TopSpin

Release Letter 3.6.0

User Manual

Version 007

Innovation with Integrity

NMR

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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 3.6.0 Installation Guide. This document is electronically available on the TopSpin DVD and at *www.bruker.com*. The detailed information is also available directly in the Help menu of the installed TopSpin program.

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

Target Audience

The Bruker Software Release Letter, in this case the Release Letter for TopSpin 3.6.0, 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 MAC OS 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 provided on the BASH DVD.

2 TopSpin - Basics

2.1 About TopSpin

TopSpin 3.6.0 is a minor update of TopSpin program package containing many improvements, new and useful features and bug fixes. This version has been tested for all AVANCE III HD and AVIII spectrometers.

Please also review section 2.5 about incompatible changes compared to earlier TopSpin versions.

2.2 License Requirements

TopSpin 3.6.0 comes as a full program version on DVD and requires a TopSpin 3 license.

Please contact your local Bruker representative for license order and more details. All addresses in detail are listed in Bruker Addresses.

2.3 TopSpin Program Versions

The TopSpin 3.6.0 DVD contains the following program versions:

- TopSpin 3.6.0
- IconNMR 5.0.8
- NMRSim 6.0.2
- NMR Guide 4.4

The following programs are part of the TopSpin 3.6.0 DVD content, but please note that they must be licensed separately in each case:

- AMIX 3.9.15
- Spectra Base 1-1-2

  (Please note that the Spectra Base is only available with AMIX and the different license types (belonging to the pH-value) and the updates must be licensed separately.)
- CMC-se 2.5.3

  CMC-se comes as part of the TopSpin installation and requires a separate license.
- CMC-assist 2.9
- InsightMR^{TM} 1.1.1 (for Windows and Linux)
- DynamicsCenter 2.5.3 (Protein Dynamics)

Please note that for the Mac a reduced collection is available. For further information please refer to Installation on Mac OS X.

2.4 Hardware Requirements

2.4.1 PC Hardware

TopSpin runs on Windows or Linux PCs.

To run TopSpin 3.6.0 the following computer hardware is recommended:

- PC (state of the art); Bruker recommends and delivers the following PC:
  HP z440, Intel Xeon Quad Core E5-1620v3 / 3.50GHz / 10MB Cache
- Memory: 16GB (2x 8GB) DDR4-2133 ECC, 8x memory slots (2x used)
- Video Card: Graphic adapter: Graphic adapter NVIDIA Quadro K620, 2GB
- Network adapters: 1x Intel I218LM PCIe on Board 10/100/1000 Mbits/s (SPECT),
  1x Intel Ethernet I210AT PCIe GbE 10/100/1000 MBits/s (NET)
- Hard Disc: 2TByte, 3Gb/s, NCQ, SATA, 7200rpm
- Optical Storage: Slim SATA SuperMulti DVD writer
- 3 button mouse or wheel mouse
- DVD device (TopSpin is delivered on DVD’s with "-R" format)

Furthermore, display resolution must be set to 1280*1024 or higher.

If your hardware does not meet these requirements, TopSpin might still run but with a much lower performance.

The installation was tested on a ’HP workstation z440’.

2.4.2 Apple Computers

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

2.5 Spectrometer Hardware Requirements

For upgrade possibilities of your spectrometer with TopSpin 3.6.0, please check with your local Bruker office.

2.5.1 AVANCE III Spectrometers

DPP1	required minimum EC Level
part # H12513f1	04

2.5.2 AVANCE III HD Spectrometers

TopSpin 3.6.0 runs on any AVANCE III HD spectrometer.

2.6 Supported Operating Systems

TopSpin 3.6.0 on spectrometer computers is supported for:

- Windows 10 (64bit)
- Windows 7 (64 bit)
- The minimum supported version is CentOS 5.11 (64 bit)
- CentOS 7 (64 bit) (Please note: The minimum required CentOS7 Version is 7.1)

All operating system updates (hot fixes and service packs) at the time TopSpin 3.6.0 was released have been tested and are supported.

Latest 64 bit distributions of Linux operating system do not contain by default 32bit libraries that are required to install and operate Topspin 3.6.0.

Bruker is not allowed to redistribute these libraries as a part of a Topspin installation. Please, use following link to get a description how to install the required components for a CentOS 7 operating system:

ftp://ftp.bruker.de/pub/nmr/CentOS/7/TopSpinInstallationRequirements.html

TopSpin 3.6.0 on data stations is supported for:

- Windows 7
- Windows 8.1
- Windows 10
- The minimum supported version is CentOS 5.11
- CentOS 7 (64 bit) (Please note: The minimum required CentOS7 Version is 7.1)
- Apple Mac OS X 10.12 or higher

Please note that a data station PC can be based on a 32 or 64 bit CPU. For the Mac OS X version a CPU capable of running 64bit instructions is required.

Although not officially supported by Bruker, users reported that TopSpin is also running and is used for data processing on other Linux systems. Bruker does not recommend and cannot support these systems for the use of TopSpin.

2.7 Software Requirements

2.7.1 Under Windows

All AVANCE III HD and AVANCE III spectrometers do not need any further software or equipment to install TopSpin.

2.7.2 Under Linux

To control a spectrometer, make sure that the following packages are installed:, tftp-server, xinetd and dhcp. If one is missing use the command: yum install <package name> to install it.

2.7.3 Under Mac OS X

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

3 TopSpin Installation

3.1 Installation on Windows and Linux

Please note that TopSpin 3.6.0 comes as a full program DVD and, as such, requires a DVD device for installation.

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

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

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

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

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

If you have already a previous TopSpin version installed, then install the TopSpin 3.6.0 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 3.6.0 usually replaces a previous version of TopSpin and, normally, you want to keep the existing configuration. The installation program automatically detects previous installations of TopSpin, prompts you to select one and then copies its configuration files. If multiple previous installations are found, you can choose which configuration you want to copy to the current installation.

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

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

help nmr_save

or refer to the Installation Guide.

3.3 Installation on macOS

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

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

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

4 Bug Fixes

The following topics describe the major fixes which come with TopSpin 3.6.0.

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 # 14366	AU program qnpset doesn't work anymore, so QNP probes don't work
• Item # 14355	The central audit file is not created when installed
• Item # 14354	The central audit log file can be deleted without administrative rights
• Item # 14348	Unresponsive Parameters, Analysis and Title popup windows in Experiment List
• Item # 14345	Automation freezes with hourglass and has to be killed
• Item # 14320	File →Import Configuration does not set various configuration items
• Item # 14317	Archiving may overwrite previously archived directory
• Item # 14303	Both Assure and CMC-Verification use Preceding Experiments window
• Item # 14298	Routine Spectroscopy background not centered in lockdown (non-supervisor) mode
• Item # 14297	MWM lockdown mode not recognized
• Item # 14243	Barcode: Samples beyond row #99 in 'Experiment Table' not wasted
• Item # 14231	Error when running deconvolution (**mdcon**)
• Item # 14212	TopSpin peak picking uses inconsistent rounding of peak values
• Item # 14210	Error in molecular weight calculation in structure editor
• Item # 14183	Central audit file not available from .exe installer
• Item # 14171	**Getprosol** does not update f4 CPD PW and power
• Item # 14168	Molfile cannot be set in certain circumstances
• Item # 14166	User defined function written in java does not work
• Item # 14160	User manager does not open
• Item # 14159	Cortab: No experiment possible if no preamp is selected
• Item # 14148	CMC Verification check runs and fails AssureSST experiments
• Item # 14136	Experiment/sample info not included in plot
• Item # 14131	T2 calculation doesn't work
• Item # 14130	Run does not start using MAS 3: mash failed

Bug Fixes

• Item # 14128	InsightMR Automation run cannot be started
• Item # 14115	Helium Logfile Scheduled Task measures multiple times per night on Windows
• Item # 14106	AssureSST User Defined Tests inoperative
• Item # 14009	Integral calibration with large numbers gives wrong values

5 New Features

5.1 General

5.1.1 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.

5.1.1.1 CodeMeter installation on not supported Linux distributions

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

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

and follow the given Installation details.

5.1.2 Exchange of FlexLM licenses

Beginning with TopSpin 3.6, TopSpin and other Bruker NMR software use the new CodeMeter licensing system, instead of the deprecated FlexLM system. We offer a possibility of a complimentary exchange of existing TopSpin 3 FlexLM licenses for corresponding CodeMeter license tickets.

The exchange is provided on the Bruker website, under

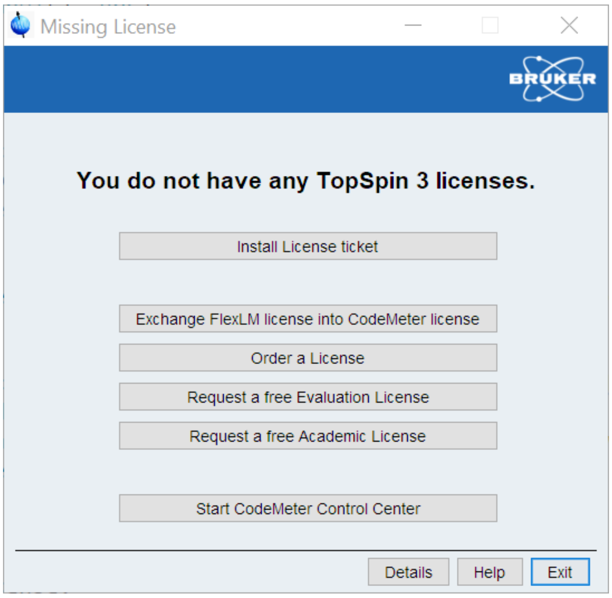
https://www.bruker.com/service/support-upgrades/software-downloads/nmr/nmr-license-exchange.html

Please note that the signed form should be sent to *License.NMR@bruker.com*.

5.1.3 TopSpin starts without license

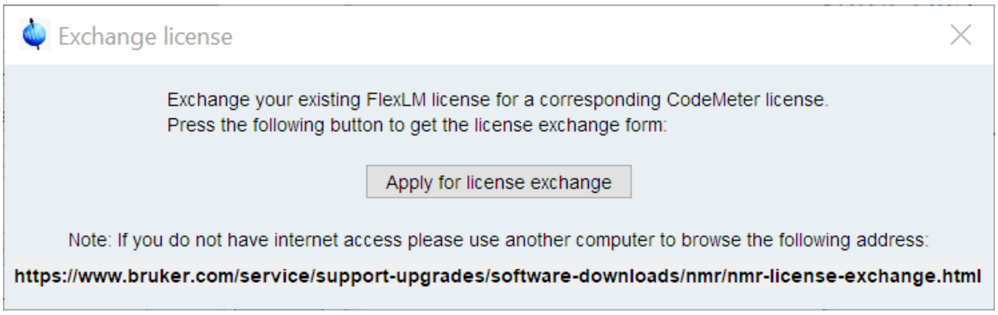
TopSpin can start even without a valid license, then informing the user with an interactive dialogue about available licensing options.

This dialog is also available within a running TopSpin instance, from menu **Help | Bruker License**.



You do not have any TopSpin 3 licenses.

Figure 5.1:



Exchange your existing FlexLM license for a corresponding CodeMeter license.
Press the following button to get the license exchange form:

Note: If you do not have internet access please use another computer to browse the following address:

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

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

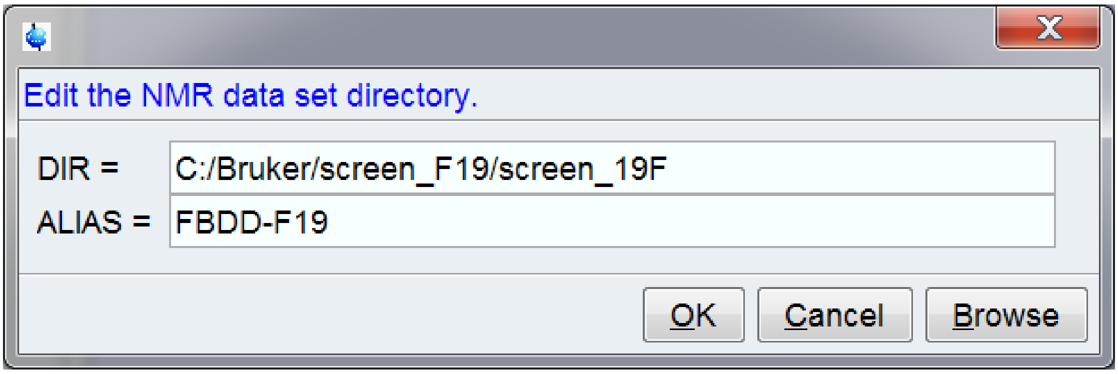
https://www.bruker.com/service/support-upgrades/license-requests/nmr-license-requests.html

5.2 User Interface

5.2.1 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.



Edit the NMR data set directory.

DIR = C:/Bruker/screen_F19/screen_19F

ALIAS = FBDD-F19

5.2.2 "Find" functionality

The integrated search functionality in the data browser tab allows to quickly filter for certain data sets. 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.

5.3 System Support

5.3.1 Linux Graphics Configuration

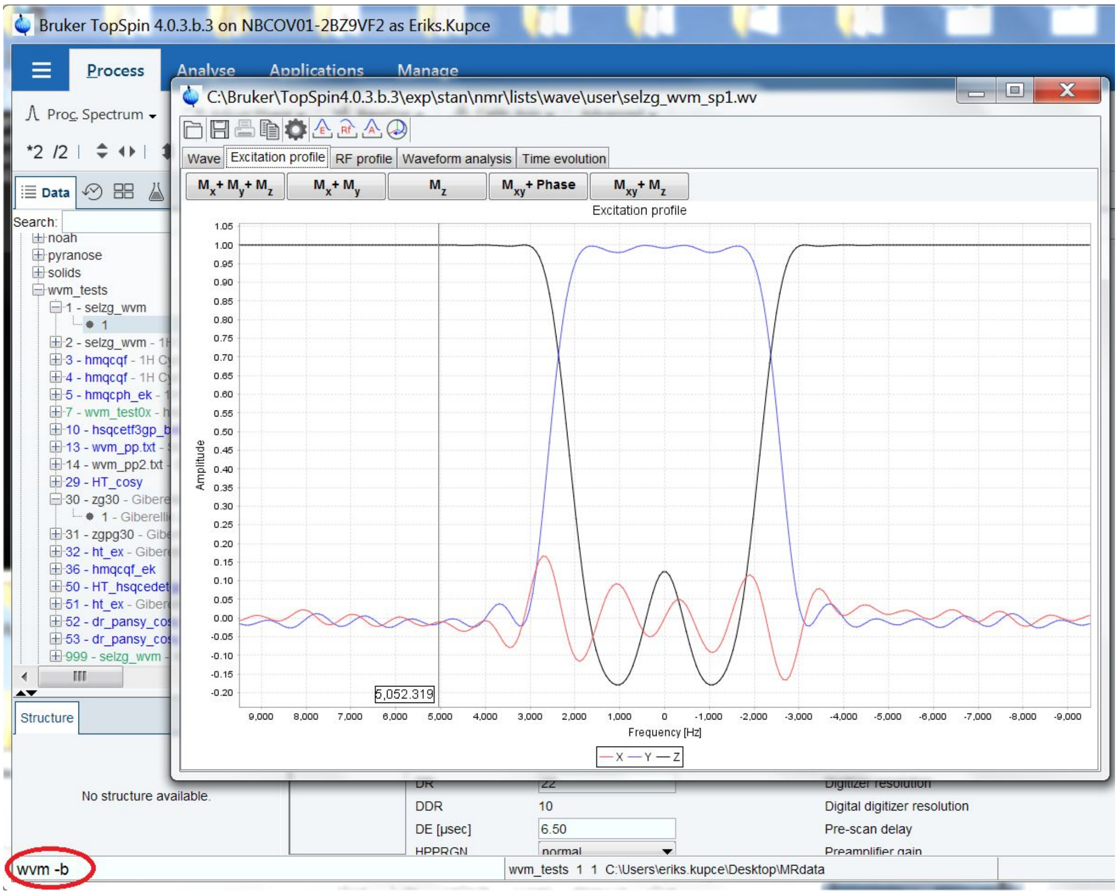
For Linux, Topspin can use OpenGL-based graphics mode as an alternative. On a number of systems instable graphics performance has been observed especially for the lock display. Enabling OpenGL mode can remove this effect on supported systems. The respective selection is configured in the file javaenv.sh which is located in the TopSpin installation directory. If you observe such graphics problems please enable the OpenGL mode by editing this file and removing the leading '#' at the beginning of the line "GRAPHICS_OPTIONS=-Dsun.java2d.opengl=True".

5.4 Acquisition

5.4.1 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).



Bruker TopSpin 4.0.3.b.3 on NBCOV01-2BZ9VF2 as Eriks.Kupce

C:\Bruker\TopSpin4.0.3.b.3\exp\stan\nmr\lists\wave\user\selzg_wvm_sp1.wv

DDR	10	Digital digitizer resolution
DE [µsec]	6.50	Pre-scan delay
HPPRGN	normal	Preamplifier gain

```
wvm -b
```

wvm_tests 1 1 C:\Users\eriks.kupce\Desktop\MRdata

Figure 5.2: The wvm-b option in WaveMaker shows the excitation profile of the shaped pulse(s).

5.4.2 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:

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

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

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

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

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

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

5.4.3 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.

5.4.4 tdmax truncates instead of rounding

When using **tdmax** it was possible that delays became negative because the values were rounded mathematically instead of truncated to the right respective value. This behavior is now corrected.

5.4.5 New Parameter for command edsp/edasp

A new Parameter for the command **edsp/edasp** has been introduced: "edsp -s" or "edsp status".

This commands show the complete routing of an experiment as it was during acquisition even on a different workstation. If the data was acquired with older TopSpin versions, the probe may be missing.

5.5 Processing

5.5.1 Handling of parameter SPECTYP changed

Parameter SPECTYP specifies the content of the processed data, is used in several application like CMC-se or FBS 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 FBS documentation.

5.5.2 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.

5.6 Automation

5.6.1 Icon NMR 5.0.8

- Mol files are now copied at measurement start
- $USER and $USERGROUP in variables available in Archive directory paths
- “Sref default calibration done” message may be removed from remarks
- Show sample/probe Temperature
- Assure SST Water Suppression Test
- Assure SST Shim Program setting for each SST Experiment

5.7 Analysis

5.7.1 CMC-assist 2.9

The GUI to set the parameters for the calculation of potency was improved.

5.8 GxP Operation

5.8.1 21 CFR Part 11 Documentation

The manual “21 CFR Part 11 Compliance Document” has been further revised and extended.

5.8.2 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.

5.8.3 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.

5.8.4 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.

5.8.5 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.

5.9 Plot Editor

5.9.1 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.

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.

Bruker BioSpin offers the following license types for TopSpin:

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

Processing-Only	Processing, Plotting, Simulation and NMR-GUIDE
	run of validity: 15 years
Student and Academia	Processing Plotting, Simulation and NMR-GUIDE
	run of validity: 15 years
	free of charge

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

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

On the same web page you can request your free license activation ticket for TopSpin 3.6.0. 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.

7 History of Changes

7.1 TopSpin 3.5.0

7.1.1 New Features

7.1.1.1 Acquisition

To set up the NMR probe, the new **edprobe** command replaces the classical **edhead**. Please note that **edprobe** is a mandatory command to be run after **cf** has completed. Please refer to the Acquisition Reference Manual for all details.

The permanent configuration data stored in the memory of the probe (PICS) is an essential input for the hardware configuration management. TopSpin’s acquisition infrastructure has been further improved in version 3.5 and strongly relies on the correctness of these data. Therefore, it may be necessary to correct/complete the PICS of certain probes that contain yet incomplete information data.

This is now easily possible, as the new **edprobe** command offers a straightforward way to write a new PICS file into the probe’s permanent memory (via Manage/FlashPics). The required signed PICS file can be obtained from Bruker. Just send the folder *conf/instr/probeheads* by email to nmr-support@bruker.com and Bruker support will provide you with the new PICS (a file with extension .spf). Please make sure that it is clear for which probe you need the new PICS, if you work with more than one probe.

Although TopSpin tries to recognize an incomplete PICS, it can nevertheless happen that an error message will be shown that is not related to an incomplete PICS. In such a case, please contact your local Bruker Hotline and provide the exact error message and details in order to allow further investigation of the source of the problem.

TopSpin now provides an integrated supervision of the CryoProbe^{TM} Prodigy probe platform

Additional user interface components (in acquisition status bar, dedicated dialog) similar to **vtudisp** allow to control and observe all important Prodigy functionalities, like e.g.

- Basic Prodigy operation (warm up, cool down, N_2 refill)
- Display of Prodigy status, residual warming/cooling time
- Display of general information
- Easy access to the Prodigy service tool
- Storing Prodigy log files
- Automatic acquisition stop if Prodigy is not cooled

Please note: Required Prodigy firmware will be available in Q1 2015.

For the Compressed Sensing (CS) processing, a new method ‚Virtual Echo‘ is introduced with this release. This method improves phase distortion problems with low number of acquired data points and leads to cleaner spectra.

CS is now the default selection for 2D-NUS (whereas the Multi-Dimensional Decomposition (MDD) method remains the default for NUS experiments with dimension of three or greater).

Status information is now displayed in separate window which allows to scroll through the messages and to check for details.

At the end of **cf** a revised list of additional setups is provided. It contains the new commands **edprobe** and **edcstm** (For further information see the following paragraphs).

The new **edcstm** command provides a central interface to store information about the customer and the spectrometer together with information about the Bruker service engineer and how to contact the local Bruker office. This should be filled in during the spectrometer installation, nevertheless you may enter any information you would like to see by use of the command **edcstm**.

A new command '**gs mas** <sideBandIndex> <scanAverage>' has been introduced.

It allows to interactively adjust the magic angle position and shows the respective adjustment data on the display of the HPPR/2 Cover 2 (HPPRII) module.

This command starts **g**s and switches into the online FT mode.

The software then determines one single value from the spectrum: The height of the <sideBandIndex>th rotation side-band (e.g. the 5th sideband). If <sideBandIndex> is > 0 the <sideBandIndex>th side band on the right side of the main peak is taken, otherwise the <sideBandIndex>th side band on the left side of the peak is used. The height of this peak will then be sent to the Cover module, together with the maximum value reached so far. Both values will be displayed as a histogram containing two vertical bars, one named 'curr' for 'current height', the other one named 'max' for 'maximum height'.

The aim of the operator will be to set the maximum height of this rotation sideband as high as possible by adjusting the rotational angle of the sample to the magic angle.

The parameter <scanAverage> is optional and may be set to average several scans before sending the peak value to the preamplifier display in order to reduce fluctuation of the displayed values. If <scanAverage> is not set a value of '4' is assumed.

TopSpin 3.5 supports the new MAS III Pneumatic Unit. For further details please refer to the MAS III manual accessible from the MAS display Help-Tab.

Script to recalculate all proton band selective shapes and power levels accordingly in BEST type experiments.

All power levels will be recalculated from p1 and pldB1 in the current dataset.

GUI usage: bestbw

Command line usage: **bestbw <new bandwidth in ppm> e.g. bestbw 4.85**

7.1.1.2 Processing

CMC-se 2.3 is a new release of Bruker structure elucidation suite. It brings following new key features:

1. Data Storage
   The CMC-se project file storage format has changed.
   The new format stores all analyzed information (peak and multiplet lists) in the project file. With this, it is possible to have several CMC-se projects working on the same set of NMR spectra.

   Any old (CMC-se 2.2 and older) projects are automatically converted to the new format when opened.
2. Fragment Editor
   Major improvements have been made in the fragment tool.

   With the combination of the general fragment editor and the CMC-se assignment tool the spectroscopist gets a powerful tool to work manually with the data.

   The new tool allows not only complex definition of fragments for the structure generation, but also draw and assign the whole structure from scratch. This means, that the new CMC-se version may be used as a structure workbook.

TopSpin 3.5 contains an updated version of the structure editor. Please refer to the updated manual for further documentation.

A new and more flexible way of automatic spectral referencing has been implemented. The new **sref_cond** statement only executes the classical **sref** command depending on the value of the processing parameter SREF_MOD. SREF_MOD is set to “yes” **sref_cond** will execute **sref** and the spectrum will be referenced.

The current release Dynamics Center 2.2.45 offers new features as compared to the previous release 2.1. Examples are Kinetics with series of 2D ASAP HSQC spectra, export of graphics objects in different formats, a method to determine optimum parameters for SOFAST experiments, optimization in multi component fitting and several GUI improvements.

Parameter objects in plot layouts can now display a customized text. If the new option “Use custom definition” is checked the text for the parameter block will not be generated automatically. Instead, the object will display the text content as edited by the user (after click on the “Edit Text…” button) and only replace certain elements by dynamic content as follows:

- <PARAMETER> will be replaced by the current value of the status parameter PARAMETER, e.g. <SI> may be replaced by the value 32768.
- The elements <NAME>, <EXPNO>, <PROCNO>, and <DISK> will be replaced by respective description of the current data set (i.e. the data set to which the parameter object in the layout has been assigned).
- The element <CREATIONDATE> will be replaced by the current date/time stamp. This is not the date of the experiment but the time the plot has been generated. It can be used e.g. to document the time/date of printing, or PDF generation on the layout.
- <$VARIABLE> will be replaced by the current value of the environment variable VARIABLE. E.g., <$USERNAME> results in the name of the logged in user on Windows systems.

An increasing number of customers use cloud storage services in their daily life. Cloud services allow e.g. to have personal data available on mobile devices like smartphones and tablet devices, or consolidate information from various sources at one common place for convenience.

TopSpin 3.5 introduces an option to interface with cloud storage services of your personal choice and provides a very easy and fast solution to “upload” information about your current data set. Once this option has been configured initially, a simple click on “Publish / Mobile” in the TopSpin’s Flow Menu will upload a compact set of files to your cloud service. Shortly after this action, you can use the tools provided by the cloud provider to view the information e.g. on your mobile device. When working in automation, IconNMR can be configured to perform such an upload after an experiment has been finished.

By default, the uploaded information includes an overview plot of your data, a picture of the molecule structure, and all PDFs that are found in the processing directory (e.g. the automation plot, any report generated by CMC or other Bruker software products). The contents can be adapted to your personal choice by the “Configure…” option, available in the Flow Menu from the "Publish/Mobile” drop-down menu. The “Mobile settings” dialog also provides configuration options for the cloud storage service that is to be used. For services like e.g. DropBox™ you need to install the synchronization software of the services which maps a local file folder to your cloud file space. The location of this “sync” folder must be entered here. Every time you click on the “Mobile” button TopSpin will dynamically generate the information package about your current data set and save it to this folder. The software tool of the cloud services then takes care for its synchronization automatically. Usually a few seconds later, the information is available the cloud storage (response time may depend on your network connectivity).

All information generated by this feature is saved below a folder named “Bruker” in your cloud storage space. In order to assist you in keeping all the information organized, TopSpin asks for a “Project” name when uploading. It stores information in a subfolder structure generated from this project name and the data set name. If you want to delete information, you can use the “Mobile / Delete Data…” command to remove data which have been uploaded before. Alternatively, you can manually remove any subfolders in your cloud storage space if you want to make information for specific data sets (or even a complete project) unavailable.

As an alternative to public services like e.g. DropBox™, WebDAV servers can be set as upload target. This option especially may be a choice in environments where “private cloud” functionality may be attractive but public services are not acceptable. Please note that setting-up a WebDAV server may require advanced experience and/or assistance of IT administrators. WebDAV scenarios have been tested successfully by Bruker with the WebDAV service feature of Microsoft Windows 7 and Apache2 web server under CentOs6. Other implementations may work as well but have not been tested so far.

Please note that it is your personal responsibility to decide whether you can use such storage options. E.g. aspects of data security should be considered before configuring and using cloud services. It may also be incompatible with policies of your work environment to do so. In order to give lab operators control over this functionality in TopSpin, access to the “Mobile Settings” dialog is protected by a request for the NMR Superuser password every time. Only users with access to the NMR Superuser password therefore can enable and/or change the storage functionality. The default installation prevents user from uploading information unintentionally.

7.1.1.3 Automation

SampleJet/SampleXpress Individual Sample Matrix ID Support

- Scan a barcoded NMR tube into Icon’s experiment setup table or easy setup window and place your sample anywhere. SampleXpress/SampleJet will find it, and Icon will add the ID information to the data set ready for an ID based search for all your samples experiments*.
- Spreadsheet/External setup supported.
- SampleTrack™/SampleXpress™/SampleJetTM supported.
- Integrated in IconNMR’s Web interface.

Configuration Import/Export

- Export/Import All/Individual configuration settings (including user settings, composites etc.) with one xml file to other IconNMR installations. See the File menu in Configuration

InsightMR™

- Monitor your reactions easily with this dedicated single interface, harnessing the full power of your Bruker NMR Instrument. Close down TopSpin and use the InsightMR shortcut on your Windows Desktop to launch the program. The shortcut icon is automatically placed on your desktop upon installation of the software. See the Quick Start guide, under the ‘Help’ menu of InsightMR, for details on how to use the program.

SmartDriveNMR

- Depending on a verification analysis by the CMC-assist algorithm, further measurements and interpretations may be triggered. Get the most out of your instrument by allowing it to decide what to measure. The ideal combination of NMR experiments for the verification task is identified and carried out. These experiments include 1D1H, HSQC, 13C, and now HMBC experiments. It is decided on-the-fly if further experiments can improve significantly the verification confidence while complying with the user’s demands concerning allocable spectrometer time and confidence. The relevant inputs are intuitive and NMR independent - only relating to the structure verification task: Desired verification confidence, Maximum measurement time, Molecular structure and Solvent

Easy setup updated

- See what experiments are available at a glance for even faster selection.
- Limit the number/type of experiments/solvents to those you want to run, irrespective of ‘User Manager’ experiment lists.

Virtual Parameter Sets

- Make new/Tweak experiments for use inside IconNMR Automation based on any TopSpin parameter set.
- Parameters may be modified or even inherited from other experiments. Alternative/ multiple Acquisition AU programs/commands may be prescribed or alternative underlying parameter sets selected.
- Eliminate the need for multiple customized parameter sets (even across multiple instruments), with only minor differences. See Configuration->Virtual Parameter Sets.

General Automation

- Improved User Interface Experience
- Use system passwords to login to Web IconNMR's HTTPS site.
- Download JDX/ZIP Files of spectra from Web-IconNMR.
- Define an Idle Temperature to use after the last sample has left the magnet.
- Accounting reports may now be generated for users which are broken down according to the different settings of a particular originator item.
- Accounting report output now available in spreadsheet format.
- Pausing a run can now remove or leave the sample in the magnet.
- Start times are copied/set automatically on follow up experiments.
- Absence of the Priority User permission no longer disables the day/night experiment switch.
- Spreadsheet files with .xlsx/.xls/.csv extensions can be imported automatically when copied to the external setup directory.
- Experiment numbers and parameter modifications can now be taken from spreadsheets.
- Send notification/data e-mails in HTML with Authentication/Encryption.
- Easily define multiple data archiving directories.
- Set ATM options coarse/exact etc. on individual experiments.
- Periodic Experiments Tool now makes full use of IconNMR’s ‘Start Time’ system.

Other New Features:

- Hidden Options from _iconnmrrc.txt are now fully accessible from the General Options Miscellaneous Tab.
- Start and Stop the run via External Setup keywords START_RUN, STOP_RUN, also available as command line options (Type iconnmr ? in TopSpin for all options).

See the Reference Guide’s ‘What's New’ section for more details on changes since your last version of IconNMR.

You can access this information any time from the 'What's new' help menu command
*) This feature may require additional hardware/firmware updates on your SampleJet.

7.1.1.4 Pulse Programming

The new shape tool features full parameterized control of waveform generation and analysis and modification.

Shapes now consist of several waveforms which can easily be worked on individually and mutually while maintaining consistency of global properties.

Furthermore particular shape parameters are allowed to be used within pulse program calculations and GS mode offers a comfortable way of offset adjustment of any compound of shapes.

Please note that a completely revised manual “pulse programming” is now available with TopSpin 3.5.0.

The new operator .max returns for several types of lists (pulse, power, delay, frequency) the maximum element of the respective list (cf. Pulse Programming Manual for further details).

To a limited extent it is now possible to use relations in CPD-programs (cf. Pulse Programming Manual for further details).

7.1.1.5 General User Interface

The horizontal and vertical axes in data windows now have interactive capabilities which allow to shift and scale axis with more comfort, without always access the toolbar. With a left-mouse-button click-and-hold action an axis can be moved. Turning the mouse wheel while placing the mouse over an axis can be used to scale it. A double-click on an axis results in a “reset” i.e. sets it back to maximum/minimum axis values for the displayed data. A double-click at any place within the spectrum will perform a reset for both horizontal and vertical axes which is identical to clicking the “Show full spectrum” button in the toolbar.

Pressing the hotkey F11 once allows to toggle between TopSpin’s current screen layout and a maximized layout, alternatively. For the maximized display, the toolbar is hidden and the data browser panel toggled.

If a data set is opened that contains acquisition data but never has been processed, TopSpin will perform a default Fourier transformation automatically if appropriate. This behavior can be switched on or off in the TopSpin user preferences.

7.2 TopSpin 3.5.1

7.2.1 New Features

7.2.1.1 Acquisition

To set up the NMR probe, the new **edprobe** command replaces the classical **edhead**. Please note that **edprobe** is a mandatory command to be run after **cf** has completed. Please refer to the Acquisition Reference Manual for all details.

7.2.1.2 Processing

Dynamics Center 2.2.5

The current release Dynamics Center 2.2.5 offers new features as compared to the previous release 2.1. Examples are Kinetics with series of 2D ASAP HSQC spectra, export of graphics objects in different formats, a method to determine optimum parameters for SOFAST experiments, optimization in multi component fitting and several GUI improvements.

7.3 TopSpin 3.5.2

The following topics describe the major fixes which come with TopSpin 3.5pl2.

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 that a user account and password is required to open this page. To login or register for a free account, please open the following web page:

http://www.bruker.com/login-customer.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 # 13170 ---- **Prosol** relations not updated automatically
- item # 13169 ---- Opening datasets in TopSpin always opens new window
- item # 13164 ---- **edprobe** fails: Unable to get tuning/matching info for token 1H/19F
- item # 13162 ---- ATM not always being used on new solvent for X Nuclei
- item # 13143 ---- Priority does not work
- item # 13120 ---- Could not set password for account nmrsu: … Unknown option –c
- item # 13112 ---- iptables: command not found
- item # 13110 ----- cannot remove */tmp/swim-4008/prog*: Is a directory
- item # 13101 ---- Acquisition aborted with PROHOMODEC
- item # 13086 ---- Parameters cannot be modified via Spreadsheet Import
- item # 13085 ---- Night Experiments fail with Barcodes/Matrix IDs
- item # 13083 ---- **topshim** fails on non-PICS probes
- item #13072 ---- Projection Reconstruction does not work
- item # 13067 ---- plot0 does not work
- item # 13025 ---- **edprobe**: the probe can’t be defined
- item # 13023 ---- topshim solvcal fails with error
- item # 13020 ---- wrong routing for F19CPD with QNP accessory
- item # 12782 ---- Wrong return value of CPR_exec(vtuselftune”, WAIT_TERM) in case of failure
- item # 12660 ---- missing reference shift correction value in **edlock**
- item # 9143 ---- **topshim** does not work without lock board

7.3.1 New Features

7.3.1.1 Acquisition

New Pulse Program classes

With TopSpin 3.5pl2 new classes of pulse sequences have been added:

Homodecoupling sequences:

reset_*: broadband homodecoupling using reset approach

*_bbhd: broadband homodecoupling using BIRD pulses

*_bshd: bandselective homodecoupling

*_zshd: broadband homodecoupling using Zangger-Sterk

*bbhd *bshd and *zshd for AVIII and AVIII HD only

New 13C detected 3D, 4D and 5D sequences:

c_*

Dual Receive sequences:

dr_*

New semi constant time (in F2 dimension) experiments:

*_sct

For details please check the file Update.info in the TopSpin subfolder *\exp\stan\nmr\lists\pp.dexam*.

New 4D and 5D Bio-NMR experiments with 1H detection. New Bio-NMR experiments with 15N detection. New homodecoupling experiments based on “psyche” building block. More “best” triple resonance experiments

With TopSpin 3.5pl2 all “best” experiments allow for the calculation of shaped pulse length and power based on offset and bandwidth.

Introduction of “tdmax” calculation for all constant time experiments.

New Pulse Assignments in Prosol

With the new version 2.000 of the Prosol relations, new pulse assignments have been introduced for the default, triple, triple_c and lcnmr class. For details please refer to the file *Update.info* in the TopSpin subfolder *exp\stan\nmr\lists\prosol\pulseassign*. This update will force a recalculation of all Prosol values based on the 90° hard pulses.

For the conversion **edprosol** must be executed otherweise **getprosol** will not work.

7.3.1.2 Processing

Identify structures with CSEARCH

As a new feature in the Structure Analysis, TopSpin offers a tool to search for known compounds in the CSEARCH database operated by the University of Vienna. The functionality is available in the menu system under “Analyse / Structures / Identify structures with CSEARCH”, or by the command **csearch_ident** alternatively. The search is based on C13 chemical shifts. A request for C13 spectra is automatically generated, and sent to CSEARCH upon confirmation by the user . The respond is given via email after a short time. The request needs C13 chemical shifts and optional knowledge like the chemical formula and the mass.

For more information about CSEARCH use the following link: *http://nmrpredict.orc.univie.ac.at/*

Dynamics Center 2.3

The current release Dynamics Center 2.3 offers new features as compared to the previous release 2.2. Examples are analysis of time domain data as created by minispec and the general possibility of providing user defined start parameters for data modelling.

CMC-se 2.4

A new feature in CMC-se offers a CSEARCH database request to match all possible structures. The request based on C13 chemical shifts uses additional information about hybridization, the chemical formula and the mass after the automatic analysis. The request will be automatically generated and the result is given via e-mail.

For more information about CSEARCH use the following link:

http://nmrpredict.orc.univie.ac.at/

Reference Deconvolution

With Reference Deconvolution TopSpin offers a new interactive tool for removing distortions in 1D spectra which might have been caused by field inhomogeneities or modulations. The functionality is available in the menu system under “Processing / Advanced / Reference Deconvolution”, or alternatively by the command **.refdcon** .

edlock / sref

Starting with TopSpin 3 the new edlock table lacks the column "Ref. Shift" from the older edlock table. In addition, some values of the column called "Reference shift" erroneously refer to the column "Ref" from the older edlock table.

With TopSpin 3.2pl7 the old column “Ref.Shift” has been reintroduced and is now named “Reference Shift Correction”. The values in the column “Reference Shift” have been corrected.

The Reference Shift Correction values help when the solvent is used as a reference substance rather than an internal reference like TMS. The default reference shift calculated on the basis of BF1 is sample dependent. C6D6, for example, does not necessarily have a default chemical shift of 7.16. To correctly identify the C6D6 peak, the default calibration done by the command **sref** may have to be slightly corrected and the Reference Shift Correction value accomplishes this.

Automated referencing of 2D spectra

In Multiple Display for 2D data it is possible to align F2 shifted data automatically. The alignment will be calculated relative to the first dataset as reference.

Introduction of LabToGo

TopSpin 3.5 offers customers the possibility to upload current results to a personal cloud storage by one-click operations (see also section “Copying Results to Personal Cloud Storage” in chapter “History of Changes”). LabToGo is a new app for iPad launched by Bruker BioSpin in the Apple AppStore. It offers the review of documents in the cloud storage in a very convenient way and fully integrates with Topspin3.5 and the newest CMC-assist release.

At the desktop, customers get a one-button solution for uploading results of their NMR analysis to their cloud storage like e.g. Dropbox. On an iPad, LabToGo and cloud access are the only things needed for reviewing reports created with TopSpin and CMC-assist, plot graphics, and more, whenever connectivity to the cloud storage is available.

Well known touch gestures allow navigating through documents. 1D NMR data can be interactively displayed. Additionally, LabToGo can even mirror the current status of automation jobs and receive continuous updates from IconNMR monitoring the lab. If configured, finished experiment reports are automatically copied to the personal cloud storage for review with the app. Conveniently, the use of cloud technologies removes the need for a direct network connection into the laboratory network (which is often impracticable).

The menu entry “Publish / Mobile / Send to mobile” has been renamed to “Send to LabToGo” accordingly.

LabToGo can be downloaded from the App Store and requires an iPad with iOS8 or newer. Apple, the Apple logo, iPad, and iOS are trademarks of Apple Inc., registered in the U.S. and other countries. App Store is a service mark of Apple Inc.

7.3.2 Bug Fixes in TopSpin 3.5pl2

The following topics describe the major fixes which come with TopSpin 3.5pl2.

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 that a user account and password is required to open this page. To login or register for a free account, please open the following web page:

http://www.bruker.com/login-customer.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 # 13170 ---- **Prosol** relations not updated automatically
- item # 13169 ---- Opening datasets in TopSpin always opens new window
- item # 13164 ---- **edprobe** fails: Unable to get tuning/matching info for token 1H/19F
- item # 13162 ---- ATM not always being used on new solvent for X Nuclei
- item # 13143 ---- Priority does not work
- item # 13120 ---- Could not set password for account nmrsu: … Unknown option –c
- item # 13112 ---- iptables: command not found
- item # 13110 ----- cannot remove */tmp/swim-4008/prog*: Is a directory
- item # 13101 ---- Acquisition aborted with PROHOMODEC
- item # 13086 ---- Parameters cannot be modified via Spreadsheet Import
- item # 13085 ---- Night Experiments fail with Barcodes/Matrix IDs
- item # 13083 ---- **topshim** fails on non-PICS probes
- item #13072 ---- Projection Reconstruction does not work
- item # 13067 ---- plot0 does not work
- item # 13025 ---- **edprobe**: the probe can’t be defined
- item # 13023 ---- topshim solvcal fails with error
- item # 13020 ---- wrong routing for F19CPD with QNP accessory
- item # 12782 ---- Wrong return value of CPR_exec(vtuselftune”, WAIT_TERM) in case of failure

- item # 12660 ---- missing reference shift correction value in **edlock**
- item # 9143 ---- **topshim** does not work without lock board

7.4 TopSpin 3.5.5

The following topics describe the major fixes which come with TopSpin 3.5pl5.

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 # 11538 ---- Misleading TopSpin error message after lock failure with HRMAS
- item # 11668 ---- 1H{19} with QNP-Accessory fails with 300MHz spectrometer
- item # 11738 ---- 2H decoupling does not work on systems with more than one receiver
- item # 13074 ---- drag and drop to plot portfolio does not work for internal plot window
- item # 13216 ---- 2H decoupling experiments on dual receiver systems
- item # 13221 ---- Selection Rectangle in 2D spectra always black
- item # 13224 ---- Usage of BEST not possible in TopSpin 3.5 with CryoProbe and CryoFit
- item # 13227 ---- **ftnd** may not work correctly with stripped data
- item # 13255 ---- Acquisition problems when running as a non "Supervisor" user
- item # 13258 ---- **gs** fails if SPNAM > 9 is used
- item # 13260 ---- Parameter modifications not correctly displayed
- item # 13268 ---- Parameter/Title modification not possible as non supervisor user
- item # 13269 ---- Auto-update of EDPROSOL puts liquids numbers in for solid state probe
- item # 13273 ---- NMR-GUIDE fails to start
- item # 13274 ---- JChemPaint can't save modified molfile - Permission denied
- item # 13276 ---- EDTE window closes on temperature change
- item # 13281 ---- Cortab for X-nuclei with cortab-box and QNP-accessory not possible
- item # 13292 ---- pulse program: **cw** in if-statements always executed
- item # 13298 ---- Error Message: image "ParCLockNDisabled" doesn't exist
- item # 13299 ---- IPSO tty 6 and 7 not available in **cf**
- item # 13305 ---- **rga**: This RG value has already been tried before
- item # 13306 ---- Diverse activation issues with priority/start time settings
- item # 13308 ---- Lock command can not open locksolv file (permission denied)
- item # 13312 ---- **topshim** fails: no acquisition running
- item # 13315 ---- **edasp** fails: Error in check_swilpso: Error at ipsoRout
- item # 13316 ---- wrong F1 axis unit when processing DOSY experiment
- item # 13318 ---- **getprosol** doesn't work if user doesn't belong to group nmrsu

- item # 13325 ---- automation does not run correctly with single peak lineshape check activated
- item # 13334 ---- acquisition status parameter TD = 0 out of range must be greater 0
- item # 13344 ---- Automation queue halts if night experiments not complete at the end of night-time
- item # 13353 ---- Diverse Problems with IconWeb configuration handling
- item # 13385 ---- FIDRES difference between Status Parameter and Plot
- item # 13386 ---- IconWeb https site inoperable with Firefox 39.0
- item # 13387 ---- calibo1p1 doesn't work
- item # 13388 ---- **edprobe** fails: Bad BIS value: ProbeAllCoils
- item # 13397 ---- **edprosol** update destroys DE stored value
- item # 13400 ---- **topshim** exceeds power limit on probe
- item # 13404 ---- not possible to use cortab box with amplifiers with output routing
- item # 13411 ---- Pulsecal fails on datasets written to network drives
- item # 13417 ----The address stated below does not conform to protocol standards: URL=
- item # 13418 ---- after import **cf** always generates a datastation
- item # 13421 ---- Missing sample down after 60 seconds
- item # 13422 ---- **cf**: SGU connections to amplifier lost
- item # 13423 ---- **atma** / **atmm** for 11B fails with RXS-1 error on AV3 HD
- item # 13425 ---- Error message: can’t read data (SubmittedList)
- item # 13428 ---- pulse program: **cpd** erroneously works like **cw**
- item # 13437 ---- Generating landscape-oriented PDF files by printing action in PlotEditor results in rotated output
- item # 13441---- AU-program calibO1p1 fails with error message
- item # 13443 ---- Barcodes not always found - measurements not performed
- item # 13446 ---- CPR program garp4.p60 is missing
- item # 13449 ---- SampleTrack - Automation hangs when normally a dialog would appear
- item # 13451 ---- pulse program: phcor not added
- item # 13454 ---- crco service installed and active by default
- item # 13464 ---- NMR-Guide not installed on MacOS
- item # 13477 ---- incorrect file size warning
- item # 13490 ---- Void error during changing the probe with BACS-60
- item # 13495 ---- TopShim failure with error "Sample failed to reach target spin rate"
- item # 13511 ---- edprobe: Addition of power limits to PICS probe fails
- item # 13533 ---- projection-spectroscopy fails with compilation error
- item # 13535 ---- **edprobe** fails: maximum allowed size exceeded
- item # 13536 ---- DATE not updated correctly after tr-command
- item # 13562 ---- User created adiabatic pulses calculate power wrongly in shape tool
- item # 13565 ---- Logged in automation user changes unexpectedly
- item # 13570 ---- Shaped pulse power cannot be adjusted in GS mode
- item #13588 ---- **Wobb** fails on NUS datasets

7.4.1 New Features in TopSpin 3.5pl5

7.4.1.1 Acquisition

New shape tool features full parameterized control of waveform generation and analysis and modification.

Shapes now consist of several waveforms which can easily be worked on individually and mutually while maintaining consistency of global properties.

Furthermore particular shape parameters are allowed to be used within pulse program calculations and GS mode offers a comfortable way of offset adjustment of any compound of shapes.

When having a solvent in the probe which cannot be locked on (no 2H or 19F), it was complicated to use the chemical shift of the solvent as a reference after the acquisition.

Therefore, there is a new feature in the solvent table. One can assign if it is a ‘lock solvent’ or not, and in both cases apply the **lock** command on that solvent. As a result, all the parameters are set in the data set (even for the non-lockable solvent), and the solvent can be applied as a reference.

A new au program set_loopval has been implemented for loop adjustments. It is a combination of the classical loopadj (loop adjust) program and the lock.1 to lock.12 macros to set the strength of the lock coupling. Set_loopval first determines automatically lock coupling for the given sample based on the signal to noise of the lock signal (given by the lock gain) and then offers a table of loop settings for modification in a graphical interface.

7.4.1.2 Processing

CS (Compressed Sensing) IST (Iterative Soft Thresholding) with disabled VE (Virtual Echo) processing of 2D data no longer requires a NUS license.

In case no NUS license is available processing of 2D NUS data automatically switches to above mode after issuing an appropriate message.

The interactive Integration Mode (Processing -> Integrate) gets a new feature for cursor-defined integrals. The interpolated baseline in the current integral region will be automatically displayed during region selection. This allows a better integration of peaks placed at the shoulder of a big peak. The baseline values are stored as a bias and slope in the standard integration region file (see the TopSpin User Manual for further information).

The datastation configuration of TopSpin is optimized for faster startup and reduced memory consumption. As a consequence the command **ased** is no longer possible with the “Default Datastation” configuration. To enable this command again execute **cf** and select the “Bruker_default_avIII600” configuration or use any other spectrometer configuration.

7.4.1.3 Automation

Include Experiment Description in EasySetup radio buttons – See experiment comments at a glance

Search forwards/backwards for first character of experiments/solvents EasySetup radio buttons

Disable EasySetup radio buttons if necessary

Switch EasySetup on/off where available from tools menu

Use variables from Data Set Name in Originator Items $DATE, $USER, $SETUP…

ATMA now can run automatically if the acquisition parameter TUBE_TYPE changes between samples

Last Sample measured with any barcode information shown in automation status line

New Barcode automation modes show live scan information in automation status line

SST System Suitability available only on demand if frequency set to zero. Tools-> Run System Suitability Test Now

Web server uses more secure TLS encryption

Switch EasySetup on/off where available from tools menu (Since TopSpin 3.5 PL2 / IconNMR 5.0.2)

InsightMR™

FlowTube Automation Mode Supported

WET Suppression experiments included

Persistent Sample feature added – When multiple samples in use – forces the current sample to remain in the magnet

After unhooking Automation when Insight experiments complete, default Automation mode becomes active

SmartDriveNMR

Show measured data sets in SmartDriveNMR Monitor (Right Click in Preceding Experiments Window)

SmartDriveNMR relevant experiments (CMC_*) always shown at top of experiment list

7.4.1.4 Analysis

CMC-se 2.5 is a new minor release with the following new key features:

3D Structure Analysis with ROESY and NOESY

NOESY and ROESY spectra were added to the list of supported experiments.

This allows the manual estimation of relative stereochemistry in CMC-se.

Correlation Highlighting in Structure Editor

The highlighting functionality discriminate different experiment types and its information content. Correlation highlighting can separate between COSY and HMBC for valid and invalid correlations. As an additional improvement, correlations can be shown between individual drawn protons, especially for correlations from ROESY and NOESY.

Interface to CSEARCH Robot Referee (Structure Assignment Check)

With CSEARCH get an assignment check ahead a publication and have it ready for the transfer in the article. The result is an email holding URLs to details about the evaluation, the spectrum prediction and the classification of the assigned structure.

Read more information in the following link:

http://nmrpredict.orc.univie.ac.at/c13robot/robot.php

With this release comes the ability to analyze HMBC data. Along with the automated analysis of a 1D1H, HSQC, and optionally 13C data, HMBC spectra can be included to further refine the verification analysis.

7.4.2 Bug Fixes in TopSpin 3.5pl5

The following topics describe the major fixes which come with TopSpin 3.5pl5.

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 # 11538 ---- Misleading TopSpin error message after lock failure with HRMAS
- item # 11668 ---- 1H{19} with QNP-Accessory fails with 300MHz spectrometer
- item # 11738 ---- 2H decoupling does not work on systems with more than one receiver
- item # 13074 ---- drag and drop to plot portfolio does not work for internal plot window
- item # 13216 ---- 2H decoupling experiments on dual receiver systems
- item # 13221 ---- Selection Rectangle in 2D spectra always black
- item # 13224 ---- Usage of BEST not possible in TopSpin 3.5 with CryoProbe and CryoFit
- item # 13227 ---- **ftnd** may not work correctly with stripped data
- item # 13255 ---- Acquisition problems when running as a non "Supervisor" user
- item # 13258 ---- **gs** fails if SPNAM > 9 is used
- item # 13260 ---- Parameter modifications not correctly displayed
- item # 13268 ---- Parameter/Title modification not possible as non supervisor user
- item # 13269 ---- Auto-update of EDPROSOL puts liquids numbers in for solid state probe
- item # 13273 ---- NMR-GUIDE fails to start
- item # 13274 ---- JChemPaint can't save modified molfile - Permission denied
- item # 13276 ---- EDTE window closes on temperature change
- item # 13281 ---- Cortab for X-nuclei with cortab-box and QNP-accessory not possible
- item # 13292 ---- pulse program: **cw** in if-statements always executed
- item # 13298 ---- Error Message: image "ParCLockNDisabled" doesn't exist
- item # 13299 ---- IPSO tty 6 and 7 not available in **cf**
- item # 13305 ---- **rga**: This RG value has already been tried before
- item # 13306 ---- Diverse activation issues with priority/start time settings
- item # 13308 ---- Lock command can not open locksolv file (permission denied)
- item # 13312 ---- **topshim** fails: no acquisition running
- item # 13315 ---- **edasp** fails: Error in check_swiIpso: Error at ipsoRout
- item # 13316 ---- wrong F1 axis unit when processing DOSY experiment
- item # 13318 ---- **getprosol** doesn't work if user doesn't belong to group nmrsu
- item # 13325 ---- automation does not run correctly with single peak lineshape check activated
- item # 13334 ---- acquisition status parameter TD = 0 out of range must be greater 0
- item # 13344 ---- Automation queue halts if night experiments not complete at the end of night-time
- item # 13353 ---- Diverse Problems with IconWeb configuration handling
- item # 13385 ---- FIDRES difference between Status Parameter and Plot

- item # 13386 ---- IconWeb https site inoperable with Firefox 39.0
- item # 13387 ---- calibo1p1 doesn't work
- item # 13388 ---- **edprobe** fails: Bad BIS value: ProbeAllCoils
- item # 13397 ---- **edprosol** update destroys DE stored value
- item # 13400 ---- **topshim** exceeds power limit on probe
- item # 13404 ---- not possible to use cortab box with amplifiers with output routing
- item # 13411 ---- Pulsecal fails on datasets written to network drives
- item # 13417 ----The address stated below does not conform to protocol standards: URL=
- item # 13418 ---- after import **cf** always generates a datastation
- item # 13421 ---- Missing sample down after 60 seconds
- item # 13422 ---- **cf**: SGU connections to amplifier lost
- item # 13423 ---- **atma** / **atmm** for 11B fails with RXS-1 error on AV3 HD
- item # 13425 ---- Error message: can’t read data (SubmittedList)
- item # 13428 ---- pulse program: **cpd** erroneously works like **cw**
- item # 13437 ---- Generating landscape-oriented PDF files by printing action in PlotEditor results in rotated output
- item # 13441---- AU-program calibO1p1 fails with error message
- item # 13443 ---- Barcodes not always found - measurements not performed
- item # 13446 ---- CPR program garp4.p60 is missing
- item # 13449 ---- SampleTrack - Automation hangs when normally a dialog would appear
- item # 13451 ---- pulse program: phcor not added
- item # 13454 ---- crco service installed and active by default
- item # 13464 ---- NMR-Guide not installed on MacOS
- item # 13477 ---- incorrect file size warning
- item # 13490 ---- Void error during changing the probe with BACS-60
- item # 13495 ---- TopShim failure with error "Sample failed to reach target spin rate"
- item # 13511 ---- edprobe: Addition of power limits to PICS probe fails
- item # 13533 ---- projection-spectroscopy fails with compilation error
- item # 13535 ---- **edprobe** fails: maximum allowed size exceeded
- item # 13536 ---- DATE not updated correctly after tr-command
- item # 13562 ---- User created adiabatic pulses calculate power wrongly in shape tool
- item # 13565 ---- Logged in automation user changes unexpectedly
- item # 13570 ---- Shaped pulse power cannot be adjusted in GS mode
- item #13588 ---- **Wobb** fails on NUS datasets

7.5 TopSpin 3.5.6

The following topics describe the major fixes which come with TopSpin 3.5pl6.

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 # 13811---- Some securemail servers reject mal connection
- Item # 13806 ---- Error when using "Run an Experiment Periodically"
- Item # 13789 ---- Popt option mash does not work vor MASIII unit
- Item # 13772 ---- command **resume** yelds "Command not implemented"
- Item # 13761 ---- User groups not visible/usable within Accounting
- Item # 13752 ---- Incorrect solvent set (CDCL3) for ASTM sample in Benzene via Assure SST
- Item # 13741 ---- InsightMR: Data are always archived to *C:\ReactionMonitoring*
- item # 13733 ---- Parameter block in plot layout should list all valid electronic signatures
- item # 13731 ---- TopSpin internal login dialog should block after multiple failed login attempts
- item # 13714 ---- AU program library function manipulateShapeC buggy
- item # 13710 ---- Error notification e-mail is blank
- item # 13707 ---- **topshim** fails when coil=29Si
- item # 13695 ---- Randomize Priority function ignored
- item # 13694 ---- Remaining time display intermittent
- item # 13693 ---- Priority reset when **expt** edited
- item # 13681 ---- Installation of 3.5pl5 does not import **gradpar** from 3.5pl4
- item # 13665 ---- Routine Spectroscopy: SampleChanger Position/Manual Lock Shim setting is ignored
- item # 13660 ---- 1H/19F **atma** fails on certain configuration
- item # 13655 ---- shapetool: internal error
- item # 13654 ---- **TopShim** fails for probe type MIC
- item # 13648 ---- UPnP device (No UPnP device info available)
- item # 13628 ---- **edte**: Unable to read the ET-PH
- item # 13619 ---- Command **'st generate ...'** fails with error 'Resolution is too small'
- item # 13598 ---- **baseop**t: **zg** fails due to invalid group delay
- item # 13569 ---- **Edprobe** should recognise, if a Cryo probe has the ATMA unit connected
- item # 13513 ---- **showpp** and **nmrsim** do not work on Mac OS 10.10/10.11
- item # 13256 ---- No concentration calculation with eretic2
- item # 11364 ---- Routing of an AMP with Output router directly to the probe not implemented

7.5.1 New Features

7.5.1.1 Acquisition

There are several news and updates in the assisted user interface to set up solid-state NMR experiments:

- novel user interface allows easier access to a new project or the import of parameters from a former project
- automated quality evaluation of magic-angle setting and probe shimming for best hardware performance
- applications on biological samples:
  - optional optimizations introduced for spectral widths (C, Ca, CO, NH) and 1H decoupling
  - missing parameters are recognized and optimized automatically
- introduction of further application fields:
  - probe setup (e.g. after repair)
  - material samples (H/X, MQMAS, 1D/2D)
- can be used with 4 and 3.2 mm DOUBLE and TRIPLE channel probes
- flexible dataset handling
- improved PDF report (including multidimensional experiments)

WaveMaker (**wvm**) is a software solution for pulse shaping that is based on waveform definitions within the pulse programs. This avoids any need to modify the PROSOL tables when new or non-standard shaped pulses and decoupling or mixing waveforms are required. It also adds flexibility to and improves portability of many standard and user developed experiments and pulse programs. Porting the WaveMaker based pulse programs to NMR systems of different field strength is straightforward and typically require no further adjustments and PROSOL updates.

For more details see the description in the acquisition reference manual under the command **wvm**.

New Python script copypars for copying parameters from one dataset to another

The utility **copypars** provides a graphical user interface to copy calibrated pulses and optimized frequencies and sweep widths from one dataset to another. After creating a new dataset, start the utility by entering **copypars** at the command line or by selecting it from the Acquire flowbar. You will be prompted to open your reference dataset. The default mode automatically copies excitation frequencies and sweep widths for matching nuclei between the two datasets. The manual mode provides an additional GUI for the manual selection of which parameters to copy from the reference dataset, and includes options for applying **getprosol** based on the calibrated 90 degree pulses in the reference dataset and selecting any other acquisition parameter to copy. Additionally, excitation frequencies and sweeps widths can be copied from either the acquisition parameters of the reference data or from the currently displayed region of a 1D or 2D spectrum.

This TopSpin release contains the initial version of the new BioTop package. BioTop supports the user in working with biological samples (currently proteins) in high resolution NMR. The package aims at providing all necessary steps to set-up bioNMR experiments in an optimized and automated way. To enter these guided experiment workflows either choose **More/BioTop** from the Acquire menu, or enter **biotop** in the command line. Please refer to the BioTop manual in TopSpin's manual collection.

7.5.1.2 Processing

The command **lockdataset** applies permission changes on the current data set. Content of the EXPNO and PROCNO directories will be protected against further overwrite/append/delete operations, and the directory objects itself will lose permissions to add file and subdirectories in it. Effectively, the directory will be frozen. It is still possible to add and process new PROCNOs for the same raw data while the initial PROCNO remains protected. This is especially useful in GxP environments and allows to implement a standard procedure like e.g. the following:

automatically acquire and process data set in PROCNO 1→ digitally sign data by command **esign**

→ apply **lockdataset** to protect against modification

→ use command **wrp 2** to create new PROCNO → change to it by **rep 2**

→ perform interactive processing there (without touching original signed data)

The command **lockdataset** can be used as part of AU scripts like e.g. the one defined by AUNMP. It is also available by interactive menu selection *Manage/Security/Lock Data Set Against Changes*

4D NUS data can now also be processed with Mdd_mod = cs (Mdd_CsALG =

IST, Mdd_CsVE = true) instead of Mdd_mod = mdd. CS processing of 4D NUS data

requires less processing time.

7.5.1.3 Automation

Decide on a per-user/group basis in the IconNMR User Manager who can use SmartDrive/FastLane features

Store “serial processing” (data set) lists from Preceding Experiments via right click for use in CMC-assist

TMS/DSS continuous lineshape check from AssureNMR now part of general AssureSST functionality

Run AssureSST Test on an unscheduled basis only with configuration setting “On Demand”

Real parameter values now shown instead of “Default”

TLS 1.2 / SHA256 support for improved https/browser security

Corrected multi browser support for experiment selection

Corrected blinking Icons in status frame

Grab individual columns from spreadsheets based on real (1st) row cell names

Use Groups as defined in User Manager or Additional Users for accounting

TS3.5pl6 comes with the new release Dynamics Center 2.4.3. As described in the corresponding release letter it offers several bug fixes and improvements.

7.5.1.4 General User Interface

User interface for NMRSim and related products (pulse program display, Bloch module) has been reworked.

The NMRSim poses now identical look and feel on all supported platforms, the installation of additional X11 server on Mac OS-X is not required anymore.

Additional new features:

- Chemical structure may be used as a spin system description for the simulation.
- Completely new implementation of NMR Wizard allows to simulate basic NMR experiments immediately from chemical structure editor:

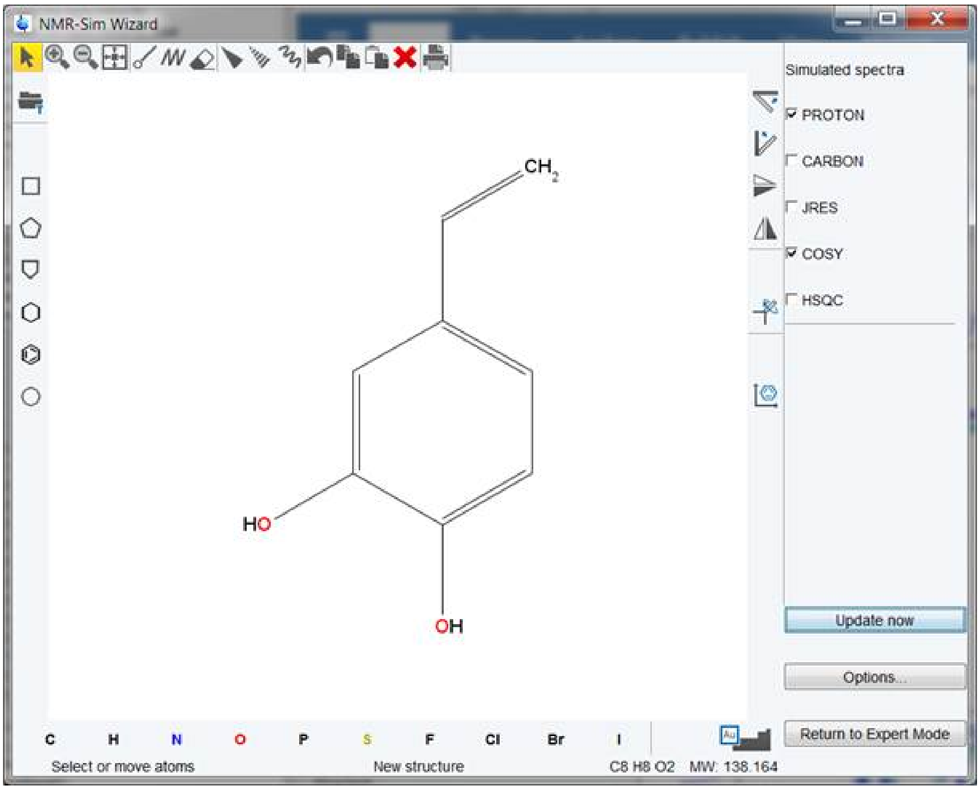


Figure 7.1: NMRwizard window

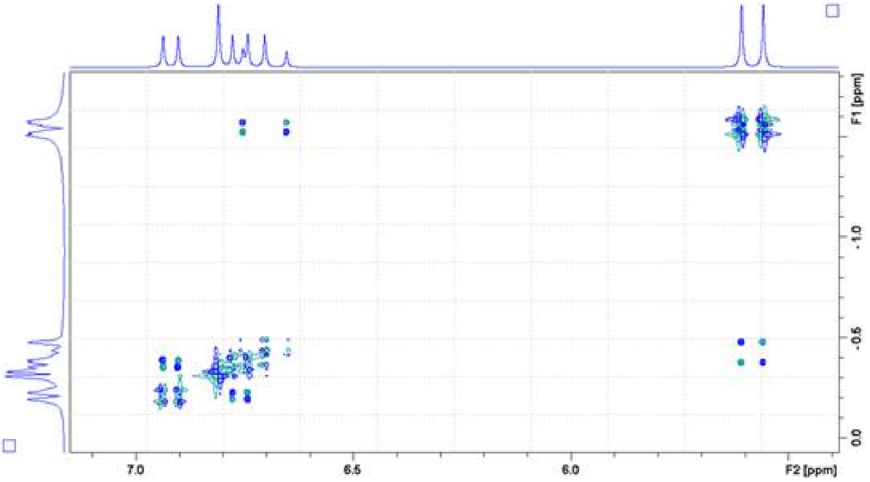
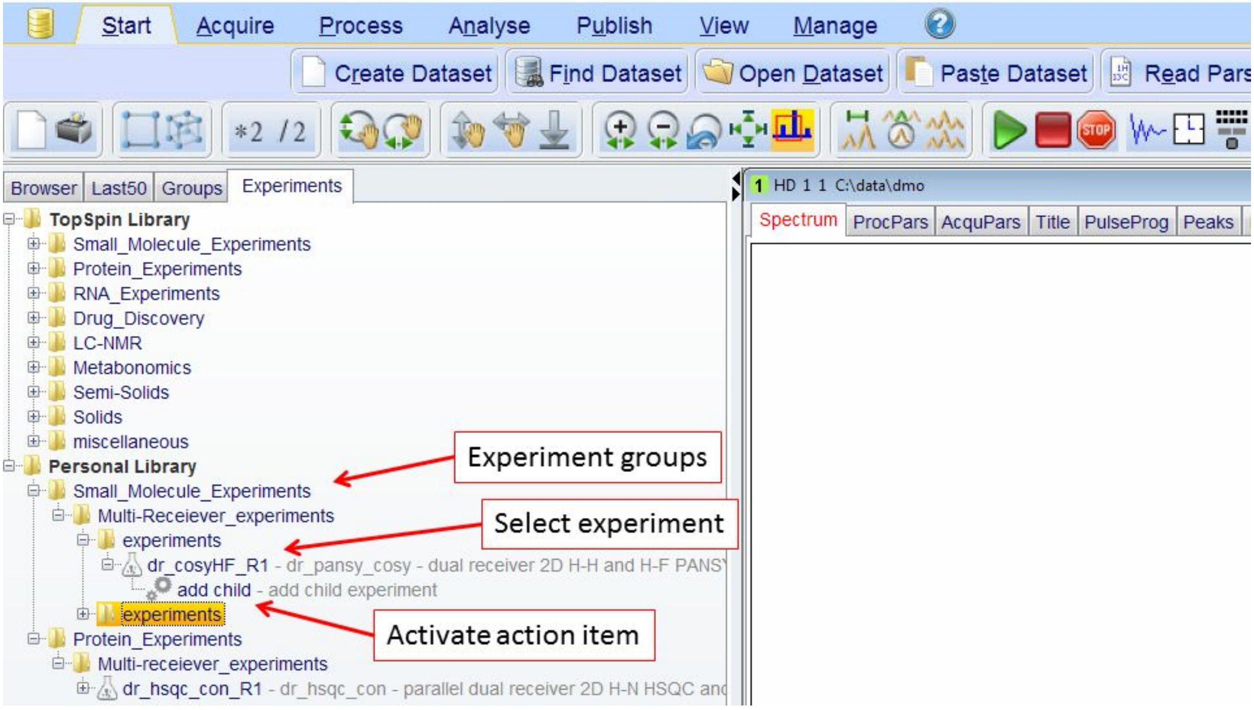


Figure 7.2: Simulate COSY spectrum

The Experiment Selector is a new user interface element introduced in TopSpin 3.5pl6. It provides an easy access to the vast experiment library of standard experiments that is available in each release of TopSpin. It is also a tool that allows the users to personalize their most frequently used standard experiments into a separate library and therefore provides a simplified overview and a quick and easy access to their most routinely used experiments. It should be pointed out that the current version of the Experiment Selector does not provide access to the user libraries, only to the standard TopSpin experiment libraries. However, the potential and functionality of the Experiment Selector is set to expand and improve in the future releases of the TopSpin making it an important and valuable tool for the TopSpin users.



The Experiment Selector window may not appear in the browser area by default and can be activated by selecting the “Browser Preferences” item from the drop-down menu pane that is activated by a right click of the mouse with the pointer in the Browser area. Once the “Show Experiments Tab” checkbox is selected click the “Apply” button and restart the TopSpin. The “Experiments” tab should now appear in the browser area.

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

The Personal Library initially is empty and can be populated by simply dragging and dropping individual experiments or groups from the standard TopSpin Library. Alternatively, the experiments can be added manually by selecting the desired group of experiments and selecting the “Create Data Set” entry from the drop down menu that is activated by a right click of the mouse:

7.5.1.5 GxP Operation

TopSpin uses a dedicated file `login.txt` for logging the activities of starting and terminating TopSpin as well as internal user login/logoff operations. This log file can be evaluated e.g. when working in regulated environments (GxP) and is now protected by checksums covering its full content. With each new entry, TopSpin automatically checks the file for consistency with existing checksums first before adding the entry and a newly calculated checksum. Any modification of the log file will be detected by TopSpin and in that case commented with a warning entry in the log (which is checksum protected again). This allows identifying if and when a 3rd party modification of the content has happened. Further entries then are correctly documented and secured again.

Data sets can now be protected against any further modification by adjusting the file/directory permissions (currently support for Windows operating systems only). The command **lockdataset** is available by choosing *Security / Lock Data Set Against Changes* from the menu *Manage*, or by entering **lockdataset** at TopSpin's command line.

The command applies permission changes on the current data set. Content of the EXPNO and PROCNO directories will be protected against overwrite/append/delete attempts, and the related directory objects will lose permissions to add file and subdirectories in it. Effectively, the directory will be frozen. It is however still possible to add new PROCNOs for the same raw data. This allows implementing a standard operation procedure e.g. in GxP environments like the following:

- automatically acquire and process data set
- apply electronic signature using command **esign**
- execute **lockdataset** to protect against modification
- copy processed data to a new PROCNO, e.g. with command **wrp 2** and switch to it for further processing steps, e.g. with command **rep 2**

The original results from automated acquisition and processing then are present for later inspection and protected against modifications while further interactive processing is possible. Note that the command **lockdataset** could be also used as part of AU scripts like e.g. the one defined by AUNMP.

TopSpin's Plot Editor allows interactive editing the Title and Parameter objects, including their text contents. In GxP environments this might be an undesired option. A new configuration option can be set to prevent the current user from editing such titles, parameter and other data related text blocks in a plot layout. The text blocks still can be marked by mouse click but the options for changing its contents are not offered. Editing of data ranges, scaling of spectra etc. remains available. In order to activate this restricted editing mode, the file `globals.prop` in the users' personal property directory should be edited and the following single line anywhere added:

```
GLP_RESTRICTIONS_ACTIVE=1
```

The restriction then will apply to the current user. The user's personal profile directory is located at `%HOMEDRIVE%%HOMEPATH%\.topspin-%COMPUTERNAME%\prop`. There is currently no option available to set this interactively in TopSpin.

7.5.2 Bug Fixes

The following topics describe the major fixes which come with TopSpin 3.5pl6.

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 # 13811---- Some securemail servers reject mal connection
- Item # 13806 ---- Error when using “Run an Experiment Periodically”
- Item # 13789 ---- Popt option mash does not work vor MASIII unit
- Item # 13772 ---- command **resume** yelds “Command not implemented”
- Item # 13761 ---- User groups not visible/usable within Accounting
- Item # 13752 ---- Incorrect solvent set (CDCL3) for ASTM sample in Benzene via Assure SST
- Item # 13741 ---- InsightMR: Data are always archived to *C:\ReactionMonitoring*
- item # 13733 ---- Parameter block in plot layout should list all valid electronic signatures
- item # 13731 ---- TopSpin internal login dialog should block after multiple failed login attempts
- item # 13714 ---- AU program library function manipulateShapeC buggy
- item # 13710 ---- Error notification e-mail is blank
- item # 13707 ---- **topshim** fails when coil=29Si
- item # 13695 ---- Randomize Priority function ignored
- item # 13694 ---- Remaining time display intermittent
- item # 13693 ---- Priority reset when **expt** edited
- item # 13681 ---- Installation of 3.5pl5 does not import **gradpar** from 3.5pl4
- item # 13665 ---- Routine Spectroscopy: SampleChanger Position/Manual Lock Shim setting is ignored
- item # 13660 ---- 1H/19F **atma** fails on certain configuration
- item # 13655 ---- shapetool: internal error
- item # 13654 ---- **TopShim** fails for probe type MIC
- item # 13648 ---- UPnP device (No UPnP device info available)
- item # 13628 ---- **edte**: Unable to read the ET-PH
- item # 13619 ---- Command **'st generate ...'** fails with error 'Resolution is too small'
- item # 13598 ---- **baseopt**: **zg** fails due to invalid group delay

- item # 13569 ---- **Edprobe** should recognise, if a Cryo probe has the ATMA unit connected
- item # 13513 ---- **showpp** and **nmrsim** do not work on Mac OS 10.10/10.11
- item # 13256 ---- No concentration calculation with eretic2
- item # 11364 ---- Routing of an AMP with Output router directly to the probe not implemented

7.6 TopSpin 3.5.7

7.6.1 Bug Fixes

The following topics describe the major fixes which come with TopSpin 3.5pl7.

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 # 14090 ---- Plot Editor may freeze after ‘Save as’ operation
- Item #14058 ---- **expset** for LC parameter sets changes cnst30 to 0
- Item # 14053 ---- Error message can’t reach $data(do_expt): no such variable appears
- Item # 14046 ---- CS processing with virtual echo fails for some large datasets
- Item # 14021 ---- Priority may not be set on an experiment
- Item # 14020 ---- Plot Editor fails to handle certain PNG files with indexed color model
- Item # 13988 ---- Topspin shows “String index out of range: -1” exception
- Item # 13978 ---- Originator item names not taken from spreadsheet columns
- Item # 13974 ---- Diverse File Formatting settings inoperable
- Item # 13970 ---- Error in graphical pulse program display
- Item # 13967 ---- Setting Disk column to read-only also prevents selection
- Item # 13947 ---- Helium Logfile is not written on Windows 10
- Item # 13923 ---- Restart experiment in SampleTrack mode inoperative
- Item # 13920 ---- **edc/new** shows wrong warning when creating new PROCNO
- Item # 13919 ---- Default Fallback when **popt** (or **poptau**) finds no optimum
- Item # 13903 ---- Data containing spaces is not useable in spreadsheet import
- Item # 13894 ---- JCONV not working on Windows workstations
- Item # 13884 ---- Automation Window doesn’t respond to commands
- Item # 13871 ---- Some pseudo parameters not correctly accessible via web interface
- Item # 13868 ---- Compatibility: History files not generated on-the-fly
- Item # 13867 ---- **edasp**: no green dots for cortab
- Item # 13864 ---- **cortab**: endless loop during attenuation adjustment

- Item # 13850 ---- **stdisp** gives error when started from FID or ACQU tab
- Item # 13846 ---- FastLane/SmartDrive Problems with Domain users
- Item # 13753 ---- shapetool does not allow the phase modulation with more than 16 offsets
- Item # 13643 ---- **plot** command doesn’t open Plot Editor with the requested reset actions or layout
- Item # 13624 ---- Impossible to copy/paste a MOL file using ISIS Draw 2.5 or Accelrys Draw 4.1 into the Plot Editor
- Item # 13579 ---- TopSpin 3.5pl3 doesn’t correctly copy prosol and lock tables during installation
- Item # 13180 ---- Eurotherm detects wrong temperature sensor
- Item # 12354 ---- Unable to paste mol file into plot editor

7.6.2 New Features

7.6.2.1 System Support

For Linux, Topspin can use OpenGL-based graphics mode as an alternative. On a number of systems instable graphics performance has been observed especially for the lock display. Enabling OpenGL mode can remove this effect on supported systems. The respective selection is configured in the file javaenv.sh which is located in the TopSpin installation directory. If you observe such graphics problems please enable the OpenGL mode by editing this file and removing the leading ‘#’ at the beginning of the line “GRAPHICS_OPTIONS=-Dsun.java2d.opengl=True”.

7.6.2.2 Acquisition

Use the command **topsolids** to open the interface directly from the TopSpin command line.

7.6.2.3 Automation

Designed to streamline potency/purity determination with a rapid and flexibly workflow from sample submission to report, Bruker’s new qNMR software is the ideal solution for both experts and non-experts working in a pharmaceutical development environment, where quality is a must.

The new workflow uses qNMR with an internal standard, which eliminates errors introduced by inherent sample differences. It starts by selecting *Internal Reference*, under *Analysis* ( ) in the *Experiment Table*, in IconNMR. The *Analysis* pop up window allows the user to choose an internal reference (R); introduce a new one *R^{+}* or a new batch (B) for an existing reference *B^{+}*.

Added functionality is the possibility of submitting multiple samples (in duplicate, triplicate…) to obtain the average potency. To use this option, right-click on the first qNMR experiment in the *Experiment Table* and select *Averaging / Copy settings to next* or alternatively, select n experiments (Ctrol key), *Averaging / Use selected experiments*. A default experiment *P_PROTON* is provided and highly recommended for optimal results when determining potency by NMR.

User intervention is possible at any time during the workflow either in IconNMR, TopSpin or CMC-assist (data visualization, analysis refinement and report).

Although there is no need for an extra license when working at the spectrometer, the new features require the activation of FastLane NMR in IconNMR [select *FastLane* under *Configuration / ->CMC-Verification*].

Potency determination by qNMR [1], also known as 'compound purity determination' and which results are expressed in % w/w, offers added functionality to the existing qNMR external standard based on the PULCON [2] method (also called by Bruker ERETIC II), which results are expressed in absolute compound concentration in mM.

7.6.2.4 Analysis

In TopSpin 3.5 pl7 we present a novel software tool for interactive analysis of NMR based screening data that is embedded within the software suite from Bruker, which now supports the workflow from data acquisition and processing to data analysis and hit reporting in the field of Fragment Based Lead Discovery (FBLD). The three most popular NMR experiments for fragment screening, Saturation Transfer Difference (STD), waterLOGSY, and relaxation based methods, are automatically identified. Reference 1D ^{1}H spectra of fragments are recognized by unique identifiers of the employed molecules and presented to the user in multi-display mode together with the screening spectra. Hits are visually identified and selected by mouse click on the display. The results are stored in a project file that is automatically loaded on program launch. The tool allows the most flexible implementation in individual laboratory environments with few restrictions with regard to data storage and preparation; for instance, no databases need to be prepared. In addition, automation routines for NMR based screening experiments that are part of the latest Topspin release are presented.

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

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

7.6.2.5 GxP Operation

The installation process in the "Customized" section provides the option "Central Audit Log File". Once this option has been installed TopSpin will maintain an additional log file at the location *<topspin_installation_directory>/prog/logfiles/master/CentralAudit.log*. This file fulfills the following specifications:

The file documents activities that are relevant for GxP regulated environments on a single central place

- login and logoff operations of TopSpin.
- Every entry that is added to data set audit files, i.e. copies of any data audit entry ever done by this TopSpin installation.
- If data sets (and their integrated audit files) would be removed from the disk or reprocessed, a copy of the original entries still exist in the central audit file. So, traces of operations applied to data sets cannot be undone by users.
- IconNMR will generate log entries to this central audit file as well, if user permissions are modified in IconNMR

The file is protected against manipulation

- Existing content cannot be overwritten or changed.
- File-append operations are the only operation possible. This is enforced by the operating system itself through permission management.
- Entries are protected and checked for consistency by time/date stamps and checksums

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[1] Webster G.K., Kumar S., Anal Chem., 86, 11474 (2014)

[2] Wider G. and Dreier L., J. Am. Chem. Soc., 128, 2571 (2006)

- Once existing, this file will never be deleted or replaced or reduced in size by TopSpin. Also new installations of TopSpin to the same directory cannot overwrite it.
- De-installation of TopSpin will not remove this file.

If the option in the installer has not been selected, the central log file will neither exist nor maintained.

This option is currently available for Windows systems only.

In the preferences dialog of TopSpin a new option “Enable GUI restrictions and protection of preferences” has been added. If this option is enabled for the current user the following restrictions apply:

- In Plot Editor, the options Cut/Copy/Paste/Delete/Duplicate are not available in the context menu and related operations are prohibited
- In Plot Editor, contents of Text objects and Parameter objects in layouts cannot be edited
- Access to the preferences dialog in TopSpin requires provision of the NMR Administration password. Active restrictions cannot be disabled without knowledge of this password.

This new option replaces the need to manually edit the property

GLP_RESTRICTIONS_ACTIVE as it has been described for TopSpin 3.5 pl6 (see section *GxP Operation [▸ 44]* in this document).

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