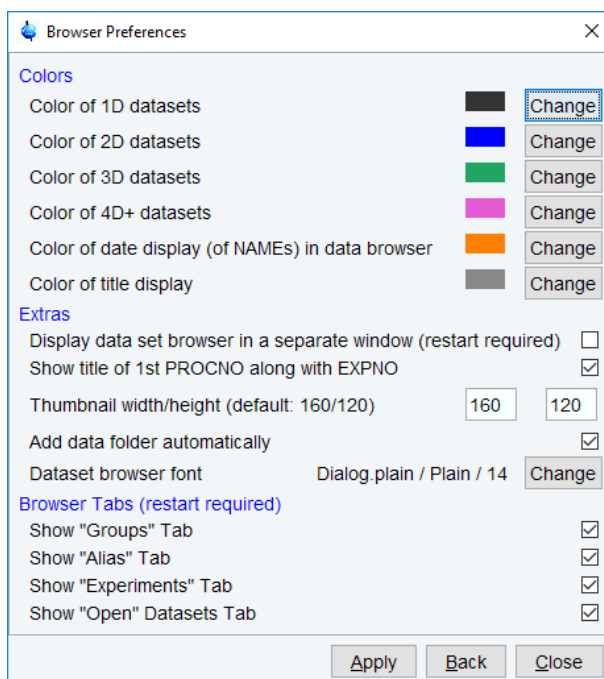


Figure 7.7: Browser Preferences to **Add data folder automatically**.

7.10.2.1.3 Online Check for Available Product Updates

Topspin can conveniently check for you whether a newer version is available. Choose the entry **Check for product updates** from the help menu in Topspin to initiate an online check, or enter the command **check_product_update** in the command line. If internet connectivity is available, information about the most recent TopSpin release will be requested from Bruker web sites and shown on the screen for your information.

7.10.2.2 Acquisition

7.10.2.2.1 FnMode Allows Odd TD Values

For a multi-dimensional experiment, odd TD values in indirect dimensions are now allowed again if FnMode is set to 'undefined'.

7.10.2.2.2 Acquisition Start Date Stored in Acquisition Status Parameters

The start date of the acquisition is now also stored in the acquisition status parameters as parameter DATE_START.

Additionally, the used experiment time is shown in the Status view of the ACQUPARS tab in the parameter EXP_TIME.

7.10.2.2.3 Support for New SampleJet Heated / Cooled

Support for new SampleJet heated / cooled. Temperatures of sample storage modules are displayed in VTU display.

7.10.2.3 Processing

7.10.2.3.1 New Command sigreg

The processing command **sigreg** finds signal regions in 1D 1H spectra using a machine learning approach.

Before running **sigreg**, the spectrum should be phase- and baseline-corrected to ensure optimal performance.

7.10.2.3.2 Improvements for Default NUS Parameters

For 3D experiments with FnTYPE=NUS, the default values of the processing parameter XDIM, which defines the submatrix / subcube sizes, have changed.

Those default values are always used when the processing is not forced via the option "xdim" to use the foreground parameters. In previous TopSpin versions the default value for XDIM in acquisition direction was always 8, leading to XDIM=8x8x4. With TopSpin 4.0.9 the default value for XDIM in acquisition direction now will be 32, if the respective SI / STSI parameter can be divided by 32 (if not, XDIM will successively be halved). In addition, the foreground XDIM in indirect dimension now also can be 1 if the respective FnMODE is non-hypercomplex (e.g. QF). In previous TopSpin versions, setting the foreground XDIM to 0 had the effect that XDIM=SI was internally used for FnMODE ≠ QF. With TopSpin 4.0.9 this is now also the case for FnMODE=QF.

7.10.2.4 Automation

Changes in IconNMR 5.1.9 (for TopSpin 4.0.9)

- Eject last sample delay – Leave the last sample in the magnet longer for possible further measurements
- SamplePro – (hr-)MAS™ Configuration support: **File | Restore Defaults and Initial Start-up settings**
- Acquisition status parameter UUID (Universally unique identifier) set on each measured experiment
- Solvents and Experiments may be restricted globally using **Configuration | Automation Window settings**
Note: This setting used only apply to Easy Setup mode solvents/experiments.
- User Manager Permissions settings streamlined

7.10.2.5 Analysis

7.10.2.5.1 CMC-assist 2.17

- NMRReData export functionality for 1D 1H data implemented.
- The list of supported journal format was significantly extended: Journal of Organic Chemistry (JOC), Journal of Medicinal Chemistry, Journal of the American Chemical Society (JACS), Angewandte Chemie, Chemistry, a European Journal, Helvetica Chimica Acta, Tetrahedron Letters, Journal of Natural Products, Analytical Chemistry, Planta Medica, Organic Letters, Phytochemistry, Fitoterapia, Bioorganic and Medicinal Chemistry Letters.

7.10.2.5.2 News in Fragment Base Screening Analysis Suite

- The FBS tool provides support to configure automatically MScreen from Mestrelab.
- The FBS tool runs without additional license when using TopSpin at the spectrometer.

7.10.2.6 Pulse Programming

7.10.2.6.1 Adjustments for List Handling

Please note that the following old commands for handling delay lists (**vd** and **ivd**) as well as pulse lists (**vp** and **ivp**) and loopcounter lists (**vc** and **ivc**) have been described as deprecated in the documentation for quite some years now.

These commands will not be supported anymore in the future versions of Topspin. Topspin 4.0.9 is the last version supporting **vc**, **ivc**, **vd**, **ivd**, **vp** and **ivp** in pulse programs.

If necessary, please adjust your pulse programs accordingly using the modern and more flexible syntax for user defined delay and pulse lists ('define list<delay>' or respectively 'define list<pulse>' or 'define list<loopcounter>').

7.10.2.6.2 Pulse Assign Adjustments

The pulse assign editor in **edprosol** supports an RFF parameter, which can be used as SQRFF for the Square tab and SHRFF for the Shape tab (since a different calculation is used in each case).

It will be saved in the pulse assign file, e.g:

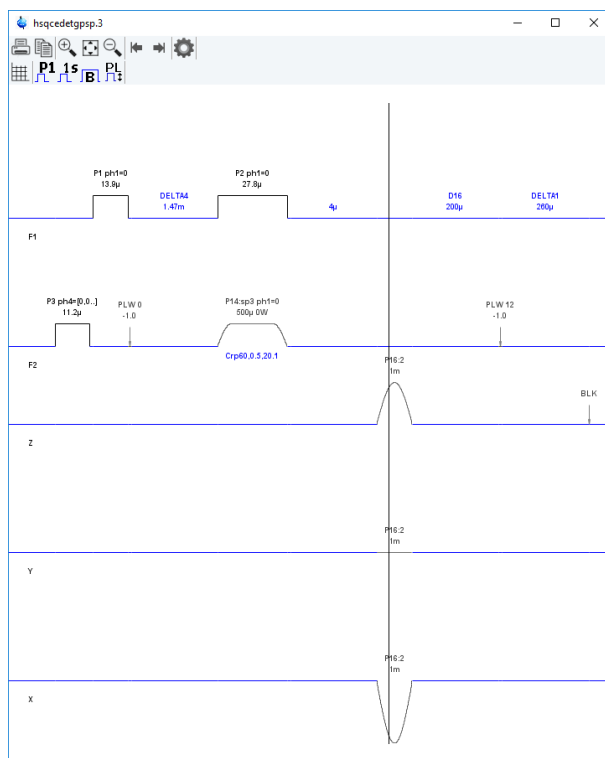
```
CNST[50]=SQRFF[2]*1.0;1
```

```
CNST[51]=SHRFF[3]*1.0;1
```

getprosol calculates the value of SQRFF and SHRFF from the appropriate formula and save it as CNST[ind].

7.10.2.6.3 Display of 3D Gradients in pulse program display

Advanced HR pulse programs using 3D magnetic field gradients can now be visualized.



7.10.2.7 GxP Operation

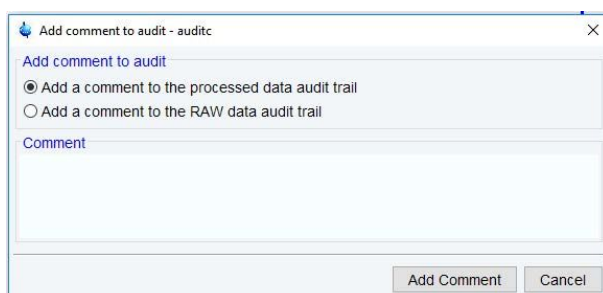
7.10.2.7.1 Data Set Audit Entries

All data set processing audit entries are now retained, even if the spectrum was completely reprocessed from scratch. So, the complete history of each data record is available.

7.10.2.7.2 Adding Comments to Audit Trail

Audit trail entries are normally generated automatically by a respective acquisition or processing command. However, a user can also add a comment manually, using the **auditc** command. This is available either from the command line, or from the menu under **Manage | Security | Add a comment to dataset audit trail (auditc)**.

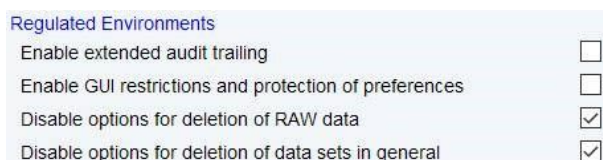
A dialog is opened allowing to enter the comment and the target component (RAW or processed data).



You may also add a comment to the raw data or processed data audit trail from an AU program, using the macros **AUDITCOMMENTA(comment)** or **AUDITCOMMENTP(comment)**, respectively.

7.10.2.7.3 Enhanced Preferences Allow Control of Data Deletion Activities

System administrators working in regulated environment often want to limit or disable software actions which allow deletion of existing NMR data. The **Preferences** dialog offers two new options **Disable options for deletion of ...**:



- With the first one active, deletion and renaming of data set NAME or EXPNO parts are prohibited. PROCNO elements are still changeable, i.e. processing data parts of data sets can be deleted. Commands **dela**, **delf**, **dels** and similar are disabled.
- With the second one active, neither NAME, EXPNO nor PROCNO elements can be deleted, or renamed. Commands **delp**, **deli**, **dels** and similar are disabled.

The related **Delete** and **Rename** actions in TopSpin's data browser are prohibited then. The command **delete** shows the dialog but with disallowed options removed.

Additionally, the activated setting **Enable GUI restrictions...** also disables the commands **expl**, **shell**, and the button **Open** in the **Files** dialog. These activities would offer access to operating system level otherwise.

7.10.2.8 Documentation

Updated documentation under Help | Manuals (docs) available for:

- Acquisition Commands & Parameters
- Processing Commands & Parameters
- Pulse Programming
- User Manual
- Fragment Based Screening Analysis Suite
- Software License Agreement – Software Copyright / License Documents
- 21 CFR Part 11 Compliance Document
- GxP – Regulatory Compliance

New documentation available in the respective additional products:

- AutoDiagnose Software User Manual
- AutoDiagnose Privacy Notice
- AutoDiagnose Terms and Conditions of Use (“Terms”)
- GoScan Software User Manual

7.11 TopSpin 4.1.0

7.11.1 Bug Fixes

7.11.1.1 Bug Fixes in TopSpin

The following topics describe the major fixes which come with TopSpin:

- **TOPS-1955 / SKB-66:**
Due to the larger dynamic range of the spectral data generated by an Avance Neo spectrometer, the au programs 'paropt' and 'parray' tended to clip peaks in the spectrum display.
- **TOPS-2286 Acquisition fails if no LOCK-board is installed**
This issue has been fixed, so that an acquisition is now possible even if there is not lock-functionality in the BSMS.
- **TOPS-2229: pulse programming: Trigger command disrupts phase cycle**
When using a trigger command in the pulse program (e.g. trignl) the phase cycle of the acquisition was not properly executed leading to suboptimal results.
- **TOPS-2220: topshim does not reactivate autoshim**
If **topshim** is executed, it should re-activate the **autoshim** algorithm when being finished in case it was running before. This was not the case in former versions.
- **TOPS-2110: FID/ser-file is not zeroed at the beginning of the acquisition**
In former versions of TopSpin, the ser-file was not zeroed when an nD-experiment was restarted on a given data set. This is not a problem if FIDs are written in consecutive sections of the ser-file (as it is normally the case), but in case some sections are intentionally skipped one would then expect a zeroed FID there instead of noise or a previously acquired signal.
- **TOPS-1797: parameter DATE was not written to acquis-file**
The acquisition parameter DATE was not updated at the end of the acquisition

- **TOPS-923: Offset for higher dimensions not updated in ased**
Changing the frequency offsets for indirect dimensions in the **ased** window had no effect in former versions of TopSpin leading to potentially confusing referencing errors during processing.

7.11.1.2 Bug Fixes in IconNMR

The following topics describe the major fixes which come with IconNMR 5.2:

- SST/External Setup Jobs will not submit
- SmartDrive turned on when using Periodic/STI and other scenarios
- HTML setup file now displays status of experiment correctly
- Biotop can't create SampleJet Rack experiments
- Automation Setup files will not load: Error: Can't read data(AnalysisTypeText,)
- Manual Lock Shim crashes the run
- AssureSST may cause AutoCalibrate to run immediately on completion
- BioTop can't send some datasets using backslashes
- Run stops on error if Remarks are generated when processing skipped

7.11.2 New Features

7.11.2.1 General

7.11.2.1.1 Background Check for Available Product Updates

TopSpin now runs a background activity which occasionally tries to contact Bruker web services and retrieve information about available product updates for TopSpin. In case of a new TopSpin version available the user is informed by an interactive message. The default time interval for such online checks can be adapted in the preference settings.

The background check can also be disabled completely. Even then, you can always perform a check manually by selecting the **Help | Check for product upgrades**.

Please note that this function only downloads upgrade information from Bruker and does not transfer any personal information about your installation to Bruker.

7.11.2.2 Operation within Regulated Environments (GxP)

With this release 4.1, TopSpin's functionalities for operation within Regulated Environments have been significantly enhanced. Laboratories will find much better support when they implement workflows oriented on Good Laboratory Practice ("GxP") and when they require to follow the 21 CFR part 11 directive of the FDA authority. This includes e.g. a centralized user identity management spanning multiple applications, a database service for tracking activities in a Central Audit Trail, and a flexible rights and roles model within the software application.

Information about GxP functionalities and configuration can be found in the new manual TopSpin GxP Quick Start Guide which is part of the online manuals, as included with a TopSpin installation.

The availability of GxP related functions is now bound to a new license option that is not part of the standard TopSpin license. Please contact your sales representative for available options, e.g. a GxP Readiness Kit package.

Any installation now requires an initial decision about the use of GxP capabilities right at the beginning. If TopSpin is installed without GxP options, the installation cannot be converted for GxP operation later. This shall ensure that the various product components are configured in the correct way. It comes also with the benefit that non-GxP installations require a smaller footprint.

7.11.2.3 Installation Procedure

The standard installation package is available for download from the Bruker website and includes the full TopSpin version, without the additional packages for GxP operation.

The extended installation package includes the full TopSpin version and the GxP extensions as described in the previous section. This package is available for download Bruker on request, as part of a product option. Additional license requirements may apply.

7.11.2.4 Acquisition

7.11.2.4.1 **ased** Improvements

In higher dimensions the offset O1 written to the status files *acqu<dimension>s* was not correctly updated if the foreground value of the respective offset in acquisition direction was changed in **ased**.

Now, the status value for O1 in a higher dimension will be the offset in acquisition direction for the same nucleus – so the algorithm takes the nucleus NUC1 specified for the respective indirect dimension and looks for that nucleus in acquisition direction and takes the respective offset specified for that nucleus for the status O1 in indirect dimension.

If this corresponding nucleus in acquisition direction cannot be found, an error message is shown.

For pseudo dimensions, i.e. FnMODE=QF(no-frequency), this nucleus look up won't be performed and the respective higher dimensional status O1 will be set to zero.

In addition, **ased** has a new section of read only parameters for each higher dimension "F<dim> indirect dimension" where currently the indirect td, indirect sweep width and o1_F<dim>, if it was assigned in the pulse program, are shown.

In **eda** window, the sections "receiver" and "nucleus" were exchanged in order – now the "nucleus" section comes before the "receiver" section because this is more useful in practice.

7.11.2.4.2 MAS Probe Rotation Rate

If the MAS is used to rotate a sample in a MAS probe, at end of acquisition the target rotation rate is stored as acquisition parameter MASR in the acquisition status parameter file.

7.11.2.4.3 Parameter AUTOPOS and HOLDER

If a sample changer is used (SampleJet or SampleCase), at end of acquisition the acquisition parameters AUTOPOS and HOLDER are written into the acquisition status parameter file now.

7.11.2.4.4 FnMode “undefined”

Acquisition with FnMode “undefined” is possible again for odd values of TD.

7.11.2.5 Pulse Programming

7.11.2.5.1 Assign Shape Name Inside the Pulse Program

The parameters SPNAM0 .. SPNAM63 as well as GPNAM0 .. GPNAM31 can now be assigned in a pulse program relation before the **ze/zd** command.

On the one hand, it is possible to perform inter-parameter assignments, e.g.

```
"spnam23=spnam42"
```

which can be useful to fixate SPNAM in the pulse program, because if an SPNAM parameter occurs on the left hand side of a relation it cannot be changed in the 'ased' - window anymore.

In addition, it is possible to assign string constants with the following syntax:

```
"spnam17 = 'Q3.1000' "
```

where it is important to enclose the string constant by single quotes '!...!'.

7.11.2.5.2 Pulse Program Manifest

A new feature, the so called "pulse program manifest" was implemented. This allows to generate formatted text (intended to be in a machine-readable language) including parameter evaluation directly inside the pulse program which then will be written into a text file *manifest.txt* in the expno directory. For more information please refer to the **Pulse Programming Manual, section 13.3.6 (Miscellaneous | Miscellaneous Statements | Generating a Manifest File)**.

7.11.2.5.3 Write FID into Multiple Data Sets

It is now possible to write the same FID into multiple data sets, e.g.

```
30m wr #0
```

```
30m wr #1
```

7.11.2.6 Automation

Changes in IconNMR 5.2 (for TopSpin 4.1.0) / New Features:

- TopSpin Bruker User (Keycloak) System supported
- User readable log entries created
- IconWeb allows for setting of Night experiments even when Priority is disabled
- Accounting may show measurement times for individual experiments

7.11.2.7 Simulation

7.11.2.7.1 NMRSim 6.4

A simulation of non uniform sampled 2D spectra (NUS) was implemented.

- supports Bruker standard pulse programs
- significantly speeds up the simulation of complex 2D experiments

7.11.2.8 Documentation

Updated documentation under Help | Manuals (docs) available for:

- Acquisition Commands & Parameters
- Processing Commands & Parameters
- Pulse Programming
- 21 CFR Part 11 Compliance Document
- GxP – Regulatory Compliance
- NMRSim Experiment Simulator

New documentation available in the respective additional products:

- TopSpin – Quick Start Guide
- TopSpin GxP – Quick Start Guide

7.12 TopSpin 4.1.1

7.12.1 Bug Fixes

7.12.1.1 Bug Fixes in TopSpin

The following topics describe the major fixes which come with TopSpin:

- **TOPS-1955 / SKB-66:**
Due to the larger dynamic range of the spectral data generated by an Avance Neo spectrometer, the au programs 'paropt' and 'parray' tended to clip peaks in the spectrum display.
- **TOPS-2286 Acquisition fails if no LOCK-board is installed**
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- **TOPS-2229: pulse programming: Trigger command disrupts phase cycle**
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- **TOPS-2220: topshim does not reactivate autoshim**
If **topshim** is executed, it should re-activate the **autoshim** algorithm when being finished in case it was running before. This was not the case in former versions.
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In former versions of TopSpin, the ser-file was not zeroed when an nD-experiment was restarted on a given data set. This is not a problem if FIDs are written in consecutive sections of the ser-file (as it is normally the case), but in case some sections are intentionally skipped one would then expect a zeroed FID there instead of noise or a previously acquired signal.
- **TOPS-1797: parameter DATE was not written to acquis-file**
The acquisition parameter DATE was not updated at the end of the acquisition
- **TOPS-923: Offset for higher dimensions not updated in ased**
Changing the frequency offsets for indirect dimensions in the **ased** window had no effect in former versions of TopSpin leading to potentially confusing referencing errors during processing.

7.12.1.2 Bug Fixes in IconNMR

The following topics describe the major fixes which come with IconNMR 5.2:

- SST/External Setup Jobs will not submit
- SmartDrive turned on when using Periodic/STI and other scenarios
- HTML setup file now displays status of experiment correctly
- Biotop can't create SampleJet Rack experiments
- Automation Setup files will not load: Error: Can't read data(AnalysisTypeText,)
- Manual Lock Shim crashes the run
- AssureSST may cause AutoCalibrate to run immediately on completion
- BioTop can't send some datasets using backslashes
- Run stops on error if Remarks are generated when processing skipped

7.12.2 New Features

7.12.2.1 General

7.12.2.1.1 Network Interface for TopSpin

TopSpin 4.1.1 introduces new programming interface (API) allowing to access TopSpin from other applications. The interface is implemented in the form of REST API. Following features are available:

- Send command to TopSpin
- Read NMR datasets (currently limited to 1D und 2D)
- Read peak lists
- Read integration regions
- Read and write data set parameters

The interface must be explicitly activated – command **start_rest_interface**. The start of the service requires administrator password.

An example python client implementation is available. This allows to build your own data analysis functionality using any python library.

The interface requires a valid license. A free evaluation license is currently available on demand, please contact NMR support NMR-Support@bruker.com.

7.12.2.1.2 New Version of CodeMeter Runtime

The TopSpin installation regularly comes with 3rd party component for license management named CodeMeter Runtime. The manufacturer WIBU has recently published the version 7.10a of this package which is also included with the current TopSpin version. During tests we occasionally observed an issue on Linux systems with CentOS 7. If the system already contains a previous version of CodeMeter Runtime, the installation will update it to the new version but might fail in restarting the CodeMeter service automatically after the update. TopSpin will not receive the required license information then and stop during program start with a dedicated message. In all reported cases a reboot of the operating system has resolved the situation.

7.12.2.2 Operation within Regulated Environments (GxP)

With this release 4.1, TopSpin's functionalities for operation within Regulated Environments have been significantly enhanced. Laboratories will find much better support when they implement workflows oriented on Good Laboratory Practice ("GxP") and when they require to follow the 21 CFR part 11 directive of the FDA authority. This includes e.g. a centralized user identity management spanning multiple applications, a database service for tracking activities in a Central Audit Trail, and a flexible rights and roles model within the software application.

Information about GxP functionalities and configuration can be found in the new manual TopSpin GxP Quick Start Guide which is part of the online manuals, as included with a TopSpin installation.

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Any installation now requires an initial decision about the use of GxP capabilities right at the beginning. If TopSpin is installed without GxP options, the installation cannot be converted for GxP operation later. This shall ensure that the various product components are configured in the correct way. It comes also with the benefit that non-GxP installations require a smaller footprint.

7.12.2.3 Acquisition

7.12.2.3.1 ased Improvements

In higher dimensions the offset O1 written to the status files *acqu<dimension>s* was not correctly updated if the foreground value of the respective offset in acquisition direction was changed in **ased**.

Now, the status value for O1 in a higher dimension will be the offset in acquisition direction for the same nucleus – so the algorithm takes the nucleus NUC1 specified for the respective indirect dimension and looks for that nucleus in acquisition direction and takes the respective offset specified for that nucleus for the status O1 in indirect dimension.

If this corresponding nucleus in acquisition direction cannot be found, an error message is shown.

For pseudo dimensions, i.e. FnMODE=QF(no-frequency), this nucleus look up won't be performed and the respective higher dimensional status O1 will be set to zero.

In addition, **ased** has a new section of read only parameters for each higher dimension "F<dim> indirect dimension" where currently the indirect td, indirect sweep width and o1_F<dim>, if it was assigned in the pulse program, are shown.

In **eda** window, the sections "receiver" and "nucleus" were exchanged in order – now the "nucleus" section comes before the "receiver" section because this is more useful in practice.

7.12.2.3.2 MAS Probe Rotation Rate

If the MAS is used to rotate a sample in a MAS probe, at end of acquisition the target rotation rate is stored as acquisition parameter MASR in the acquisition status parameter file.

7.12.2.3.3 Parameter AUTOPOS and HOLDER

If a sample changer is used (SampleJet or SampleCase), at end of acquisition the acquisition parameters AUTOPOS and HOLDER are written into the acquisition status parameter file now.

7.12.2.3.4 FnMode “undefined”

Acquisition with FnMode “undefined” is possible again for odd values of TD.

7.12.2.4 Processing

7.12.2.4.1 Command sigreg: Enhanced Options

The processing command **sigreg** which finds signal regions in 1D 1H spectra using machine learning can now be customized using the **-add**, **-expand**, and **-setsize** options in order to adjust the size of the resulting signal regions.

The same options can also be used to modify existing signal regions, independently of whether they were defined manually or by using any other TopSpin command.

7.12.2.5 Pulse Programming

7.12.2.5.1 Pulse Program commands **vc/ivc/times c**, **vd/ivd** and **vp/ivp** No Longer Supported

The pulse program commands **vc/ivc/times c**, **vd/ivd** and **vp/ivp** are no longer supported since they have been declared as obsolete for several years now. They can be replaced by the corresponding modern list syntax **\$VCLIST**, **\$VPLIST** and **\$VDLIST**. In case of pulse programs using the old syntax an error message is shown which explains in detail how the old syntax can be replaced by the new syntax, as in the following example. Please note that you cannot use the old command names as replacement because the acquisition software detects them as not supported and shows the error message described above.

Example pulse program using the old syntax (old commands shown in bold letters):

```
ze
1 d0

2 p1
vd
vp
lo to 2 times c

1u ivc
1u ivd
1u ivp
go = 1
exit
```

Same pulse program using the new syntax (changes shown in bold letters):

```
define list<loopcounter> vclist = <$VCLIST> ; required for variable loop
counter list
define list<delay> vdlist = <$VDLIST> ; required for variable pulse list
define list<pulse> vplist = <$VPLIST> ; required for variable delay list
```

```
ze
1 d0
2 p1
vdlist ; replaces "vd"
vplist ; replaces "vp"
lo to 2 times vclist ; replaces "times c"

1u vclist.inc ; replaces "ivc"
1u vdlist.inc ; replaces "ivd"
1u vplist.inc ; replaces "ivp"
go = 1
exit
```

In case of pulse programs using the old syntax an error message is shown which explains in detail how the old syntax can be replaced by the new syntax.

7.12.2.6 Automation

Changes in IconNMR 5.2 / New Features:

- TopSpin Bruker User (Keycloak) System supported
- User readable log entries created
- IconWeb allows for setting of Night experiments even when Priority is disabled
- Accounting may show measurement times for individual experiments

7.12.2.7 Simulation

7.12.2.7.1 NMRSim 6.4

A simulation of non uniform sampled 2D spectra (NUS) was implemented.

- supports Bruker standard pulse programs
- significantly speeds up the simulation of complex 2D experiments

7.12.2.8 Documentation

Updated documentation under Help | Manuals (docs) available for:

- Pulse Programming
- Software License Agreement

7.13 TopSpin 4.1.3

7.13.1 Bug Fixes

7.13.1.1 Bug Fixes in TopSpin

The following topics describe the major fixes which come with TopSpin:

- **SKB-61:** IconNMR can try to create data in an already used expno
- **SKB-63:** Non-ideal behavior when clicking a holder in Sample Holder Overview
- **SKB 175:** Field with electronic signature not shown on 2D plots
- **SKB-191:** AU programs do not link under macOS 11 (Big Sur)
This issue could not be resolved. However, there is a workaround available (see the section [Installation on macOS \[▶ 19\]](#))
- **SKB-193:** Macros and python scripts can only be executed by one user
- **SKB-214:** Externally generated composite experiments with F1/F2 References do not acquire
- **SKB-219:** Topspin sets wrong data set name as window title
- **SKB-226:** SampleCase and set&check temp before insertion may lead to "Cannot remove sample from BST since BST is empty"
- **SKB-240:** Automatic processing works on wrong dataset
- **TOPS-1759 :** The selected slider sensitivity in GS is now correctly considered by the software
- **TOPS-2191: expinstall** prints: Error in setting hspec, ret=-1
- **TOPS-2397:** popt yields Null Pointer exception
- **TOPS-2587:** solvents with umlauts in the description do not lead to an error in sref anymore
- **TOPS-2654:** Fix file type check in installer packer
- **TOPS-2642: rser** on nD experiments does not fail anymore if automatic data processing is active
- **TOPS-2694:** Commandline Entries cannot be edited
- **TOPS-2735: spdisp** does not fail with an error anymore if the pulse program contains lists.
-

7.13.1.2 Bug Fixes in IconNMR

The following topics describe the major fixes which come with IconNMR 5.2.3:

- SampleJet error on sample insertion - An error message of the form expected integer but got "2 A1 - 201" appears
- Experiments do not submit - Error message can't read "data(AnalysisTypeText,)"
- "Start-Times" ignored, experiments run in sequence after an unexpected delay time
- SampleCase and Set&check temp before insertion may lead to "Cannot remove sample from BST since BST is empty"
- Additional experiments sometimes set incorrect names when "Spectrum Number Filename" used
- Watchdog can detect hang-up after idle temperature is set

- File -> "Save as" missing in IconNMR Configuration
- Externally generated composite experiments with F1/F2 References do not acquire
- Incorrect second and third experiments entered in edc2 on composites
- InsightMR on Linux will not start
- Holder Positions not shown in SampleJet (SampleTrack) Automation mode
- InsightMR starts with an error message: X Error of failed request: BadMatch (invalid parameter attributes)
- ASSURE-SST does not start if disk and subdirectories are restricted
- qPQ Performance Quantification SST Test fails if AssureNMR activated
- Various Problems in 'Routine Spectroscopy'
- SKB-273 Temperature set incorrectly after SampleXpress Barcode Search
- SKB-272 Archiving fails - permission problems
- SKB-271 Run may halt if data set name with trailing "." submitted
- SKB-265 Changing an experiment in IconWeb throws an error: key "edsn" not known in dictionary

7.13.2 New Features

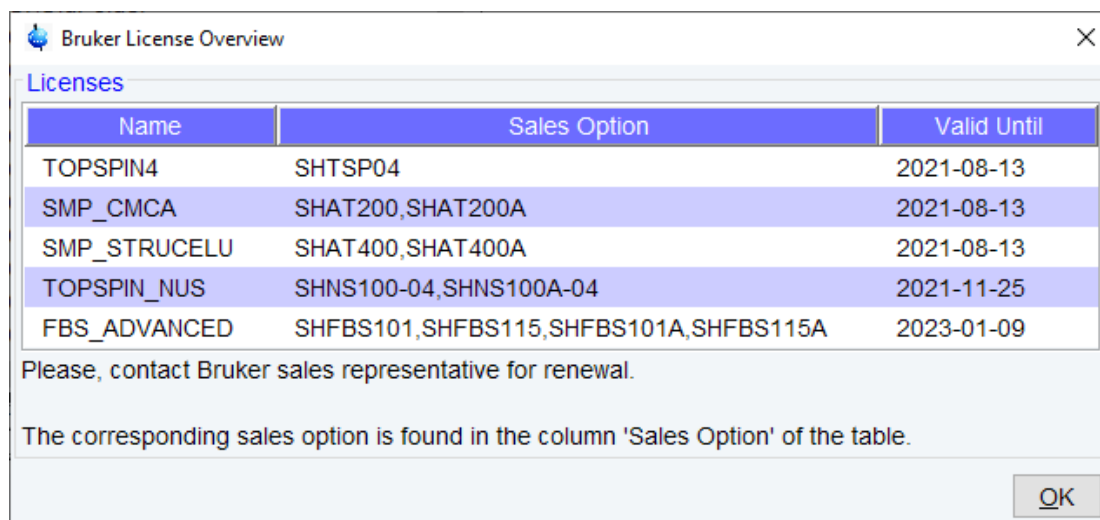
7.13.2.1 General

7.13.2.1.1 Time Formats Standardization

A TopSpin installation uses several log files including time/date stamps for the tracking of events and support purposes. The format of these time markers has been unified over the logs (acquisition, dataserer, cpr server, cpr history, history_j) to be in the form of yyyy-MM-dd hh:mm:ss.SSS

7.13.2.1.2 License Expiration Dialog

The list of available licenses with their expiration dates is now available from the Topspin Help menu (**Help | Bruker License Overview**).



Name	Sales Option	Valid Until
TOPSPIN4	SHTSP04	2021-08-13
SMP_CMCA	SHAT200,SHAT200A	2021-08-13
SMP_STRUCELU	SHAT400,SHAT400A	2021-08-13
TOPSPIN_NUS	SHNS100-04,SHNS100A-04	2021-11-25
FBS_ADVANCED	SHFBS101,SHFBS115,SHFBS101A,SHFBS115A	2023-01-09

Please, contact Bruker sales representative for renewal.

The corresponding sales option is found in the column 'Sales Option' of the table.

OK

7.13.2.1.3 Python 3.9 Part of TopSpin Installation

Python is a very popular programming language and has attracted high interest within the scientific community. Topspin yet includes a Jython interpreter which is based on the Python 2.7 language standard. However, this component has only very limited access to external Python packages. Bruker likes to support customers programming with the most recent Python features and now includes the latest Python 3.9 interpreter with the Topspin installation. Packages allow to access Topspin and Bruker data sets, and to write your own python scripts and utilize any external python package for. Example scripts are also included.

The communication with Topspin is based on the REST interface which operation requires a valid license. A free evaluation license is currently available on demand, please contact NMR support NMR-Support@bruker.com

7.13.2.1.4 Embedded Molecule Viewer Upgraded

TopSpin uses JMol as a component for molecule display. This was upgraded to the version **Jmol 14.31.24**

7.13.2.1.5 AutoDiagnose Covers Fourier Instruments

The AutoDiagnose system had been introduced for Avance NEO instruments with TopSpin 4.0.9. Now Fourier spectrometers are supported as well.

7.13.2.1.6 AvanceCore Functionality

- Added Temperature Correction pane to the Temperature Control Suite for FoodScreener Essential license package.
- The full BSMS display functionality in TopSpin is available for the FoodScreener Essential license package.
- TopSpin is regularly checking for newer versions which are validated for AvanceCore systems. This may not be every new version of TopSpin in the future.

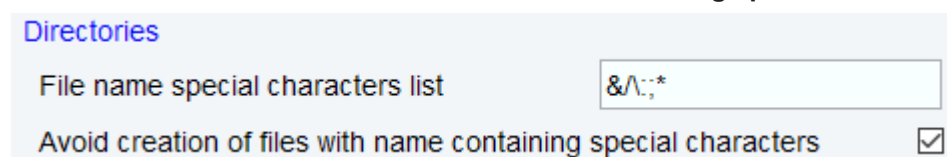
7.13.2.1.7 WaveMaker Functionality

WaveMaker accepts 2D peak lists and supports two-dimensional encoding. Encoding matrices can be defined and supplied by the user. The B1comp parameter allows compensation for B1 variations in Hadamard encoding experiments.

7.13.2.2 General User Interface (GUI)

7.13.2.2.1 Protection Against Use of Incompatible File Names

TopSpin allows to prohibit the creation of files that contain potentially problematic characters in the file name. This option can be configured in the **Directories** section of Topspin Preferences: **Avoid creation of files with name containing special characters.**



The unwanted characters can be specified in the field "File name special characters list". The default setup avoids creation of names which could harm the functionality of TopSpin. The check is applied to any file created interactively like e.g. names of data set or parameter sets.

7.13.2.3 Operation within Regulated Environments (GxP)

Please review the important information about TopSpin GxP for release 4.1 (also copied in this document below). Beginning with TopSpin 4.1.3 the installation routine for TopSpin GxP is now split into two complementing parts. This allows for installation scenarios where user management and audit trail are used as central, common components for multiple instruments in a lab. For non-GxP installations still the compact installer package can be used. More information for GxP users can be found in the TopSpin GxP Quick Start Guide ([Help | Manuals | TopSpin Quick Start Guide](#)).

Note that the functionalities **User Management** and **Apply Electronic Signature** are available as part of a TopSpin GxP installation only, but not with non-GxP installations. Operation in GxP mode is bound to a specific product license.

7.13.2.4 Acquisition

7.13.2.4.1 Delete Solvent Specific Tables

The prosol tool supports the option to delete solvent specific tables.

7.13.2.4.2 Check Spectrometer Configuration Before Import

When performing a Datastation import in **cf**, the specified folder will be checked whether it is a valid spectrometer configuration before importing.

7.13.2.4.3 Improved Attenuator

Improved attenuator switching on the transmitter unit.

7.13.2.4.4 New Behavior For Saving Non-Bruker Files

nrmrsave does not save non-Bruker files in *exp/stan/nmr/par* and *exp/stan/nmr/py* anymore since these directories are reserved for vendor-provided files. Content of the */user* folders in those directories is still included, of course.

7.13.2.4.5 ATMA / ATTM Starting Simultaneously

ATMA or ATMM is now started on more than one channel simultaneously if possible.

7.13.2.4.6 Added Support For The LT-MAS Unit

7.13.2.4.7 Expinstall Performs Automatic Backup

Bruker supplies parameter files, AU-programs, pulseprograms and other files in particular folders. **Expinstall** now moves these folders to *<TopSpin installation dir.>/exp/stan/nmr/_expinstall_automatic_backup* and installs new copies.

7.13.2.4.8 Cf Detects ELCB Firmware Status

cf will now show a warning if the installed ELCB firmware is too old.

7.13.2.4.9 TopShim

The algorithm of **topshim** has been improved for better results and more stability. It now takes the used current into account during optimization and should not run into the current limits anymore.

While the main concept remains similar and in average the results are better, some minor difference may occur, especially, when special parameters are used.

The following new features and modifications have been implemented for the present version:

- By default, **ordmax** is set to automatic detection of shims to use.
- A new parameter **initial** is introduced to simplify the procedure of a probe change or to start from an initial bad shim
- A **topshim 3d** will automatically include a final **topshim 1d**.
- The parameter **TCORR** allows to set offsets in Z and Z2 gradients due to temperature gradient in solvents with temperature dependent chemical shifts.

7.13.2.5 Processing

7.13.2.5.1 Deep Learning Technology for 1D 1H Spectra

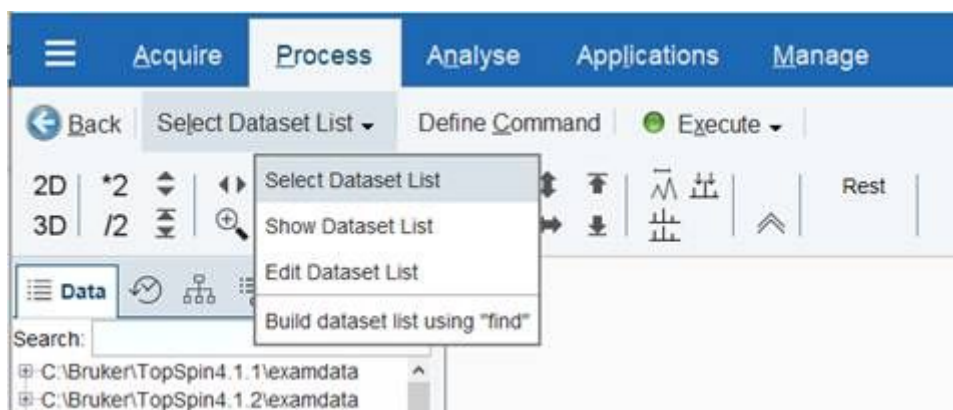
A new algorithm has been developed for the automatic phase and baseline correction of one-dimensional ¹H spectra without solvent suppression. The algorithm uses deep learning technology for the detection of the baseline and can be accessed with the existing command **apbk**. More information can be found in the processing manual (**1D Processing Commands | apbk**).

7.13.2.5.2 Parameter DTYP

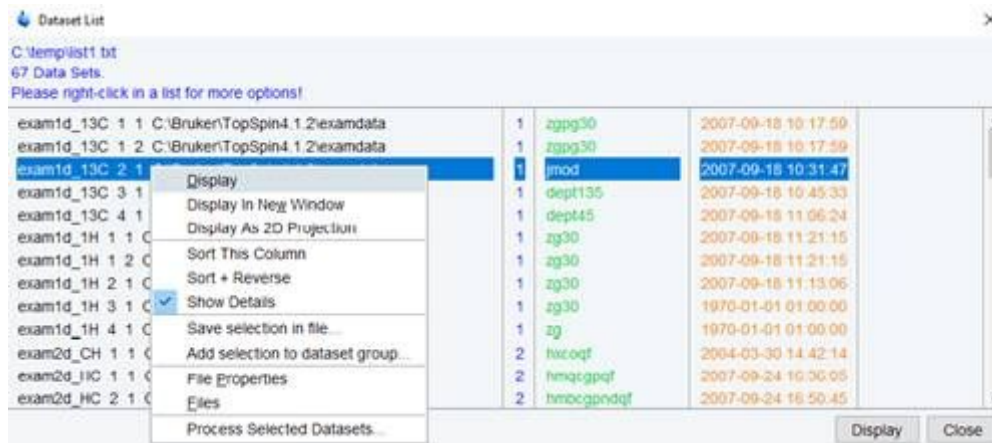
The parameter **DTYP** is now displayed with the status parameters on the PROCPARS page.

7.13.2.5.3 Improved Handling of Data Set Lists

The data set lists used for serial processing may be now reopened from the data list menu.



The list is shown in the same dialog as a result of the data search.



7.13.2.5.4 Command Line Helper

The new panel **command line helper** was added. If the tab is selected, TopSpin commands matching the command line input are shown on the fly. The corresponding command description is also included. The listed commands may be executed, the corresponding help page may be also opened from the popup menu in the command column.

Command	Description
xf1	Process data, including FT, in F1 (2D)
xf1m	Calculate magnitude spectrum in F1 (2D)
xf1ps	Calculate power spectrum in F1 (2D)
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)
xfb	Process data, including FT, in F2 and F1 (2D)
xfbm	Calculate magnitude spectrum in F2 and F1 (2D)
xfbp	Phase correction in F2 and F1 (2D)
xfbps	Calculate power spectrum in F2 and F1 (2D)
xf	

7.13.2.6 Pulse Programming

7.13.2.6.1 Command (UN)BLKGRAD Unified

The handling of the **(UN)BLKGRAD** command has been modified in several selective 1D pulseprograms and hence unified. The default position of the **BLKGRAD** command is prior to the go statement. To obtain the previous behavior (with the **BLKGRAD** before D1) the experiment should be started with the ZGOPTNS parameter set to -DFLAG_BLK. In any case should the lockphase be properly adjusted e.g. using the enhanced lock level algorithm (to be set in the **edlock** table).

7.13.2.7 Automation

Changes in IconNMR 5.2.3 / New Features:

- NOAH and PSYCHE Experiments now shown automatically in 'Preceding Experiments' Window
- Automation Preceding Window can show any .pdf file in expno/procno directories via the <Right Click> Context Menu
- More "Space" in the User Manager - Scroll down for all options
- [Automatic] External Setup Holder definition, to use Icon's position suggest system to allocate a suitable sample position
- Window Display and sizes, full-screen settings now remembered on Windows Workstations
- Latin-1 Names (non-ASCII characters) now functional for Solvent names
- Minispec/Formcheck App:
Longest Delay Calculation now optional
Daily Check now optional
- Potential Incompatibility:
"Generate Spectrum PS/PDF file in data set for possible dispatch to Email recipient" now prevents deletion of pdf/png files automatically generated in data sets;
Previously such files were always deleted

7.13.2.8 Documentation

Updated documentation under Help | Manuals (docs) available for:

- Acquisition Commands and Parameters – User Manual
- Processing Commands and Parameters – User Manual
- User Manual
- Python Programming in TopSpin
- NMR Pulse Programming for AVANCE NEO and Fourier 80
- TopSpin GxP – Quick Start Guide
- Insight MR – User Manual (Version 1.1.4)
- AU Programming – User Manual

New documentation under Help | Manuals (docs) available for:

- TopShim Automatic Shimming – User Manual

8 Contact

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Website: <http://www.bruker.com>

WEEE DE43181702

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<https://www.bruker.com/service/information-communication/helpdesk.html>

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