

IconNMR (>TopSpin 3.0)



Dr. Sven Augner
Bruker BioSpin, Rheinstetten, Germany





How to start an IconNMR set

IconNMR

Select the respective holder



IconNMR: Automation Mar09-2014-1610-BRUKER-augn

File Run Holder View Find Parameters Options Tools Help

Start [Icons] i

Experiment Table

Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
▶ 1		Available											
▶ 2		Available											
▶ 3		Available											
▶ 4		Available											
▶ 5		Available											
▶ 6		Available											
▶ 7		Available											
▶ 8		Available											
▶ 9		Available											

2x

Submit Cancel Edit Delete Add 1 Copy 1 Change User

Preceding Experiments

Search Preceding include previous runs

SampleXpress Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: BRUKER\augn

IconNMR

Select the disk



The screenshot shows the IconNMR software interface. The 'Experiment Table' is visible with columns: Hol..., Type, Status, Disk, Name, No., Solvent, Experiment, Pri, Par. Row 1 is highlighted, showing '1 Available' in the Status column and 'C:\' in the Disk column. A yellow box highlights the 'Disk' column header and the 'C:\' entry. A red arrow points from this area to a callout box. A mouse cursor is also present near the callout.

Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par
1	1	Available	C:\						
2		Available							
3		Available							
4		Available							
5		Available							
6		Available							

Callout Box:

Disk	Name	No.
C:\		

Selected Path: C:\Bruker\TopSpin3.2p15

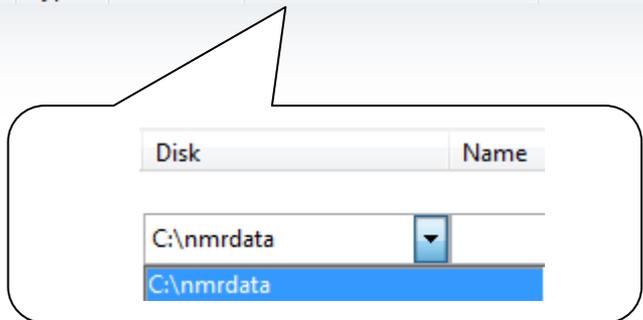
- Base directory for data storage
- Drop down list, can be edited.
- Setup: → IconNMR Configuration → User Manager (if no directory is entered in the configuration box the data will be stored under <topspinhome>/data)

The 'Data Directories' window is shown, which is currently empty. It features a toolbar with icons for adding (+), removing (-), creating a new directory (folder), and editing (pencil).

IconNMR Disk options



Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------



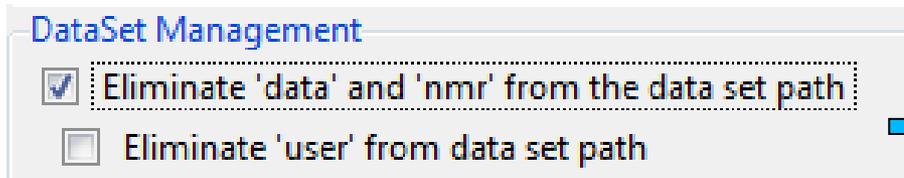
Resulting data path

TopSpin < 3.0:

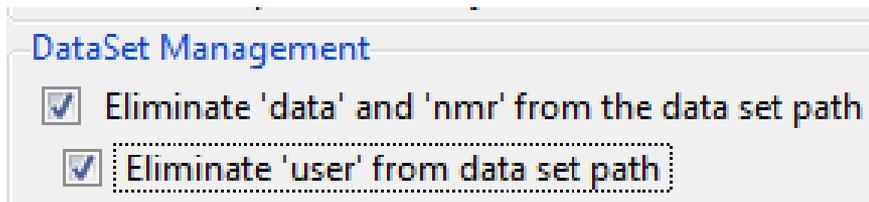
C:\nmrdata\data\user\nmr\name

IconNMR configuration: “Master Switches”:

TopSpin ≥ 3.0:



C:\nmrdata\user\name



C:\nmrdata\name

IconNMR Name



Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------

Callout box showing a dropdown menu for the 'Name' column. The menu is open, showing a list of pre-defined names:

- Mar09-2014
- Mar09-2014-BRUKERaugn
- 03092014
- 1-09-03-BRUKERaugn
- 09032014-BRUKERaugn

Configuration options:

Free entry of "Name" for an user if "Data Set Name Edit" is enabled.

Pre-defined names can be defined in the User manager.

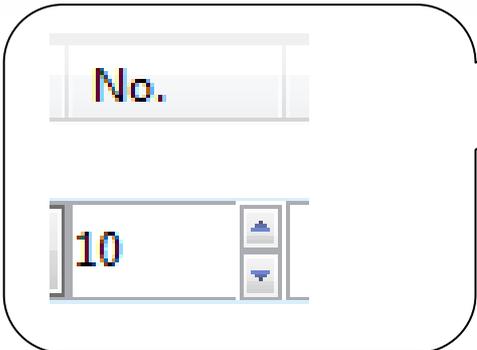
Data Set Names

- ↑ \$DATE
- ↓ \$DATEUSER
- ↓ \$NUMERICDATE
- 📄 \$HOLDER-%d-%m-\$data(UserN: %d%m%Y-\$data(Username)
- ✎



IconNMR Experiment Number

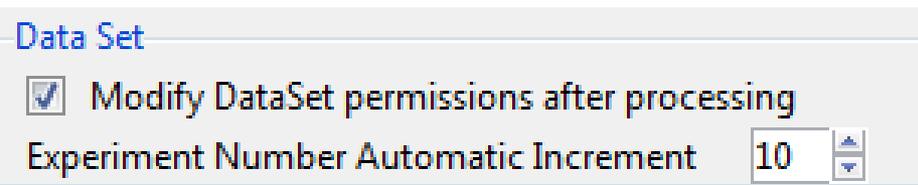
Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------



The experiment number of the dataset

Historical idea:
Samples numbered with increment 10
Experiments within each sample get increments of one.

Configuration:
General options: Experiment number
Automatic Increment





IconNMR Solvent

Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------

Solvent	Experiment	Pri	Par	Title/Orig
Acetic	acetic acid-d4			
Acetone	acetone-d6			
C6D6	benzene-d6			
CD2C12	methylenchloride-d2			
CD3CN	acetonitrile-d3			
CD3CN_SPE	LC-SPE Solvent (Acetonitrile)			
CDC13	chloroform-d			
CH3CN+D2O	HPLC Solvent (Acetonitril/D2O)			
CH3OH+D2O	HPLC Solvent (Methanol/D2O)			
D2O	deuteriumoxide			

Solvent list will be created based on the information entered in TopSpin (edsolv / edlock).

Additional Option: "Automation Window"

Default Solvents and Experiments

Default Solvent: CDC13 chloroform-d

Default Experiment: PROTON

Specify the most used solvent as default solvent

IconNMR Experiment



Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------

Experiment	Pri	Par	Title/Orig
<div style="display: flex; align-items: center;"> ▼ ☐ Application </div>			
N PROTON			1H experiment
N C13CPD			13C experiment; 1024 scans
N C13DEPT135			DEPT 135 experiment; 256 scans
N WATERSUP			1H with water suppression
C COSYGPSW			Gradient selected COSY
C COSYGPDPHPSW			Gradient selected double quantu
C HMBCGP			1H-13C HMBC with gradient selec
C HMBCETGPL3ND			1H-13C HMBC with gradient selec
C HMBCGP_15N			1H-15N HMBC with gradient selec
C HSQC_TOCSY_ADIA			1H-13C HSQC-TOCSY with gradient

This list will be defined in the User Manger.

This list based on the parameter sets (available via "rpar") in TopSpin or the "Composite Experiment" (marked with the leading "C") in IconNMR.

Additional Option: "Automation Window"

Default Solvents and Experiments

Default Solvent: CDC13 chloroform-d

Default Experiment: PROTON

Specify the most used experiment as default experiment

IconNMR Priority

Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------

I want my sample measured a.s.a.p during daytime (sun)

No hurry, please measure during nighttime (moon)

Configuration: many options.

User dependent:

Night-Time Experimente

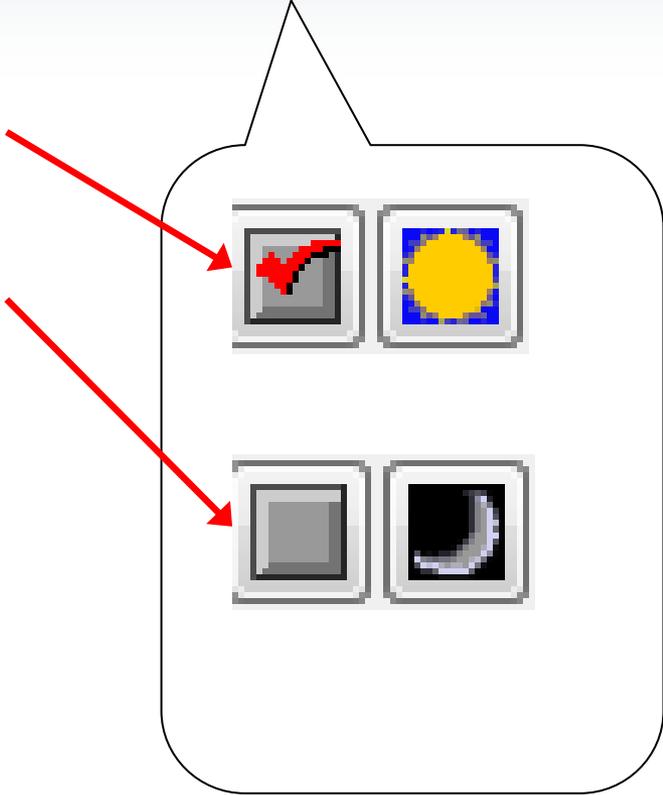
Global:

„Priority on/off, day/night“

Definition of night and weekend

„Night time experiments during daytime when idle“

„First come/First served“ or ...



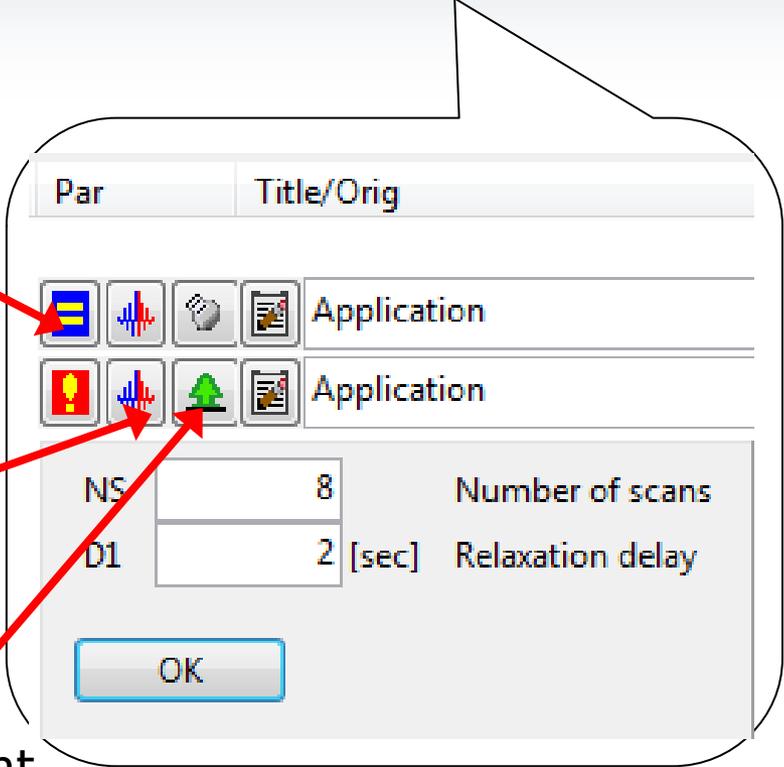
IconNMR Parameters

Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------

A simple parameter editor. Each user can have his own set of parameters

Change lock/shim/ATM parameters per sample. Should be enabled for the user

Produce paper or environment-friendly
Icon-nmr helps to protect the environment



Par	Title/Orig
   	Application
   	Application
NS	8 Number of scans
D1	2 [sec] Relaxation delay

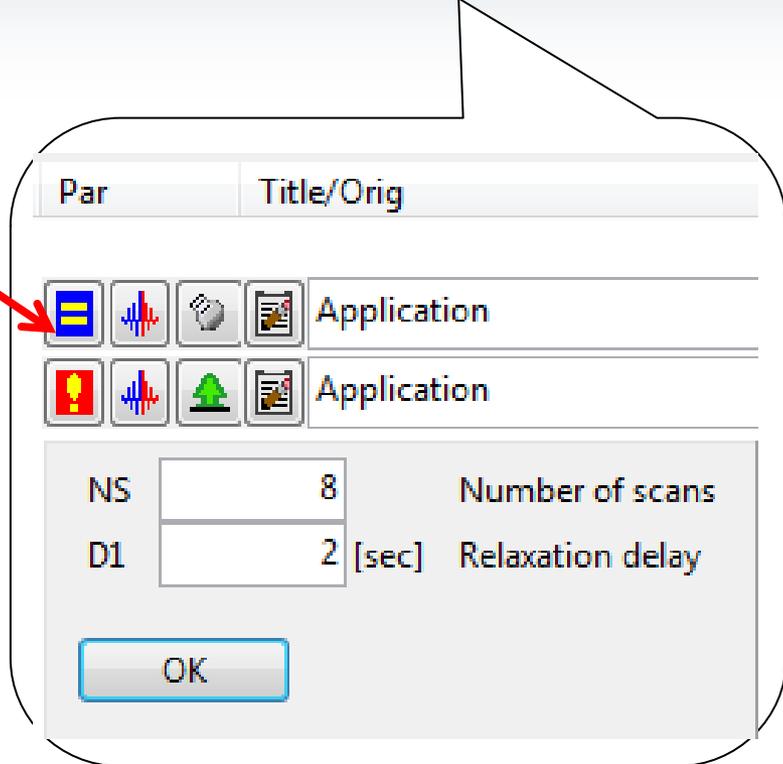
OK

IconNMR Parameters

Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------

This tiny parameter editor is called in the configuration:
User specific Parameters/**Commands**

User Specific Parameters/Commands		
↑	ns	Number of scans
	d1	Relaxation delay
↓	xpy SetupQuant	Setup quantitative analysis for produ



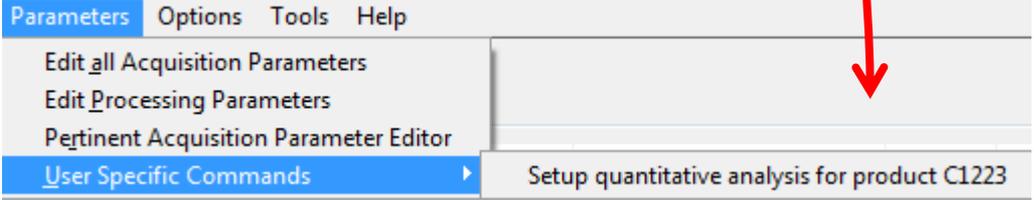
A dialog box titled 'User Specific Parameters/Commands' with a table and input fields. The table has columns 'Par' and 'Title/Orig'. It contains two rows of icons and text. Below the table are input fields for 'NS' (value 8) and 'D1' (value 2 [sec]). An 'OK' button is at the bottom.

Par	Title/Orig
[Equal sign icon]	Application
[Warning icon]	Application

NS Number of scans
D1 [sec] Relaxation delay

OK

And look into the Parameters menu:
of the setup window.



A menu titled 'Parameters' with several options. The 'User Specific Commands' option is highlighted and has a submenu open showing 'Setup quantitative analysis for product C1223'.

- Edit all Acquisition Parameters
- Edit Processing Parameters
- Pertinent Acquisition Parameter Editor
- User Specific Commands**
 - Setup quantitative analysis for product C1223

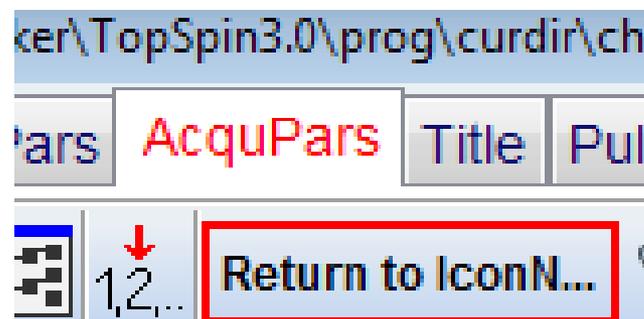
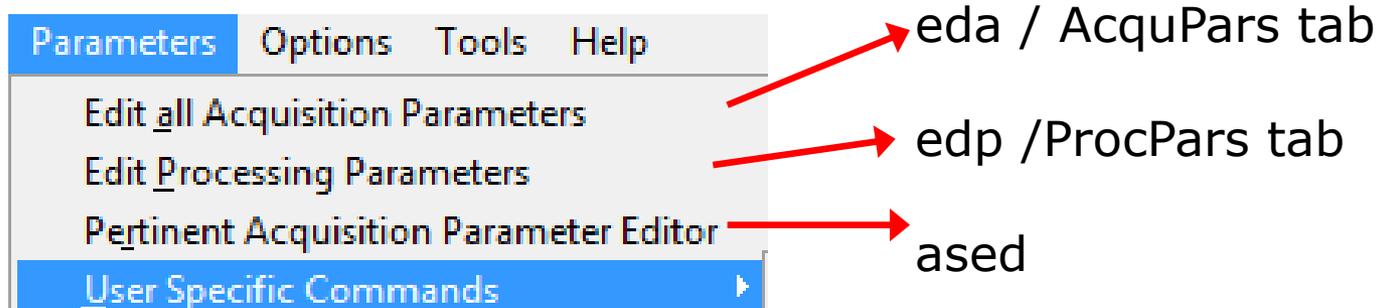
So: execute arbitrary procedures on the dataset

IconNMR Parameters



Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------

With the option: "Parameter Edit" switched on:



Use "Return to IconNMR" to go back from the TopSpin Parameter editor to IconNMR

IconNMR Title/Orig



Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------

Title / Originator Info

The screenshot shows a dialog box titled "Title / Originator Info". At the top, there is a table with columns: "Title/Orig", "Time", "User", and "St". Below the table is a text input field with a pencil icon on the left and a "BRUKER" label on the right. Underneath the input field is a large empty text area with a vertical scrollbar on the right. At the bottom of the dialog, there are two buttons: "Set Title" and "Set & Copy Title". A callout line from the "Title/Orig" column of the table above points to the dialog box.

IconNMR Start time



Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------

TopSpin \geq 3.0:

Start time for experiments

A screenshot of the Bruker software interface. The main window shows a table with columns for 'User' and 'Start Time'. A row is highlighted in light blue, containing the text 'BRUKER' and a button labeled 'Set Start Time' with a clock icon. A tooltip box is overlaid on the button, containing the text 'Select the time at which the experiment should run'.

User	Start Time
BRUKER	

Select the time at which the experiment should run

IconNMR Set up experiment



IconNMR: Automation Mar09-2014-1610-BRUKER-augn

File Run Holder View Find Parameters Options Tools Help

1 2 3 4 5 6 7

H...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	Available	Available	C:\Bruker\TopSpin3.2p15	Mar09-2014	10	benzene-d6	1H experiment			Sample 123		BRUKER	18:09 Sun
2	Available	Available											
3	Available	Available											
4	Available	Available											

Submit Cancel Edit Delete Add 1 Copy 1 Change User

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title/Orig
---	------	--------	------	-----	------------	------	-----	----------	------	------	-----	------	------	------	------------

Search
Preceding include previous runs

SampleXpress Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: BRUKER\augn

IconNMR

Set up experiment



IconNMR: Automation Mar09-2014-1610-BRUKER-augn

File Edit View Options Tools Help

9 - Only once to start the run

Start

Experiment Table

H...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	←	1Queued											
1	←	Queued	C:\Bruker\TopSpin3.2p15	Mar09-2014	10	C6D6	ben N PROTON	1H		Sample 123	00:01:5	BRUKER	18:09 Sun Ma
2		Available											
3		Available											
4		Available											

8

Submit Cancel Edit Delete Add 1 Copy 1 Change User

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title/Orig
---	------	--------	------	-----	------------	------	-----	----------	------	------	-----	------	------	------	------------

Search Preceding include previous runs

SampleXpress Busy until: Sun 18:39 Day Experiments: 00:01 Night Experiments: 00:00 User: BRUKER\augn



A journey through IconNMR

A journey through IconNMR

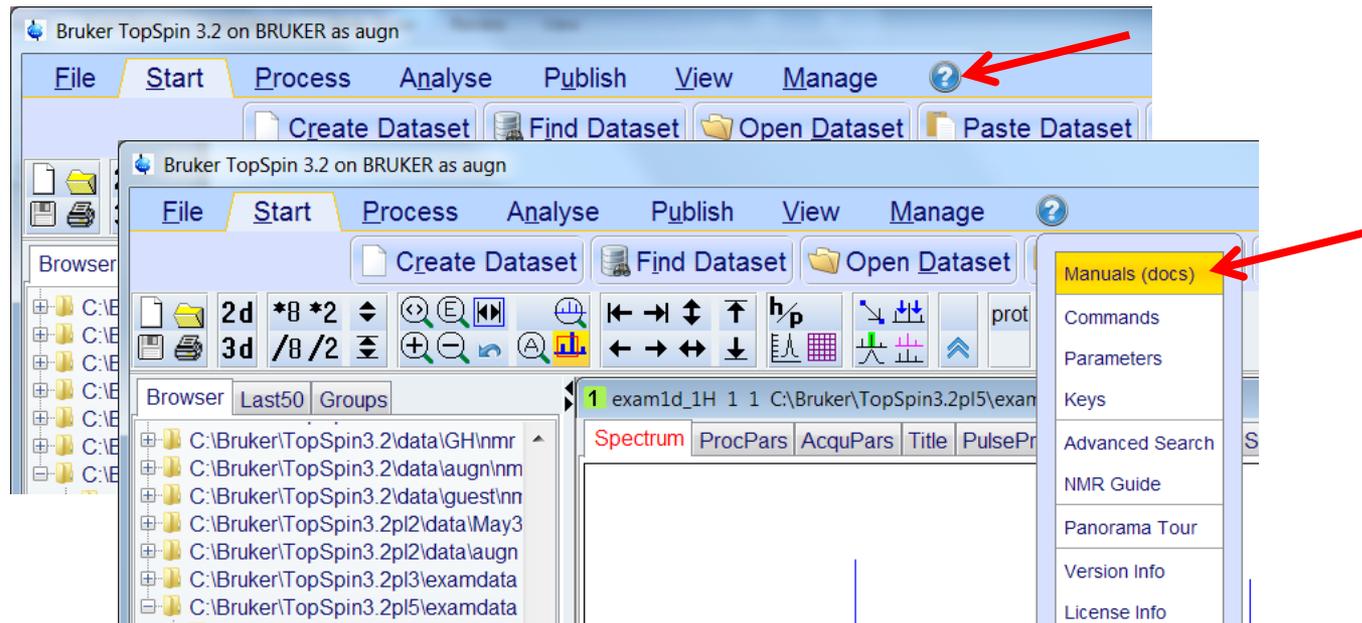


- The development of IconNMR has been started 1995.
- In 1996 the first customers starts working with IconNMR.
- This course deals with new features in IconNMR (starting with TopSpin 3.0).
Therefore this new features will be available for AVANCE II, AVANCE III, AVANCE III HD and Fourier 300 Spectrometer.
- 49 new features.

Where do I find information what's new in IconNMR?

Where do I find information what's new in IconNMR?

- „?“-button, hot key <Alt-h> or TopSpin-command docs



Where do I find information what's new in IconNMR?



Where do I find information what's new in IconNMR?

- „?“-button, hot key <Alt-h> or TopSpin-command docs

The screenshot shows the Bruker TopSpin 3.2 software interface. The menu bar includes File, Start, Process, Analyse, Publish, View, and Manage. A red arrow points to a question mark icon in the menu bar. A dialog box titled 'Software And Application Manuals' is open, displaying a list of manuals on the left and their descriptions on the right. The 'Automation and Plotting' section is highlighted with a green box. The dialog box also includes a 'Close this dialog when a manual is opened' checkbox and buttons for 'Multi-Doc Search', 'Books', and 'Close'.

Manual Title	Description
Acqu. Commands & Parameters	A description of all acquisition and acquisition related commands and parameters.
Proc. Commands & Parameters	A description of all processing and analysis commands and parameters.
Edprosol Manual	How to set up probe and solvent dependent parameters
Edlock Guide	A description of how to setup solvent and lock dependent parameters.
Pulse Program Catalogue, 1D/2D	A graphical presentation of the Bruker supplied pulse programs, 1D and 2D experiments.
Pulse Program Catalogue, BIO	A graphical presentation of the Bruker supplied pulse programs, biomolecular experiments.
NUS Parameters	A description of the parameter setup for Non Uniform Sampling
Automation and Plotting	
ICON-NMR Automation Interface	A description of the Icon driven interface for routine spectroscopy, automation, accounting and BEST-NMR.
Plotting	A description of creating and manipulating plots, interactively and in automation.
Analysis and Simulation	
Structure Analysis Tools	Describes structure analysis utilities such as Multiplet Analysis, Structure Editor/Viewer, Solids Line Shape Analysis
NMR-SIM Experiment Simulator	A description of the simulation of NMR experiments (1D/2D/3D FIDs) based on pulse sequence and Spin systems
Daisy	A description of the simulation of NMR spectra based on chemical shifts and coupling constants.
DNMR	A description of Dynamic NMR Line Shape Analysis to study slow nuclear exchange processes including conformational exchange
Structure Elucidation	Introduction into Small Molecule Structure Elucidation with TopSpin
Multiplet Analysis Tutorial	How to use the first order multiplet analysis tools

Where do I find information what's new in IconNMR?



The screenshot shows the Adobe Reader interface. On the left, the 'Lesezeichen' (Bookmarks) pane displays a table of contents for the document 'all.pdf'. The entry '1.2 What's new in IconNMR 4.7' is highlighted with a red rectangle. The main window displays page 2 of the document, titled 'Introduction'. The section '1.2 What's new in IconNMR 4.7' is also highlighted with a red rectangle. The text under this section states: 'IconNMR 4.7 is part and parcel of TopSpin 3.2 which is based on the TopSpin 3.1 backbone. For this reason, only minor modifications are contained within this version. Standby for a multitude of useful new features in an upcoming release!'. Below this, there are three sub-sections: 'New Features:', 'iPad Support', and 'CMC-Assist / Fast Lane Improvements'. Each of these sub-sections contains a list of bullet points, all of which are enclosed in a red rounded rectangle.

1.2 What's new in IconNMR 4.7

IconNMR 4.7 is part and parcel of TopSpin 3.2 which is based on the TopSpin 3.1 backbone. For this reason, only minor modifications are contained within this version. Standby for a multitude of useful new features in an upcoming release!

New Features:

- Take initial Title from Parameter set. Set this in General Options to always have the title initially taken from the parameter set.
- Access to different Linux Themes directly from IconNMR. Change the appearance of the program from the general options page. Note: Under Microsoft windows theme control is available from the Desktop->Personalize menu.

iPad Support

Web IconNMR interface now updated to handle the iPad. Login to the Web IconNMR Automation interface from your iPad and add an WebApp Icon to your Home Screen for easy optimized access to all your NMR measurements.

CMC-Assist / Fast Lane Improvements

- Known Impurities may be added to the CMC-PROTON setup experiment definition for improved Analysis results. Click on the "IMP" button under "Structure/Processing"
- Access to the CMC-Assist viewer directly from IconNMR's Preceding Experiments window. Right click on the experiment or set the standard action to CMC-Viewer in configuration.
- Access to CMC Fast lane Reports via IconNMR's web interface and Preceding

A selection of new features in TopSpin 3.0



TopSpin 3.0

IconNMR 4.5

28 new features

- **Start time may be set individually on experiments**

The time at which an experiment should start may be set. The system will modify the order of the run queue such that the experiment may be run at the set time. If it is not possible for the instrument to run the experiment at the time (due to another experiment already in progress or running at a set time with too long a duration), the setup table will show the time the experiment is expected to run.

- **Experiment Quotas**

Time quotas of experiments for users limiting total experiment time and maximum individual experiment time. Users can be allotted a maximum total time for their day or night experiments on a daily basis. Submission of individual experiments which exceed a maximum time will be prohibited.

- **Data set path now fully flexible**

For any standard Bruker data set path, the data/<user>/nmr may be completely/partially (only data & nmr) removed.

- **User Manager**

Users may be separated into groups for easier copying of settings to multiple users.

Start time for experiments



Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------	------	------	------------

A callout box with a white background and a black border, pointing to the 'Set Start Time' button in the table above. Inside the callout, there is a smaller table with two columns: 'User' and 'Start Time'. Below this, the text 'BRUKER' is followed by a blue button with a clock icon and the text 'Set Start Time'. A yellow mouse cursor with a red starburst effect is pointing at the button. Below the button is a yellow-bordered text box containing the instruction: 'Select the time at which the experiment should run'.

Time limit



In the **User Manager** a user-specific time limit can be defined.

If there are to “many” ^{13}C -NMR-measurements on your system...
→ Use ^{13}C -NMR-experiments with S/N-option!

Day Time Limit 01:00 Night Time Limit 02:30 Max. Duration of a daytime experiment 00:30

Day Time Limit 01:00 Night Time Limit 02:30 Max. Duration of a daytime experiment 00:30

IconNMR – time limit



IconNMR: Automation Nov01-2013-1721-BRUKER-augn

File Run Holder View Find Parameters Options Tools Help

Start [Pause] [Stop] [Info]

Experiment Table

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Pr	Par	Title/Orig	Time	User	Start Time
1	[Red Arrow]	1Queued											
	[Red Arrow]	Queued	C:\nmrdata								00:01:07	BRUKER	17:48 Fri Nov 01 2013
2	[Red Arrow]	1Available											
	[Red Arrow]	Available	C:\nmrdata	UKERaugn	20	acetone-d6	experiment			Sample 1743	00:01:07	BRUKER	17:49 Fri Nov 01 2013
3	[Blue Arrow]	Available											
4	[Blue Arrow]	Available											
5	[Blue Arrow]	Available											
6	[Blue Arrow]	Available											
7	[Blue Arrow]	Available											
8	[Blue Arrow]	Available											
9	[Blue Arrow]	Available											
10	[Blue Arrow]	Available											
11	[Blue Arrow]	Available											
12	[Blue Arrow]	Available											
13	[Blue Arrow]	Available											
14	[Blue Arrow]	Available											
15	[Blue Arrow]	Available											
16	[Blue Arrow]	Available											

[Submit] [Cancel]

IconNMR

This experiment exceeds the permitted time!
Try submitting it as a night experiment

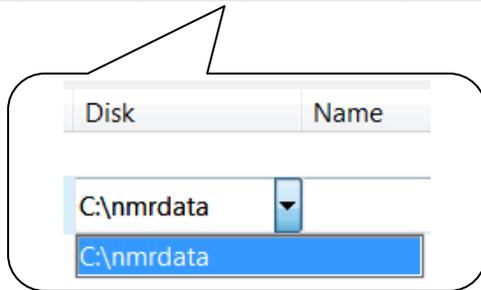
OK

Note: A mouse cursor is pointing to the Submit button in the background interface.

Data set management

TopSpin 3.0

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
--------	------	--------	------	------	-----	---------	------------	-----	-----	------------	------	------	------------



resulting data path:

TopSpin < 3.0:

C:\nmrdata\data\user\nmr\name

TopSpin ≥ 3.0:

IconNMR configuration: “Master Switches”:

DataSet Management

Eliminate 'data' and 'nmr' from the data set path



C:\nmrdata\user\name

Eliminate 'user' from data set path

DataSet Management

Eliminate 'data' and 'nmr' from the data set path



C:\nmrdata\name

Eliminate 'user' from data set path

Group names



Show/Hide Group names

Group users together for convenient copying to users in the same group. Click on the User's Group header in any user list to sort the list accordingly

User ID	User's Full Name
Administrator	Administrator
Guest	Guest
bob	bob
disk	disk
edv-	edv-
robin	robin
susan	susan
sven	sven
SamTrack	Sample Track Default User

Experiment List

Mode	Name	Experiment Comment
↑	NMRBTON	1H experiment

Experiment List

Mode	Name
●	C COSYGPSV
●	C HSQCEDE
●	C HMBCGPM

Other Settings

Spectrum Number File name: Archiving Directory:

Target E-mail Address: Umask: rw-rw-r-- User: f NmrUser: f Everyone: r

Day Time Limit: 2:00 Night Time Limit: 4:00 Max. Duration of a daytime experiment: 1:00

Commands

Save Default Delete Update Experiment List

Group names



The screenshot displays the 'IconNMR: Configuration' window. The 'Users' section is highlighted with a red box, showing a list of users and their groups. The 'Current User' field is set to 'susan' and the 'Group' dropdown is set to 'PC'. A blue callout box contains the text: 'User can be allocated convenient to groups.'

User ID	User's Group	User's Full Name
Administrator		Administrator
Guest		Guest
bob	OC	bob
diskless_user_sys		diskless_user_sys
edv-admin		edv-admin
robin	OC	robin
susan	PC	susan
sven	PC	sven
SamTrack		Sample Track Default User

Current User: susan Group: PC

Group names



The user configuration is more convenient and quicken.

User ID	User's Group	User's Full Name
Administrator		
Guest		
bob	OC	bob
diskless_user_sys		diskless_user_sys
edv-admin		edv-admin
robin	OC	robin
susan	PC	susan
sven	PC	sven
SamTrack		Sample Track Default User

- Permissions**
- | | |
|--|--|
| <input checked="" type="checkbox"/> Priority | <input checked="" type="checkbox"/> Parameter Edit |
| <input type="checkbox"/> Archive Data | <input checked="" type="checkbox"/> Exit (IconNMR) |
| <input checked="" type="checkbox"/> Supervisor | <input checked="" type="checkbox"/> Data Set Name Edit |
| <input type="checkbox"/> Essential Originator | <input checked="" type="checkbox"/> Originator |
| <input checked="" type="checkbox"/> Manual Lock/Shim | <input checked="" type="checkbox"/> Mail Spectrum PDF/PS |
| <input type="checkbox"/> E-mail Notification | <input type="checkbox"/> JDX DataMail |
| <input type="checkbox"/> JDX Copy | <input type="checkbox"/> Edit Lock/Shim/ATM |
| <input type="checkbox"/> ZIP Copy | <input type="checkbox"/> ZIP DataMail |
| <input type="checkbox"/> Print Spectrum | <input checked="" type="checkbox"/> Control Printing |

- Data Set Names**
- \$DATE
 - \$DATEUSER
 - \$NUMERICDATE
 - \$HOLDER-%d-%m-\$data(UserName)
 - %d%m%Y-\$data(UserName)
- User Specific Originator Info**
- Institute :
 - Project-No

- Data Directories**
- C:\Bruker\nmrdata
- User Specific Parameters/Commands**
- | | |
|------|-----------------------------|
| td | Size of fid |
| ns | Number of scans |
| p1 | Pulse |
| plw1 | Power level in Watt |
| te | Required Sample temperature |

Other Settings

Spectrum Number File name: _____ Archiving Directory: _____

Target E-mail Address: _____ Umask: rw-rw-r-- User:f NmrUser:f Everyone:r

Day Time Limit 2:00 Night Time Limit 4:00 Max. Duration of a daytime experiment 1:00

Commands

Save Default Delete Update Experiment List

IconNMR: Configuration

File Help

- User Settings
 - User Manager
 - Composite Experiments
 - Additional Users
 - Originator Items
- Automation
 - Master Switches
 - Automation Window
 - Lock/Shim Options
 - Solvent/Probe Dependencies
 - Tuning/Matching
 - Priority
 - Temperature Handling
 - LC-NMR Options
 - SampleTrack Options
 - Fail Safe / Error Handling
 - Web Interface
- General Options
- 'Assure'
- ToolBox Setup
- Accounting

Search

Group names



Entry Box

Originator Item: Project-No

Originator Value: [Empty]

Buttons: Append, Modify, Delete, Update User Files, Close

Permissions

<input checked="" type="checkbox"/> Priority	<input checked="" type="checkbox"/> Parameter Edit
<input type="checkbox"/> Archive Data	<input checked="" type="checkbox"/> Exit (IconNMR)
<input checked="" type="checkbox"/> Supervisor	<input checked="" type="checkbox"/> Data Set Name Edit
<input type="checkbox"/> Essential Originator	<input checked="" type="checkbox"/> Originator
<input checked="" type="checkbox"/> Manual Lock/Shim	<input checked="" type="checkbox"/> Mail Spectrum PDF/PS
<input type="checkbox"/> E-mail Notification	<input type="checkbox"/> JDX DataMail
<input type="checkbox"/> JDX Copy	<input checked="" type="checkbox"/> Edit Lock/Shim/ATM
<input type="checkbox"/> ZIP Copy	<input type="checkbox"/> ZIP DataMail
<input type="checkbox"/> Print Spectrum	<input checked="" type="checkbox"/> Control Printing

Data Set Names

- \$DATE
- \$DATEUSER
- \$NUMERICDATE
- \$HOLDER-%d-%m-\$data(UserName)
- %d%m%Y-\$data(UserName)

User Specific Originator Info

- Institute :
- Project-No :

Data Directories

- C:\Bruker\nmrdata

User Specific Parameters/Commands

td	Size of fid
ns	Number of scans
p1	Pulse
plw1	Power level in Watt
te	Required Sample temperature

Other Settings

Spectrum Number File name: [Empty] Archiving Directory: [Empty]

Target E-mail Address: [Empty] Umask: rw-rw-r-- User:f NmrUser:f Everyone:r

Day Time Limit: 2:00 Night Time Limit: 4:00 Max. Duration of a daytime experiment: 1:00

Commands

Save, Default, Delete, Update Experiment List

Group names



Update User Files

Update list for these users to current values

User ID	User's Group	User's Full Name
SamTrack		Sample Track Default User
bob	OC	bob
robin	OC	robin
susan	PC	susan
sven	PC	sven

Update Close

IconNMR: Conf...
File Help
User Settings
User Manage
Composite E
Additional U
Originator It
Automation
Master Switc
Automation
Lock/Shim O
Solvent/P
Depender
Tuning/Matc
Priority
Temperature
LC-NMR Opt
SampleTrack
Fail Safe / Er
Web Interfac
General Options
'Assure'
ToolBox Setup
Accounting

Search
Commands
Save Default Delete Update Experiment List

ers/Commands
of scans
el in Watt
Sample temperature
Everyone

Group names



IconNMR: Configuration

File Help

User Settings

- User Manager
- Composite Experiments
- Additional Users
- Originator Items

Automation

- Master Switches
- Automation Window
- Lock/Shim Options
 - Solvent/Probe Dependencies
- Tuning/Matching
- Priority
- Temperature Handling
- LC-NMR Options
- SampleTrack Options
- Fail Safe / Error Handling
- Web Interface

General Options

- 'Assure'
- ToolBox Setup
- Accounting

Users

User ID	User's Group	User's Full Name
Administrator		
Guest		
bob	OC	bob
diskless user sys		diskless user sys
edv-admin		edv-admin
robin	OC	robin
susan	PC	susan
sven	PC	sven
SamTrack		Sample Track Default User

Current User bob Group OC

Experiment List

Mode	Name	Experiment Comment
↑	N PROTON	1H experiment
↓	N C13CPD	13C experiment with decoupling, 1024 scans, 235 ppm
📄	N C13DEPT135	13C DEPT135, CH3/CH positive, CH2 negative, 256 scans, 160 ppm
📄	C COSYGPSW	Gradient selected COSY
📄	C HSQCDETGPD	sw opt. edited HSQC with gradients (e/a TPPI)
📄	C HMBCGPND	sw opt. HMBC with gradients

Permissions

<input checked="" type="checkbox"/> Priority	<input checked="" type="checkbox"/> Parameter Edit
<input type="checkbox"/> Archive Data	<input checked="" type="checkbox"/> Exit (IconNMR)
<input checked="" type="checkbox"/> Supervisor	<input checked="" type="checkbox"/> Data Set Name Edit
<input type="checkbox"/> Essential Originator	<input checked="" type="checkbox"/> Originator
<input checked="" type="checkbox"/> Manual Lock/Shim	<input checked="" type="checkbox"/> Mail Spectrum PDF/PS
<input type="checkbox"/> E-mail Notification	<input type="checkbox"/> JDX DataMail
<input type="checkbox"/> JDX Copy	<input checked="" type="checkbox"/> Edit Lock/Shim/ATM
<input type="checkbox"/> ZIP Copy	<input type="checkbox"/> ZIP DataMail
<input type="checkbox"/> Print Spectrum	<input checked="" type="checkbox"/> Control Printing

Data Set Names

- \$DATE
- \$DATEUSER
- \$NUMERICDATE
- \$HOLDER-%d-%m-%data(UserName)
- %d%m%Y-%data(UserName)

Data Directories

- C:\Bruker\nmrdata

User Specific Originator Info

- Institute :
- Project-No :

User Specific Parameters/Commands

- td Size of fid
- ns Number of scans
- p1 Pulse
- plw1 Power level in Watt
- te Required Sample temperature

Other Settings

Spectrum Number File name Archiving Directory

Target E-mail Address Umask rw-rw-r-- User:f NmrUser:f Everyone:r

Day Time Limit 2:00 Night Time Limit 4:00 Max. Duration of a daytime experiment 1:00

Commands

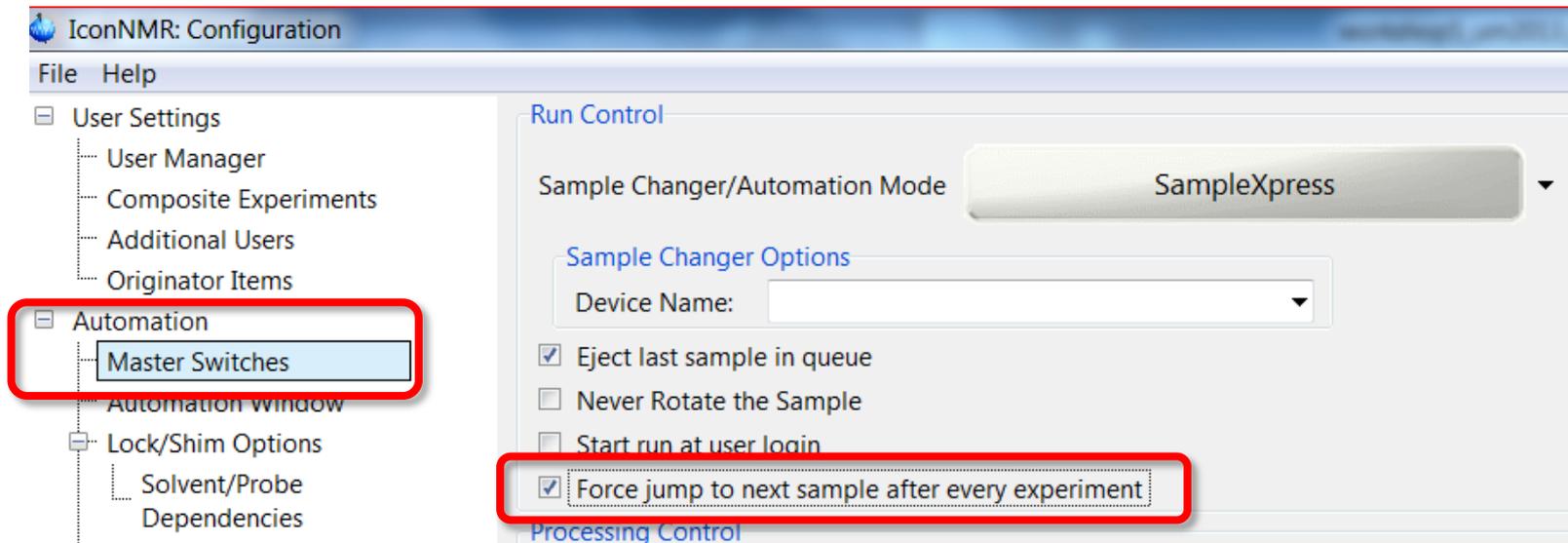
Save Default Delete Update Experiment List

„jump to next sample“



TopSpin 3.0

- jump-to-next-sample :
 - This option is now available via the IconNMR-configuration:



„jump to next sample“



IconNMR: Automation - Oct31-2013-1401-nmrslu

Processing started

Experiment Table

Hol...	Type	Status	Disk	Name	No.	Solvent
16	3	Finished	C:\Bruker\nmrdata	Kinetics_111	10	CDCB
		Finished	C:\Bruker\nmrdata	Kinetics_111	11	CDCB
		Finished	C:\Bruker\nmrdata	Kinetics_111	12	CDCB
17	3	Finished	C:\Bruker\nmrdata	Kinetics_222	10	CDCB
		Finished	C:\Bruker\nmrdata	Kinetics_222	11	CDCB
		Finished	C:\Bruker\nmrdata	Kinetics_222	12	CDCB
18	3	Finished	C:\Bruker\nmrdata	Kinetics_333	10	CDCB
		Finished	C:\Bruker\nmrdata	Kinetics_333	11	CDCB
		Finished	C:\Bruker\nmrdata	Kinetics_333	12	CDCB

Preceding Experiments

#	Date	Holder	Name
9	2013-10-31 14:46:51	18	Kinetics_333
8	2013-10-31 14:42:18	17	Kinetics_222
7	2013-10-31 14:37:40	16	Kinetics_111
6	2013-10-31 14:32:48	18	Kinetics_333
5	2013-10-31 14:27:50	17	Kinetics_222
4	2013-10-31 14:22:38	16	Kinetics_111
3	2013-10-31 14:18:24	18	Kinetics_333
2	2013-10-31 14:13:52	17	Kinetics_222
1	2013-10-31 14:08:53	16	Kinetics_111

Preceding Experiments (Detailed)

#	Date	Holder	Name	No.	Experiment	Load
9	2013-10-31 14:46:51	18	Kinetics_333	12	PROTON	✓
8	2013-10-31 14:42:18	17	Kinetics_222	12	PROTON	✓
7	2013-10-31 14:37:40	16	Kinetics_111	12	PROTON	✓
6	2013-10-31 14:32:48	18	Kinetics_333	11	PROTON	✓
5	2013-10-31 14:27:50	17	Kinetics_222	11	PROTON	✓
4	2013-10-31 14:22:38	16	Kinetics_111	11	PROTON	✓
3	2013-10-31 14:18:24	18	Kinetics_333	10	PROTON	✓
2	2013-10-31 14:13:52	17	Kinetics_222	10	PROTON	✓
1	2013-10-31 14:08:53	16	Kinetics_111	10	PROTON	✓

Submit Cancel Edit Delete Add 1

Search Preceding include previous runs

SampleExpress Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: nmrsu

A selection of new features in TopSpin 3.1



TopSpin 3.0

TopSpin 3.1

IconNMR 4.6

12 new features

- **Automation window reads spreadsheets in .xls/.xlsx format with support for multiple workspaces.**
- **Experiments may be submitted, cancelled with <Alt-s>, <Alt-c> etc. directly from the Sample Holder Overview window.**
- **Assure™ - SST (System Suitability Test)**
This is now an integral part of IconNMR and includes acquisition and analysis of NMR standards for 1H line shape, 1H sensitivity, 13C sensitivity, 19F sensitivity, 31P sensitivity, and temperature calibration. This software automatically:
 - Validates the instrument performance for line shape and sensitivity
 - Performs temperature calibration and adjustment
 - Includes an automated 'Stop' criteria to prevent user standard acquisition upon specification failure
 - Generates a PDF report of all SST results. Tests are performed regularly at user defined intervals, requiring no instrument interaction and without interrupting Automation.

ASSURE-SST System Suitability Test (SST)



TopSpin 3.0

TopSpin 3.1

IconNMR: Configuration

File Help

- User Settings
 - User Manager
 - Composite Experiments
 - Additional Users
 - Originator Items
- Automation
 - Master Switches
 - Automation Window
 - Lock/Shim Options
 - Solvent/Probe Dependencies
 - Tuning/Matching
 - Priority
 - Temperature Handling
 - LC-NMR Options
 - SampleTrack Options
 - Fail Safe / Error Handling
 - Web Interface
- General Options
 - 'Assure'
 - ToolBox Setup
 - Accounting

Options System Suitability Test (SST) Raw Material Screening

System Suitability Test

Enable System Suitability Test (Requires ASSURE-SST License)

Perform test every: 24 hours SST User Administrator

System Suitability Log Directory: C:\Bruker\TopSpin3.1pl7\users\Administrator\topspin-

Load/Save shim set before/after first test

Stop system test after any failure (implies no reports from other test samples)

Report Options

Print the report

Company/Institution:

System ID:



Available Tests

Test Name	Perform Test	Sample Position	Linewidths	Resolution Halfwidth	Left Plot Limit	Right Plot Limit	Signal region	Noise region	Noise delta	S/N
1H Lineshape Hump test	<input checked="" type="checkbox"/>	1	Linewidth at 0.55% of signal height < 1 Hz Linewidth at 0.11% of signal height < 12 Hz	0.6 Hz	8.64 ppm	7.44 ppm				
1H Sensitivity Test	<input checked="" type="checkbox"/>	2					Left limit 3 ppm Right limit 2 ppm	Left limit 7 ppm Right limit 2.8 ppm	2 ppm	135 :1
13C Sensitivity Test	<input checked="" type="checkbox"/>	3								
F19 Sensitivity Test	<input checked="" type="checkbox"/>	4								

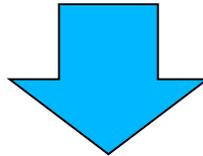
Automation window reads spreadsheets in .xls/.xlsx format

TopSpin 3.0

TopSpin 3.1

Up to TopSpin 3.0 the “.CSV” format was:

	A	B	C	D	E	F
1	Disk	Name	Solvent	Experiment	Sample ID	Plottitle
2	C:\bruker\topspin3.0\examdata	test.001	CDCI3	PROTON	SAM000001	This is the title exp 1
3	C:\bruker\topspin3.0\examdata	test.002	CDCI3	PROTON	SAM000002	This is the title exp 2
4	C:\bruker\topspin3.0\examdata	test.003	CDCI3	C13CPD32	SAM000003	This is the title exp 3
5	C:\bruker\topspin3.0\examdata	test.004	DMSO	C13DEPT4	SAM000004	This is the title exp 4



Save as “.CSV” file.

```
Disk;Name;Solvent;Experiment;Sample ID;Plottitle
C:\bruker\topspin3.0\examdata;test.001;CDCI3;PROTON;SAM000001;This is the title exp 1
C:\bruker\topspin3.0\examdata;test.002;CDCI3;PROTON;SAM000002;This is the title exp 2
C:\bruker\topspin3.0\examdata;test.003;CDCI3;C13CPD32;SAM000003;This is the title exp 3
C:\bruker\topspin3.0\examdata;test.004;DMSO;C13DEPT4;SAM000004;This is the title exp 4
```

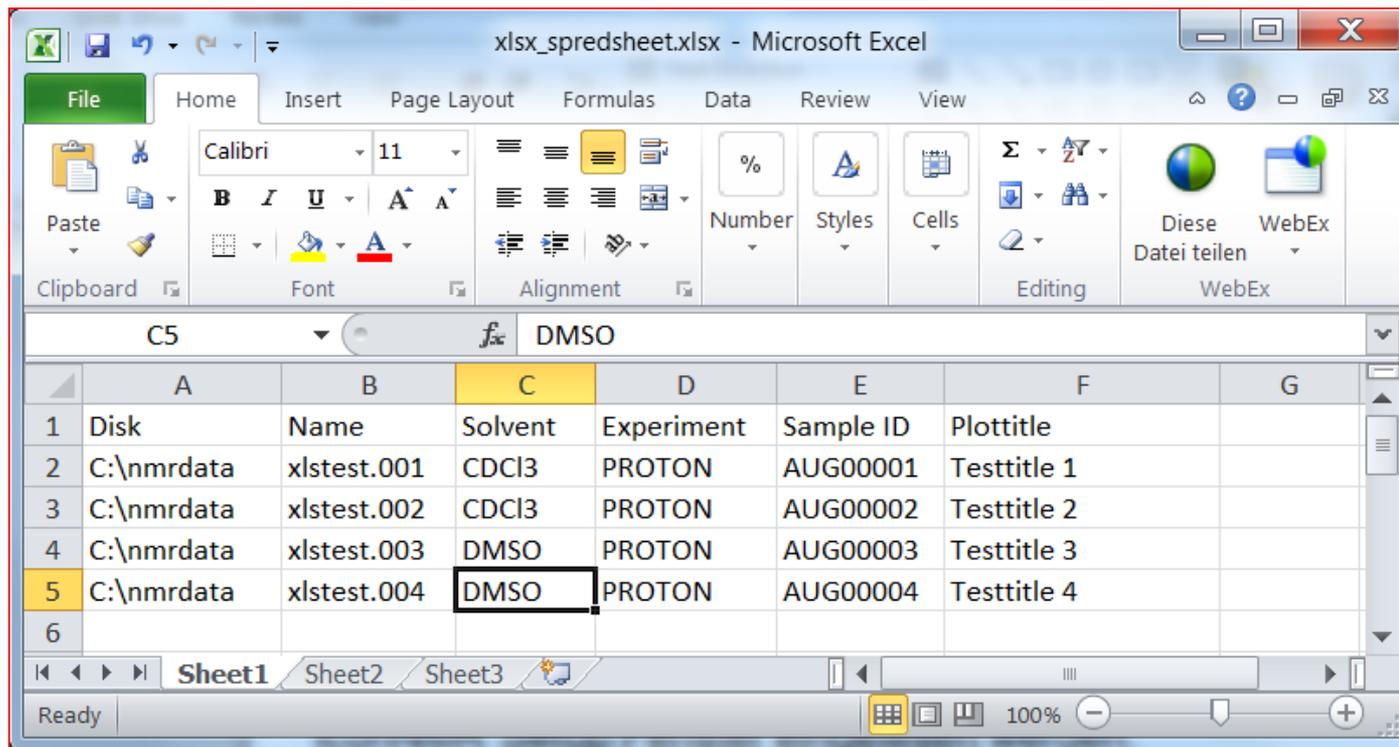
Because of different language settings the “.CSV” file can consist different characters. The columns must be divided by semicolon!

Automation window reads spreadsheets in .xls/.xlsx format

TopSpin 3.0

TopSpin 3.1

Since TopSpin 3.1 a spreadsheet can be read in “.XLS/.XLSX” format.



Save as
“.XLS/.XLSX”



Store this file in the folder <topspinhome>\prog\tmp (default location).

Automation window reads spreadsheets in .xls/.xlsx format



TopSpin 3.0

TopSpin 3.1

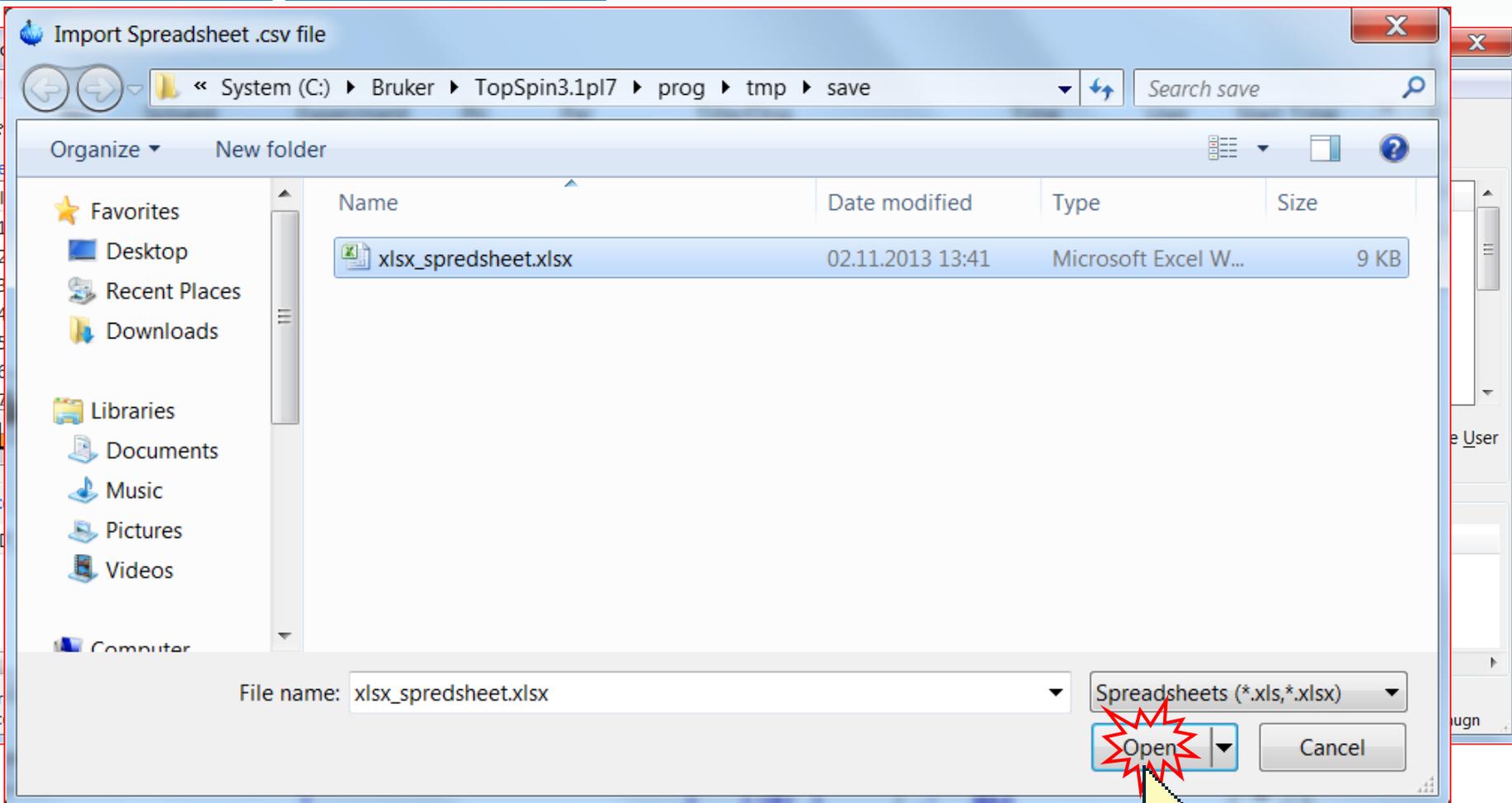
The screenshot shows the Bruker TopSpin 3.1 Automation window. The title bar reads "NonNMR: Automation Nov02-2013-1325-BRUKER-augn". The menu bar includes File, Run, Holder, View, Find, Parameters, Options, Tools, and Help. The File menu is open, showing options: New, Save, Save as external setup, Import Spreadsheet file (highlighted with a red starburst), Print (List Setup), Print History File, a list of recent files (Nov02-2013-1320-BRUKER-augn.set, Nov02-2013-1039-BRUKER-augn.set, Nov21-2012-1626-ahof.set), Close, and Close All. A red starburst also highlights the 'Import Spreadsheet file' option. The main window contains a table with columns: No., Solvent, Experiment, Pri, Par, Title/Orig, Time, User, Start Time. Below the table are buttons for Edit, Delete, Add, Copy, and a Change User button. At the bottom, there is a 'Preceding Experiments' section with a table with columns: #, Date, Holder, Name, No., Experiment, Load, ATM, Lock, Shim, Acq, Proc, User, Disk, Title/Orig. The status bar at the bottom shows search options, a search icon, and system information: SampleXpress/Pro Webservice, Busy until: No Jobs!, Day Experiments: 00:00, Night Experiments: 00:00, User: BRUKER\augn.

Automation window reads spreadsheets in .xls/.xlsx format



TopSpin 3.0

TopSpin 3.1



Automation window reads spreadsheets in .xls/.xlsx format



TopSpin 3.0

TopSpin 3.1

IconNMR: Automation Nov02-2013-1325-BRUKER-augn

File Run Holder View Find Parameters Options Tools Help

Start [Icons]

Experiment Queue

Hol...	Type	Status	Disk	Na...
▶ 1	U	Available		
▶ 2	U	Available		
▶ 3	U	Available		
▶ 4	U	Available		
▶ 5	U	Available		
▶ 6	U	Available		
▶ 7	U	Available		

Submit Cancel

Preceding Experiments

#	Date	Holder
---	------	--------

Search Preceding [Input] [Icon] include previous runs

SampleXpress/Pro Webservice Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: BRUKER\augn

Choose workspace

This spreadsheet contains multiple workspaces.

Please select the required workspace

Select Workspace:

Sheet1

OK Cancel

Automation window reads spreadsheets in .xls/.xlsx format



TopSpin 3.0

IconNMR: Import Spreadsheet .csv file

Load Setup from Spreadsheet .csv/.xls(x) File

Data Set Name

Disk [COL_A]

Sample Name [COL_B]

Barcode ID [COL_E]

Solvent / Experiment

Solvent [COL_C]

Experiment [COL_D]

Spread Sheet Extraction

Begin at Sample Position 1

Begin at CSV File Row 2

Stop at CSV File Row Last

Include the following columns in title/originator information [COL_F]

Load into Setup Window

Generate External Setup File

Generate BACS/SampleJet Barcode Orders

Close

IconNMR: Automation Nov02-2013-1325-BRUKER-a

File Run Holder View Find Parameters Options

Start

Experiment Queue

Hol...	Type	Status	Disk	Name
1	U	Available		
2	U	Available		
3	U	Available		
4	U	Available		
5	U	Available		
6	U	Available		
7	U	Available		

Submit Cancel

Preceding Experiments

#	Date	Holder	Name
---	------	--------	------

Search Preceding include previous

Time User Start Time

Change User

Proc	User	Disk	Title/Orig
------	------	------	------------

00:00 Night Experiments: 00:00 User: BRUKER\augn

Automation window reads spreadsheets in .xls/.xlsx format



TopSpin 3.0

TopSpin 3.1

IconNMR: Automation Nov02-2013-1325-BRUKER-augn

File Run Holder View Find Parameters Options Tools Help

Start [Icons] i

Experiment Queue

Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	1Queued	Queued	C:\nm	xlstest.001	10	CDCI3	PROTON	[Icons]	[Icons]	Plottitle Testtitle 1	00:01:07	BRUKER	14:18 Sat N
2	1Queued	Queued	C:\nm	xlstest.002	10	CDCI3	PROTON	[Icons]	[Icons]	Plottitle Testtitle 2	00:01:07	BRUKER	14:23 Sat N
3	1Queued	Queued	C:\nm	xlstest.003	10	DMSO	PROTON	[Icons]	[Icons]	Plottitle Testtitle 3	00:01:07	BRUKER	14:28 Sat N
4	1Queued	Queued	C:\nm	xlstest.004	10	DMSO	PROTON	[Icons]	[Icons]	Plottitle Testtitle 4	00:01:07	BRUKER	14:33 Sat N

Submit Cancel Edit Delete Add 1 Copy 1 Change User

Preceding Experiments

#	Date	Holder	Name	No.	Experiment	Load	ATM	Lock	Shim	Acq	Proc	User	Disk	Title/Orig
---	------	--------	------	-----	------------	------	-----	------	------	-----	------	------	------	------------

Search Preceding [Input] [Icon] include previous runs SampleXpress/Pro Webservice Busy until: Sat 14:38 Day Experiments: 00:04 Night Experiments: 00:00 User: BRUKER\augn

A selection of new features in TopSpin 3.2



TopSpin 3.0

TopSpin 3.1

TopSpin 3.2

IconNMR 4.7

9 new features

- **Additional Users**

IconNMR's Additional user list may now be generated externally together with plain text passwords which the program encrypts on first display.

New in TopSpin 3.2 pl5 (IconNMR 4.7.5):

- ASSURE-SST:
 - Run SST every 0-365 days! (=> "0" means: Queued on demand.)
 - 4 user defined experiments can be configured.
- New in 3.2 PL4. Configure Automation to start without the Identify User Window.

Password for Additional User

TopSpin 3.0

TopSpin 3.1

TopSpin 3.2

- The user name are stored in:
<topspinhome>/conf/instr/<spect>/inmrusers/.nmrusers
as ASCII file.
- The file format is very convenient and can be modified externally. Each user is entered in a new line with name, ID and Password (divided by colon):
Max Musterman:mmu:<Encrypted Password>
or
Max Musterman:mmu:NULL
if no password is entered.

```
.nmrusers
1 #
2 #           Nmr Users File modified by ICON-NMR
3 #           Last Changed by Configuration on 1553-Nov02-2013
4 #
5 #NMR_USER_ID:nmrstu
6 sven:sven:IwOEBF90LzTWO
7 bob:bob:NULL
8 susan:susan:NULL
9 robin:robin:NULL
```

Password for Additional User

TopSpin 3.0

TopSpin 3.1

TopSpin 3.2

- If the file will be created externally, the respective password can be entered plaintext. IconNMR will convert this plaintext password, when the “Additional Users” configuration page will be opened for the first time after an IconNMR restart.
- After that the configuration must be saved to renew the “.nmrusers” file.
- The following format must be used for the plaintext password:
Full Name:ID:PLAIN_TEXT_PASSWORD:Password
- “Password” is here the example password to convert.
- The key word “PLAIN_TEXT_PASSWORD” informs the software to convert the following term.

```
.nmrusers
1 #
2 #           Nmr Users File modified by ICON-NMR
3 #           Last Changed by Configuration on 1553-Nov02-2013
4 #
5 #NMR_USER_ID:nmrstu
6 sven:sven:IwOEBF90LzTWO
7 bob:bob:PLAIN_TEXT_PASSWORD:topspin
8 susan:susan:PLAIN_TEXT_PASSWORD:Password
9 robin:robin:PLAIN_TEXT_PASSWORD:12_Ra_34
```

Password for Additional User



The screenshot shows the 'IconNMR: Configuration' application window. The 'Additional Users' section is selected in the left-hand navigation pane. The main area displays the 'Options' and 'Additional User Setup' sections. The 'Options' section includes a text field for 'NMR Super User' containing 'BRUKER\augn' and a dropdown menu for 'Additional User's Effective User ID' set to 'nmrsu'. The 'Additional User Setup' section has two text input fields: 'Additional User's Full Name' (with the example 'e.g. Bob Smyth') and 'User ID e.g. bs'. Below these fields are three buttons: 'Add new', 'Modify', and 'Delete'. To the right of the input fields is a table with two columns: 'User ID' and 'User's Full Name'. The table contains the following entries:

User ID	User's Full Name
sven	sven
bob	bob
susan	susan
robin	robin

Overlaid on top of the configuration window is a smaller dialog box titled 'Passwords Converted'. It features a yellow warning triangle icon and the text 'Plain text passwords were converted to real passwords!'. An 'OK' button is located at the bottom right of the dialog box.

Password for Additional User



IconNMR: Configuration

File Help

- User Settings
 - User Manager
 - Composite Experiments
 - Additional Users**
 - Originator Items
- Automation
 - Master Switches
 - Automation Window
 - Lock/Shim Options
 - Solvent/Probe Dependencies

Options

NMR Super User: BRUKER\augn

Additional User's Effective User ID: nmrsu

Additional User Setup

Additional User's Full Name: robin
e.g. Bob Smyth

User ID e.g. bs: robin

This account has a password.

User ID	User's Full Name
sven	sven
bob	bob
susan	susan
robin	robin

```
.nmusers
1 #
2 #      Nmr Users File modified by ICON-NMR
3 #      Last Changed by Configuration on 1553-Nov02-2013
4 #
5 #NMR_USER_ID:nmrsu
6 sven:sven:IwOEBF90LzTWO
7 bob:bob:PLAIN_TEXT_PASSWORD:topspin
8 susan:susan:PLAIN_TEXT_PASSWORD>Password
9 robin:robin:PLAIN_TEXT_PASSWORD:12_Ra_34
```

```
.nmusers
1 #
2 #      Nmr Users File modified by ICON-NMR
3 #      Last Changed by Configuration on 1620-Nov02-2013
4 #
5 #NMR_USER_ID:nmrsu
6 sven:sven:IwOEBF90LzTWO
7 bob:bob:VdPTIAAUK6SWY
8 susan:susan:NzMlgbK..aBoQ
9 robin:robin:AdxuODhR.Ai0U
```



New in TopSpin 3.2 pl5: Improved functionalities in ASSURE-SST



TopSpin 3.0

TopSpin 3.1

TopSpin 3.2

TopSpin 3.2pl5

The screenshot displays the 'System Suitability Test (SST)' configuration window in TopSpin 3.2pl5. The window is divided into several sections:

- System Suitability Test (V. 2.0):** Includes checkboxes for 'Enable System Suitability Test (Requires ASSURE-SST)', 'Load/Save shim set before/after first test', and 'Print the report (Suitable Adobe Reader Installed)'. A yellow mouse cursor is pointing at the 'Enable System Suitability Test' checkbox, which is highlighted with a red starburst.
- Report Options:** Includes 'Print the report (Suitable Adobe Reader Installed)' checkbox, 'Company/Institution: BBIO', and 'System ID: HH003007'.
- Available Tests:** Includes 'Standard' and 'User Defined' tabs. Under 'User Defined', '1H Lineshape HumpTest' is selected with a checked 'Perform Lineshape Test' option. Below this, '13C Sensitivity Test' is also selected with a checked 'Perform 13C Sensitivity Test' option.
- General Options:** A red box highlights the 'Assure' option under the 'General Options' section.
- ToolBox Setup:** Shows signal region and noise region parameters for 13C and 31P tests.

Test	Left limit (ppm)	Right limit (ppm)	Noise region (ppm)	Noise delta (ppm)	S/N
13C Sensitivity Test	140	120	100	40	130 :1
31P Sensitivity Test	124	80	102	104	103 :1
Temperature Test/Automatic Adjustment					

New in TopSpin 3.2 pl5: Improved functionalities in ASSURE-SST

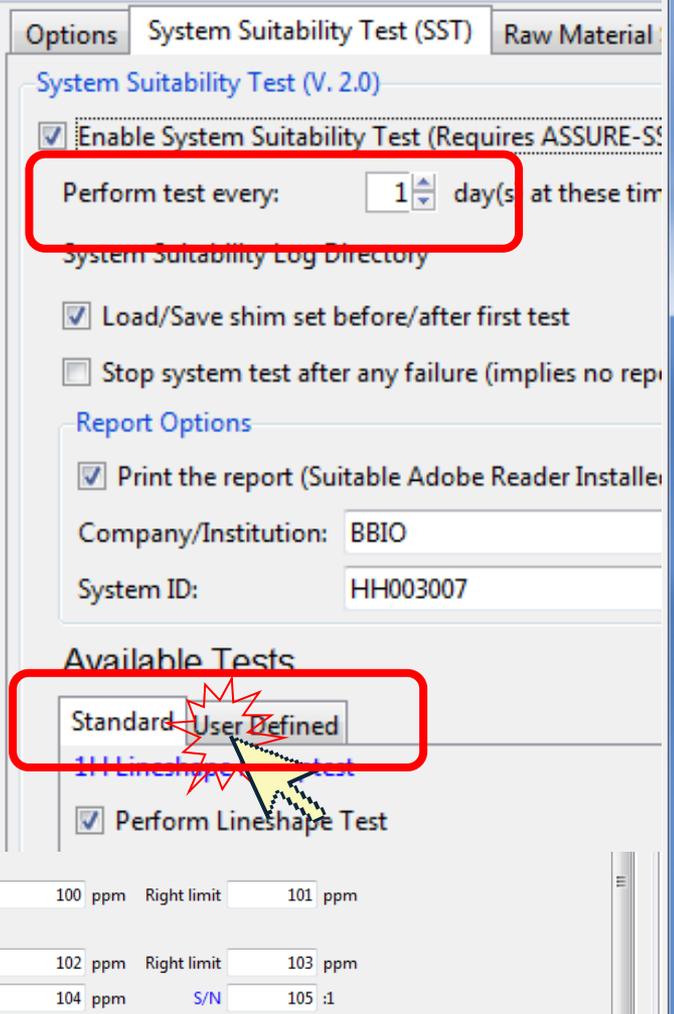
TopSpin 3.0

TopSpin 3.1

TopSpin 3.2

TopSpin 3.2pl5

These test can be performed in a range of 0 to 365 days.
4 user defined experiments can be set up for SST.



Options System Suitability Test (SST) Raw Material

System Suitability Test (V. 2.0)

Enable System Suitability Test (Requires ASSURE-SST)

Perform test every: 1 day(s) at these times

System Suitability Log Directory

Load/Save shim set before/after first test

Stop system test after any failure (implies no report)

Report Options

Print the report (Suitable Adobe Reader Installed)

Company/Institution: BBIO

System ID: HH003007

Available Tests

Standard User Defined

Perform Lineshape Test

New in TopSpin 3.2 pl5: Improved functionalities in ASSURE-SST



TopSpin 3.0

TopSpin 3.1

TopSpin 3.2

TopSpin 3.2pl5

Options System Suitability Test (SST) Raw Material Screening

System Suitability Test (V. 2.0)

Enable System Suitability Test (Requires ASSURE-SST License)

Perform test every: day(s) at these times: (hh:mm, hh:mm,...) SST User

System Suitability Log Directory

Load/Save shim set before/after first test

Stop system test after any failure (implies no reports from other test samples)

Report Options

Print the report (Suitable Adobe Reader Installed) Paper Size A4 Letter

Company/Institution:

System ID:



Available Tests

Standard User Defined

User Defined Lineshape Test1

Perform User Defined Lineshape Test1

Description

Solvent

Parameter Set

Sample Position

Linewidths

Linewidth at 0.55% of signal height < Hz

Linewidth at 0.11% of signal height < Hz

Resolution Halfwidth < Hz

Left Plot Limit ppm Right Plot Limit ppm

User Defined Sensitivity Test1

Perform User Defined Sensitivity Test1

Description

Solvent

Parameter Set

Sample Position

Signal region

Left limit ppm Right limit ppm

Noise region

Left limit ppm Right limit ppm

Noise delta ppm S/N :1

New in TopSpin 3.2 pl5: Improved functionalities in ASSURE-SST

TopSpin 3.0

TopSpin 3.1

TopSpin 3.2

TopSpin 3.2pl5

User Defined Lineshape Test2

Perform User Defined Lineshape Test2

Description

Solvent

Parameter Set

Sample Position

Linewidths

Linewidth at 0.55% of signal height < Hz

Linewidth at 0.11% of signal height < Hz

Resolution Halfwidth < Hz

Left Plot Limit ppm Right Plot Limit ppm

User Defined Sensitivity Test2

Perform User Defined Sensitivity Test2

Description

Solvent

Parameter Set

Sample Position

Signal region

Left limit ppm Right limit ppm

Noise region

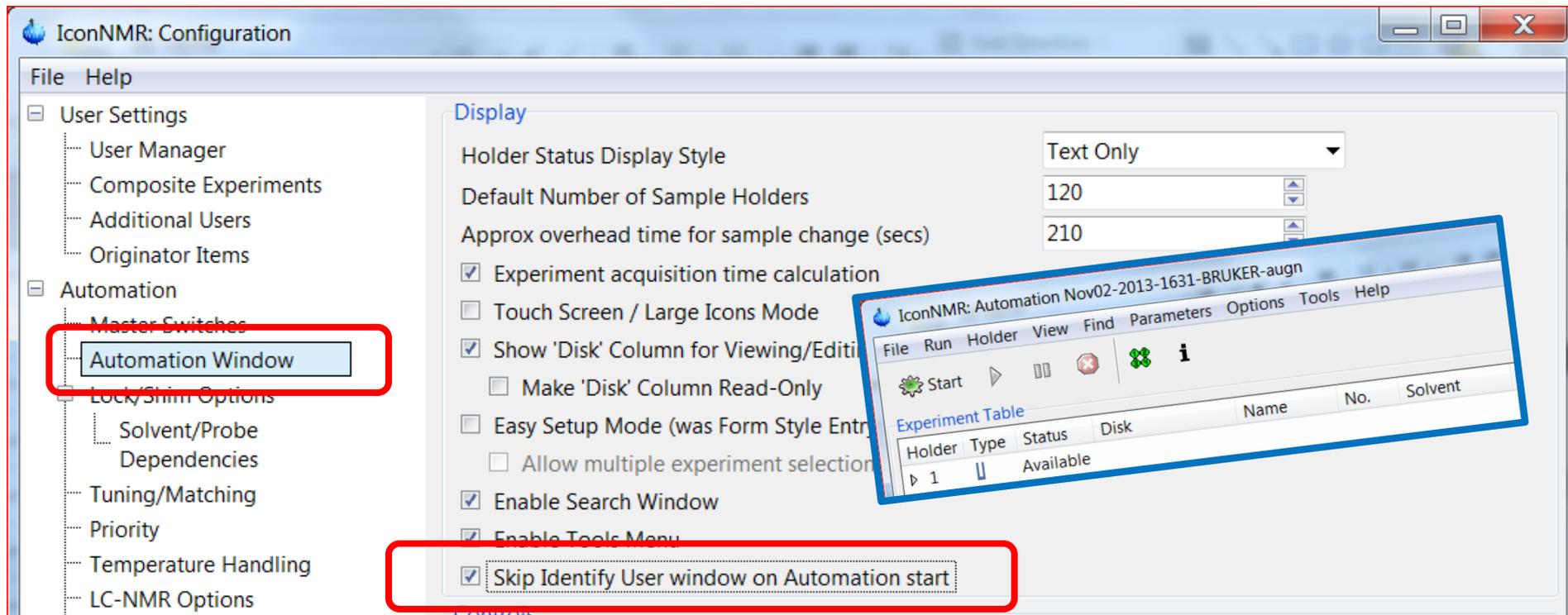
Left limit ppm Right limit ppm

Noise delta ppm S/N :1

Please adapt these setting according to your system.

New in TopSpin 3.2 pl5: Skip Identify User window

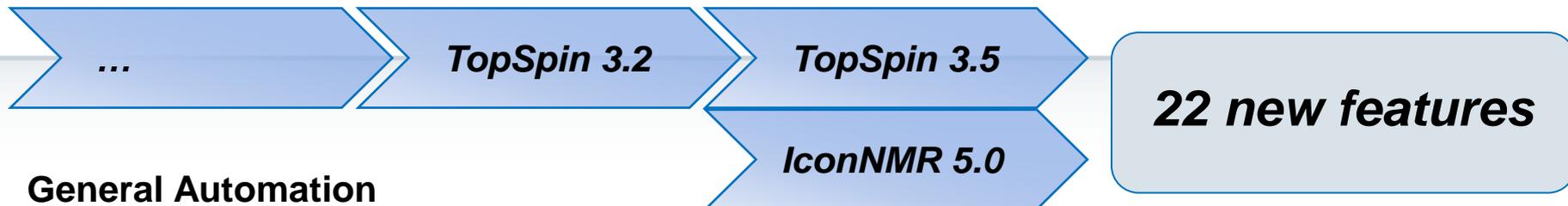
Selecting this option will start the IconNMR set with the User ID of the logged-in operating system user.



The screenshot shows the 'IconNMR: Configuration' window. The 'Automation' section is expanded, and the 'Automation Window' option is highlighted with a red box. In the 'Display' section, the 'Skip Identify User window on Automation start' checkbox is checked and highlighted with a red box. An inset window titled 'IconNMR: Automation Nov02-2013-1631-BRUKER-augn' is also shown, displaying an 'Experiment Table' with the following data:

Holder	Type	Status	Disk	Name	No.	Solvent
1		Available				

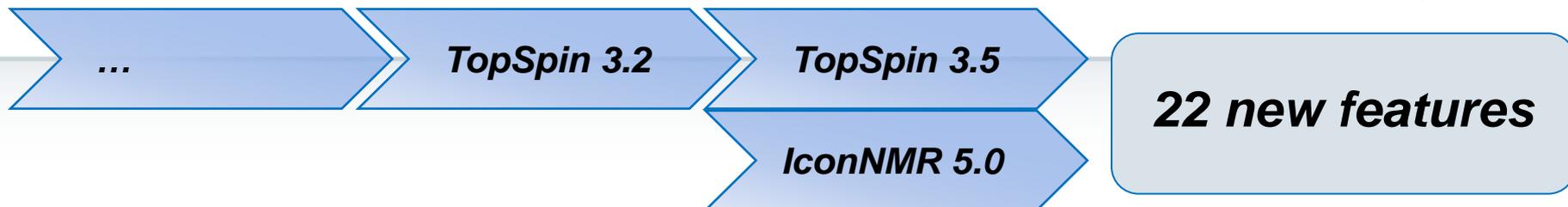
A selection of new features in TopSpin 3.5



General Automation

- Use system passwords to login to IconNMR's https site
- 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 remove or leave the sample in the magnet
- Start times are copied/set automatically to/on follow up experiments
- Absence of the Priority User permission no longer disables the day/night experiment switch
- Spreadsheet files with .XLXS / .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 Emails in HTML with Authentication/Encryption
- Easily define multiple data archiving directories
- Configure Automation to start without User Identification. See **Configuration → Automation Window**
- Periodic Experiments Tool now makes full use of IconNMR's 'Start Time' system

A selection of new features in TopSpin 3.5



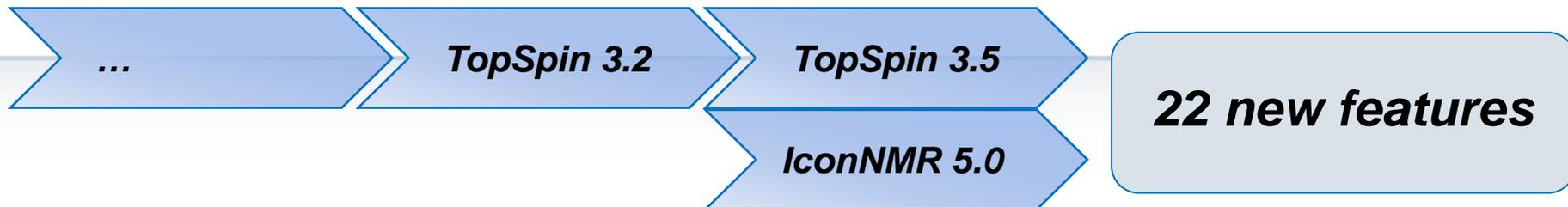
Easy setup updated

- See what experiments are available at a glance for even faster selection.
- Limit the number/type of experiments 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 by 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**

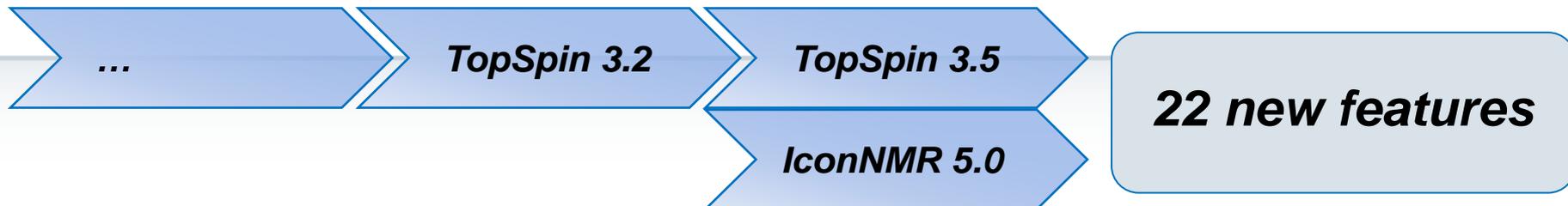
A selection of new features in TopSpin 3.5



Other New Features:

- 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
- Hidden Options from `_iconnmrrc.txt` are now fully accessible from the **Options Resource File Settings** 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)

A selection of new features in TopSpin 3.5



SampleJet Individual Sample MatrixID Support

Scan a barcoded nmr tube into Icon's experiment setup table or easy setup window and place your sample anywhere. 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*

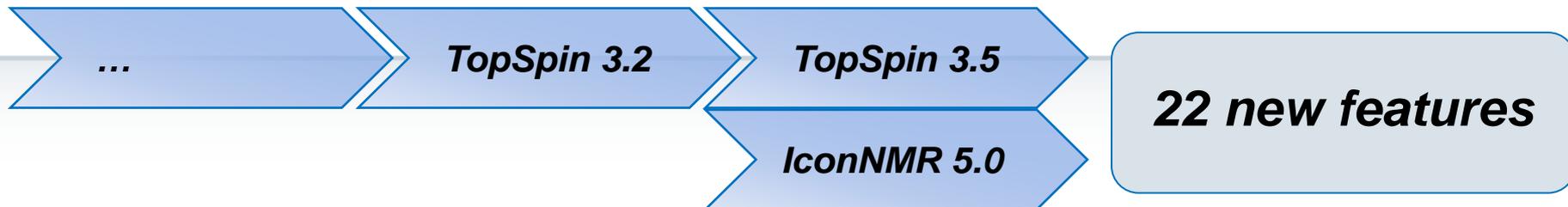
- Spreadsheet/External setup supported
- SampleTrack/SampleJet supported
- Integrated in IconNMR's Web interface

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.

A selection of new features in TopSpin 3.5



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. It is decided *on-the-fly* if further experiments can improve significantly the verification confidence while complying with the user's demands concerning allocatable 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

For more information consult your CMC documentation.

Easy setup – easy



Limit the automation to a dedicated number of experiments and solvents:
e.g. for production control or Open-Access Systems:

The screenshot shows the 'IconNMR: Configuration' window. The left sidebar has 'Automation Window' selected. The main panel shows the 'Display' section with 'Easy Setup Mode' checked and highlighted by a red box. Below this is a table of restricted experiments.

Enable	Experiment Name	Experiment Comment
<input checked="" type="checkbox"/>	N PROTON128	1H experiment 128 scans
<input checked="" type="checkbox"/>	N C13CPD32	13C experiment with decoupling, 32 scans, 235 ppm
<input checked="" type="checkbox"/>	C COSY90SW	sw opt. COSY90 (magn. mode)

Easy setup – easy



1. Select **Name**
2. Select **Solvent**
3. Select **Experiment**
4. Enter the **Title**
5. Queue Experiment → The System Administrator can arrange a customized help information.

Ho...	Type	Status	Disk	Name	No.	Solvent	Title/Orig	Time	User	Start Time
1		Available								

SampleJet /SampleXpress Barcode Support



IconNMR Setup can now handle Barcode
 – ID's instead of Holder-Numbers!

#	Tube ID	Ho...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig
1	140010		1	Available								
				Available	C:\	Jan09-2015	10	CDCI3	N PROTO	★	☀ = 🇺🇸 🇩🇪 🇫🇷	
2	170250		1	Available								
				Available	C:\	01092015	20	D2O	N PROTO	★	☀ = 🇺🇸 🇩🇪 🇫🇷	

Open Access!

EASY Setup Mode –Barcode/Tube ID

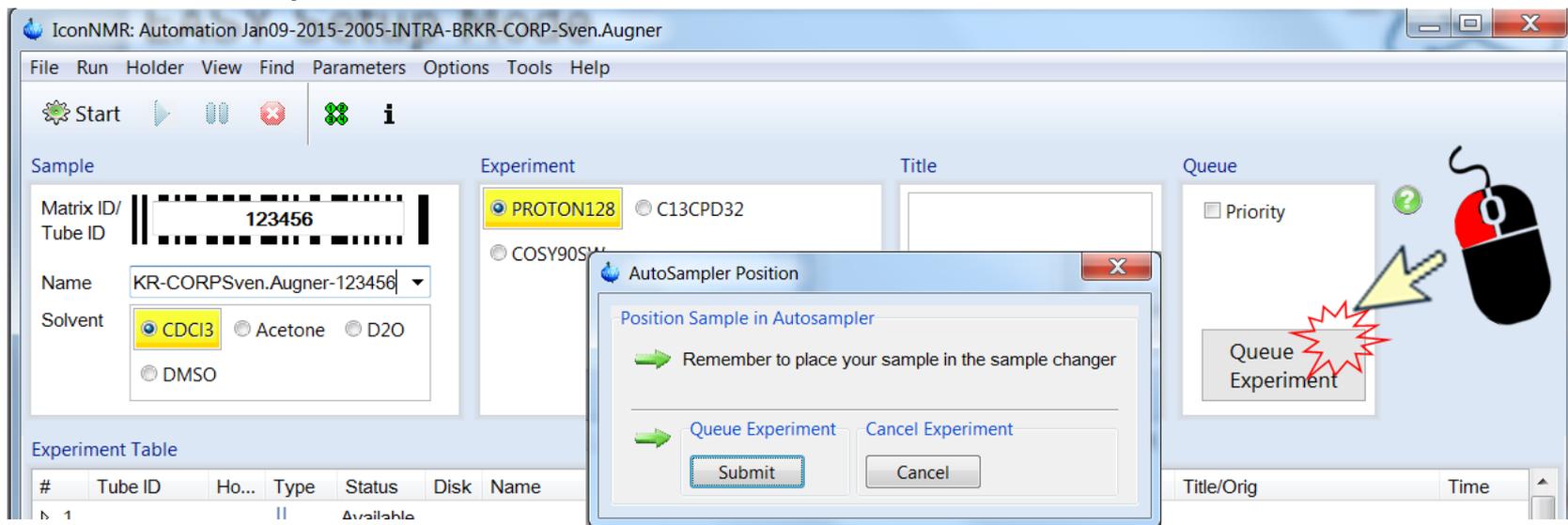
TopSpin 3.0

TopSpin 3.1

TopSpin 3.2

TopSpin 3.5

- Barcode/Tube ID based operation possible, too.
- Enter Barcode ID/Tube ID of the respective NMR tube
- *Optional: Adaption of the automatically generated data set name*
 - e.g. Username+“_”+Tube ID
- Select Solvent and Experiment
- „Queue experiment“



- Place the sample on any (free) holder in the SampleChanger



Virtual Parameter Sets



Virtual Parameter Sets

Enable Virtual Parameter Sets

Make new or Modify experiments for use inside IconNMR Automation based on any TopSpin parameter set. Click on the boxes to see example settings. Leave cells blank for default behaviour.

Parameters may be modified or easily transferred between experiments.
Alternative/multiple AU programs may be prescribed or alternative underlying parameter sets specified.
Eliminate the need for multiple customized parameter sets (even across multiple instruments) containing only minor differences.
All 'Virtual' Experiments defined in the 'Experiment Name' column may be used inside IconNMR Configuration as required.

	Enable	Experiment Name	Comment	Underlying Parameter Set	Command after dataset creation	Command At Acquisition (AUNM)
+	<input checked="" type="checkbox"/>	PROTON64	1H 64 scans	PROTON	SETPAR ns 64	
-	<input checked="" type="checkbox"/>	C13Bilev	C13 with Bilev	C13CPD	SETPAR cpdprg2 bi_waltz16_32	

- Virtual Parameter Sets can be based on Bruker or customized Parameter sets
- Parameter modification will be defined under "Command after dataset creation".

Virtuelle Parametersätze



TopSpin 3.0

TopSpin 3.1

TopSpin 3.2

TopSpin 3.5

Enable	Experiment Name	Comment	Underlying Parameter Set	Command after dataset creation	Command At Acquisition (AUNM)
<input checked="" type="checkbox"/>	PROTON-IconNMR	Modified Proton Experiment used inside IconNMR	PROTON	SETPAR ns 8 td 1k;	
<input checked="" type="checkbox"/>	PROTON	Proton to save RG and O1	PROTON		XAUA;SAVEPARS rg o1; #Run acquisit
<input checked="" type="checkbox"/>	PROTON	Proton uses RG and O1 from previous exp	PROTON		GETPARS rg o1;XAUA; #Get rg and o1

Carry over of parameters from the first to the next experiments
e.g. to set up a series of experiments with the same RG or O1 values

Commands for the acquisition (AUNM)

Blank: executes "xaua"

First experiment : XAUA;SAVEPARS rg o1

Next experiment: GETPARS rg o1;XAUA

In older IconNMR versions please use AU Programs:
e.g. with saveprofpars/getprofpars

IconNMR Configuration



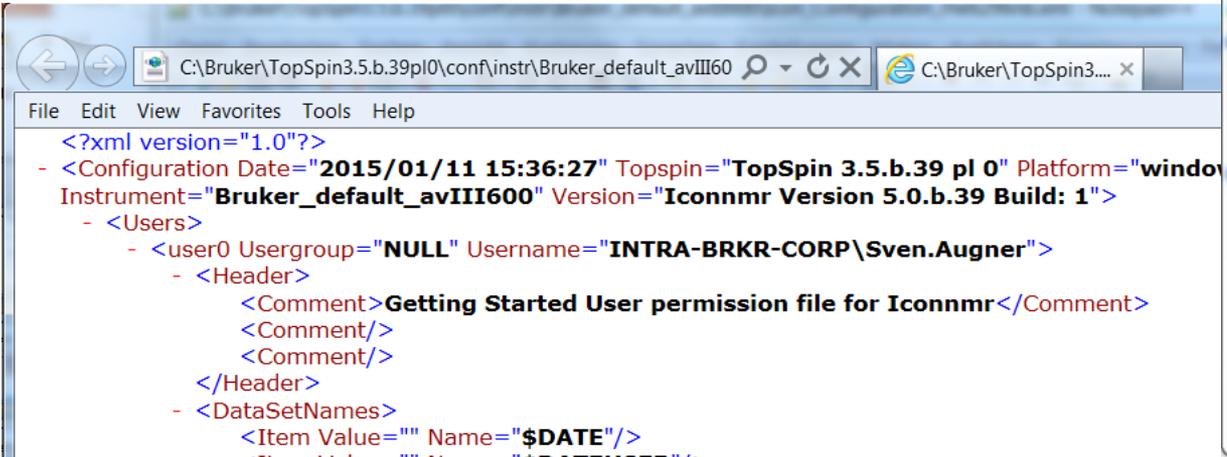
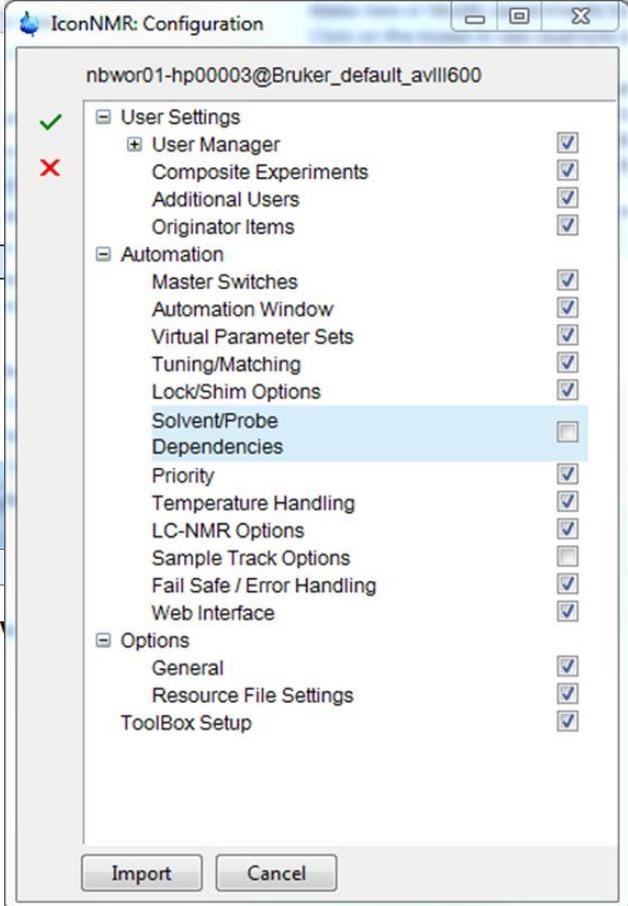
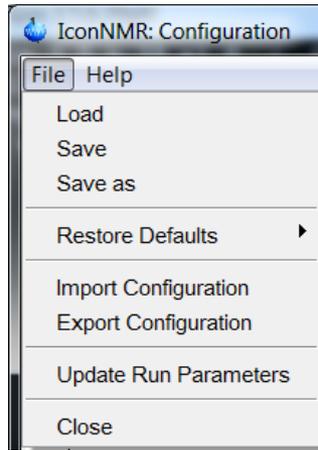
New option in IconNMR to import and export the configuration.

IconNMR Configuration:

File -> Export Configuration

Generates a XML file including:

- User Setting
- Composite Experiments
- Additional Users
- Originators
- Automation configuration
- **Virtual Parameter Sets**



IconNMR : E-mail



Your IT Department requires a secured SMTP Server for sending e-mails:

No problem for / with IconNMR!

Mail

SMTP Mail Server	<input type="text" value="smtp.company.com"/>	"From:" Address	<input type="text" value="iconnmr@company.com"/>
Security Type	<input type="text" value="TLS/SSL Encryption"/>	Port	<input type="text" value="25"/>
User Name	<input type="text" value="nmr"/>	Password	<input type="text" value="*****"/>

Send Mail in HTML



Accounting in IconNMR

Accounting



- IconNMR assists you by the accounting of the measurements.
- This can be done user specific (“Additional-User“ or operating system user) or via Originator-infos.

The screenshot displays the IconNMR software interface with several key sections highlighted by red boxes:

- Users:** A table listing system users. The user 'bob' is selected, with 'OC' as the group and 'bob' as the full name.
- Experiment List:** A table of recorded experiments, including 'N PROTON', 'N C13CPD', 'N C13DEPT135', 'C COSYGPSW', 'C HSQCDETGPD', and 'C HMBCGPND'.
- Permissions:** A list of user permissions, with 'Priority', 'Supervisor', 'Manual Lock/Shim', and 'Print Spectrum' checked.
- Data Set Names:** A list of variables used in file naming, such as '\$DATE', '\$DATEUSER', '\$NUMERICDATE', '\$HOLDER-%d-%m-\$data(UserName)', and '%d%m%Y-\$data(UserName)'. The 'User Specific Originator Info' section below it is also highlighted, showing 'Institute' and 'Project-No' fields.
- Data Directories:** A list of storage paths, including 'C:\Bruker\nmrdata'.
- User Specific Parameters/Commands:** A list of parameters like 'td' (Size of fid), 'ns' (Number of scans), and 'p1' (Pulse).

Accounting



- Example: Accounting per user
(two possible options: "All" or the respective user)

IconNMR: Configuration

File Help

User Settings

- User Manager
- Composite Experiments
- Additional Users
- Originator Items

Automation

- Master Switches
- Automation Window
- Lock/Shim Options
 - Solvent/Probe Dependencies
- Tuning/Matching
- Priority
- Temperature Handling
- LC-NMR Options
- SampleTrack Options
- Fail Safe / Error Handling
- Web Interface

General Options

- 'Assure'
- ToolBox Setup
- Accounting**

File Report

Accounting for:

- User
- Group
- Originator

Accounting mode

Accounting Period 01 01 2000 12 31 2013
M D Y M D Y

Unit Price per hour (day) 25

Unit Price per hour (night) 19:01 - 08:00 15

Unit Price per 1 GByte disk space 10

Currency EUR

List the experiments

Remove entries before this date from accounting file

START

Accounting



- Example: Accounting per user

```
Temporary location in: C:/Users/nmrsu/AppData/Local/Temp/file.tmp
Accounting File: C:/Bruker/TopSpin3.2p15/conf/instr/spect/inmrsusers/Inmracct.br
Accounting mode: per Experiment
Temporary location in: C:/Users/nmrsu/AppData/Local/Temp/file.tmp
weekend: 0 6
```

```
User: bob
Accounting Period: from 01/01/2000 to 12/31/2013
Spectrometer time (day): 0 h 23 min
Spectrometer time (night): 0 h 0 min
Disk space total: 0.13 Mbyte
Unit Price per hour (day): 25 EUR
Unit Price per hour (night): 15 EUR
Night time: from 19:01 to 08:00
Unit Price per 1 GByte disk space: 10 EUR
```

```
Number of experiments: 2
List of experiments:
  1 x C HSQCEDETPG sw opt. edited HSQC with gradients (e/a TPPI)
  1 x N PROTON 1H experiment
Item price time: 9.85 EUR
Item price disk: 1.27 EUR
Total price: 11.12 EUR
Temporary location in: C:/Users/nmrsu/AppData/Local/Temp/file.tmp
weekend: 0 6
```

```
User: nmrsu
Accounting Period: from 01/01/2000 to 12/31/2013
Spectrometer time (day): 308 h 58 min
Spectrometer time (night): 727 h 18 min
Disk space total: 142.30 Mbyte
Unit Price per hour (day): 25 EUR
Unit Price per hour (night): 15 EUR
Night time: from 19:01 to 08:00
Unit Price per 1 GByte disk space: 10 EUR
Number of experiments: 2496
List of experiments:
  38 x N C13CPD 13C experiment with decoupling, 1024 scans, 235 ppm
  59 x C13SENS
  4 x N C13DEPT135p 13C DEPT135, CH3/CH positive, CH2 negative, 235 ppm
  310 x PROTON
  4 x N C13DEPT45 13C DEPT45, all positive, 235 ppm
  2 x C13DEPT90
  6 x C13CPD
  238 x COSYGPSW
  65 x PROHUMP
  2 x C13DEPT135p
```

```
User: robin
Accounting Period: from 01/01/2000 to 12/31/2013
Spectrometer time (day): 0 h 37 min
Spectrometer time (night): 0 h 0 min
Disk space total: 0.38 Mbyte
Unit Price per hour (day): 25 EUR
Unit Price per hour (night): 15 EUR
Night time: from 19:01 to 08:00
Unit Price per 1 GByte disk space: 10 EUR
```

```
Number of experiments: 6
List of experiments:
  3 x N PROTON 1H experiment
  3 x C COSYGPSW Gradient selected COSY
Please note: Incomplete experiments:
  1 x N PROTON 1H experiment
```

```
Item price time: 15.72 EUR
Item price disk: 3.81 EUR
Total price: 19.53 EUR
Temporary location in: C:/Users/nmrsu/AppData/Local/Temp/file.tmp
weekend: 0 6
```

```
User: sven
Accounting Period: from 01/01/2000 to 12/31/2013
Spectrometer time (day): 0 h 27 min
Spectrometer time (night): 0 h 0 min
Disk space total: 0.88 Mbyte
Unit Price per hour (day): 25 EUR
Unit Price per hour (night): 15 EUR
Night time: from 19:01 to 08:00
Unit Price per 1 GByte disk space: 10 EUR
```

```
Number of experiments: 7
List of experiments:
  7 x N PROTON 1H experiment
Item price time: 11.38 EUR
Item price disk: 8.75 EUR
Total price: 20.13 EUR
```

```
All Users, Spectrometer time (day) : 310 h 27 min
All Users, Spectrometer time (night) : 727 h 18 min
All Users, Total price: 20107.90 EUR
```

Accounting



- Example: Accounting per Originator-Item

The screenshot shows the 'IconNMR: Configuration' window. The left sidebar contains a tree view with categories: 'User Settings' (User Manager, Composite Experiments, Additional Users, Originator Items), 'Automation' (Master Switches, Automation Window, Lock/Shim Options, Tuning/Matching, Priority, Temperature Handling, LC-NMR Options, SampleTrack Options, Fail Safe / Error Handling, Web Interface), and 'General Options' ('Assure', ToolBox Setup). The 'Accounting' option under 'ToolBox Setup' is highlighted with a red box. The main panel shows the 'Accounting for:' section, which is also circled in red. It includes radio buttons for 'User', 'Group', and 'Originator' (selected). Below are dropdown menus for 'All', an empty dropdown, and 'Institute' (with a dropdown menu open showing 'Institute' and 'Project-No'). The 'Accounting mode' dropdown is also open, showing 'Institute' and 'Project-No'. The 'Accounting Period' is set to '01 01 2000' to '12 31 2013'. Below this are input fields for 'Unit Price per hour (day)' (25), 'Unit Price per hour (night) 19:01 - 08:00' (15), and 'Unit Price per 1 GByte disk space' (10). The 'Currency' is set to 'EUR'. There is a checked checkbox for 'List the experiments' and a 'REMOVE' button next to a date input field. A yellow mouse cursor points to a 'START' button at the bottom, which is surrounded by a red starburst effect.

Accounting



- Example: Accounting per Originator-Item

```
Temporary location in: C:/Users/nmrsu/AppData/Local/Temp/file.tmp
Accounting File: C:/Bruker/TopSpin3.2p15/conf/instr/spect/inmrusers/Inmracct.brief
Accounting mode: per Experiment
Temporary location in: C:/Users/nmrsu/AppData/Local/Temp/file.tmp
weekend: 0 0
Originator: Institute PC
Accounting Period: from 01/01/2000 to 12/31/2013
Spectrometer time (day): 0 h 27 min
Spectrometer time (night): 0 h 0 min
Disk space total: 0.88 Mbyte
Unit Price per hour (day): 25 EUR
Unit Price per hour (night): 15 EUR
Night time: from 19:01 to 08:00
Unit Price per 1 GByte disk space: 10 EUR

Number of experiments: 7
List of experiments:
    7 x N PROTON 1H experiment

Item price time:          11.38 EUR
Item price disk:          8.75 EUR
Total price:             20.13 EUR
```



Accounting in TopSpin

Accounting in TopSpin



- Accounting in TopSpin has to be activated manually once.

The screenshot shows the Bruker TopSpin 3.2 software interface. The main window title is "Bruker TopSpin 3.2 on AVIII300Z420W7 as nmrsu / Sven". The menu bar includes "Start", "Acquire", "Process", "Analyze", "Publish", "View", and "Manage". Below the menu bar is a toolbar with various icons. A red starburst highlights the "Preferences" button in the toolbar. A "User preferences" dialog box is open, showing a list of categories on the left: "Administration items", "Window settings", "Text editors", "Miscellaneous", "Remote connection", "Directories", "Acquisition", and "More preferences". The "Acquisition" category is highlighted with a red box. The "Acquisition" section in the dialog box is also highlighted with a red box and contains the following settings:

- File menu: Show "File" text rather than icon (restart!)
- Fonts and colors
- Size of tool bar icons [pixels] 24
- Use TopSpin 2.1 icons instead of TopSpin 3.0 icons
- Open new internal windows "cascaded" rather than "maximized"
- Configure cascaded windows
- 'Arrange' internal windows is only applied to dataset windows
- Minimum visible command lines 1
- Maximum visible command lines 3
- Tabbed pane layout
- Acquisition
- Show "ased" parameter selection with "eda"
- Overwrite existing FID without inquiry (ZG safety off)
- Display digital resolution in FID display window
- Auto open acquisition window after 'zg'
- Configure accounting & data archiving after 'zg'
- Automatically perform getprocal during rparfcd/mrsw

Below the "Acquisition" section, there are several other preference categories, each with a "Change" button:

- More preferences
- Spectra Display Preferences
- Spectra Printing Preferences
- Browser Preferences
- Status Bar Preferences
- Lock Display Preferences
- BSMS Display Preferences

A yellow arrow points to the "Change" button for "Configure accounting & data archiving after 'zg'", which is also highlighted with a red starburst.

Accounting in TopSpin



- Accounting in TopSpin has to be activated manually once.

The screenshot shows the Bruker TopSpin 3.2 interface. A dialog box titled "Setup Auto-Archiving & Accounting" is open in the foreground. The dialog box contains the following text and settings:

When acquisition ('zg') is finished, TopSpin allows you to

- write accounting info to be evaluated by the command 'account'
- to copy the acquired dataset to a desired archiving directory.

When 'zg' is executed multiple times on the same dataset, TopSpin will increment the EXPNO while archiving so as to never override already archived data. You may specify an additional EXPNO offset for this case.

The accounting info is stored in the following directory, one file per day:
"<topspin homedir>/prog/curdir/acqhistory"

The archiving directory may contain the following tags:
\$USERHOME or \$USER. They are replaced by the login user's home directory or name, respectively, at archiving time.

Auto-archive after 'zg' = no

Archiving directory = C:\Users\nmrsu

EXPNO offset = 1000

Write accounting info after 'zg' = yes

Buttons: Browse, OK, Cancel

In the background, the TopSpin main window is visible with a menu bar (Start, Acquire, Process, Analyze, Publish, View, Manage) and a toolbar. A red starburst graphic highlights the "Preferences" option in the menu. Another red starburst graphic highlights the "Change" button in the background window's settings panel.

Accounting in TopSpin



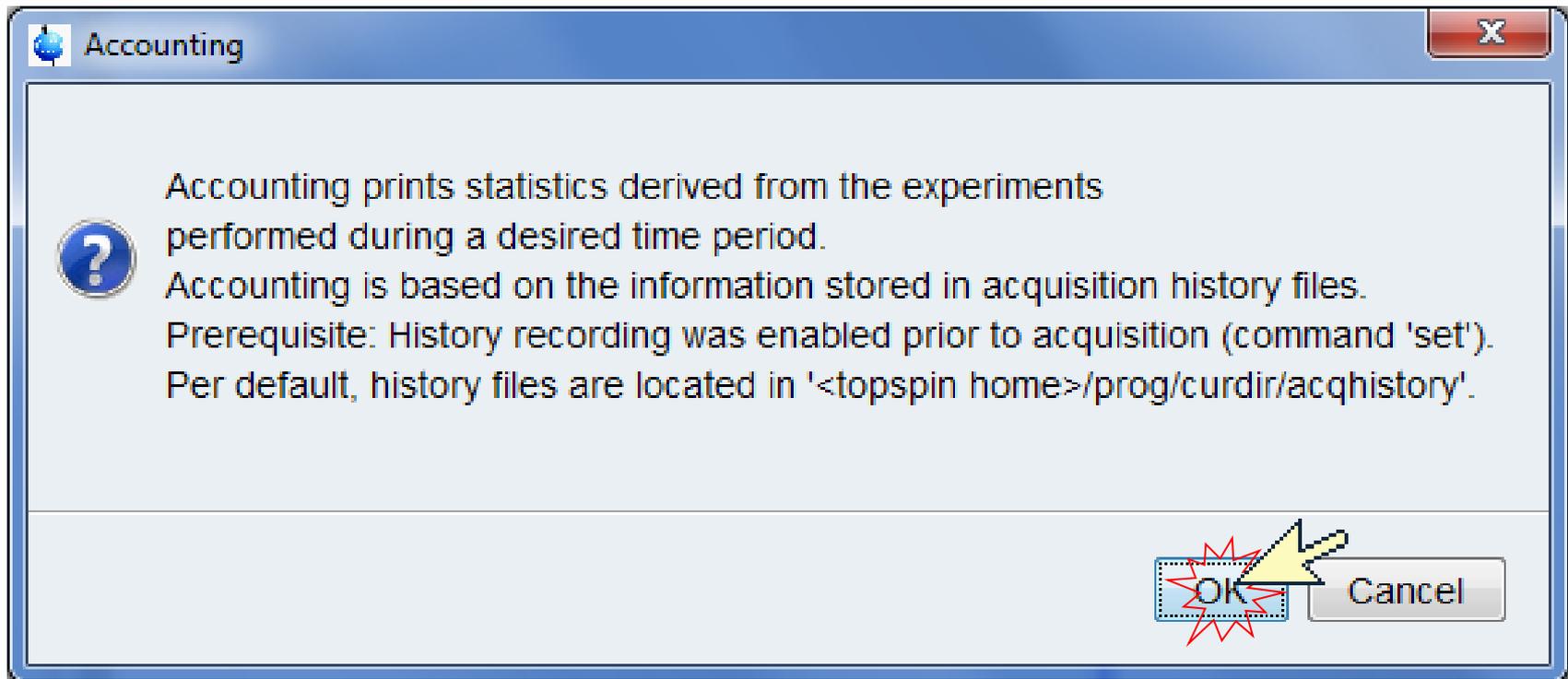
- The accounting file (a file per day; XML format) will be stored in the <topspinhome>/prog/curdir/acqhistory directory.
- The accounting file can be opened via Manage → Spectrometer → Spectrometer Usage (account)



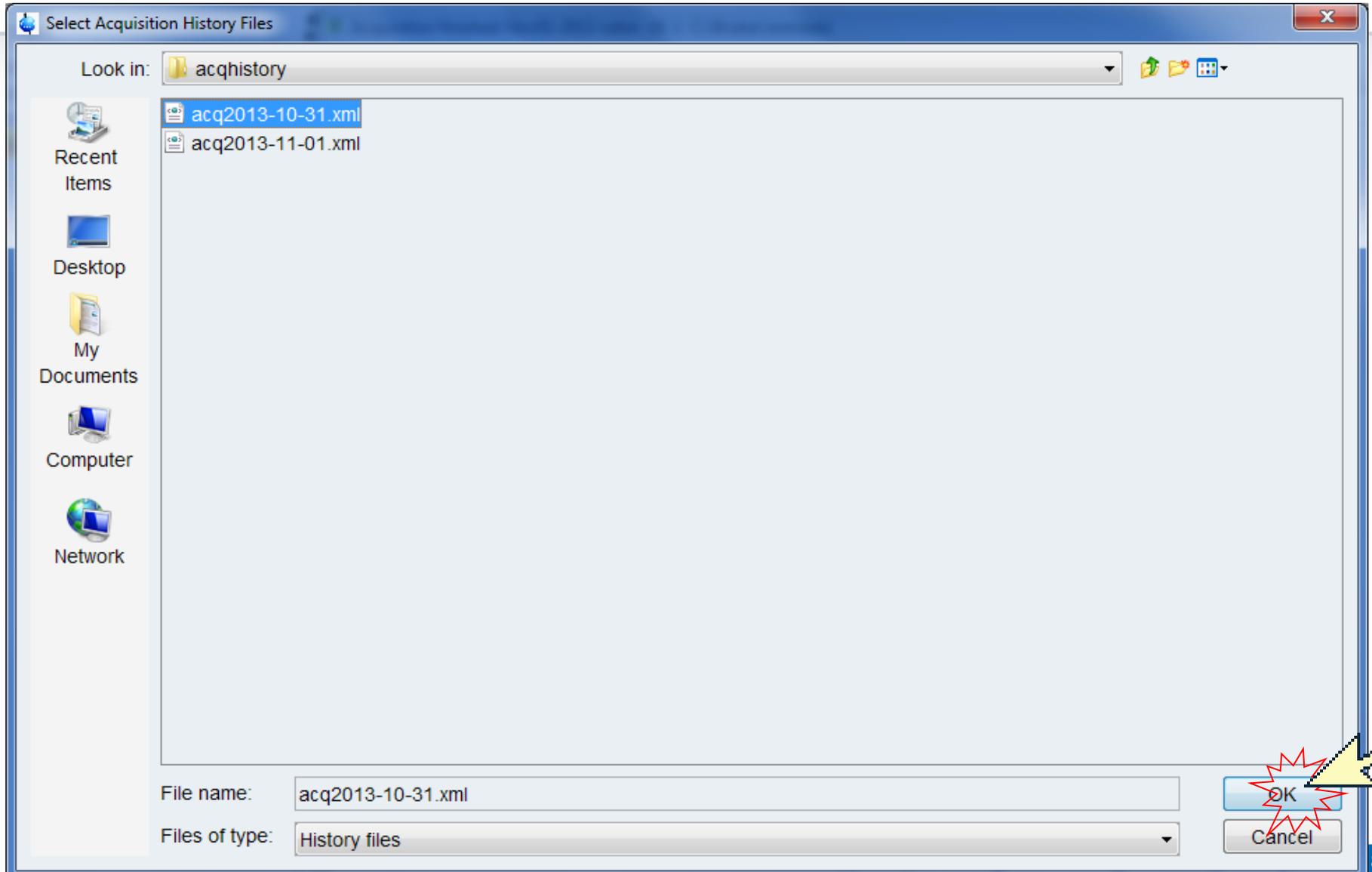
- or the TopSpin command ***account***



Accounting in TopSpin



Accounting in TopSpin



Accounting in TopSpin



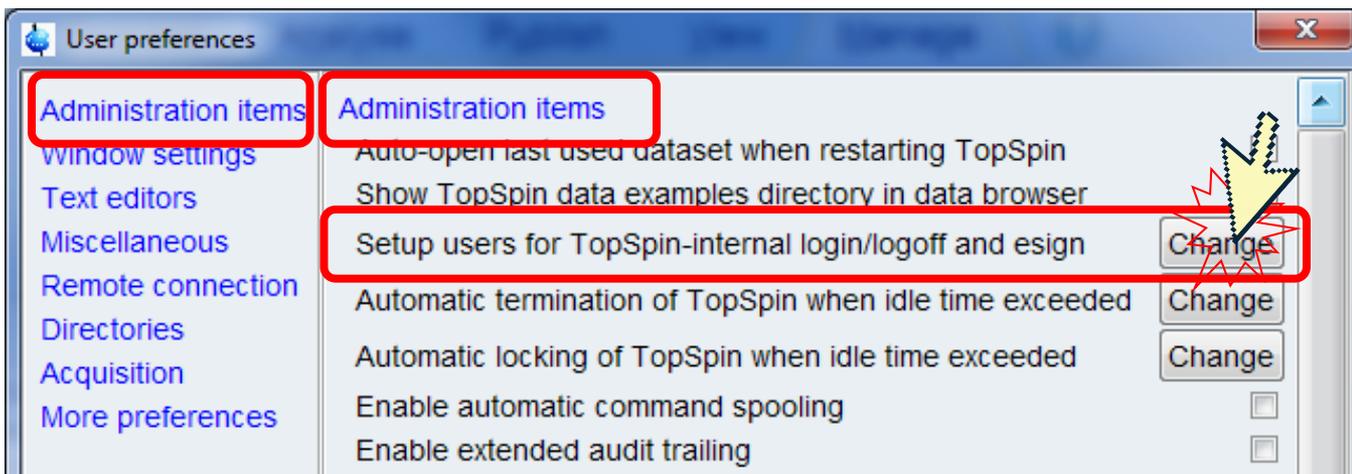
```
Accounting Protocol
File Edit Search
1 Accounting Protocol
2 Created: 2013-11-01 17:46:14 CET
3 TopSpin: 3.2
4
5 User: nmrsu / Sven
6 #Datasets  Dim    Exp.Time  Failed
7          4      1      3.30 min    0
8          0      2      0.00 sec    0
9          0     >2      0.00 sec    0
10 Sum =
11          4    Any      3.30 min    0
12
13
14 Period
15 From: 2013-11-01 17:29:51 CET
16 To:   2013-11-01 17:36:36 CET
17
18
```

1 : 1

Accounting in TopSpin



- Using TopSpin-internal users you are able to account user-specific.



Accounting in TopSpin



- Using TopSpin-

User Administration - uadmin

Enforce "login" for working with TopSpin

User ID	User Name	Allowed Signature Meanings
Robin	Robin	Operator
Sven	Sven	Operator

Add User Change Meanings Remove User Passwd Length

Save Save+Close Help Cancel

Bruker TopSpin 3.2 on AVIII300Z420W7 as nmrsu / Sve

Start Acquire Process

*8 *2 /8 /2 ppm

User preferences

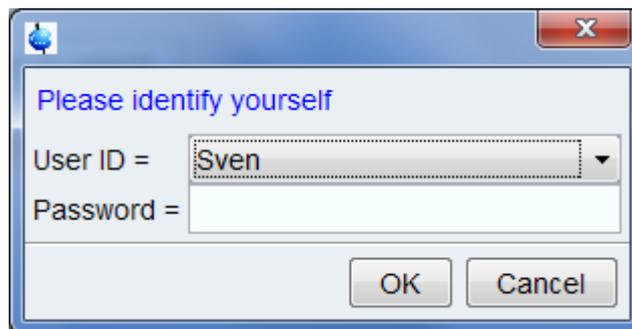
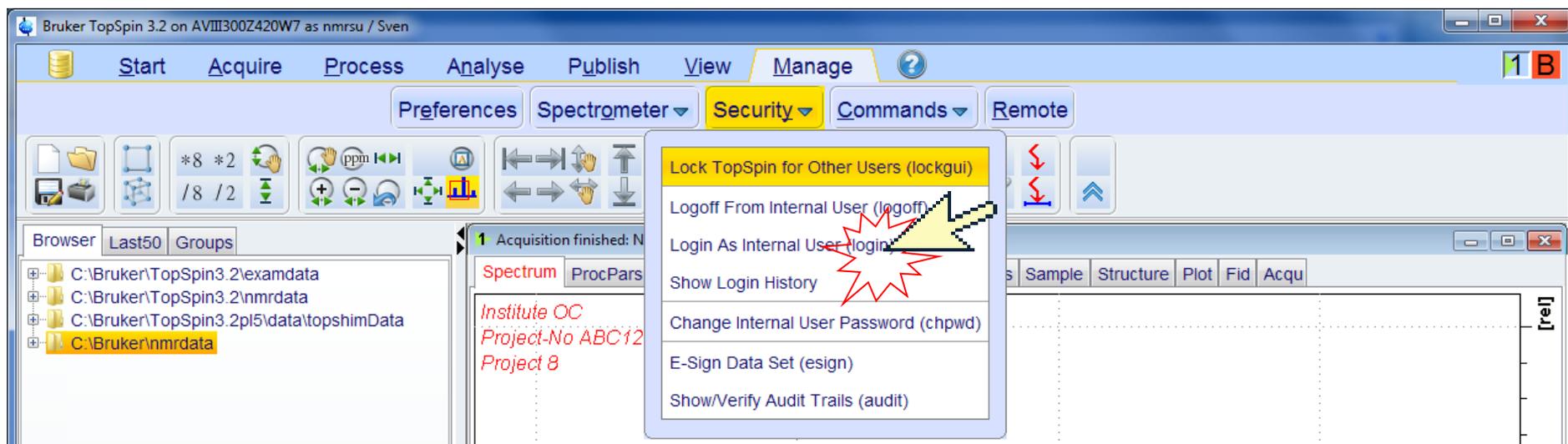
- Administration it
- Window settings
- Text editors
- Miscellaneous
- Remote connect
- Directories
- Acquisition
- More preference

1 B

Accounting in TopSpin



- Switching the user can be executed with the commands “login” / “logoff”.



Accounting in TopSpin

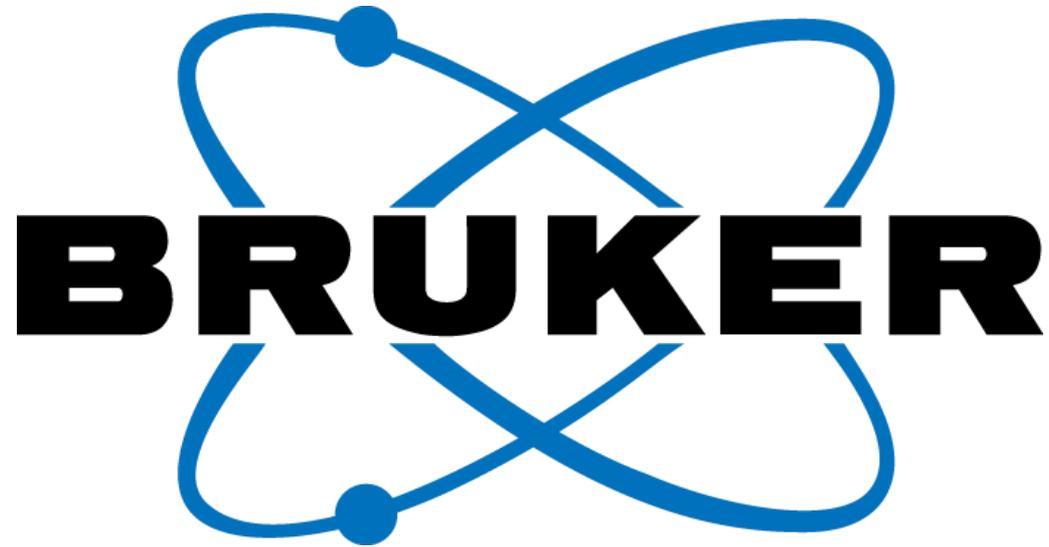


```
Accounting Protocol
File Edit Search
1 Accounting Protocol
2 Created: 2013-11-01 17:44:16 CET
3 TopSpin: 3.2
4
5 User: nmrsu
6 #Datasets  Dim      Exp.Time  Failed
7           2       1       1.07 min  0
8           0       2       0.00 sec  0
9           0      >2       0.00 sec  0
10 Sum =
11          2      Any       1.07 min  0
12
13
14 Period
15 From: 2013-10-31 16:44:10 CET
16 To:   2013-10-31 16:48:33 CET
17
18
19 -----
20
21
22 User: nmrsu / Robin
23 #Datasets  Dim      Exp.Time  Failed
24           4       1       1.59 min  1
25           0       2       0.00 sec  0
26           0      >2       0.00 sec  0
27 Sum =
28          4      Any       1.59 min  1
29
30
31 Period
32 From: 2013-10-31 16:50:28 CET
33 To:   2013-10-31 16:51:44 CET
34
35 The following datasets had "acquisition failed" status:
36
37 C:\Bruker\nmrdata\Oct31-2013-robin\16\pdata\1
38 failed: Raw data file 'fid' not found: No such file or directory Oct31-2013-robin 16 1 C:\Bruker\nmrdata
39
40 -----
```

Accounting in TopSpin



- Accounting will not work with ***multizg***.
- To use accounting for multiple experiments please use ***multicmd*** and set up the measurements with the spooler.
- To use accounting in combination with AU Programs please insert instead of the term
ZG
the term
XCMD("sendgui zg");



Innovation with Integrity