


TopSpin

- Release Letter 3.5.6
User Manual
Version 007



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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 3.5 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 3.5pl6, 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 3.5pl6 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 3.5pl6 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 3.5pl6 DVD contains the following program versions:

- TopSpin 3.5.6
- IconNMR 5.0.6
- NMRSim 6.0
- NMR Guide 4.4

The following programs are part of the TopSpin 3.5pl6 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
CMC-se comes as part of the TopSpin installation and requires a separate license.
- CMC-assist 2.5
- InsightMR™ 1.0.6 (for Windows and Linux)
- DynamicsCenter 2.4.3 (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 3.5pl6 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
("Intel Core 2 Duo" processor type or newer. Note that "Intel Core Duo" procesors used in the first Intel Macs are not running 64bit instructions.)
- Apple mouse or any 3 button or wheel mouse
- DVD device (TopSpin is delivered on DVD's with "-R" format)

2.5 Spectrometer Hardware Requirements

For upgrade possibilities of your spectrometer with TopSpin 3.5pl6, please check with your local Bruker office.

2.5.1 AVANCE III Spectrometers

DPP1	required minimum EC Level
part # H12513f1	04

BVT3000 and older VTUs are currently not fully supported by TopSpin 3.5, see Bug #13180.

2.5.2 AVANCE III HD Spectrometers

TopSpin 3.5pl6 runs on any AVANCE III HD spectrometer.

2.6 Supported Operating Systems

TopSpin 3.5pl6 on spectrometer computers is supported for:

- Windows 10 (64bit)
- Windows 7 (64 bit)
- CentOS 5 (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 3.5pl6 was released have been tested and are supported.

TopSpin 3.5pl6 on data stations is supported for:

- Windows Vista
- Windows 7
- Windows 8.1
- Windows 10
- CentOS 5
- CentOS 7 (64 bit) (Please note: The minimum required CentOS7 Version is 7.1)
- Apple Mac OS X 10.8 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 these systems for the use of TopSpin. Please note that Bruker cannot support the use of above named systems.

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, tftp-server, xinetd, dhcp, portmap, bootparamd and nfs-utils. 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 in Windows and Linux

Please note that TopSpin 3.5pl6 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 or Linux. 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 3.5pl6 program in a different directory. This will allow you to utilize and enjoy the new features without affecting your current installation.

3.2 Installation on Mac OS X

3.2.1 Installation

Please note that there is no separate installation guide available for the Mac OS X because the installation process on an Apple computer is very easy and straightforward.

Insert the DVD and use Finder to inspect its contents. TopSpin for Mac OS X comes as a DMG file that is located in the root folder of the DVD. Double click the file *TopSpin-3.5.dmg* to open it. When the DMG is opened for the very first time, Mac OS X will verify its checksum. Due to the rather large size (around 500 MB) this may take a while (usually 30s on an iMac, probably longer on MacBook or MacMini). But the verification will happen only once. It is recommended to wait and let the system finish the check. Mac OS X will then mount the disk image and automatically display a Finder window with the Release Letter and the installation package file.

Double-click the installation package and follow the instructions given on screen in order to complete the installation. The installation takes only a few minutes.

3.2.2 License Handling

3.2.2.1 TopSpin processing software is free for academia and governmental institutions only

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 special software distribution package that does not require a license file for operation. It is available from the Bruker website at the following address:

<https://www.bruker.com/nc/service/support-upgrades/software-downloads/nmr/free-topspin-processing/download-page.html>

Note that the distribution package provided by DVD and at the standard download location requires a license file for operation. The download and use of the free software for commercial organizations or companies is prohibited.

3.2.2.2 Getting the License

Once the installation has finished successfully, use Finder and go to Applications. You will find the TopSpin icon there. For your convenience you may want to draw this icon also to the dock.

Double-clicking the TopSpin icon will start TopSpin. At first start a message will notify you about the hostid of this machine and a missing license file.

Use to the hostid displayed here for your license request. If you are connected to the internet you may press the button "Go to web page" which gets you directly to the license request forms at Bruker web site. Or contact Bruker license department by email with your details.

3.2.2.3 Installing the License

Once you have received the e-mail with the license file attached, save the attachment to a location of your choice (e.g. the Mac OS desktop). Now use Finder and open "TopSpin Utilities" in Applications. Double-click on "Install License". You are asked to locate the license file. The license gets installed automatically then and no further user action is required.

Double click the TopSpin icon again. TopSpin now should start normally.

3.2.2.4 Differences in License Handling in Mac OS X

For use of TopSpin on a Mac only node-locked licenses are available, i.e. a license is bound to a particular Mac computer (but not to a particular user). Floating licenses are currently not available for TopSpin on a Mac.

Please note that license files used on Mac OS X installations are different from those used on other platforms. License files issued for a Mac cannot be used on Windows/Linux systems and vice versa.

3.2.3 Differences of the Mac Version Compared to Other Platforms

In accordance to the guidelines for Mac applications, no target directory can be chosen during the installation. Unlike on other platforms, a parallel installation of several TopSpin instances is not supported. Installation is possible only on the root volume.

TopSpin on Mac OS X is a processing-only installation. Support for NUS (non-uniform sampling) data is fully implemented and available. NMRsim and the full NMR Guide are available as well.

There is no acquisition support, nor IconNMR present.

Example Data Sets

On Mac OS X, the TopSpin installer currently installs a subset of the full example data sets only. If required, you can find the full set on the TopSpin DVD in the following file:

```
/noarch/pack/nmrdata.tar.xz
```

Use a Finder window to navigate to the sub folder *mac/bin* of the DVD and double-click *nmrdata-extract*. This opens a window and asks for a folder where to extract the data. The program *nmrdata-extract* can alternatively be run in a terminal.

3.2.4 TopSpin Utilities

Completing the installation, the "Applications" folder contains the TopSpin icon as well as a separate folder "TopSpin Utilities". You can find the following tools there:

- "Install License": used to install the license file as already described above
- "SaveLogs": used to collect log files and more required information for support incidents
- "Terminate TopSpin": in case TopSpin does not start as expected, components of the application may not have been terminated correctly from the last session and may still be active in memory. Use this tool to stop all running components. TopSpin should start normally after that.
- "Uninstall TopSpin": this tool will remove the TopSpin installation from your harddisk. Use this only if you want to delete TopSpin completely. Security questions will protect you from an unintentional use.

3.2.5 Additional Notes

During the release testing it has been observed that the presence of at least one virus scanning tool for Mac OS X may delay the start of TopSpin significantly (up to a couple of minutes). If you notice similar behavior we recommend to temporarily disable the virus scanner. TopSpin should start very fast then.

When starting TopSpin for the first time, the firewall of Mac OS may ask whether you want to allow or deny "access to cprclient". This request is displayed only once and we suggest to choose "Deny". (The installation procedure cannot do that automatically for you.)

3.3 Using a Previous Configuration (TopSpin)

TopSpin 3.5pl6 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.

3.4 Compatibility with TopSpin 3.0 and Earlier

Data sets that have been opened or modified with TopSpin 3.1 or newer will lose some acquisition parameters. These data sets may not be usable in TopSpin 3.0 and earlier versions.

The format of the acquisition parameter files has been changed with respect to the parameters CPDPRG1..8, GPNAM0..63 and SPNAM0..63, which have been converted from single to array parameters CPD-PRG[1..8], GPNAM[0..63], and SPNAM[0..63], respectively.

Parameter files generated with previous versions will automatically be converted to the new format when modified within the new version. The modified files are no longer usable in the older versions.

AU programs which use the parameters need not be modified and can use the old syntax:

```
STOREPAR ("SPNAM15", "gauss1.100");
```

as well as the new one:

```
STOREPAR ("SPNAM 15", "gauss1.100");
```

4 Bug Fixes

The following topics describe the major fixes which come with TopSpin 3.5p16.

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** yields "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 3.5p15 does not import **gradpar** from 3.5p14
- 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

Bug Fixes

- item # 13256 ---- No concentration calculation with eretic2
- item # 11364 ---- Routing of an AMP with Output router directly to the probe not implemented

5 New Features

5.1 Acquisition

5.1.1 TopSolids 2.0

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)

5.1.2 Introduction of WaveMaker (wvm)

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**.

5.1.3 New Python Script cypars

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

The utility **cypars** 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 **cypars** 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.

5.1.4 New package for working with Biological Samples - BioTop

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.

5.2 Processing

5.2.1 New command lockdataset available

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 GLP 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*

5.2.2 Mdd_mod CS processing now available for 4D NUS data

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.

5.3 Automation

5.3.1 CMC-Verification

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

5.3.2 AssureSST

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"

5.3.3 IconNMR Web Interface

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

5.3.4 Spreadsheet Import

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

5.3.5 Accounting

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

5.3.6 Dynamics Center 2.4.3

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.

5.4 General User Interface

5.4.1 NMRSim - New User Interface For NMRSim

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:

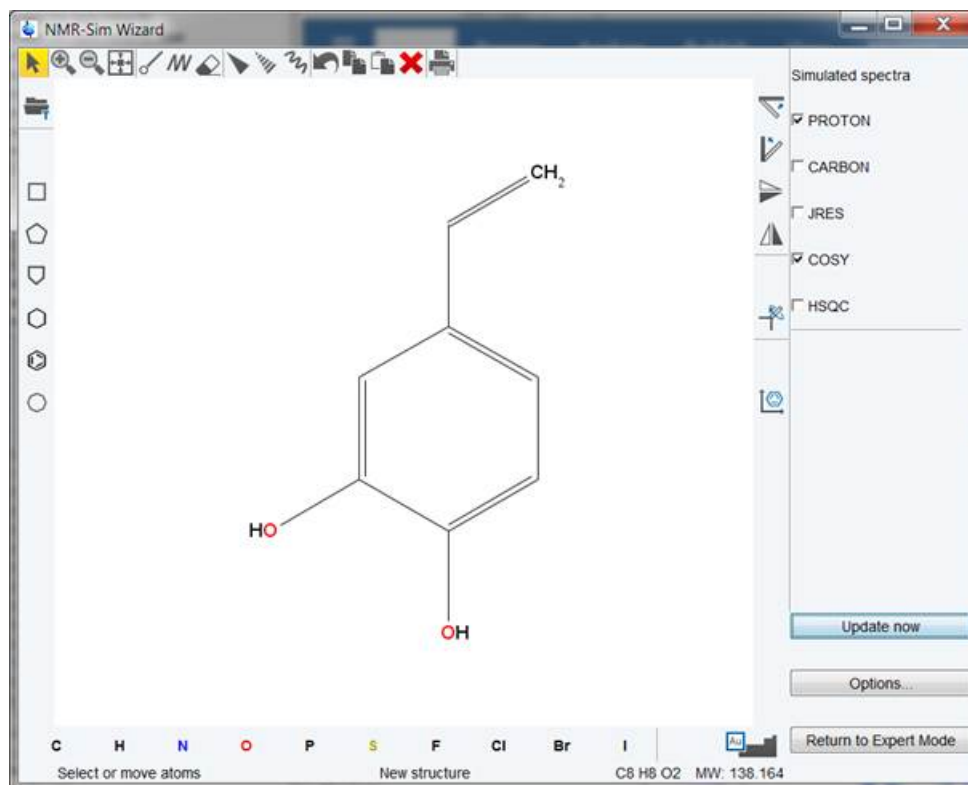


Figure 5.1: NMRwizard window

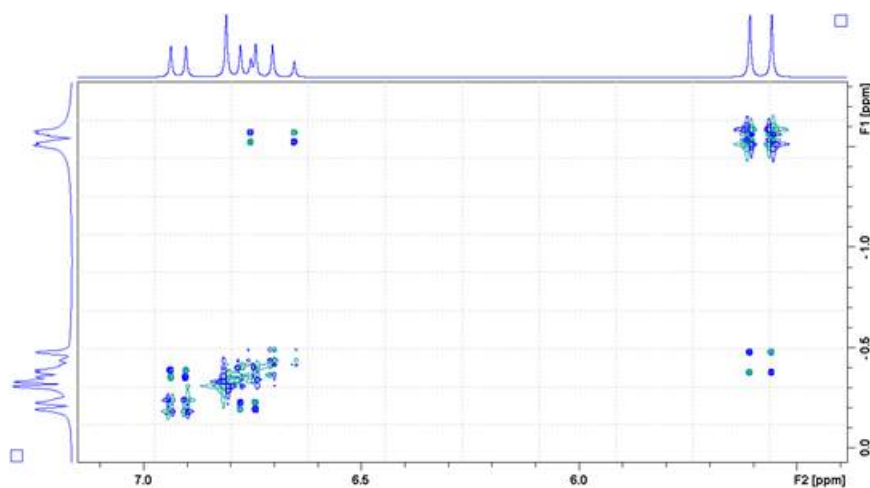
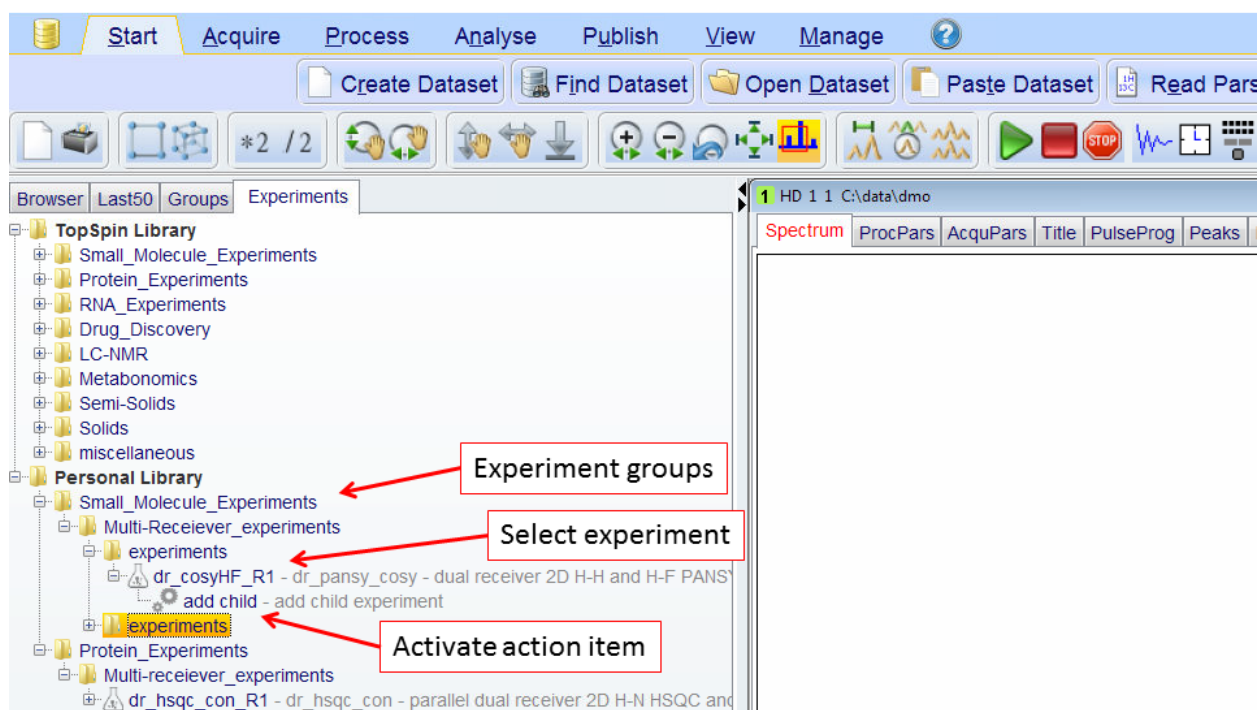


Figure 5.2: Simulate COSY spectrum

5.4.2 New interactive tool "Experiment Selector"

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

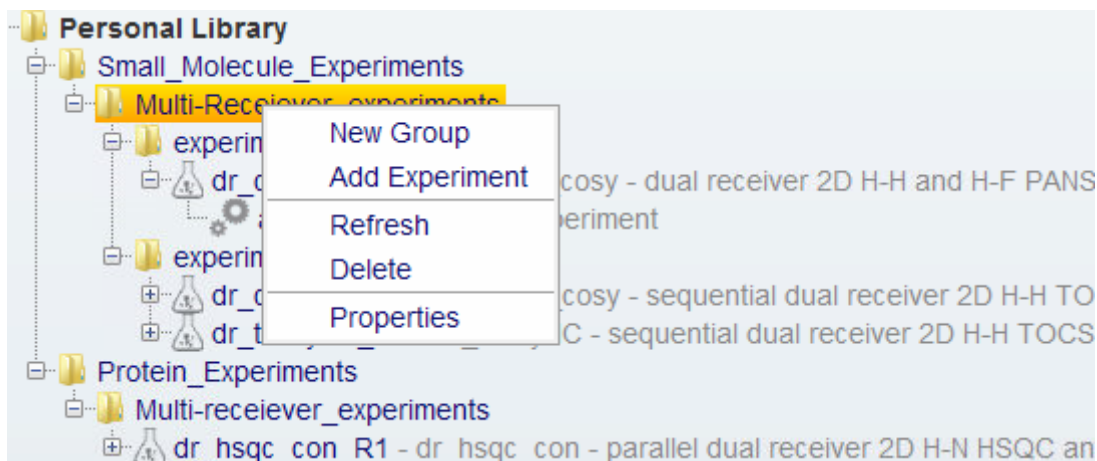
access to the user libraries, only to the standard TopSpin experiment libraries. However, the potential and functionality of the Experiment Selector is set to expand and improve in the future releases of the TopSpin making it an important and valuable tool for the TopSpin users.



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:



5.5 GLP Operation

5.5.1 Login Auditing

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 (GLP) 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.

5.5.2 Data Set Protection

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 GLP 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.

5.5.3 Restrictions in Plot Editor

TopSpin's Plot Editor allows interactive editing the Title and Parameter objects, including their text contents. In GLP 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.

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
	no restrictions
Demo	Acquisition, Processing, Automation (IconNMR), Plotting, Simulation and NMR-GUIDE
	run of validity: 3 months
	node locked, uncounted, free of charge
Processing-Only	Processing and Plotting
	run of validity: 15 years
	no restrictions
Student and Academia	Processing, Plotting, Simulation and NMR Guide
	run of validity: unlimited. Current special download version is free until March 31, 2017 and will be updated again with free version.
	Node locked

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 special software distribution package that does not require a license file for operation. It is available from the Bruker website at the following address:

<https://www.bruker.com/nc/service/support-upgrades/software-downloads/nmr/free-topspin-processing/download-page.html>

Note that the distribution package provided by DVD and at the standard download location requires a license file for operation. The download and use of the free software for commercial organizations or companies is prohibited.

7 History of Changes

7.1 TopSpin 3.5

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* and the file *conf/instr/probehead* by email to nmr-support@bruker.de 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™ 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, N₂ 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 **gs** 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™/SampleJet™ 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.

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 3.5p1

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 3.5pl2

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(vtuseftune", 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 otherwise **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.

7.4 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 ---- $^1\text{H}\{19\}$ 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_swilps0: 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>

History of Changes

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.

8 Contact

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NMR Hotlines

Contact our NMR service centers.

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