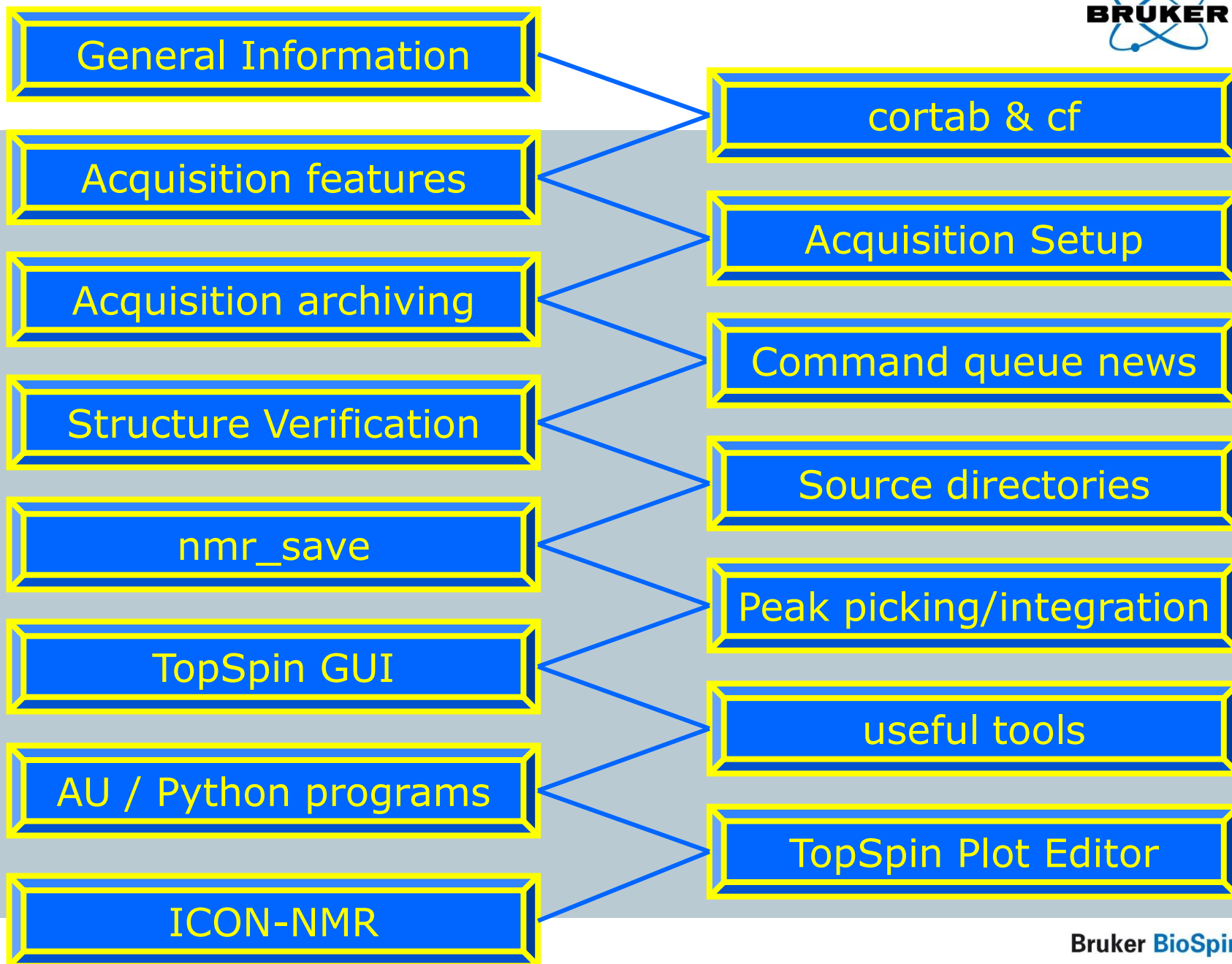


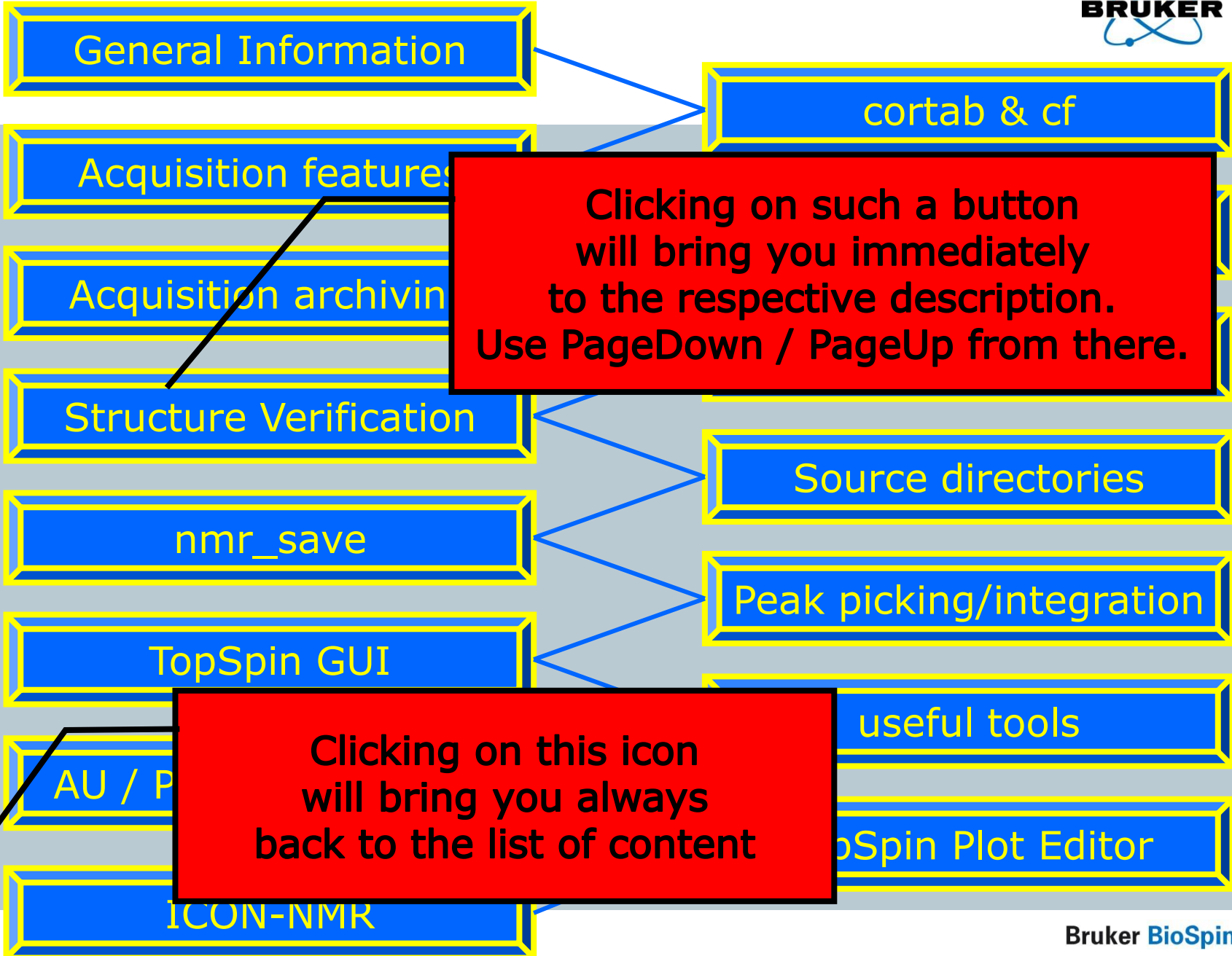
# Release Letter TopSpin 2.1

## Picture Presentation

# Content



# How to use this document



# How to use this document

General Information

cortab & cf

Acquisition features

Clicking on such a button will bring you immediately to the respective description. Use PageDown / PageUp from there.

Acquisition archiving

Structure Verification

Tip:  
Acrobat Reader offers nice full screen view  
→ press ‚Ctrl‘ and ‚L‘  
(press ‚Esc‘ to exit)

Directories

Peak picking/integration

TopSpin GUI

useful tools

AU / P

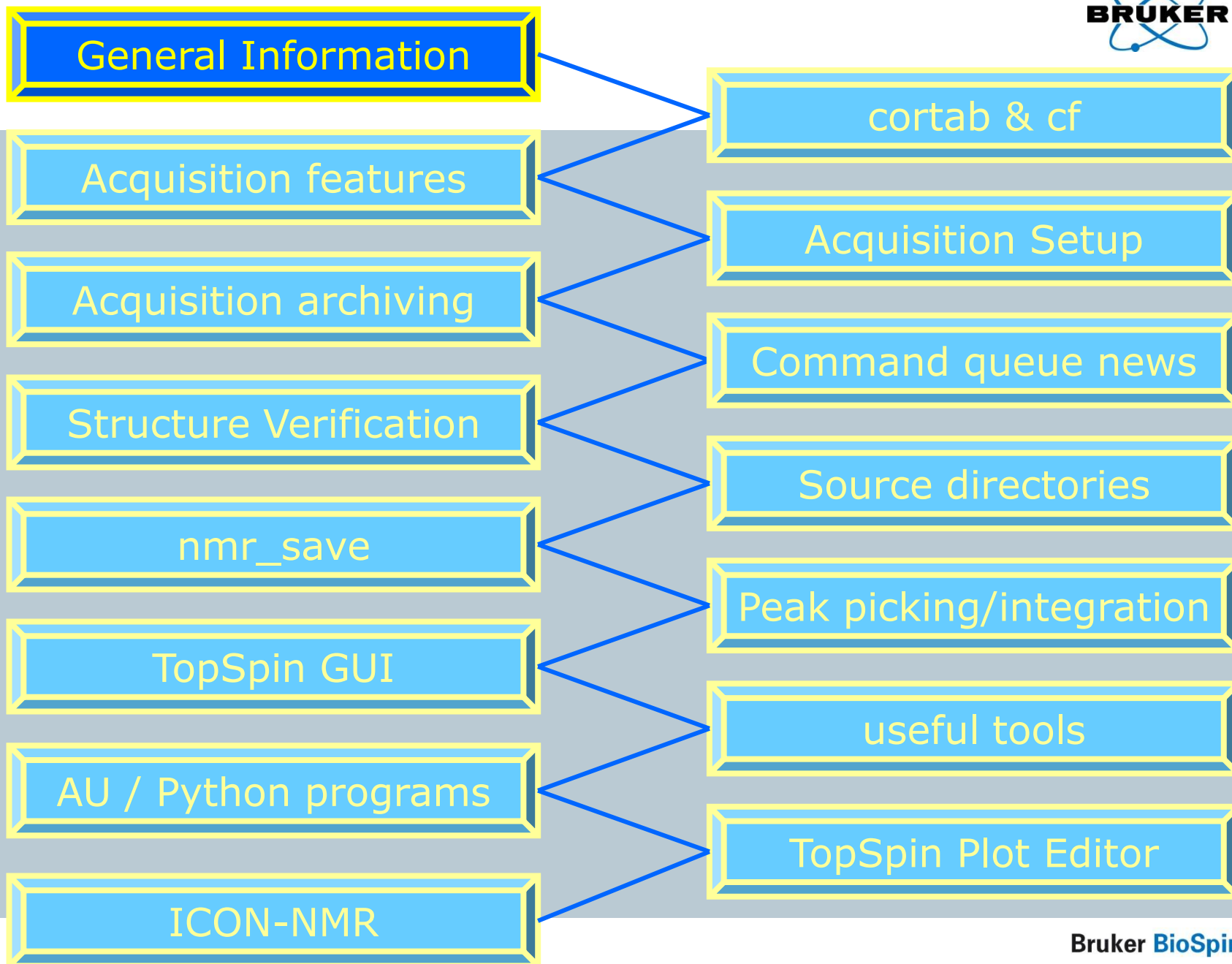
Clicking on this icon will bring you always back to the list of content

TopSpin Plot Editor

ICON-NMR



# Content



# Spectrometer support - TopSpin



	Avance III	Avance II	Avance I	D*X
TopSpin 2.1	✓	✓	✓	-
TopSpin 2.0	✓	✓	✓	-
TopSpin 1.3	-	✓	✓	✓
TopSpin 1.2	-	-	✓	-
TopSpin 1.1	-	-	-	-

# OS support - TopSpin 2.1



	RHEL WS 3	RHEL WS 4	RHEL WS 5	W2k	Win XP	Win Vista
Processing	✓	✓	✓	✓	✓	✓
Acquisition	✓	✓	-	-	✓	✓

32 bit version

# Support – Spectrometer/TopSpin/OS



	D*X	AVI	AVII	AVIII
TopSpin 1.3	✓	✓	✓	✓
TopSpin 2.0	-	✓	✓	✓
TopSpin 2.1	-	✓	✓	✓
Windows 2000	✓	✓ (1.3)	✓ (1.3)	-
Windows XP	✓	✓	✓	✓
Windows Vista	-	✓ (2.1)	✓ (2.1)	✓ (2.1)
RHEL WS 3	✓	✓	✓	✓
RHEL WS 4	✓ (1.3pl6)	✓ (2.0)	✓ (2.0)	✓
RHEL WS 5	-	-	-	-

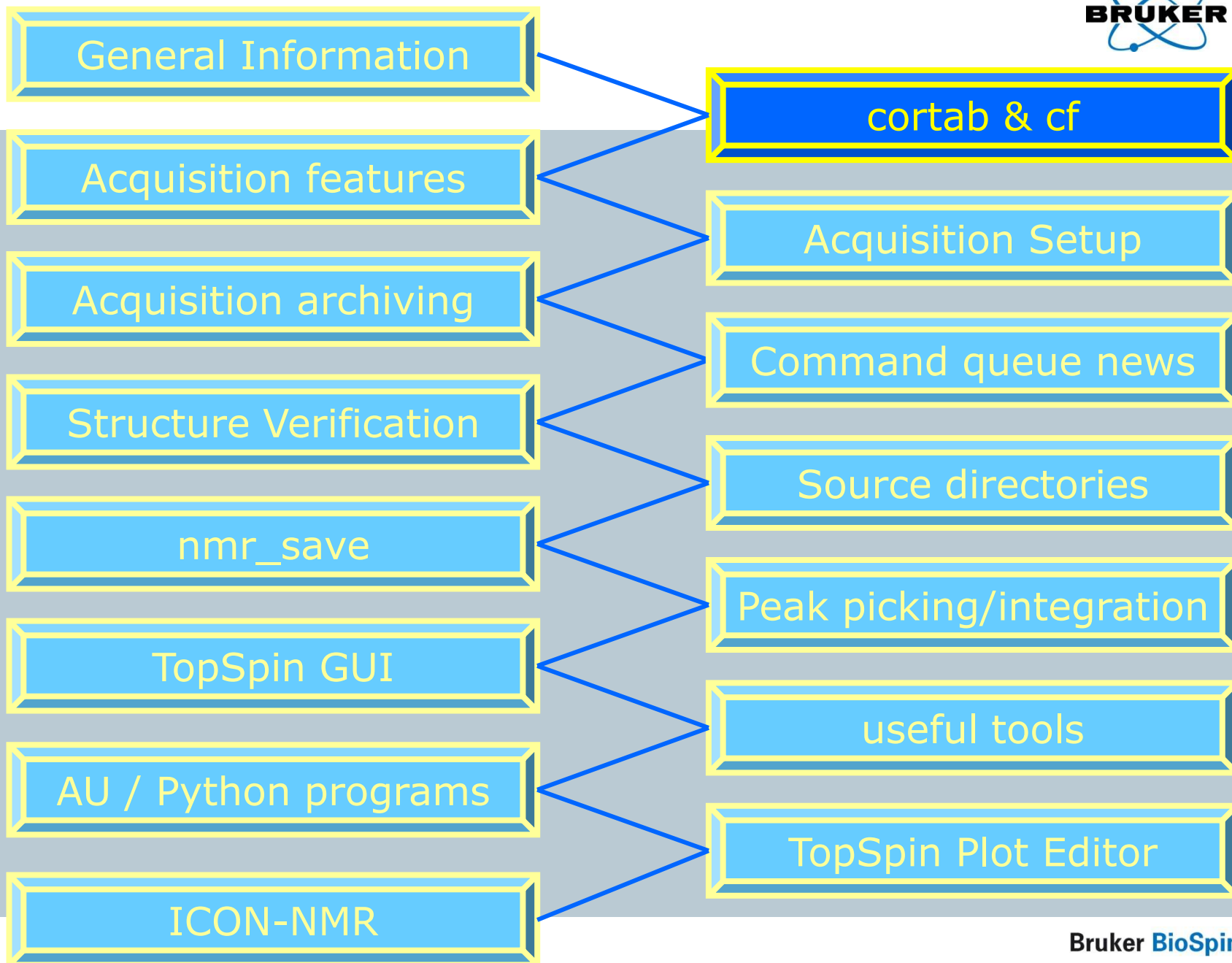
TopSpin 2.1 is a minor upgrade from 2.0

All you need is:

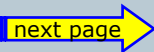
 a TopSpin 2.0 license

 a TopSpin 2.1 DVD

# Content



New procedure to correct  
phase dependency of receiver gain

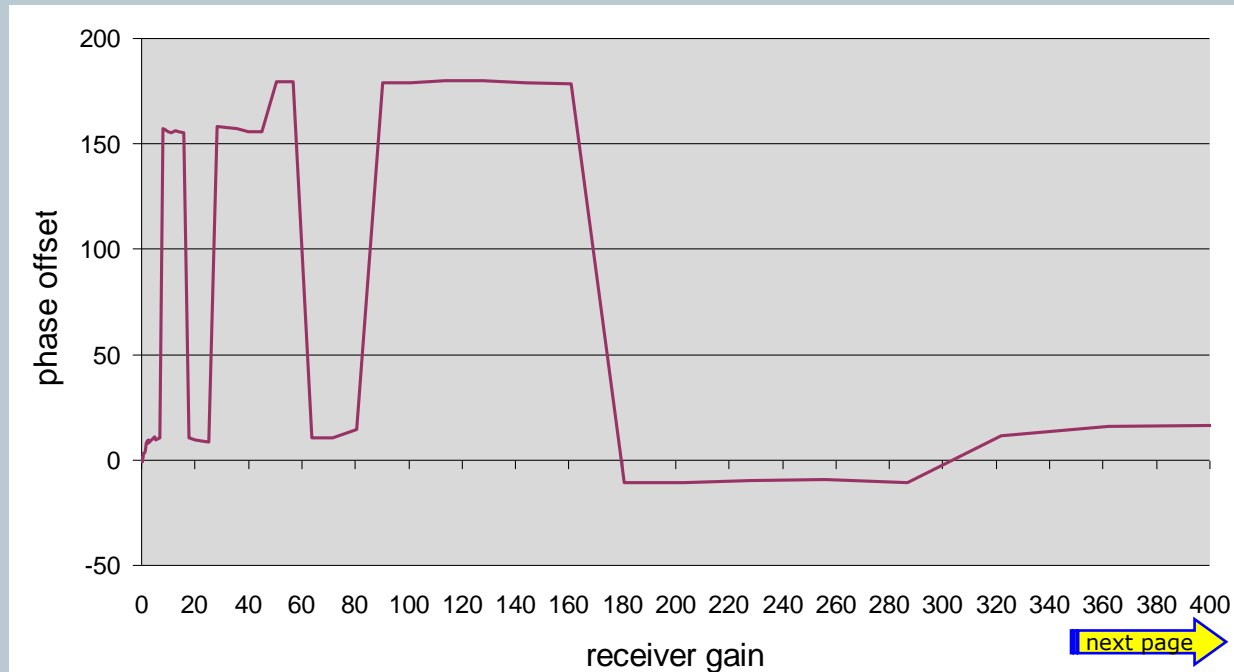
next page 




Because of the phase dependency of the RG value there is a phase offset if a 2D phasing is done on a basis of a 1D with different RG.

Cortab offers new functionality **REC Phase Linearization** which corrects this situation.

With TopSpin 2.1 the receiver phase correction should be done together with every new cortab.



[next page](#) 

If the receiver gain adjustment for a certain nucleus fails during a multiple-experiment session (three experiments or more), the failed experiment will be skipped and the system continues with the next nucleus.

The skipped nuclei are collected and displayed at the end of the linearization procedure.

New button that allows editing of amplifier peak power values in an existing cortab table.

Cortab now allows the user  
to set up a queue of experiments  
easily and quickly.

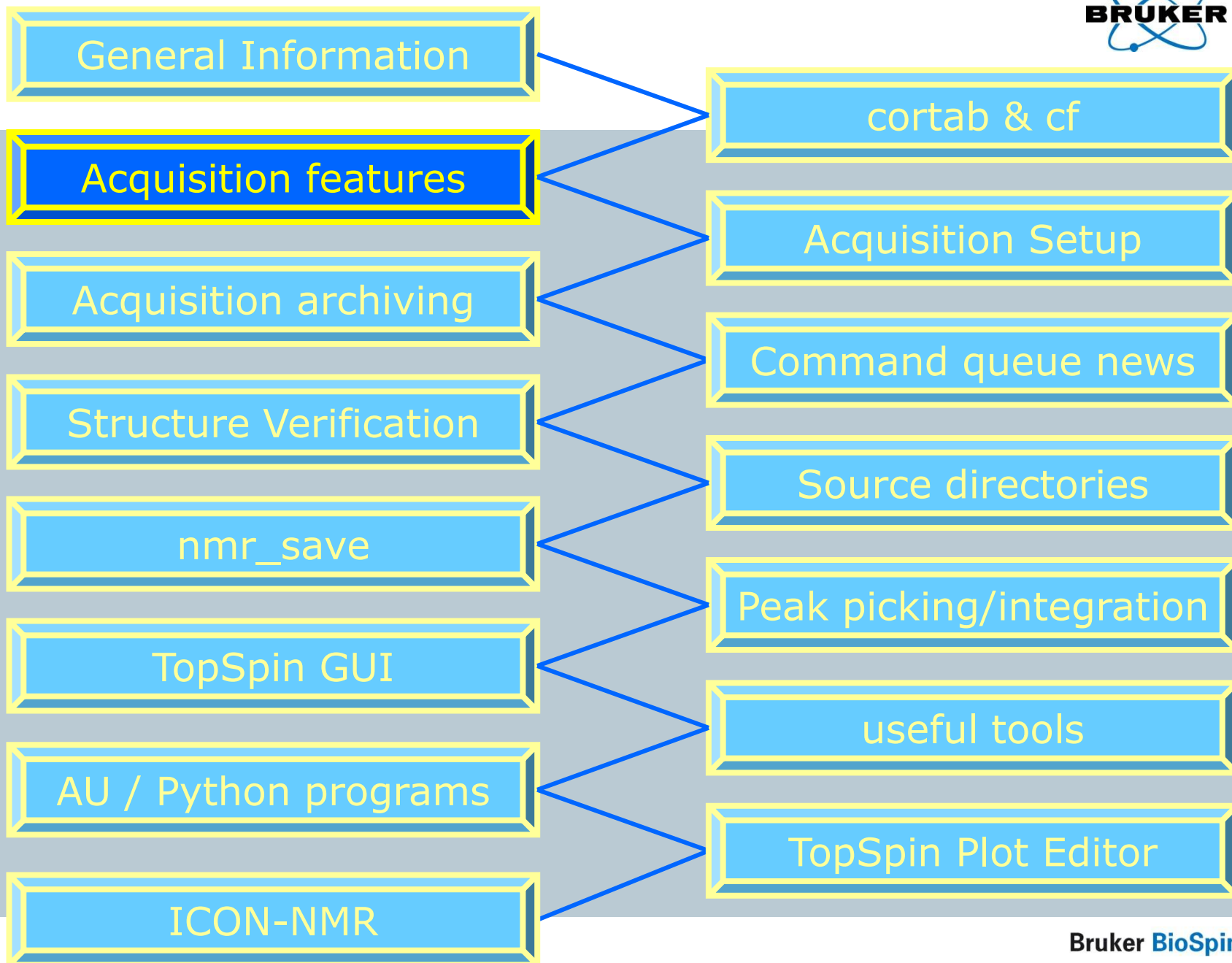
cf supports broad band type amplifier modules  
as BB (not X or H)

cf supports  $^{19}\text{F}$  lockswitch

Wobble is now able to switch  
the switchbox between Proton and  $^{19}\text{F}$



# Content



# Pulse program syntax enhancement - 1



The power setting after a shape pulse remains as it was in the last point of the shape.

In previous TOPSPIN versions this was reset to the default power of the channel where the shape was executed.

# Pulse program syntax enhancement - 2



**go=nn cpd2:f2 finally do:f2**

"**do**" (decoupler off) is no longer needed at the place where the "**go**" loops back to and in the code following

# Pulse program syntax enhancement - 3



Now power calculations like:  
**pl5=sp23; pl3=cnst23;**  
are possible

# Pulse program syntax enhancement - 4



cpd following cpd without **'do'** (decoupler off) in  
between

# Pulse program syntax enhancement - 5



Two new parameters:

## **PLSTRT** and **PLSTEP**

enable the automatic replacement of setting the pulse power level via slow analog attenuators by fast and artifact free amplitude setting using the digital modulation of the SGU.

TopSpin 2.1 supports the fast NMR method APSY  
(Automated Projection Spectroscopy)

APSY can be started under:

**Spectrometer → Fast Acquisition Methods**

APSY requires a separate license. A free demo license can be ordered anytime under:

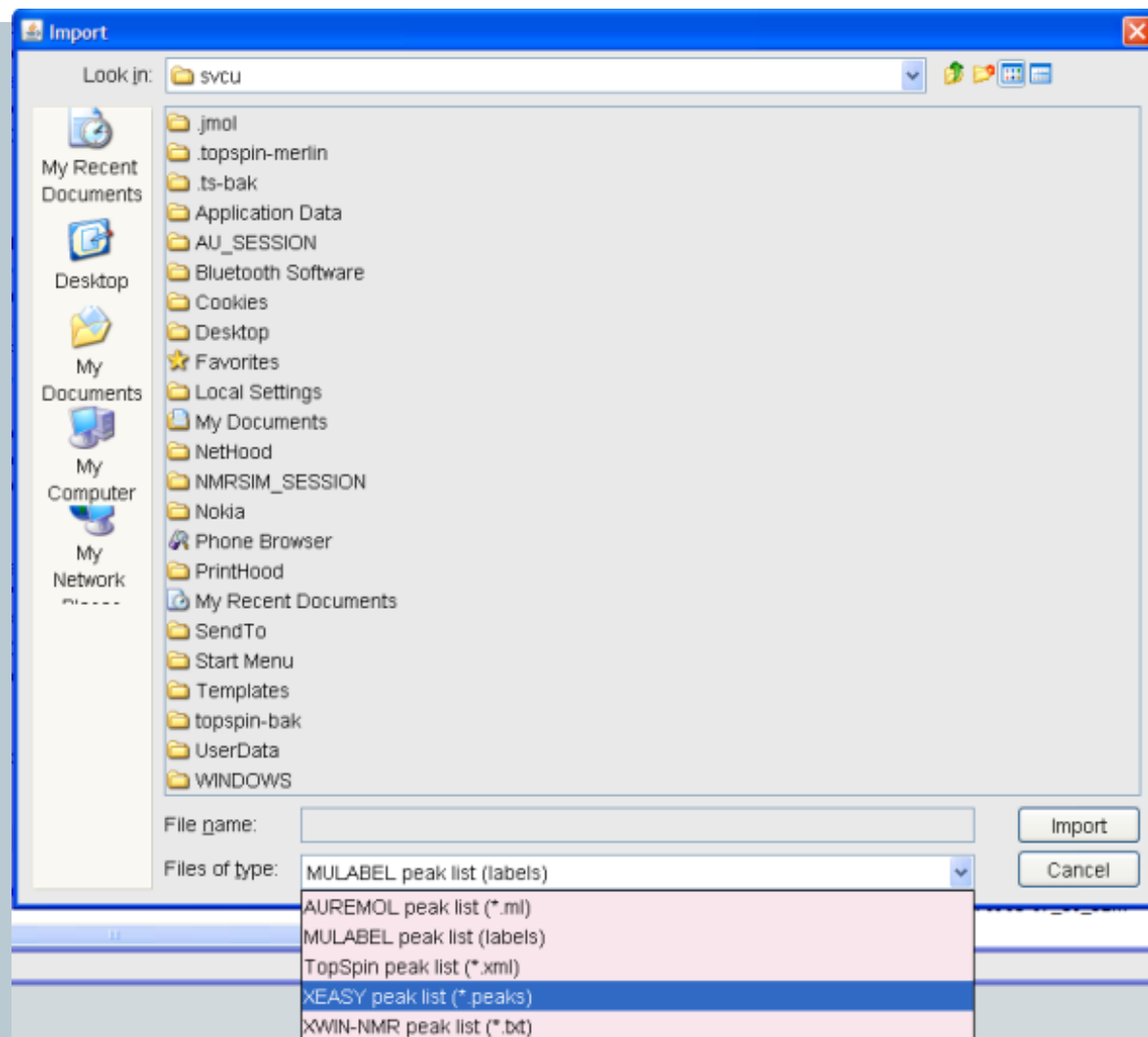
[www.bruker-biospin.com](http://www.bruker-biospin.com)



# XEASY peak list files can be im/exported



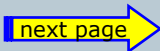
XEASY peak lists  
are the result of  
the fast NMR  
method **APSY**



TopSpin 2.1 allows comfortable multiple receiver acquisition.

Functionality of software routing has been enhanced by adding respective receiver setup.

For detailed information enter **help AVIIMultiReceive** in TOPSPIN 2.1 command line.



# Multiple Receiver



**Edit Spectrometer Parameter**

frequency	logical channel	amplifier	preamplifier	receiver	observe channel
BF1 500.13 MHz	NUC1	X 300 W	1H LNA	REC1	NUC1
SFO1 500.132249 MHz	F1		XBB19F 2HS		F1
OFS1 2249.21 Hz	1H				1H
BF2 500.13 MHz	NUC2	H/F 1000 W	2H		NUC2
SFO2 500.133088 MHz	F2	H 150 W	HPHP 19F/1H	REC2	F2
OFS2 3088.51 Hz	off				off
BF3 500.13 MHz	NUC3	X 300 W			NUC3
SFO3 500.133088 MHz	F3				F3
OFS3 3088.51 Hz	off				off

Legend:  
— : cable wiring  
- - : possible RF routing

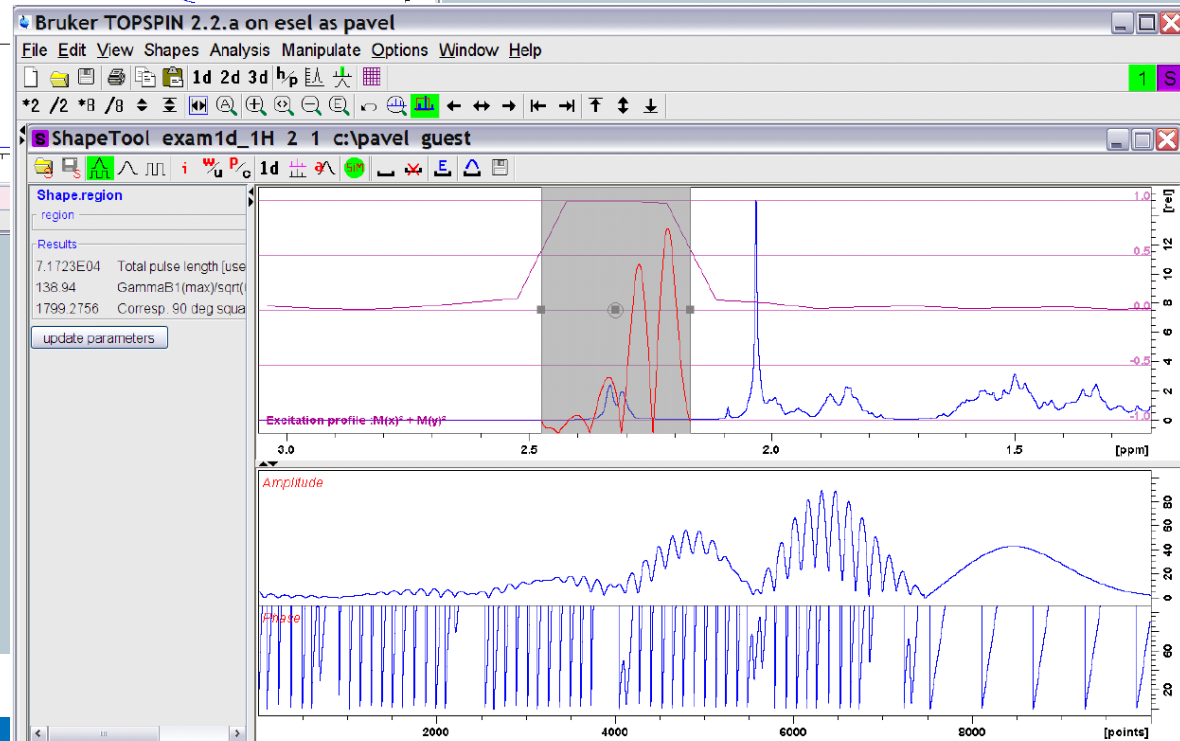
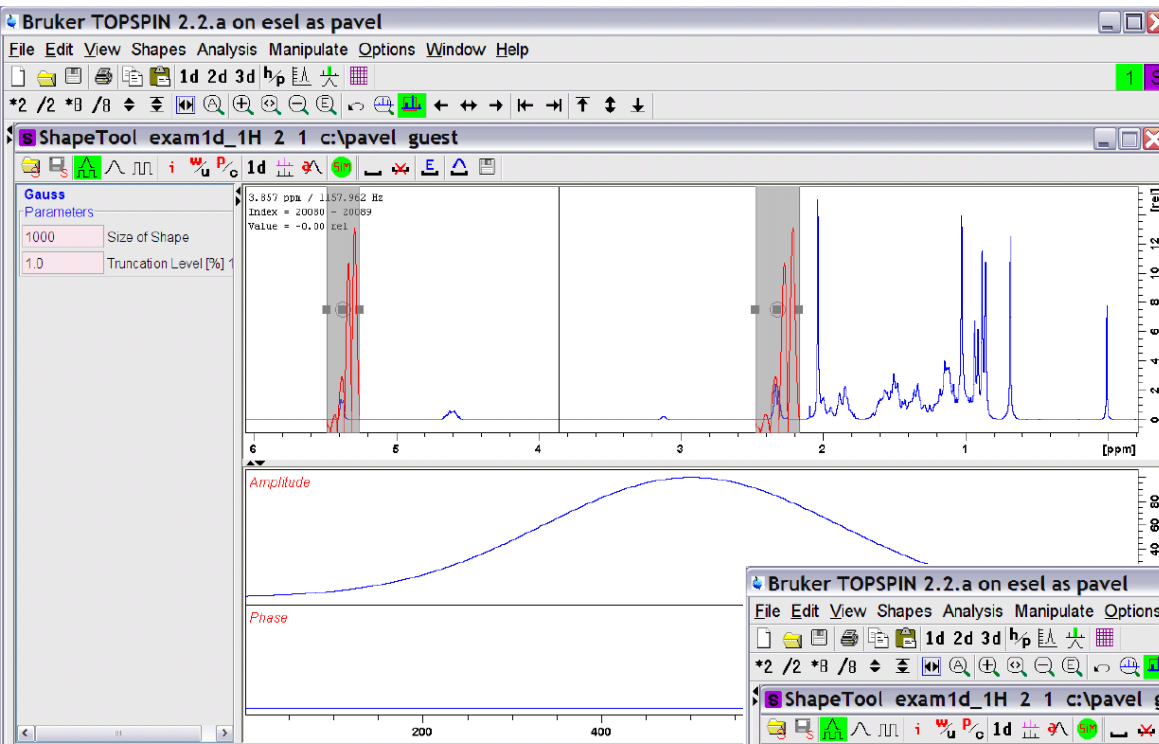
Settings:  
 show receiver routing  
 show RF routing

Buttons: Save, Switch F1/F2, Switch F1/F3, Add a logical channel, Remove a logical channel, Default, Info, Param, Close

New feature allows interactive definition of excitation regions in Shape-Tool.

All parameters, such as power level, pulse length and the excited region, are coupled together for easy setup of selective experiments.

# Shape tool



The Eretic channel can be defined during spectrometer configuration.

Eretic setup is now enabled for all AVANCE systems by the command  
**edasp**

**Edit Spectrometer Parameter**

frequency	logical channel	amplifier	preamplifier
BF1 0.0 MHz	NUC1		
SFO1 0.0 MHz	<input type="button" value="F1"/>	<input type="button" value="SGU1"/>	
OFS1 0.0 Hz			
BF2 0.0 MHz	NUC2		
SFO2 0.0 MHz	<input type="button" value="F2"/>	<input type="button" value="SGU2"/>	
OFS2 0.0 Hz			

**Diagram:** X 300 W, 1H 100 W, 2H 150 W (amplifiers) connected to 1H/2H 1H, 1H/2H 2H, XBB19F 2HS (preamplifiers).

settings

- show receiver routing
- add eretic

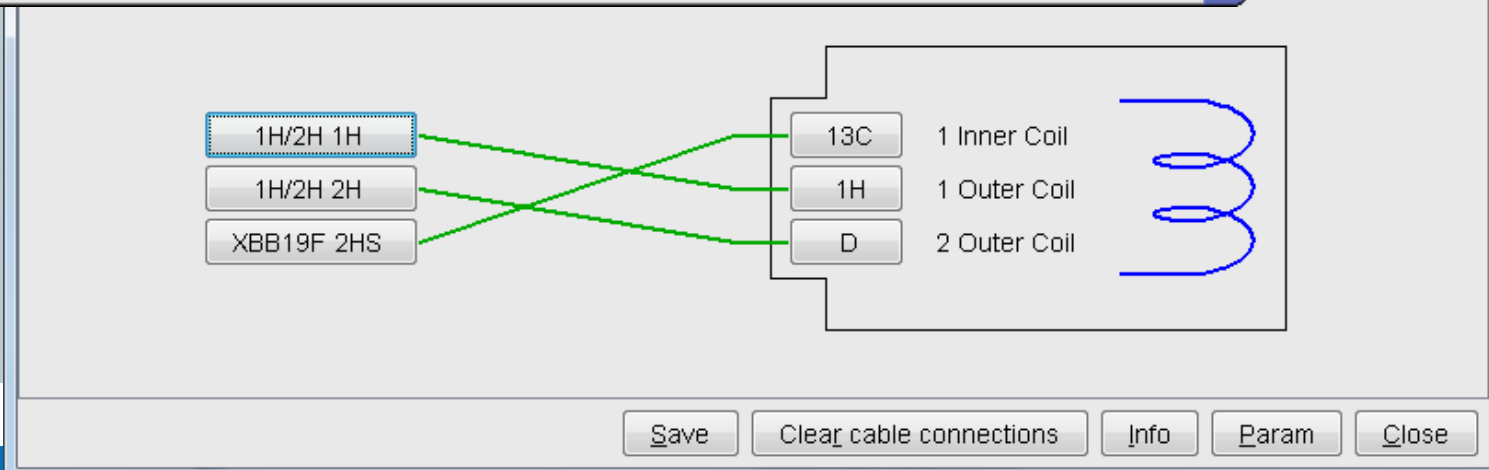
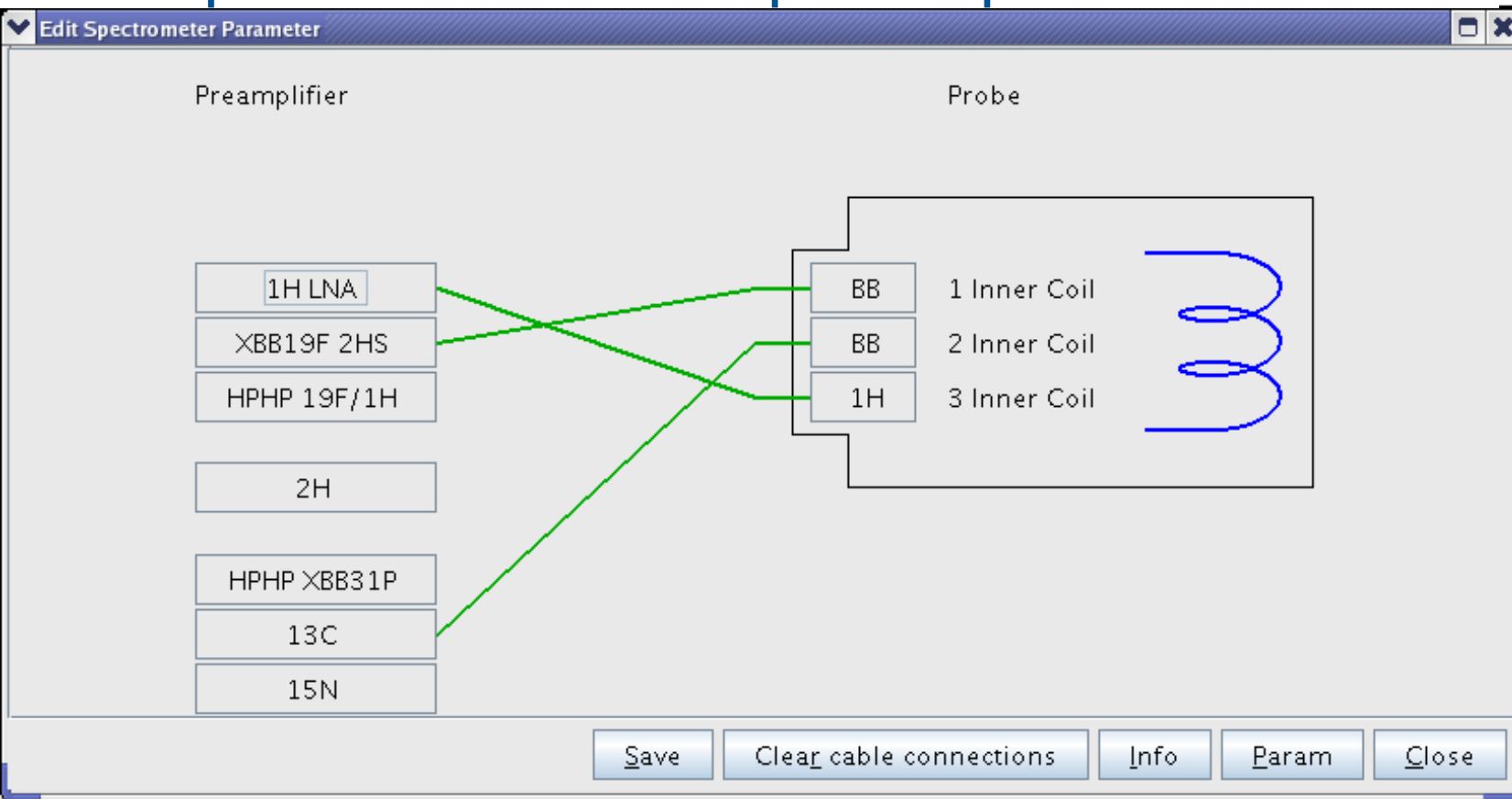


**paropt** can now be stopped  
with the command **stop**

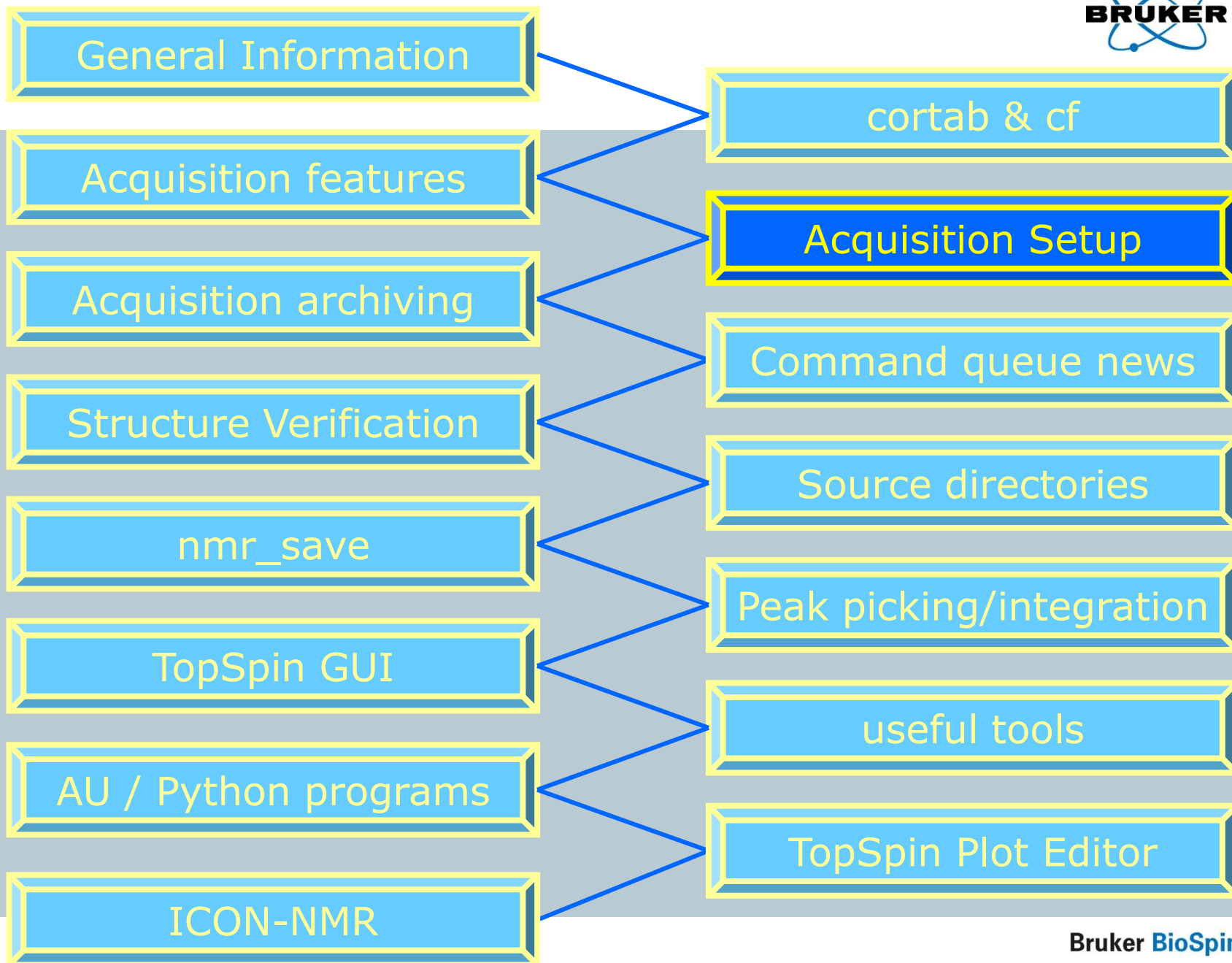
When exiting **edhead** it displays a new window where the preamp-probe connection can be defined.

This is used for power check to find out the correct peak power limit of the probe (e.g. in case of a TBI probe for the  $^{13}\text{C}$  selective input or the BB input, respectively).

# Examples for edhead preamp connection



# Content



# Acquisition and processing up to 8D is supported

The screenshot displays the Bruker TopSpin software interface. A red arrow points from the text 'Acquisition and processing up to 8D is supported' to a '1,2,...' button in the 'ProcPars' tab. A warning dialog box titled 'parmode' is overlaid on the interface, displaying the following text:

**Warning!**

You are about to change the dimension of the current dataset. As a consequence an existing FID will be deleted!

Change acquisition dimension of dataset from 1D to **2D**

The dialog box includes 'OK' and 'Cancel' buttons. A dropdown menu is open, showing options from 2D to 8D. The main interface shows the 'ProcPars' tab with the following parameters:

Parameter	Value	Description
PULPROG	zgpg30	Current pulse program
AQ_mod	DQD	Acquisition mode
TD	65536	Size of fid
NS	256	Number of scans
DS	4	Number of dummy scans
TD0	1	Loop count for 'td0'
▼ Width		
SW [ppm]	236.5959	Spectral width
SWH [Hz]	17857.143	Spectral width
AQ [s]	1.8350580	Acquisition time
FIDRES [Hz]	0.272478	Fid resolution
FW [Hz]	90000.00	Filter width
▼ Receiver		
RG	32768	Receiver gain
DW [μs]	28.000	Dwell time
DWOV [μs]	3.500	Oversampling dwell time
DECIM	8	Decimation rate of digital filter
DSPFIRM	rectangle	DSP firmware filter

# Acquisition and processing up to 8D is supported



The screenshot displays the Bruker TopSpin software interface. A warning dialog box titled "parmode" is open, displaying the following text:

**Warning!**

You are about to change the dimension of the current dataset. As a consequence an existing FID will be deleted!

Change acquisition dimension of dataset from 1D to **5D**

Buttons: **OK**, **Cancel**

The background interface shows the "exam1d\_13C" experiment parameters window. The "Experiment" section includes:

- PULPROG: zgpg30
- AQ\_mod: DQD
- TD: 65536
- NS: 256
- DS: 4
- TD0: 1

The "Width" section includes:

- SW [ppm]: 236.5959
- SWH [Hz]: 17857.143
- AQ [s]: 1.8350580
- FIDRES [Hz]: 0.272478
- FW [Hz]: 90000.00

The "Receiver" section includes:

- RG: 32768
- DW [μs]: 28.000
- DWOV [μs]: 3.500
- DECIM: 8
- DSPFIRM: rectangle

The "Installed probe" is listed as "5 mm Multinuclear inverse Z-grad".

# Acquisition and processing up to **8D** is supported



TopSpin 2.1 now provides examples for  
4D experiments (HSQC-NOESY-HSQC):

- 4D parameter sets (ending with 4D)  
and
- 4D pulse programs (ending with 4d).

# Acquisition and processing up to 8D is supported



Bruker TopSpin on merlin as svcu

File Edit View Spectrometer Processing Analysis Options Window Help

\*2 /2 \*8 /8 \*X ± 1

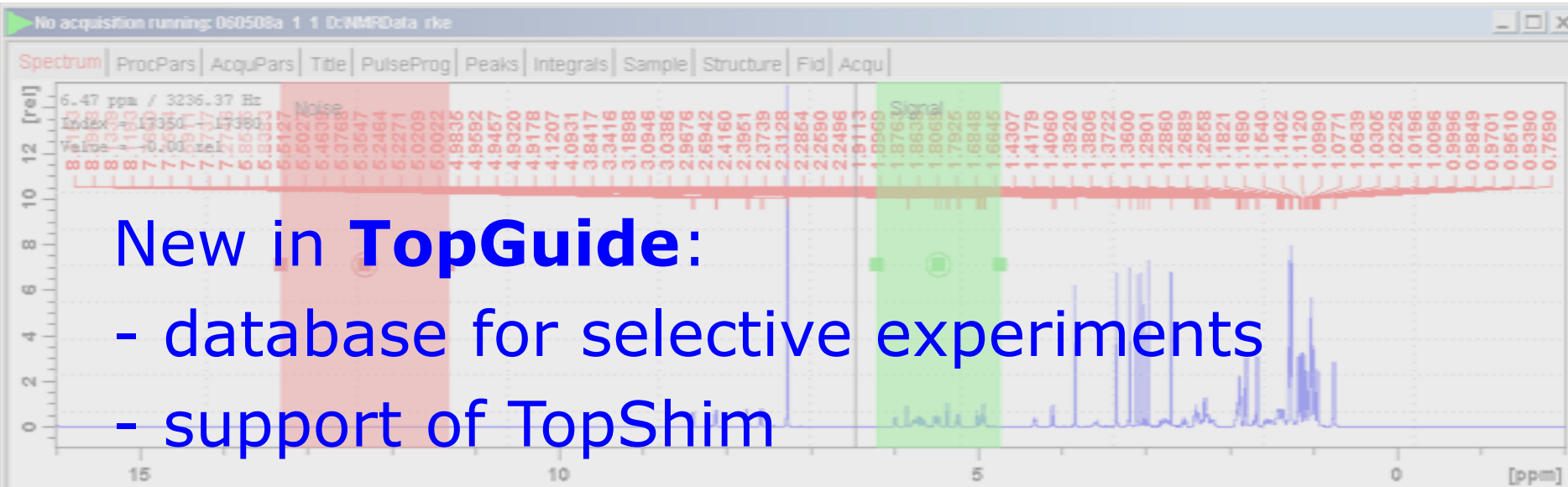
exam1d\_13C 1 8 F:\Bruker\topspin2.0 guest

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Fid

Installed probe: 5 mm Multinuclear inverse Z-grad

	F5	F4	F3	F2	F1	Frequency axis
Experiment						
Width						
Receiver						
Nucleus						
Durations						
Power						
Program						
Probe						
Lists						
Wobble						
Lock						
Automation						
Miscellaneous						
User						
Routing						
	PULPROG: zgpg30					Current pulse
	AQ_mod: DQD					Acquisition mc
	FnMODE: undefined					Acquisition mc
	TD: 65536	256	256	256	256	Size of fid
	NS: 256					Number of sca
	DS: 4					Number of dur
	TD0: 1					Loop count fo
	SW [ppm]: 236.5959					Spectral width
	SWH [Hz]: 17857.143					Spectral width
	IN_F [μs]: 322.61096191					Increment for
	AQ [s]: 1.8350580					Acquisition tirr
	FIDRES [Hz]: 0.272478					Fid resolution
	FW [Hz]: 90000.00					Filter width
	RG: 32768					Receiver gain
	DW [μs]: 28.000					Dwell time





## New in TopGuide:

- database for selective experiments
- support of TopShim

Define reference signal for signal to noise determination ...

Left limit of noise region	13.321
Right limit of noise region	11.321
Left limit of signal region	6.21
Right limit of signal region	4.739

Current signal/noise 681.63

Determine the signal to noise (S/N) of your reference spectrum. The region around the highest signal (green) neglecting the solvent and a noise region (red) of up to 2 ppm are pre-selected.

You should select the signal(s) (green region) you are mainly interested in. The calculated S/N is shown above. It will be used for all further experiments with this sample to estimate a necessary NS (number of scans).

GO

STOP

# Acquisition parameters



Only these nuclei are shown

$^{13}\text{C}$   $\{^1\text{H}\}$

which are used in the pulse program.

All others are collapsed automatically.

The screenshot shows the Bruker TopSpin software interface. The main window is titled "Bruker TopSpin on merlin as svcu". The menu bar includes File, Edit, View, Spectrometer, Processing, Analysis, Options, Window, and Help. The toolbar contains various icons for file operations and data processing. The main window is divided into several panes:

- Browser:** A tree view showing the file structure. The path is C:\NMR data > F:\Bruker\topspin1.3pl6 > F:\Bruker\topspin2.0 > guest > exam1d\_13C > 1 - zgpg30. Other folders like exam1d\_1H, exam2d\_CH, exam2d\_HC, exam2d\_HH, exam3d, exam\_DNMR\_Me, exam\_DNMR\_ipr, and svcu are visible but collapsed.
- AcquPars:** A table of acquisition parameters for two nuclei.

Parameter	Value
Experiment	NUC1
Width	13C
Receiver	O1 [Hz]
Nucleus	O1P [ppm]
Durations	SFO1 [MHz]
Power	BF1 [MHz]
Program	
Probe	
Lists	
Wobble	
Lock	
Automation	
Miscellaneous	
User	
Routing	

The table shows the following values:

- NUC1: 13C
- O1 [Hz]: 7546.77
- O1P [ppm]: 100.000
- SFO1 [MHz]: 75.4752958
- BF1 [MHz]: 75.4677490
- NUC2: 1H
- O2 [Hz]: 1200.52
- O2P [ppm]: 4.000
- SFO2 [MHz]: 300.1312005
- BF2 [MHz]: 300.1300000

# Current probe



The screenshot shows the Bruker TopSpin software interface. The 'AcquPars' tab is active, displaying various parameters for the current experiment. A red box highlights the 'eda' icon in the top toolbar, and another red box highlights the text 'Installed probe: 5 mm Multinuclear inverse Z-grad' in the top right area of the 'AcquPars' window. The 'Experiment' section shows parameters such as PULPROG (zg), AQ\_mod (DQD), TD (65536), NS (16), and DS (4). The 'Receiver' section shows parameters such as RG (32), DW (83.200), DWOV (2.600), DECIM (32), DSPFIRM (sharp(standard)), and DIGTYP (HADC+).

Parameter	Value	Description
PULPROG	zg	Current pulse program
AQ_mod	DQD	Acquisition mode
TD	65536	Size of fid
NS	16	Number of scans
DS	4	Number of dummy scans
RG	32	Receiver gain
DW	83.200	Dwell time
DWOV	2.600	Oversampling dwell time
DECIM	32	Decimation rate of digital filter
DSPFIRM	sharp(standard)	DSP firmware filter
DIGTYP	HADC+	Digitizer type

Current probe is now displayed in **eda**  
→ usage of **getprosol** icon is safer





A status monitor is available for external amplifiers on Avance III systems.

# Amplifier status monitor



Bruker TOPSPIN 2.1.a on titanic as nmrsu

File Edit View Spectrometer Processing Analysis Options Window Help

ACQ: es 1 1 /opt/alpha es

Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Fid Acqu

File: zgpg30 (/opt/alpha/exp/stan/nmr/lists/pp/user)

```
;$CLASS=HighRes
;$DIM=1D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

;$OWNER=Bruker
#include <Avance.incl>
#include <Delay.incl>

"d11=30m"

"DELTA=d1-100m"

1 ze
d11 p112:f2
2 30m do:f2
10u p113:f2
d11 cpd2:f2
DELTA
4u do:f2
10u p112:f2
100m cpd2:f2
p1*0.33 ph1
go=2 ph31
30m do:f2 p113:f2 mc #0 to 2 F0(zd)
exit

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

next page

Amplifier Control  13C 1H	Acquisition information scan: 54 / 1024 residual time: 1h2m41s experiments: 1 / 1	Fid Flash 	Lock 	Sample 	POWCHK 	Spooler running: 0 queued: 0 delayed: 0	BSMS status message <b>Δ Z3 -3</b> Autoshim ✓ Locked ✓ Error	Time 15:58 Jan 03
---------------------------------	--	---------------	----------	------------	------------	--	--	-------------------------

## Amplifier Control



# Amplifier status monitor



The screenshot shows the Bruker TOPSPIN 2.1.a software interface. The main window displays acquisition parameters for a 13C NMR experiment. The acquisition is currently running, as indicated by the 'STOP' button being disabled. The status bar at the bottom shows the current scan (93 / 1024) and the residual time (1h0m9s). The status bar also displays the current acquisition parameters (13C, 1H) and the current status (Running, Locked, Error).

**Acquisition Information:**

- PULPROG = zgpg30
- NUC1 = 13C
- SW = 298.823
- SMH = 18028.8
- TD = 65536
- EXPERIMENTS = 1/1
- SCANS = 93/1024
- RES. TIME = 1h0m9s/1h6m13s

**Status Bar:**

- Amplifier Control: 13C 1H
- Acquisition information: scan: 93 / 1024, residual time: 1h0m9s, experiments: 1 / 1
- Fid Flash: [Indicator]
- Lock: [Indicator]
- Sample: [Indicator]
- POWCHK: [Indicator]
- Spooler: running: 0, queued: 0, delayed: 0
- BSMS status message:  $\Delta Z2 -2$
- Time: 16:00 Jan 03



Show routing information of current acquisition (edsp)  
Stop acquisition

Show routing information of current acquisition (edsp)  
Stop acquisition

# Autoshim on/off



The screenshot displays the Bruker TOPSPIN 2.1.b.13 software interface. A context menu is open over the BSMS status monitor, listing several options. A yellow callout box highlights the text: "Autoshim on/off available from context menu of BSMS status monitor." The BSMS status monitor at the bottom right shows a red "Z -2" and "Autoshim" with a checkmark, indicating it is on.

**Autoshim on/off available from context menu of BSMS status monitor.**

- Toggle between  $^1\text{H}$  and difference mode
- Show status message
- Show last error message
- Clear error message
- Toggle autoshim mode (command autoshim on/off)
- Toggle lift on /off (command ej/ij)
- Toggle sample rotation (command ro on/off)

zg: stored TD(F1)=53 into /opt/ts21b13/data/nmrstu/n

Amplifier Control 1H	Acquisition information scan: 16 / 16 residual time: 2h18m17s experiments done: 53 / 256	Fid Flash	Lock	Sample	POWCHK X	VTU [Celsius] 26.7	BSMS status message $\Delta Z -2$ Autoshim <input checked="" type="checkbox"/> Locked <input checked="" type="checkbox"/> Error	Time 07:21 Oct 16
-------------------------	---	-----------	------	--------	-------------	--------------------------	---	-------------------------

# Autoshim on/off



The screenshot displays the Bruker TOPSPIN 2.1.b.13 software interface. A yellow callout box highlights the text: **Eject / Insert available from context menu of BSMS status monitor.** A red-bordered context menu is open over the BSMS status monitor panel, listing the following options:

- Toggle between  $^1\text{H}$  and difference mode
- Show status message
- Show last error message
- Clear error message
- Toggle autoshim mode (command autoshim on/off)
- Toggle lift on /off (command ej/ij)
- Toggle sample rotation (command ro on/off)

The BSMS status monitor panel at the bottom right shows the following information:

BSMS status message	
$\Delta Z$	-2
Autoshim	✓
Locked	✓
Error	

Other panels visible include:

- Amplifier Control:** Shows a green bar and "1H".
- Acquisition information:** scan: 16 / 16, residual time: 2h18m17s, experiments done: 53 / 256.
- Fid Flash:** Shows a red waveform.
- Lock:** Shows a grid of colored squares.
- Sample:** Shows a blue icon of a sample tube.
- POWCHK:** Shows a red 'X'.
- VTU [Celsius]:** 26.7.
- Time:** 07:21 Oct 16.



# Autoshim on/off



The screenshot displays the Bruker TOPSPIN 2.1.b.13 software interface. A yellow callout box highlights the text: "Rotation on/off available from context menu of BSMS status monitor." A red-bordered context menu is open over the BSMS status monitor, listing several options:

- Toggle beam ... and difference mode
- Show status ...
- Show last error ...
- Clear error mes ...
- Toggle autoshim ... (command autoshim on/off)
- Toggle lift on /off ... (command ej/ij)
- Toggle sample rotation (command ro on/off)

The BSMS status monitor at the bottom right shows the following information:

BSMS status message	
$\Delta Z$	-2
Autoshim	✓
Locked	✓
Error	

Other interface elements include a file browser on the left showing a directory tree under /opt, a status bar at the bottom with acquisition information (scan: 16 / 16, residual time: 2h18m17s, experiments done: 53 / 256), and a time display (07:21 Oct 16).

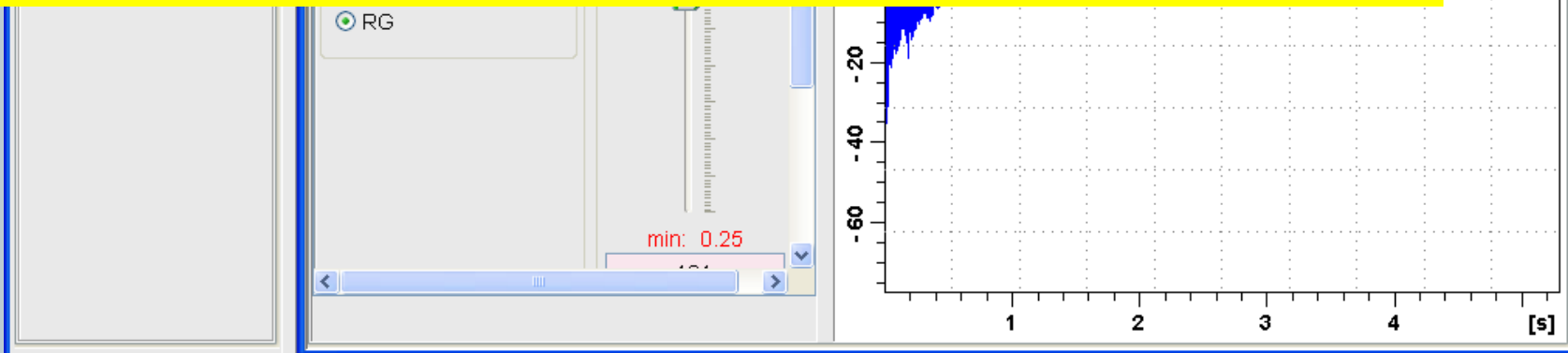
BSMS display supports N2 sensor, if available.

The daily helium measurement will also check and protocol N2 if the N2 sensor is available.





Bruker TOPSPIN 2.1.a on Leda2 as nmrsu

Acquisition status bar offers many possibilities for your convenience:

- screen resolution of 1280x1024 is required
- status line appears above status bar



gs: acquisition running, modify parameters via sliders or keyboard

Acquisition information	Fid Flash	Lock	Sample	POWCHK	Spooler	BSMS status message	Time
fid area: 44274823 scan: 7					running: 0 queued: 0 delayed: 0	<b>Δ Z -2</b> Autoshim ✓ Locked ✓ Error	12:39 Jan 03

# FID display



Default: Every FID is automatically scaled:

scaling FID  
on one dataset ...

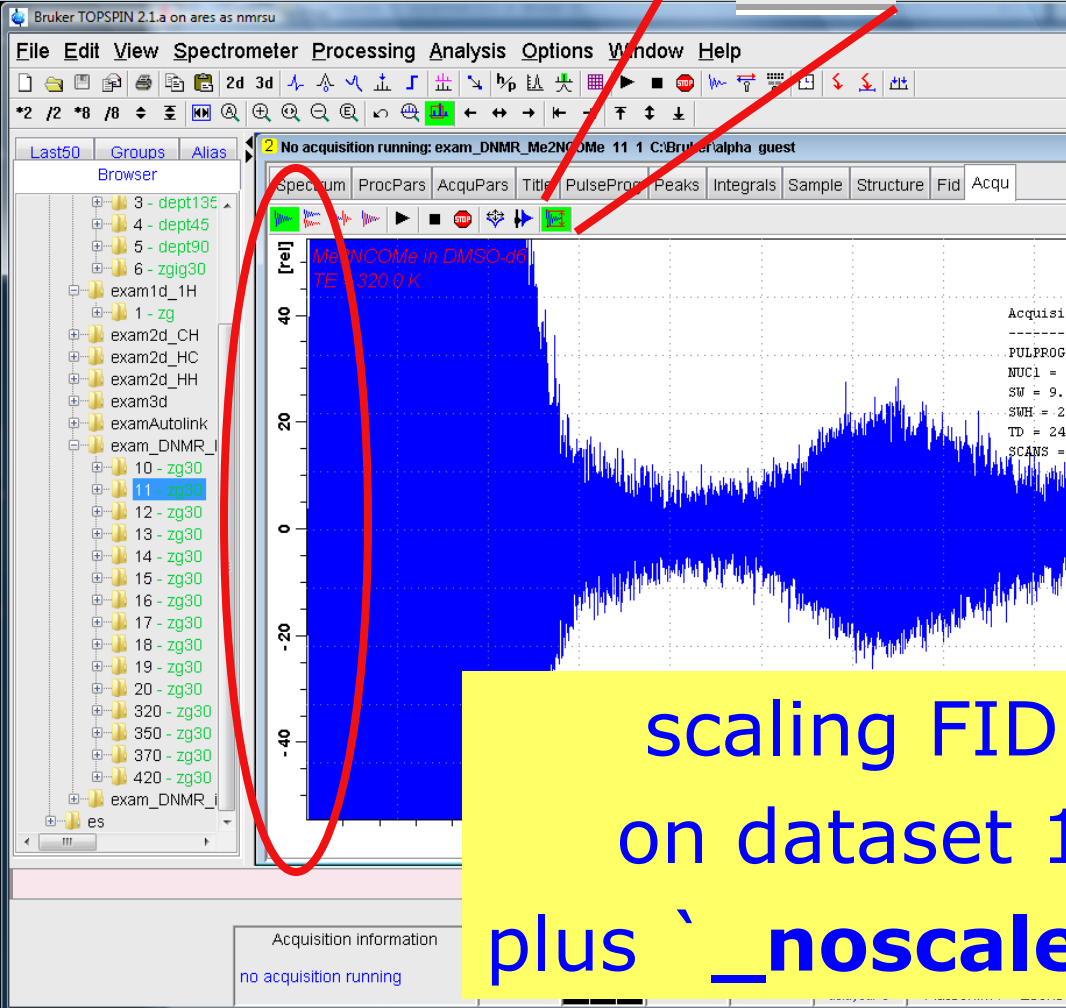
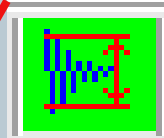
... optimised  
scaling  
on next  
dataset

next page

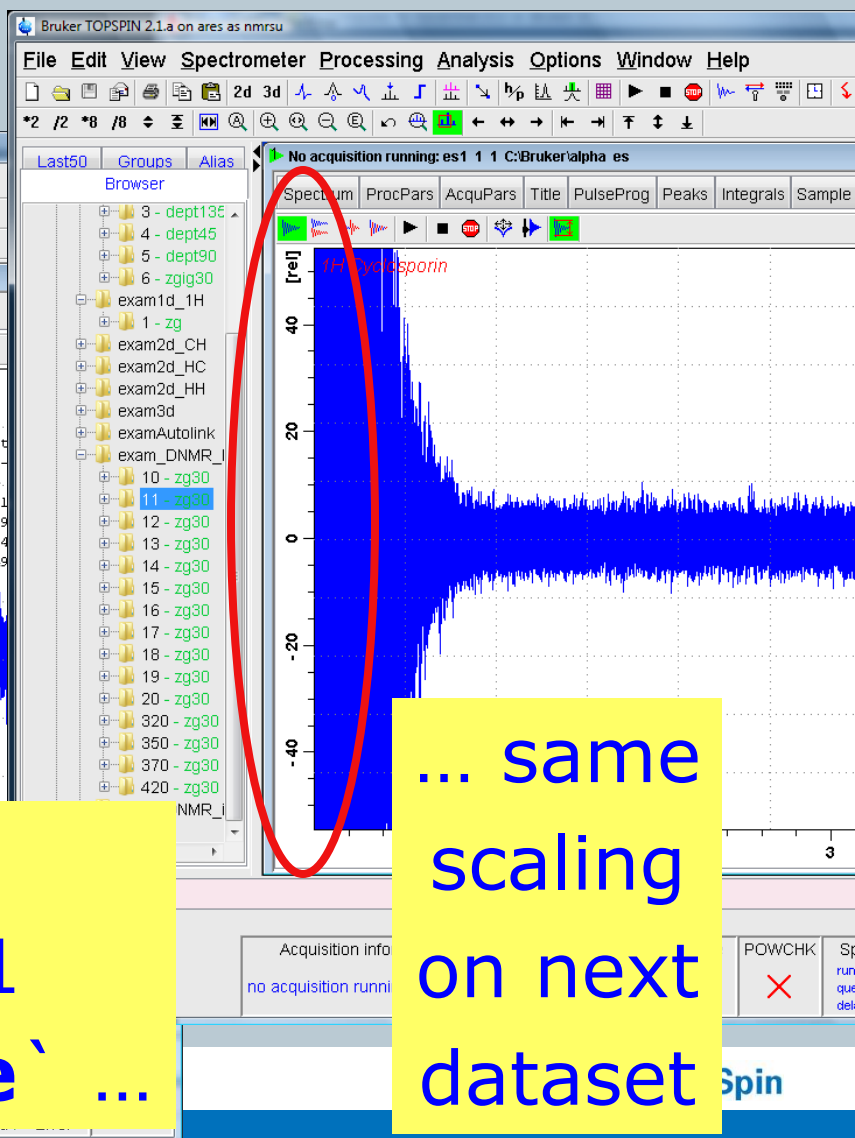
# FID display



New feature: The FID scaling can be fixed:

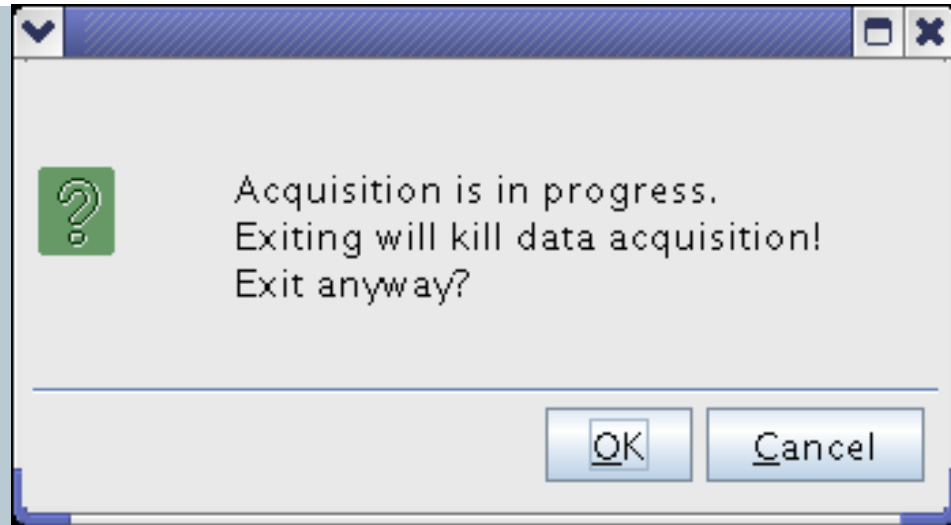


scaling FID  
on dataset 1  
plus ` \_noscale` ...

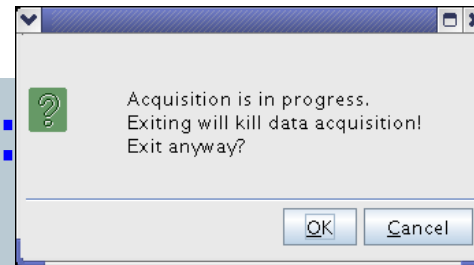


... same  
scaling  
on next  
dataset

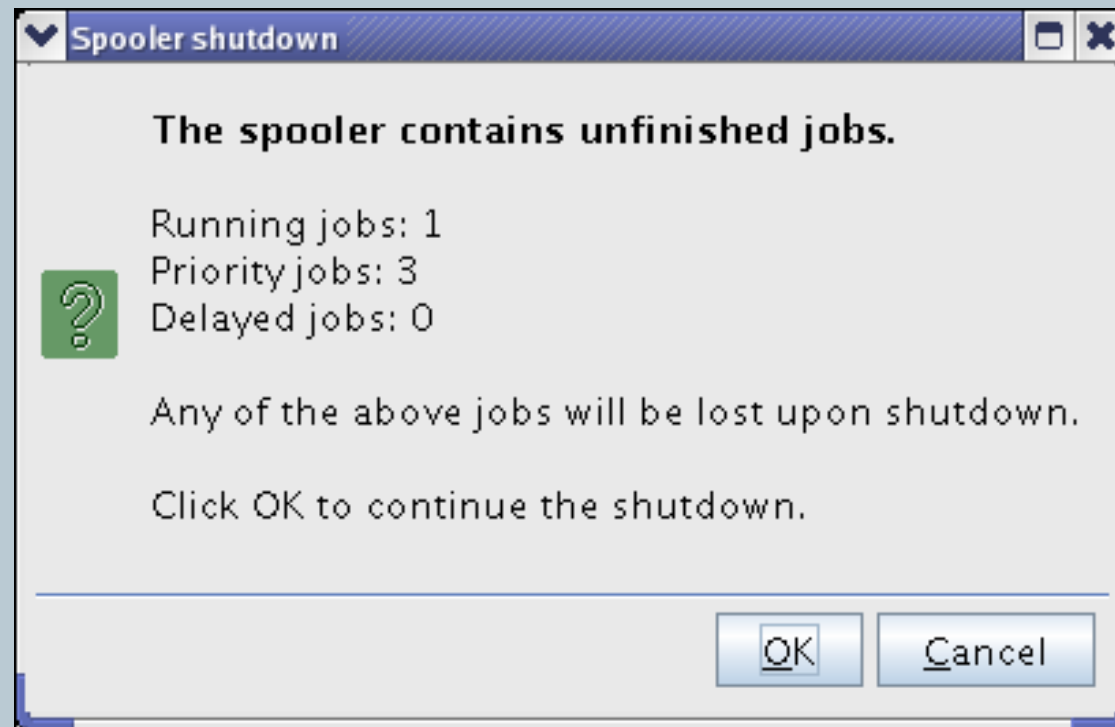
## 1. Acquisition is running:



1. Acquisition is running:



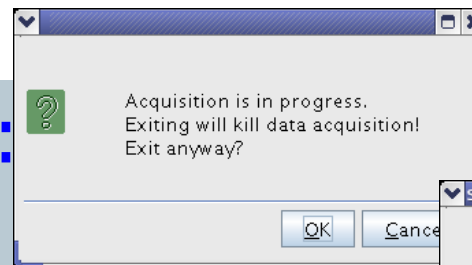
2. Spooler contains unfinished jobs:



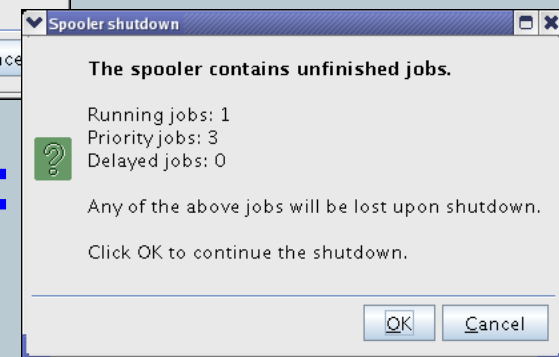
# TopSpin exit messages



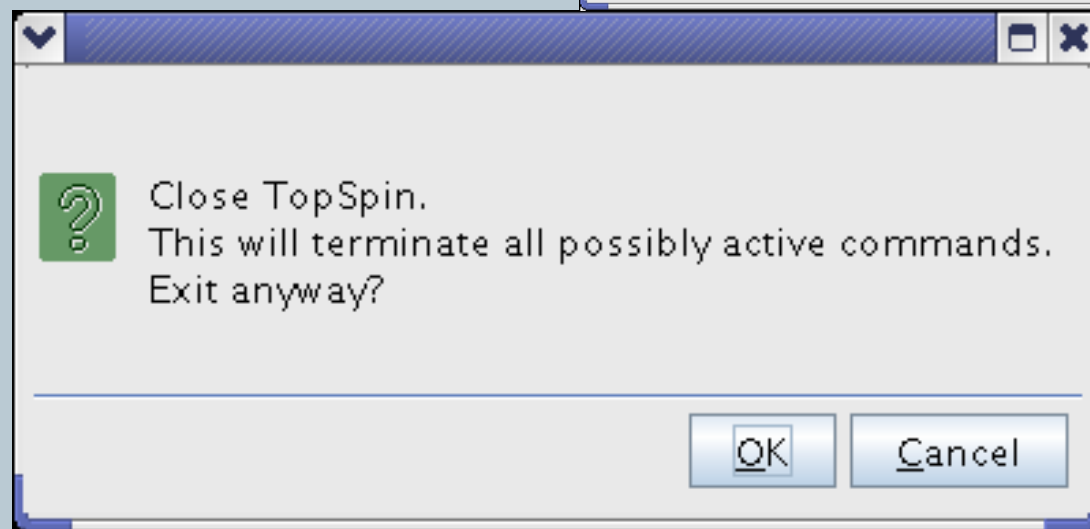
1. Acquisition is running:



2. Spooler contains unfinished jobs:



3. Default message:

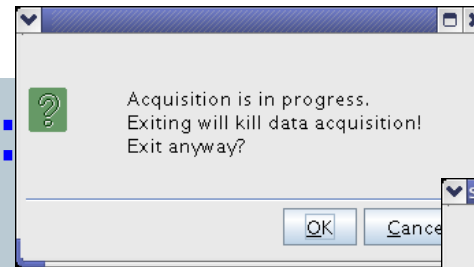




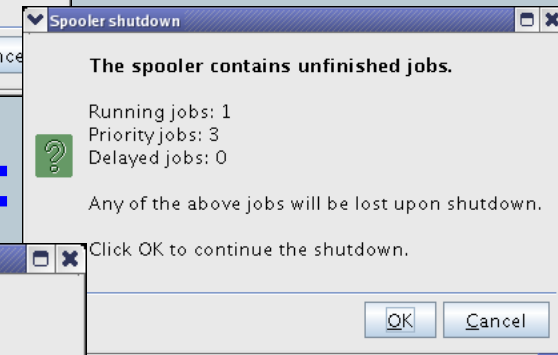
# TopSpin exit messages



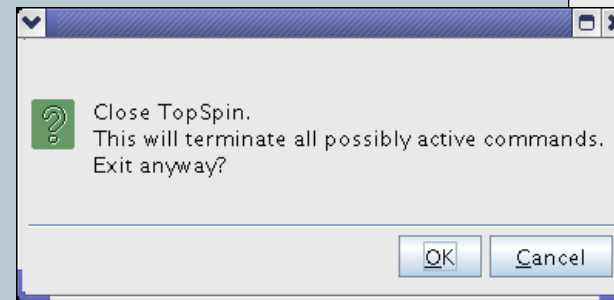
1. Acquisition is running:



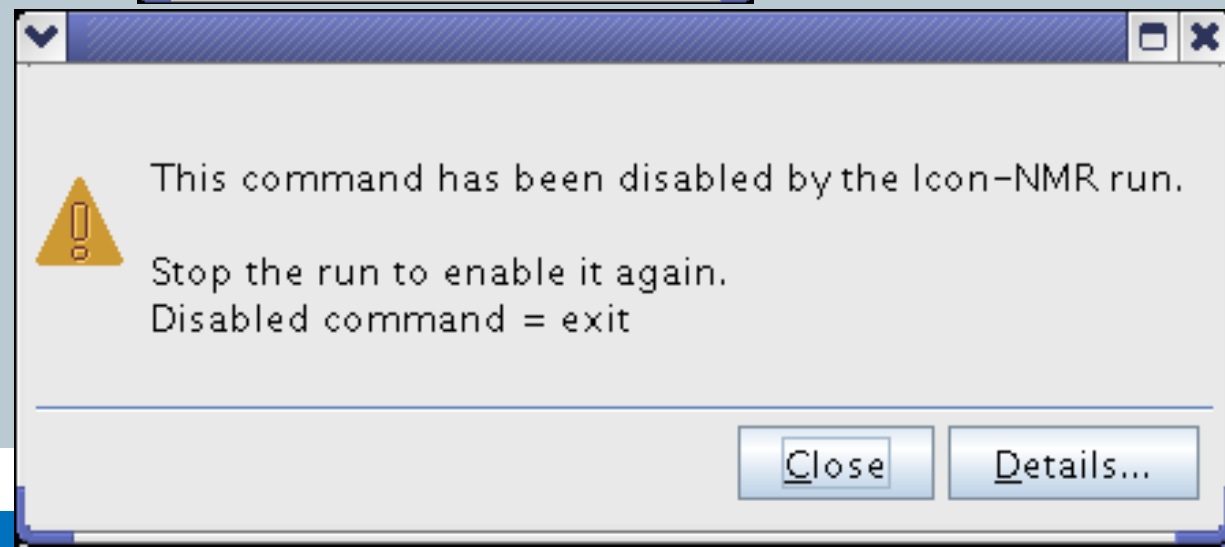
2. Spooler contains unfinished jobs:



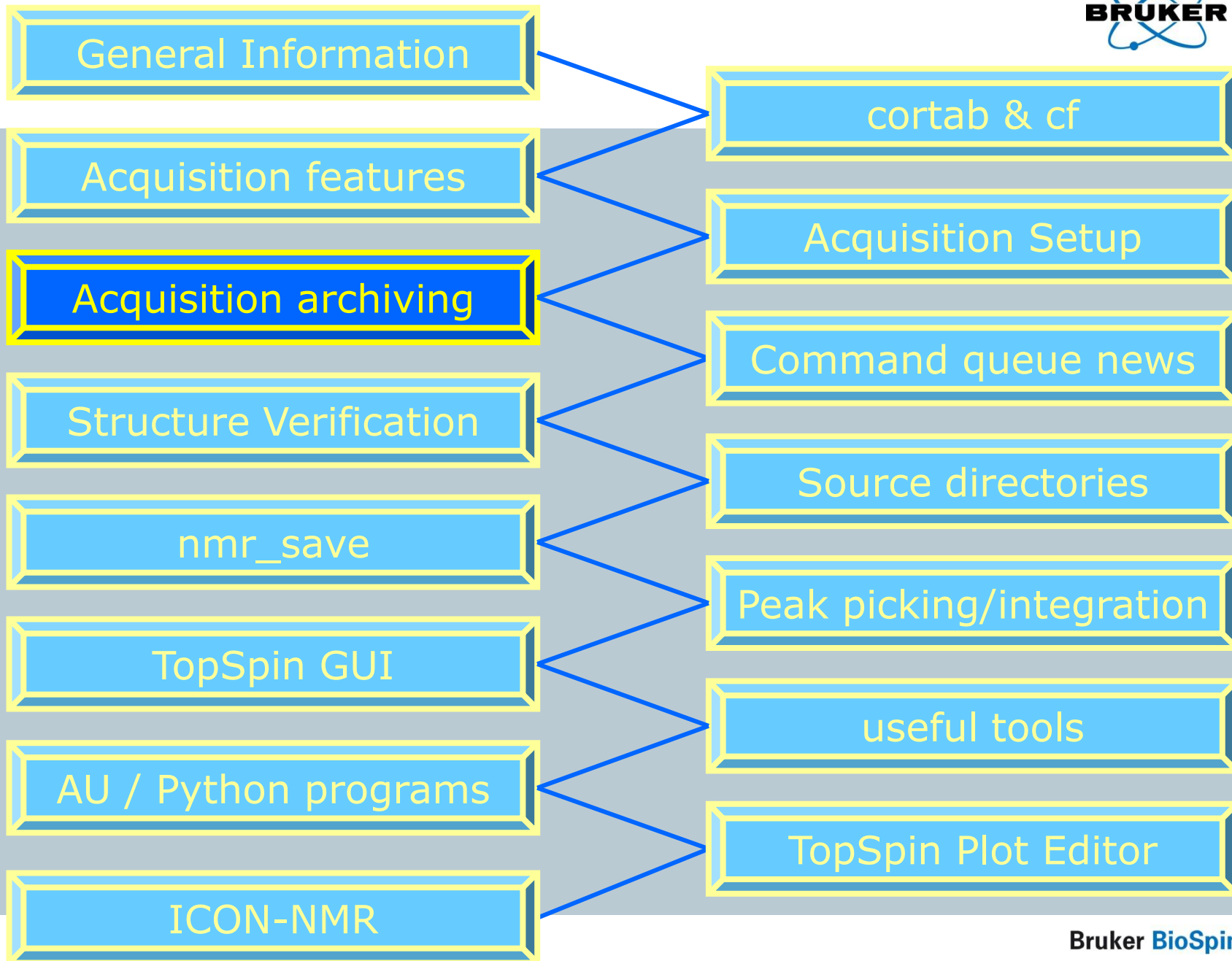
3. Default message:



4. No exit during an active ICON-NMR run:



# Content



# Archiving and accounting in TopSpin

## Configuration tool:

**User preferences**

Administration items | Text editor for edpul, edmac, edpy, ... always in foreground

Spectrum | Setup remote systems pdv-400

Contour plot | Configure remote access

Spectrum title | Language (change requires program restart!) English

Spectrum cursor | Define right-click action on a menu item

---

**Acquisition**

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'

---

Include spectra

Include time

Include sample temperature

Include acquisition status

Include acquisition indicator

Include lock signal

Include MAS spinning rate

Include peak power check (POWCHK) indicator

Include sample state

Include BSMS status

Include amplifier control

---

**Acquisition**

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'

---

**BSMS display**

Auto open BSMS display

# Archiving configuration



**Setup Auto-Archiving & Accounting**

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 following directory, one file per day:  
"<topspin homedir>/proq/curdir/acqhistory"

Auto-archive after 'zg' =

Archiving directory =

EXPNO offset =

Write accounting info after 'zg' =

Like archive option in ICON-NMR

- will archive each acquisition which has been started from within TopSpin GUI

next page

(for AU programs: use **'XCMD("sendgui zg")'**)

# Archiving configuration



**Setup Auto-Archiving & Accounting**

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 following directory, one file per day:  
"<topspin homedir>/prog/curdir/acqhistory"

Auto-archive after 'zg' =

Archiving directory =

EXPNO offset =

Write accounting info after 'zg' =

If an experiment is executed second time

- dataset in the archive can be overwritten or a new expno can be added. Increment is user-specific.

next page

# Accounting configuration



**Setup Auto-Archiving & Accounting**

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 following directory, one file per day:  
"<topspin homedir>/prog/curdir/acqhistory"

Auto-archive after 'zg' =

Archiving directory =

EXPNO offset =

Write accounting info after 'zg' =

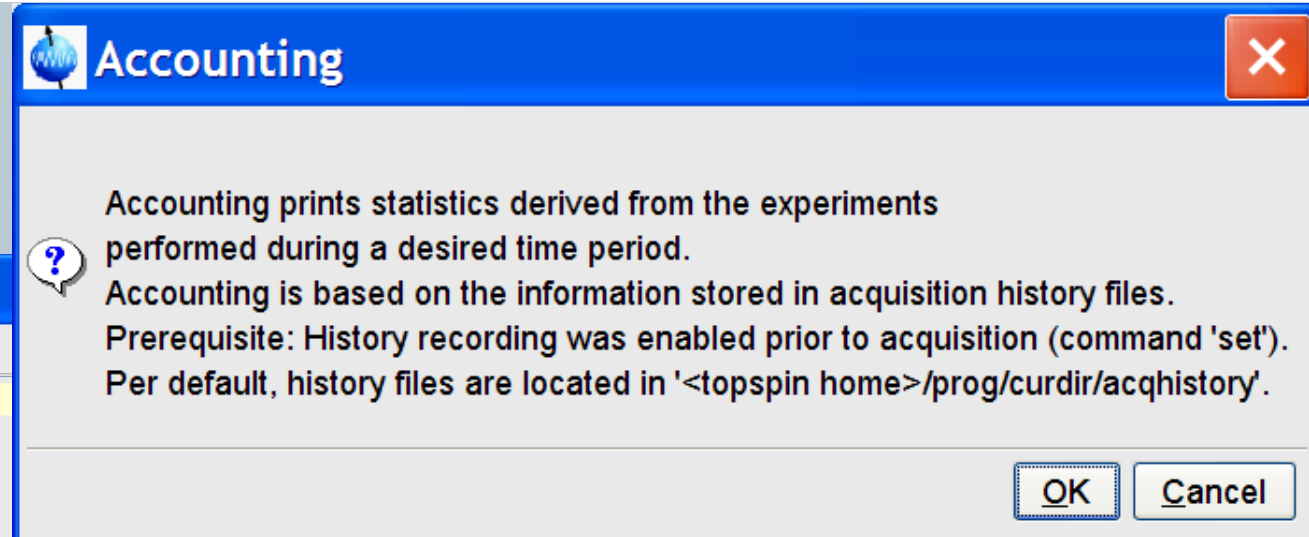
New command **account** is implemented

that checks the acquisition history file.

next page

## New TopSpin command **account** :

```
Accounting Protocol
File Edit Search
1 Accounting Protocol
2 Created: 2007-02-16 09:49:39 CET
3 TopSpin: 2.1.a
4
5 User: bg
6 #Datasets Dim Exp.Time Failed
7 3 1 3.55 sec 1
8 6 2 21.86 sec 0
9 5 >2 7.08 sec 0
10 Sum =
11 14 Any 32.49 sec 1
12
13
14 Period
15 From: 2007-01-31 14:49:47 CET
16 To: 2007-02-02 10:44:57 CET
17
18 The following datasets had "acquisition failed" status:
19
20 c:\bruker\topspin\data\guest\nmr\exam1d_13C\1\pdata\1
21 failed xxx
22
23 -----
24
25
```



**Accounting**

Accounting prints statistics derived from the experiments performed during a desired time period.

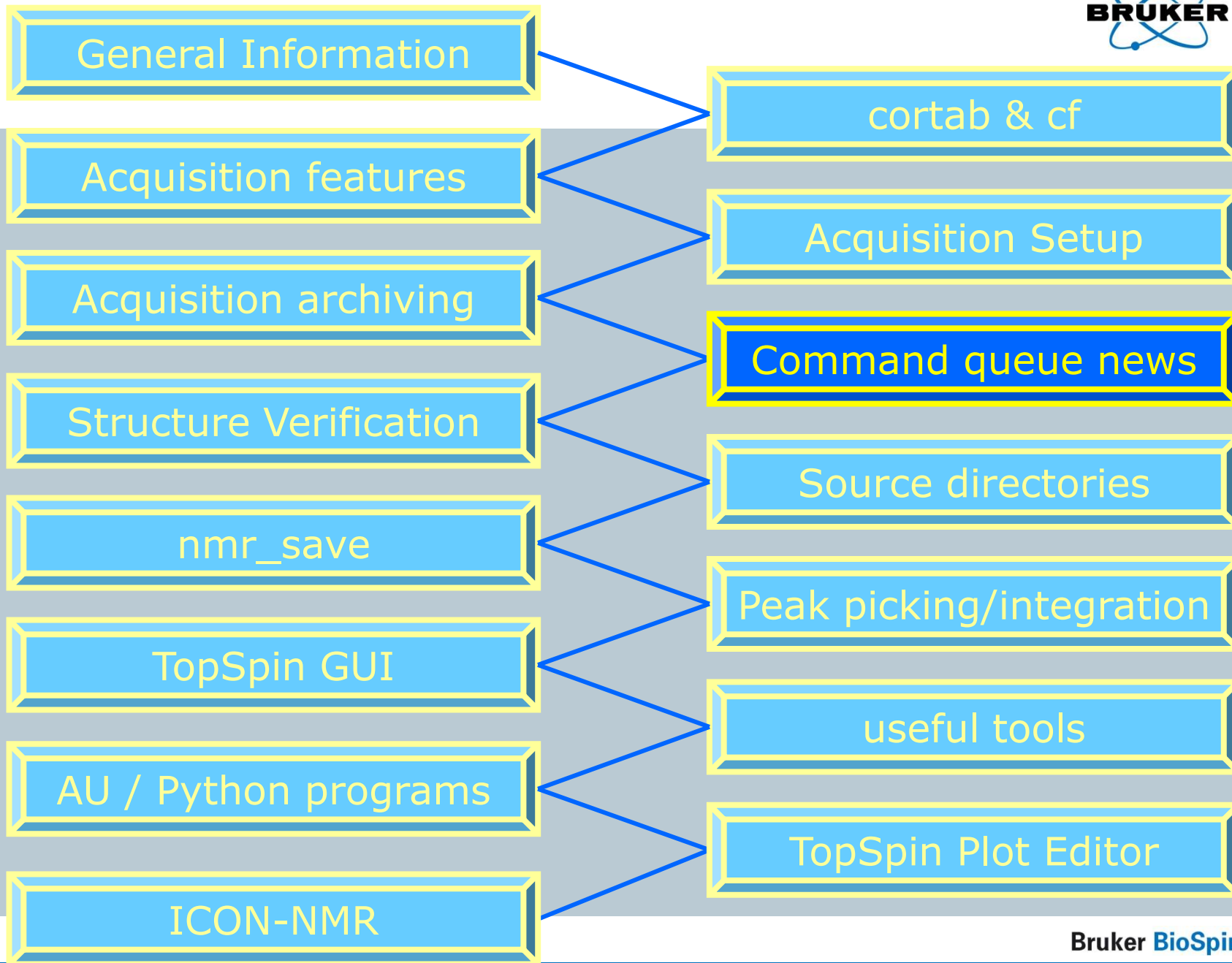
Accounting is based on the information stored in acquisition history files.

Prerequisite: History recording was enabled prior to acquisition (command 'set').

Per default, history files are located in '<topspin home>/prog/curdir/acqhistory'.

OK Cancel

# Content





It is now possible to define the experiment number on which a command should be queued:

qumulti

atmulti

File Edit View Processing Analysis Options Window Help

Browser Last50 Groups Alias

exam1d\_1H 1 1 F:\Bruker\topspin2.0 guest

Peaks Integrals Title ProcPars AcqPars

exam\_DNMR\_Me2NCOME  
exam\_DNMR\_ipr2sic  
svcu

6  
4  
2  
0

10 8

6  
4  
2  
0

0 [ppm]

New job

Job

Command

Experiment IDs

1  
 3  
 4  
 11

OK Cancel

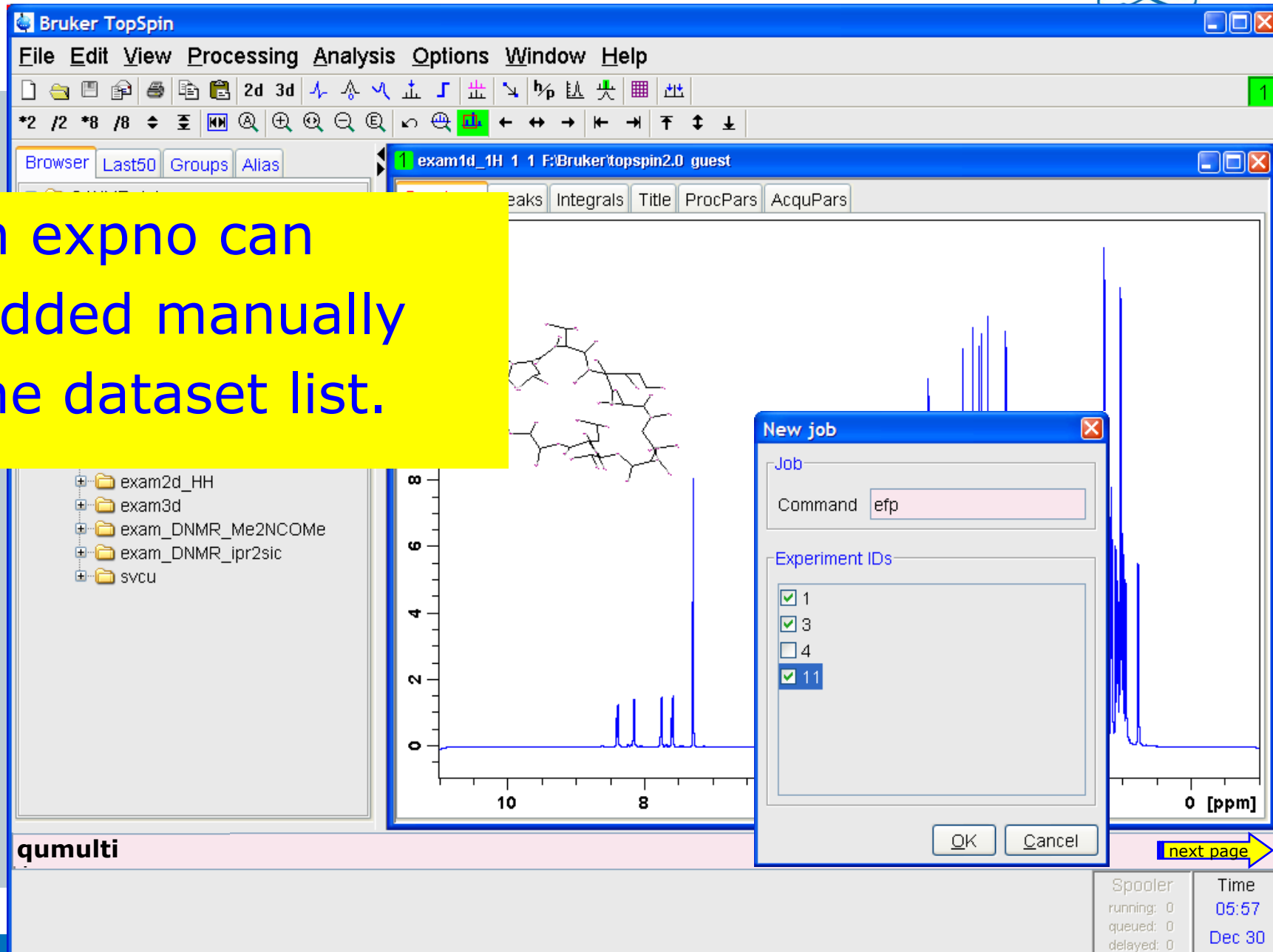
next page

qumulti

Spooler running: 0  
queued: 0  
delayed: 0

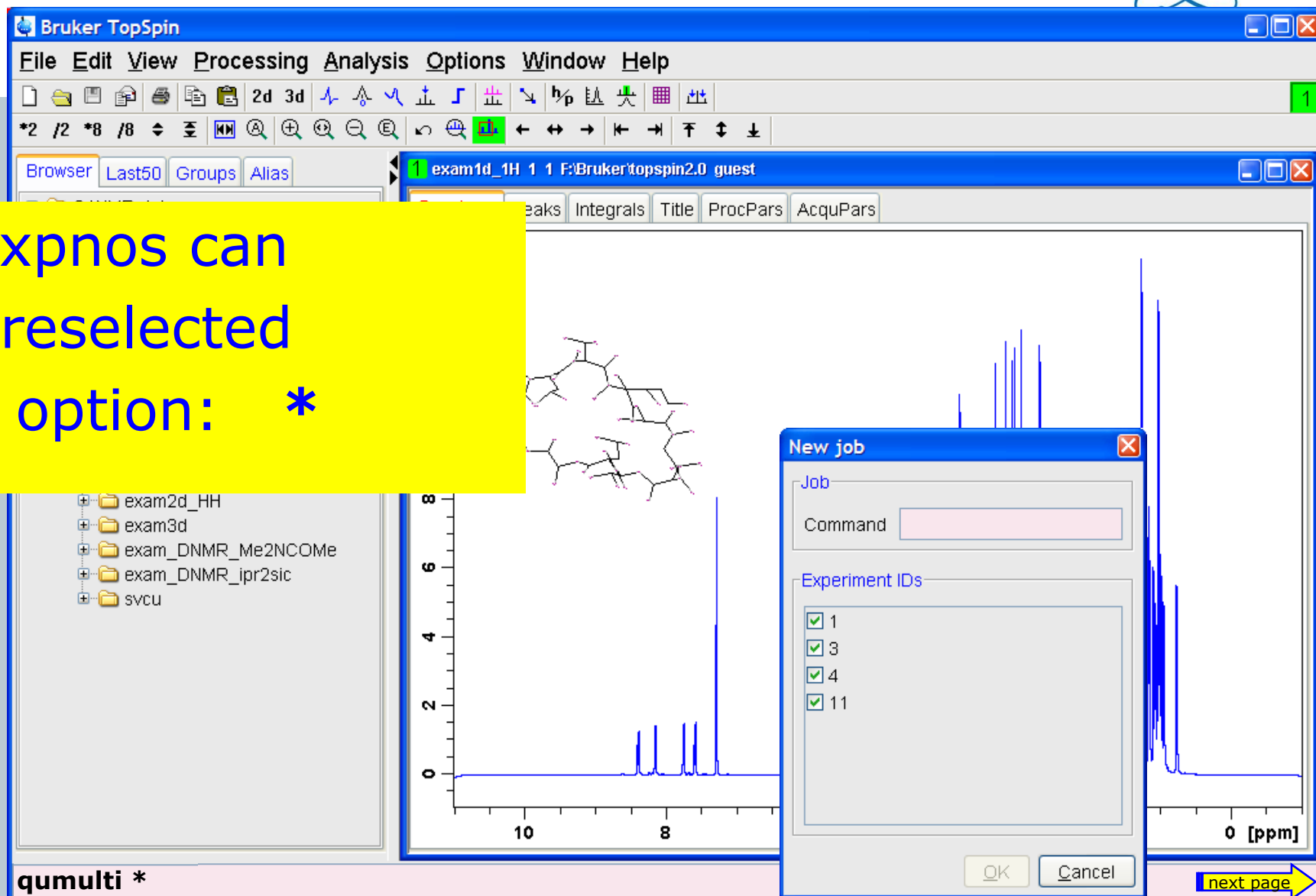
Time 05:57  
Dec 30

The current dataset is automatically enabled in the list of expnos.



The screenshot displays the Bruker TopSpin software interface. The main window shows a dataset list on the left with folders: exam2d\_HH, exam3d, exam\_DNMR\_Me2NCOME, exam\_DNMR\_ipr2sic, and svcu. The central area features a chemical structure of a complex organic molecule and a 1D NMR spectrum with peaks at approximately 8.5, 8.2, 7.8, and 7.5 ppm. A 'New job' dialog box is open, showing the 'Command' field set to 'efp' and the 'Experiment IDs' list with checkboxes for 1, 3, 4, and 11. The '11' checkbox is selected. The 'OK' and 'Cancel' buttons are visible at the bottom of the dialog. The status bar at the bottom right shows 'Spooler running: 0', 'Time 05:57', and 'Dec 30'. A yellow arrow labeled 'next page' points to the right.

Each expno can be added manually to the dataset list.



The screenshot displays the Bruker TopSpin software interface. The main window shows a 1D NMR spectrum with a chemical structure overlay. A 'New job' dialog box is open, showing the 'Experiment IDs' section with checkboxes for 1, 3, 4, and 11, all of which are selected. The 'Command' field is empty. The 'Job' field is also empty. The 'OK' and 'Cancel' buttons are visible at the bottom of the dialog box.

File Edit View Processing Analysis Options Window Help

Browser Last50 Groups Alias

exam1d\_1H 1 1 F:\Bruker\topspin2.0 guest

peaks Integrals Title ProcPars AcqPars

exam2d\_HH  
exam3d  
exam\_DNMR\_Me2NCOME  
exam\_DNMR\_ipr2sic  
svcu

8  
6  
4  
2  
0

10 8

0 [ppm]

New job

Job

Command

Experiment IDs

1  
 3  
 4  
 11

OK Cancel

next page

All expnos can  
be preselected  
with option: \*

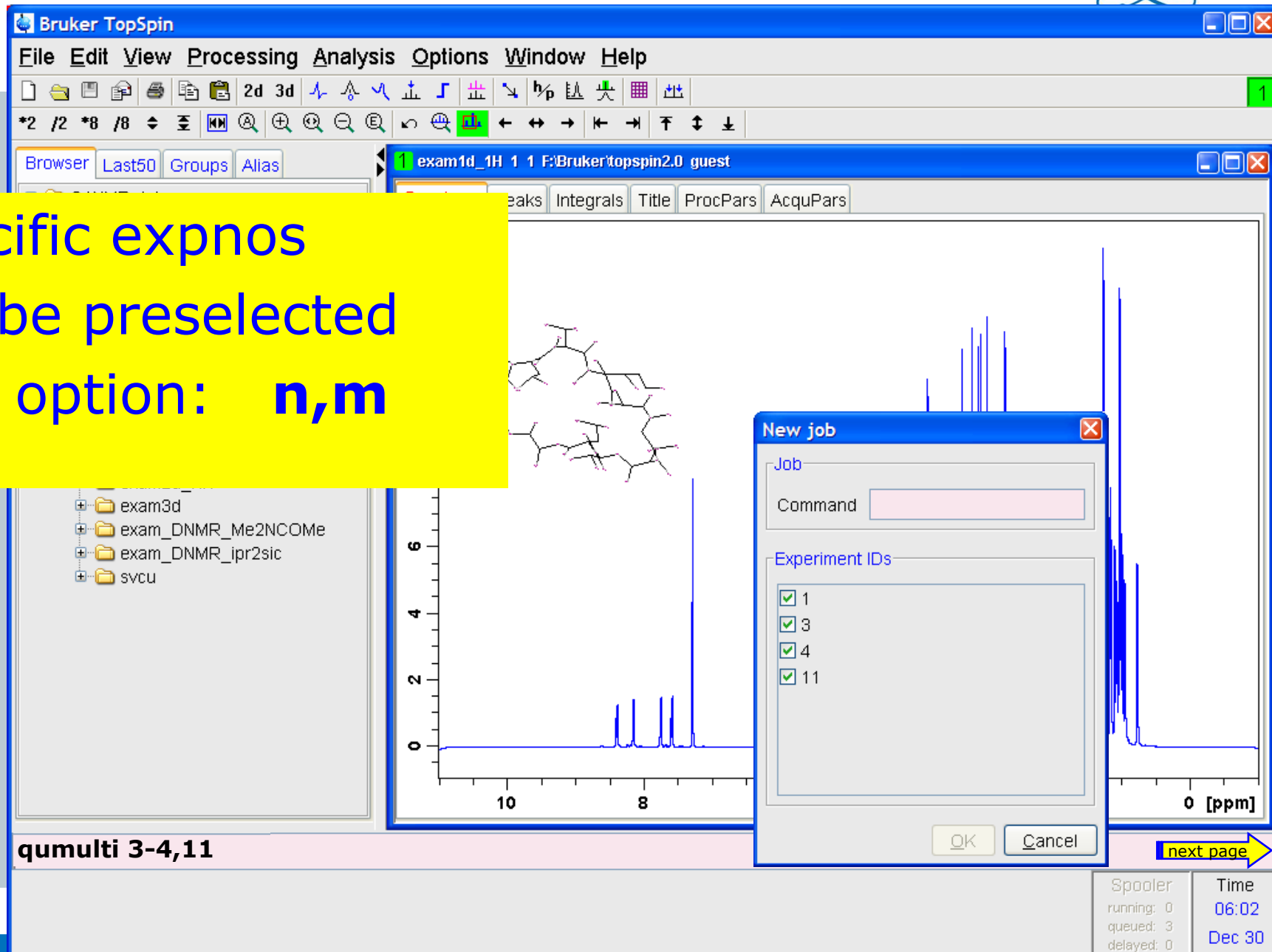
qumulti \*

The screenshot displays the Bruker TopSpin software interface. At the top, there is a menu bar (File, Edit, View, Processing, Analysis, Options, Window, Help) and a toolbar with various icons. Below the toolbar, a file browser shows a directory structure with folders like 'exam12u\_nn', 'exam3d', 'exam\_DNMR\_Me2NCOME', 'exam\_DNMR\_ipr2sic', and 'svcu'. In the center, a chemical structure is shown. To the right, two NMR spectra are displayed, one with a chemical structure overlaid. A 'New job' dialog box is open in the foreground, showing a 'Job' section with a 'Command' field and an 'Experiment IDs' section with a list of IDs: 1, 3, 4, and 11. The checkboxes for 1, 3, and 4 are checked, while the checkbox for 11 is unchecked. The dialog box has 'OK' and 'Cancel' buttons at the bottom.

A range of expnos can be preselected with option: **n-m**

qumulti 3-4

[next page](#)



The screenshot displays the Bruker TopSpin software interface. The main window shows a 1D NMR spectrum with a chemical structure overlay. A 'New job' dialog box is open, showing the 'Experiment IDs' section with checkboxes for 1, 3, 4, and 11, all of which are selected. The 'Command' field is empty. The 'Job' field is also empty. The 'OK' and 'Cancel' buttons are visible at the bottom of the dialog box.

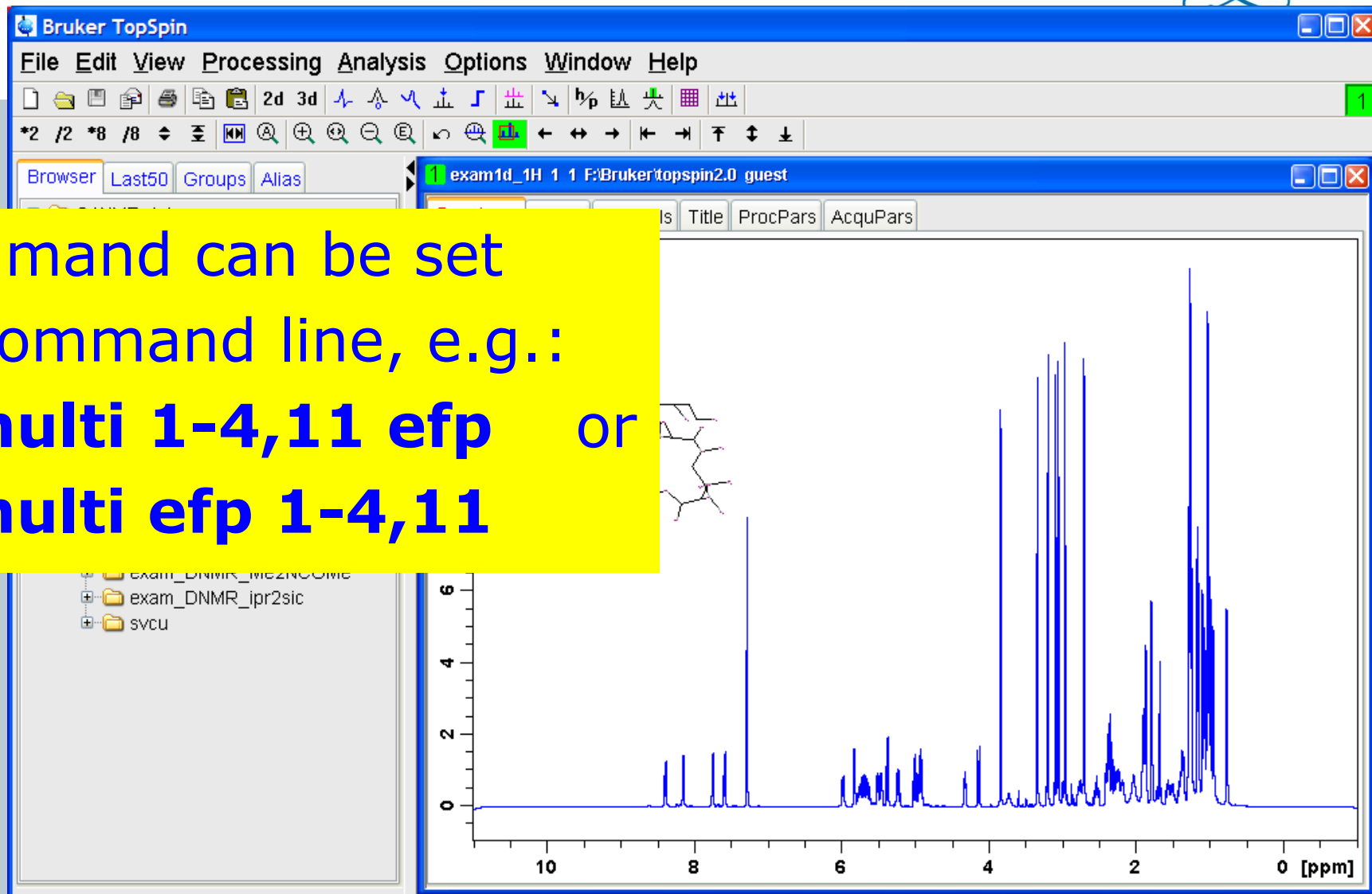
**Specific expnos can be preselected with option: **n,m****

qumulti 3-4,11

next page


Spooler running: 0  
queued: 3  
delayed: 0

Time 06:02  
Dec 30




Command can be set  
on command line, e.g.:  
**qumulti 1-4,11 efp** or  
**qumulti efp 1-4,11**

**qumulti 3-4,11 efp**


[next page](#) 


Same functionalities  
are available for the  
list of delayed jobs  
with command:  
**atmulti**

**New schedule** 

Schedule

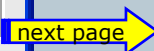
Command

Time  

Date  

Experiment IDs

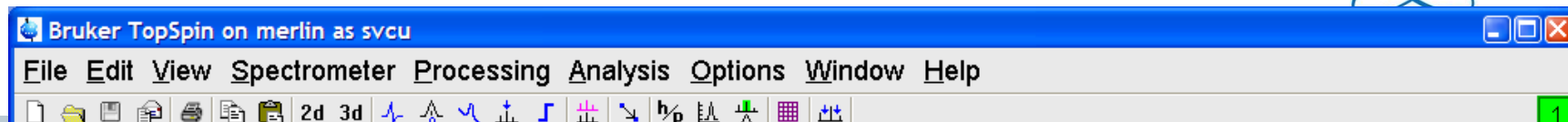
- 1
- 3
- 4
- 11



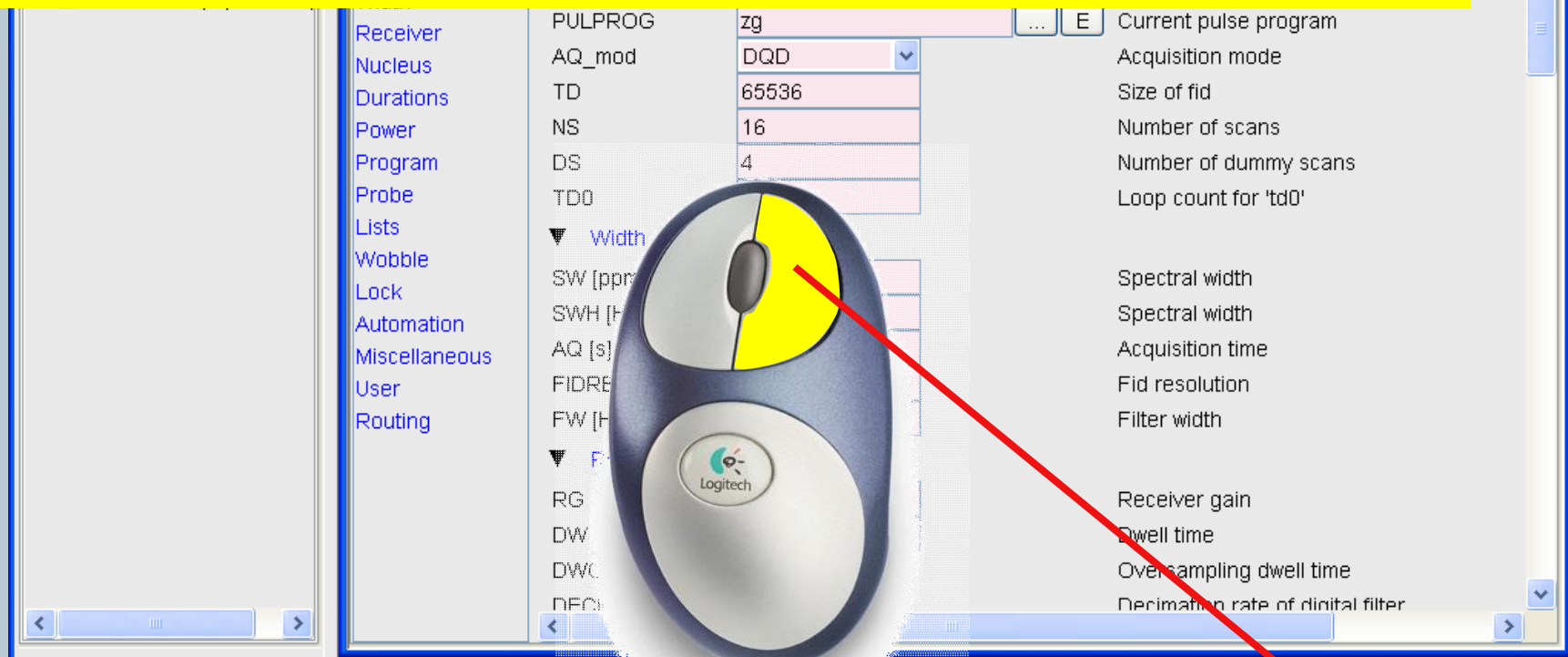
next page



# Command queue log file



The command spooler now contains easy access to the log files



next page

Spooler	Time
queued: 0	18:01
delayed: 0	
cron: 2	May 08

# Command queue log file



The screenshot shows the Bruker TopSpin software interface. A context menu is overlaid on the main window, listing several actions: Show, Suspend, Remove all jobs, Show spooler report, and Show spooler log. The 'Show spooler log' option is highlighted in blue. A red box highlights the menu, and a red arrow points from the menu to a smaller version of the menu in the bottom right corner. The background shows the software's main window with a file browser on the left and a parameter table on the right.

Parameter	Value
SWH [Hz]	6009.615
AQ [s]	5.4527283
FIDRES [Hz]	0.091699
FW [Hz]	125000.00
Receiver	
RG	32
DW [μs]	83.208
DWOV [μs]	2.600
DECIM	32

next page →

# Command queue log file



Bruker TopSpin on merlin as svcu

File Edit View Spectrometer Processing Analysis Options Window Help

2d 3d

Spooler logger

Timestamp	Message
January 2, 2007 6:16:42 AM CET	Spooler state changed to RUNNING.
January 2, 2007 6:16:56 AM CET	Spooler state changed to STOPPED.
January 2, 2007 6:17:08 AM CET	Removing state AUTO_STOPPED due to queue request.
January 2, 2007 6:17:08 AM CET	Added priority job to priority queue: PriorityJob[id=1, command=efp, priority=0, dataObject=F:/Bruker/topspin2.1-alpha/data/guest/nmr/exam1d_1H/1/pdata/1]
January 2, 2007 6:17:08 AM CET	Added priority job to priority queue: PriorityJob[id=2, command=efp, priority=0, dataObject=F:/Bruker/topspin2.1-alpha/data/guest/nmr/exam1d_1H/4/pdata/1]
January 2, 2007 6:17:08 AM CET	Added priority job to priority queue: PriorityJob[id=3, command=efp, priority=0, dataObject=F:/Bruker/topspin2.1-alpha/data/guest/nmr/exam1d_1H/6/pdata/1]
January 2, 2007 6:17:08 AM CET	Added priority job to priority queue: PriorityJob[id=4, command=efp, priority=0, dataObject=F:/Bruker/topspin2.1-alpha/data/guest/nmr/exam1d_1H/7/pdata/1]
January 2, 2007 6:17:08 AM CET	Started watching for job property update events.

Show spooler report  
Show spooler log

A list of all Spooler events of the current TopSpin session

Automation	SWH [Hz]	6009.615
Miscellaneous	AQ [s]	5.4527283
User	FIDRES [Hz]	0.091699
Routing	FW [Hz]	125000.00
	Receiver	
	RG	32
	DW [μs]	83.208
	DWVOV [μs]	2.600
	DECIM	32
	Dwell time	
	Oversampling dwell time	
	Decimation rate of digital filter	

- Show
- Suspend
- Remove all jobs
- Show spooler report
- Show spooler log

next page

# Command queue report file



The screenshot shows the Bruker TopSpin software interface. A context menu is open over a job entry, listing the following options:

- Show
- Suspend
- Remove all jobs
- Show spooler report
- Show spooler log

The 'Show spooler report' option is highlighted in blue. A red box highlights the entire menu, and a red arrow points from the menu to a smaller version of the menu in the bottom right corner. A yellow arrow labeled 'next page' points to the right.

Parameter	Value
SWH [Hz]	6009.615
AQ [s]	5.4527283
FIDRES [Hz]	0.091699
FW [Hz]	125000.00
Receiver	
RG	32
DW [μs]	83.208
DWOV [μs]	2.600
DECIM	32

Parameter	Value
Current pulse program	E
Acquisition mode	
Size of fid	
Number of scans	
Number of dummy scans	
Loop count for 'td0'	
Spectral width	
Acquisition time	
Fid resolution	
Filter width	
Receiver gain	
Dwell time	
Oversampling dwell time	
Decimation rate of digital filter	

# Command queue report file



File Edit View Spectrometer Processing Analysis Options Window Help

exam1d\_1H 1 1 F:\Bruker\topspin2.1-alpha guest

Browser

- C:\NMR data
- F:\Bruker\topspin1.3pl6
- F:\Bruker\topspin2.0
- F:\Bruker\topspin2.1-alpha

peaks Integrals Sample Structure Fid

Installed probe: 5 mm Multinuclear inverse Z-grad

Current pulse program  
Acquisition mode  
Size of fid  
Number of scans  
Number of dummy scans  
Loop count for 'td0'

Result	Timestamp	Command	Data object	Owner
✖	June 19, 2007 8:47:15 AM CEST	zg	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu
?	June 19, 2007 8:46:45 AM CEST	xfb	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu
✔	June 19, 2007 8:42:56 AM CEST	efp	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu
✔	June 19, 2007 8:42:58 AM CEST	ehs	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu
✔	June 19, 2007 8:44:46 AM CEST		/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu
✔	June 19, 2007 8:44:46 AM CEST	efp	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu

A list of all finished jobs, ever done in TopSpin.

# Command queue report file



A screenshot of the Bruker TopSpin software interface. The title bar reads "Bruker TopSpin on merlin as svcu". The menu bar includes File, Edit, View, Spectrometer, Processing, Analysis, Options, Window, and Help. The toolbar contains various icons for file operations and analysis. The main window is titled "exam1d\_1H 1 1 F:\Bruker\topspin2.1-alpha guest" and shows a "Browser" panel on the left with folders for "C:\NMR data" and "F:\Bruker\topspin2.1-alpha". A context menu is overlaid on the right side, containing the following items: "Show", "Suspend", "Remove all jobs", and "Show spooler report". A red arrow points from the "Show spooler report" option to the "Spooler report" window in the foreground.

The "Spooler report" window displays a table of command queue entries. The table has columns for Result, Timestamp, Command, Data object, and Owner. A yellow callout bubble points to a row with a yellow question mark icon, indicating that selected protocol entries can be easily deleted.

Result	Timestamp	Command	Data object	Owner
✗	June 19, 2007 8:47:15 AM CEST	zg	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
?	June 19, 2007 8:46:45 AM CEST	xfb	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
✓	June 19, 2007 8:42:56 AM CEST	efp	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		abs	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		apk	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		efp	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
		efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/1/pdata/1	svc_u
	September 6, 2007 11:12:27 AM CEST	efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/4/pdata/1	svc_u

Selected protocol entries can be easily deleted

- Display
- Delete
- Copy
- Export...
- Import...
- Print...
- Print preview...
- Table properties...

# Command queue report file



File Edit View Spectrometer Processing Analysis Options Window Help

exam1d\_1H 1 1 F:\Bruker\topspin2.1-alpha guest

Browser

- C:\NMR data
- F:\Bruker\topspin1.3pl6
- F:\Bruker\topspin2.0
- F:\Bruker\topspin2.1-alpha

peaks Integrals Sample Structure Fid

Installed probe: 5 mm Multinuclear inverse Z-grad

Current pulse program  
Acquisition mode  
Size of fid  
Number of scans  
Number of dummy scans

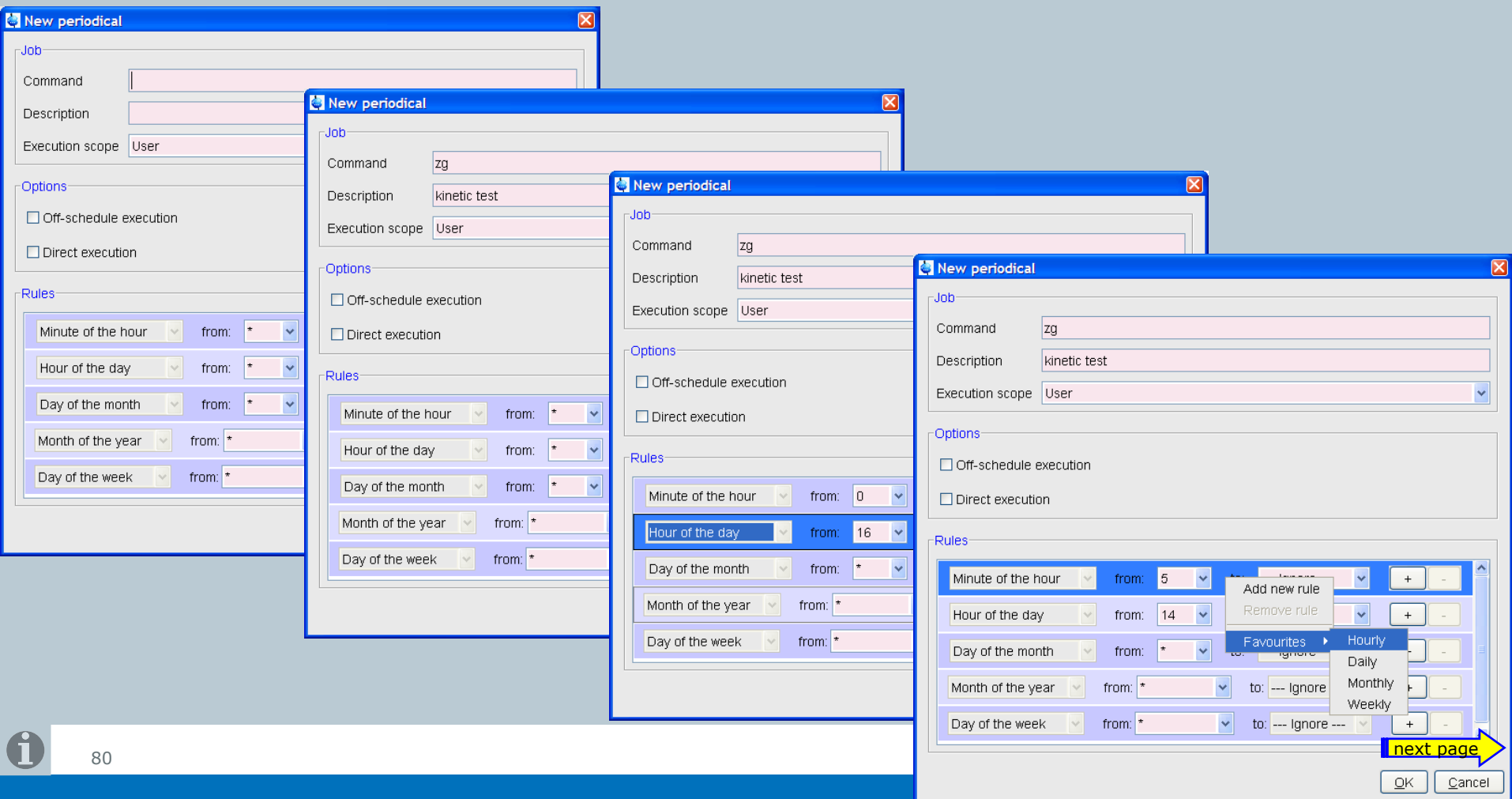
Result	Timestamp	Command	Data object	Owner
✘	June 19, 2007 8:47:15 AM CEST	zg	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu
?	June 19, 2007 8:46:45 AM CEST	xfb	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu
✔	June 19, 2007 8:42:56 AM CEST	efp	/bruker/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu
✔	June 19, 2007 8:42:58 AM CEST		er/topspin/data/guest/nmr/exam1d_13C/1/pdata/1	svcu
✔	June 19, 2007 8:44:46 AM CEST		er/topspin/	
✔	June 19, 2007 8:44:46 AM CEST			
✔	September 6, 2007 11:12:25 AM CE		ruker/	
✔	September 6, 2007 11:12:47 AM CE		ruker/Top	
✔	September 6, 2007 11:18:01 AM CE		ruker/Top	
✔	September 6, 2007 11:18:05 AM CE		ruker/Top	
✔	September 6, 2007 11:18:02 AM CE		ruker/Top	
✔	September 6, 2007 11:12:26 AM CE		ruker/TopS	
✔	September 6, 2007 11:12:48 AM CE		ruker/TopSpin/data/guest/nmr/exam1d_13C/3/pdata/1	svcu
✔	September 6, 2007 11:18:02 AM CE		ruker/TopSpin/data/guest/nmr/exam1d_13C/3/pdata/1	svcu
✔	September 6, 2007 11:12:27 AM CEST	efp	F:\Bruker\TopSpin\data/guest/nmr/exam1d_13C/4/pdata/1	svcu

Display  
Delete  
Copy  
Export...  
Import...  
Print...  
Print preview...  
Table properties...

Associated datasets can be easily opened

# New command: **cron**

**cron** allows executing a TopSpin command periodically at a specific time/date:



The image displays four overlapping "New periodical" dialog boxes, illustrating the configuration of a cron job. Each dialog box contains the following fields and options:

- Job:** Command, Description, Execution scope (User).
- Options:**  Off-schedule execution,  Direct execution.
- Rules:** Minute of the hour, Hour of the day, Day of the month, Month of the year, Day of the week, each with a "from" field.

The bottom-right dialog box shows a context menu over the "Hour of the day" field, with the "Hourly" option selected. The menu options are: Add new rule, Remove rule, Favourites, and a sub-menu containing Hourly, Daily, Monthly, and Weekly.

80 next page

OK Cancel



# New command: cron



## 'Execution Scope'

- user** - defines a job for the current logged in user
- TopSpin** - defines a job which should be executed independent of the current logged in user (requires NMR Administration Password)

The screenshot displays the Bruker software interface for configuring a 'cron' command. The main window shows the 'Job' configuration with the following details:

- Job:** Command: zg, Description: kinetic test, Execution scope: User
- Options:**  Off-schedule execution,  Direct execution
- Rules:** Minute of the hour (from: \*), Hour of the day (from: 16), Day of the month (from: \*), Month of the year (from: \*), Day of the week (from: \*)

A yellow callout box titled "'Execution Scope'" provides the following information:

- user** - defines a job for the current logged in user
- TopSpin** - defines a job which should be executed independent of the current logged in user (requires NMR Administration Password)

A context menu is open over the 'Hour of the day' rule, showing options: 'Add new rule', 'Remove rule', 'Favourites' (with sub-options: 'Hourly', 'Daily', 'Monthly', 'Weekly'), and 'to: --- Ignore ---'. The 'Hour of the day' rule is currently set to 'from: 16'.

# New command: cron



## 'Off-schedule execution'

- Jobs are executed only when TopSpin is up and running.
- The last one of a series which could not be executed because TopSpin did not run, will be executed when TopSpin is started.

Rules

Minute of the hour from: \*

Hour of the day from: \*

Day of the month from: \*

Month of the year from: \*

Day of the week from: \*

Options

Off-schedule execution

Direct execution

Rules

Minute of the hour from: \*

Hour of the day from: \*

Day of the month from: \*

Month of the year from: \*

Day of the week from: \*

Description kinetic test

Execution scope User

Options

Off-schedule execution

Direct execution

Rules

Minute of the hour from: 0

Hour of the day from: 16

Day of the month from: \*

Month of the year from: \*

Day of the week from: \*

Options

Off-schedule execution

Direct execution

Rules

Minute of the hour from: 5

Hour of the day from: 14

Day of the month from: \*

Month of the year from: \* to: --- Ignore

Day of the week from: \* to: --- Ignore

next page

# New command: cron



## 'Direct execution'

- Commands are send to the queue when it is time.
- Commands are executed directly when it is time.

# New commands: **edcron edqu edat**



Spooler

Spooler Queue Job Tools

Queued jobs (0) Scheduled jobs (0) Cron jobs (1)

Command	Minute of the hour	Hour of the day	Day of the month	Month of the year	Day of the week	Data object	Owner	Estimated time	Description
.nmrsave -dat...	2	16	8	*	*	none	TopSpin	n/a	Execute NMR...

next page

# New commands: edcron

Spooler Queue Job Tools

Queued jobs (0) Scheduled jobs (1)

Command Minute of the day Day of the month Month of the year

nmrsave -dat... 16

**New...**

**Delete**

**Properties...**

Properties of periodical job 'zg'

Status

Command zg

Description kinetic test

Data object F:\Bruker\TopSpin\data\guest\nmr\exam1d\_1H\1pdata\1

Owner svcu

Created Tue May 08 17:53:31 CEST 2007

Sent Tue May 08 17:53:31 CEST 2007

Last execution n/a

State Waiting

Options

Off-schedule execution

Direct execution

Rules

Minute of the hour	from: 0	to: --- Ignore ---	+ -
Minute of the hour	from: 10	to: --- Ignore ---	+ -
Minute of the hour	from: 20	to: --- Ignore ---	+ -
Minute of the hour	from: 30	to: --- Ignore ---	+ -
Minute of the hour	from: 40	to: --- Ignore ---	+ -
Minute of the hour	from: 50	to: --- Ignore ---	+ -
Hour of the day	from: 16	to: 17	+ -
Day of the month	from: *	to: --- Ignore ---	+ -
Month of the year	from: *	to: --- Ignore ---	+ -
Day of the week	from: *	to: --- Ignore ---	+ -

next page

OK Cancel Apply

# Spooler in acquisition status bar



The screenshot shows the Bruker TopSpin software interface. On the left is a file browser with a tree view of folders. The main window displays a spectrum plot with a peak at 5.87 ppm. A red box highlights a 'Spooler' status window overlaid on the plot. The status window contains the following information:

Spooler		Time	
queued:	9	09:35	
delayed:	0		
cron:	1	May 11	

next page

Spooler	Time
queued: 9	09:35
delayed: 0	
cron: 1	May 11

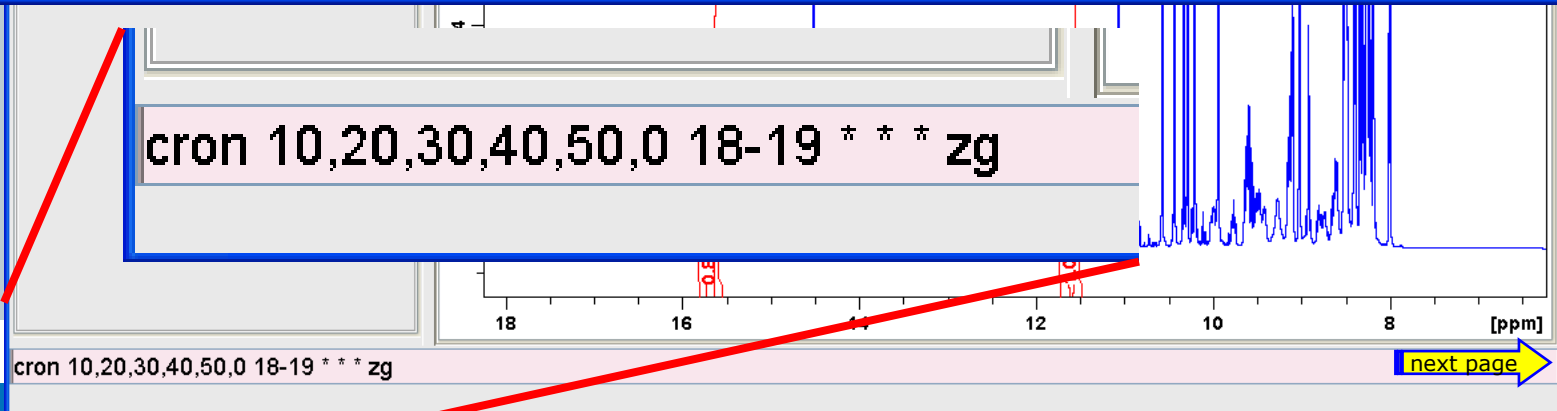
# cron: command line options



Spooler Job Tools

Queued jobs (0) Scheduled jobs (0) Cron jobs (2)

Command	Data object	Owner	Description	Minute of the hour	Hour of the day	Day of the month	Month of the year	Day of the week
zg	F:/Bruker/TopSpin/data/guest/...	svcu	kinetic test	0,10,20,30,40,50	16-17	*	*	*
zg	F:/Bruker/TopSpin/data/guest/...	svcu		10,20,30,40,50,0	18-19	*	*	*



# cron usage – an example



**New periodical**

Job

Command: zg

Description: kinetic test

Execution scope: User

Options

Off-schedule execution

Direct execution

Rules

Minute of the hour	from: 0	to: --- Ignore ---	+	-
Minute of the hour	from: 10	to: --- Ignore ---	+	-
Minute of the hour	from: 20	to: --- Ignore ---	+	-
Minute of the hour	from: 30	to: --- Ignore ---	+	-
Minute of the hour	from: 40	to: --- Ignore ---	+	-
Minute of the hour	from: 50	to: --- Ignore ---	+	-
Hour of the day	from: 16	to: 17	+	-
Day of the month	from: *	to: --- Ignore ---	+	-
Month of the year	from: *	to: --- Ignore ---	+	-
Day of the week	from: *	to: --- Ignore ---	+	-

OK Cancel

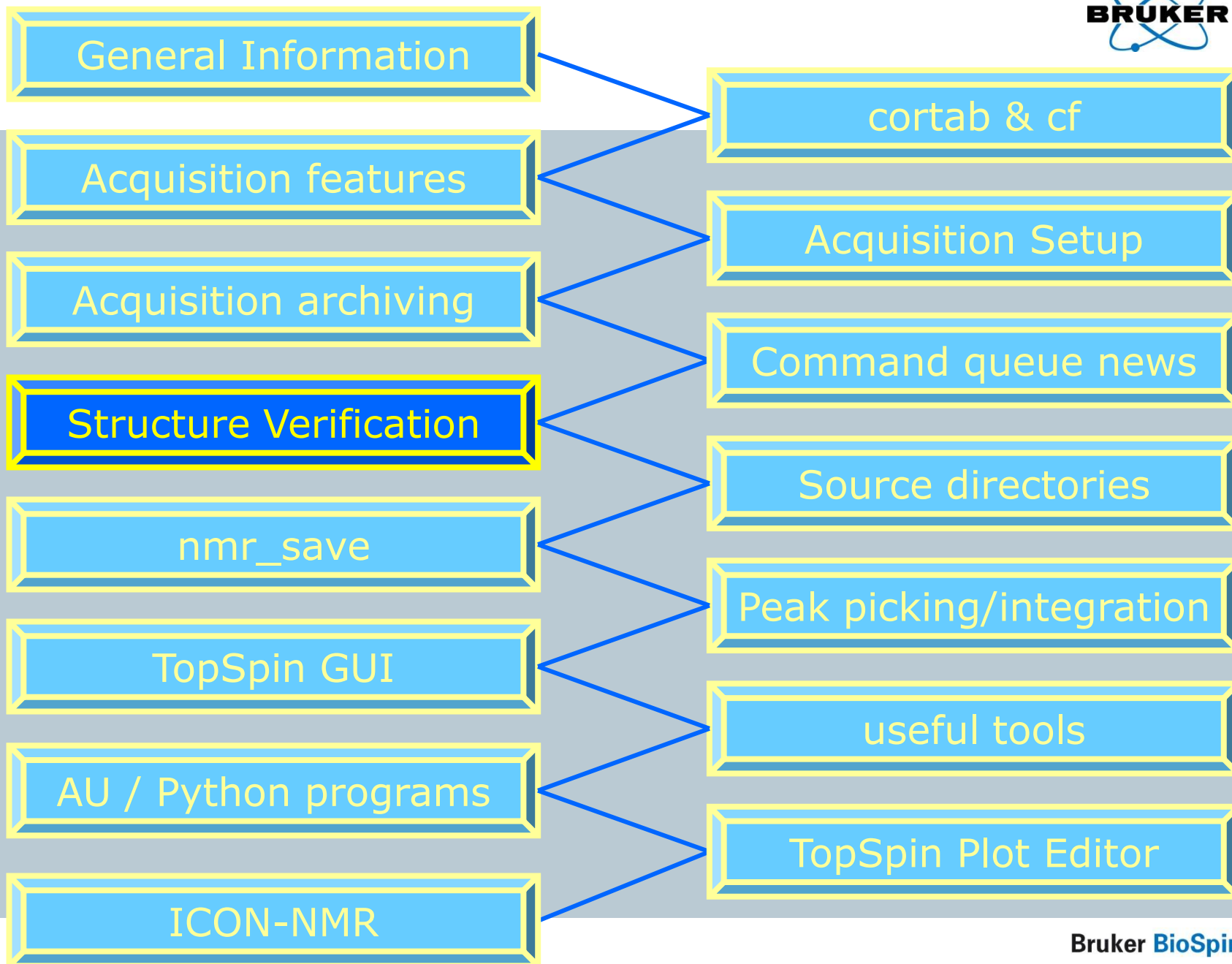
**zg** on current dataset will be executed every 10 minutes between 4 pm and 5 pm.

**another example later on**

next page →

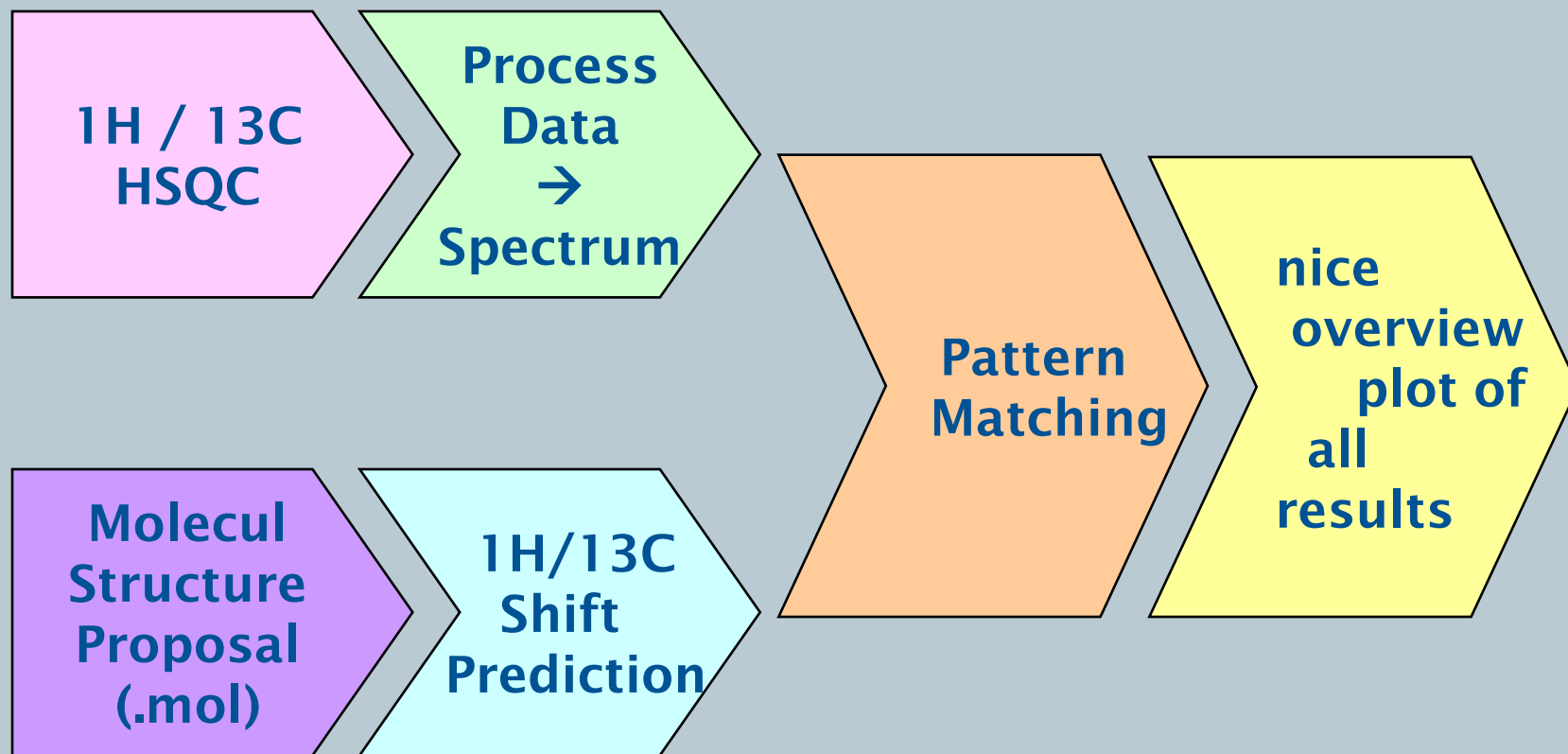


# Content



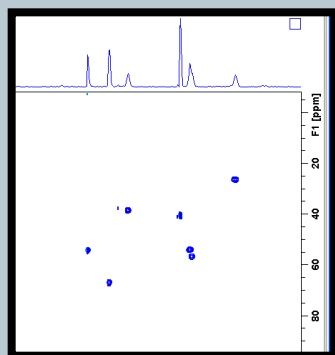
# Teamwork:

## TopSpin/Perch\*/AMIX/TS Plot Editor

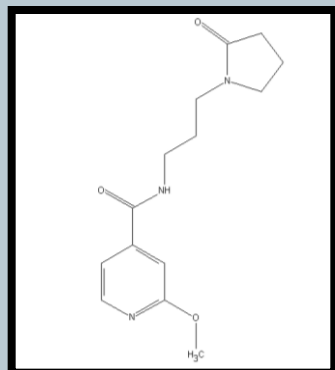


# Teamwork:

## TopSpin/Perch\*/AMIX/TS Plot Editor

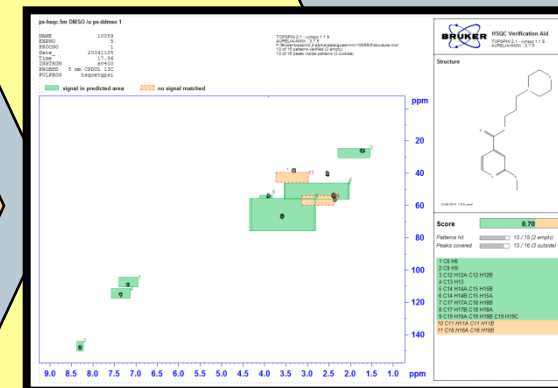


Process  
Data  
→  
Spectrum



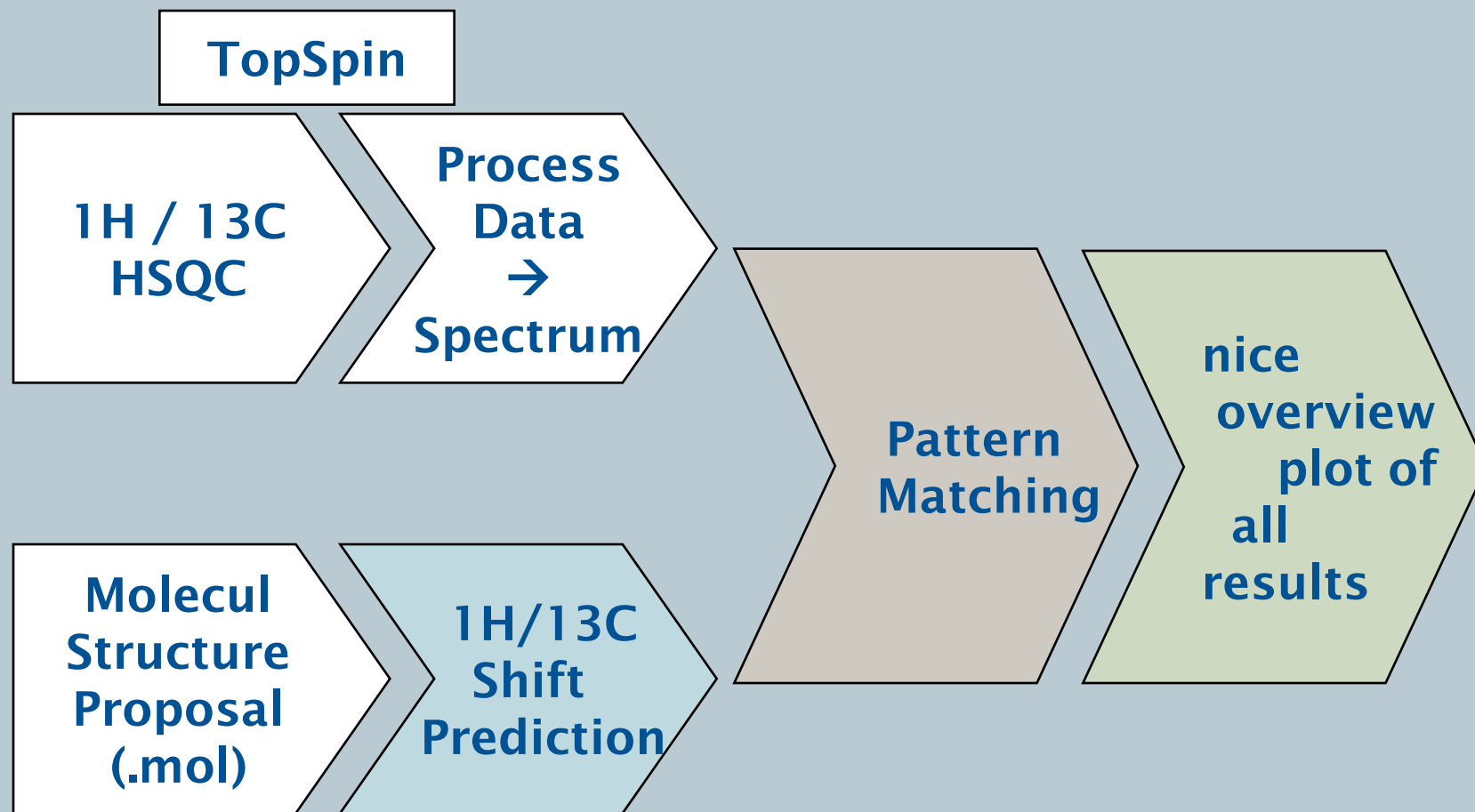
$^1\text{H}/^{13}\text{C}$   
Shift  
Prediction

Pattern  
Matching



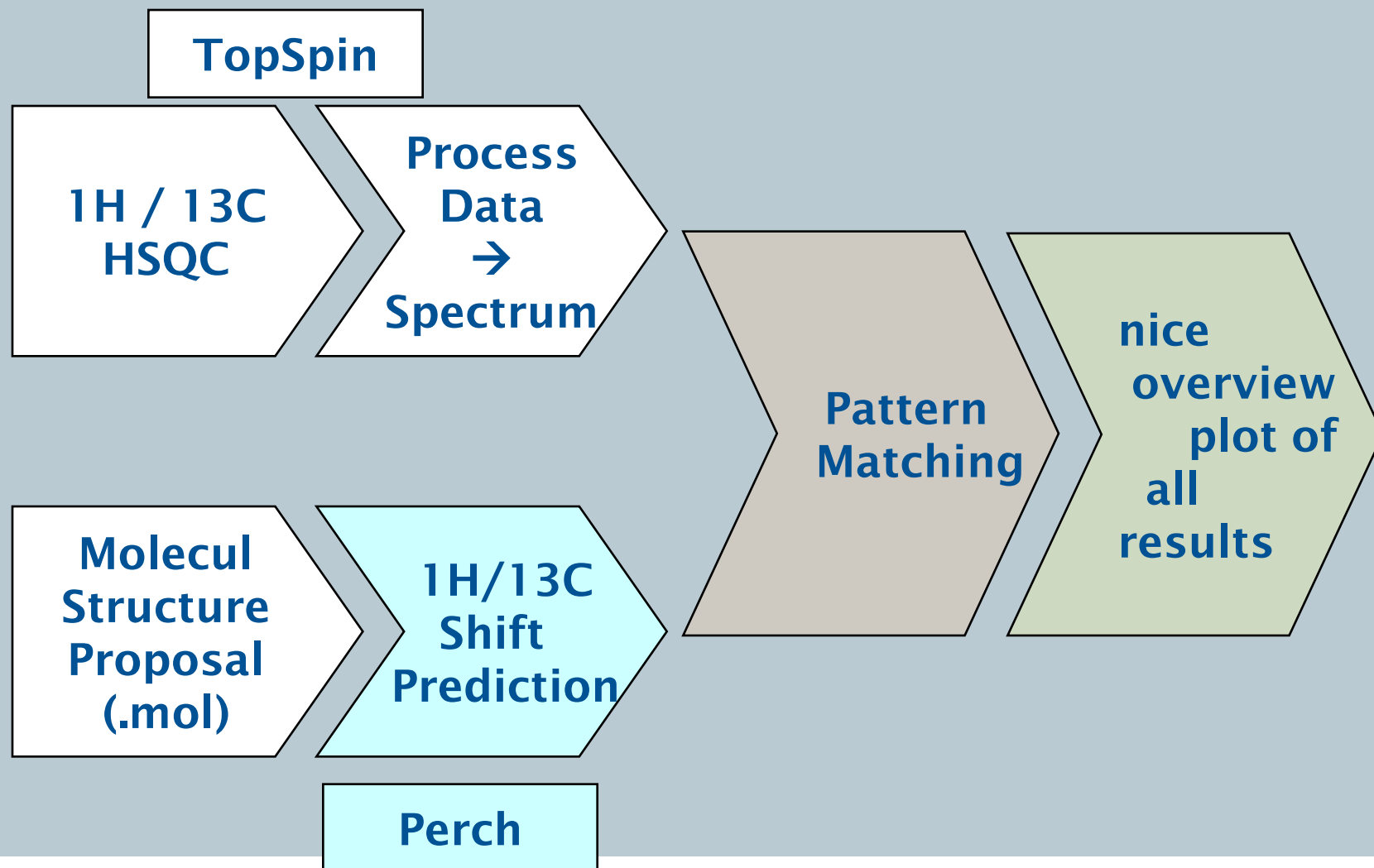
# Teamwork:

## TopSpin/Perch\*/AMIX/TS Plot Editor



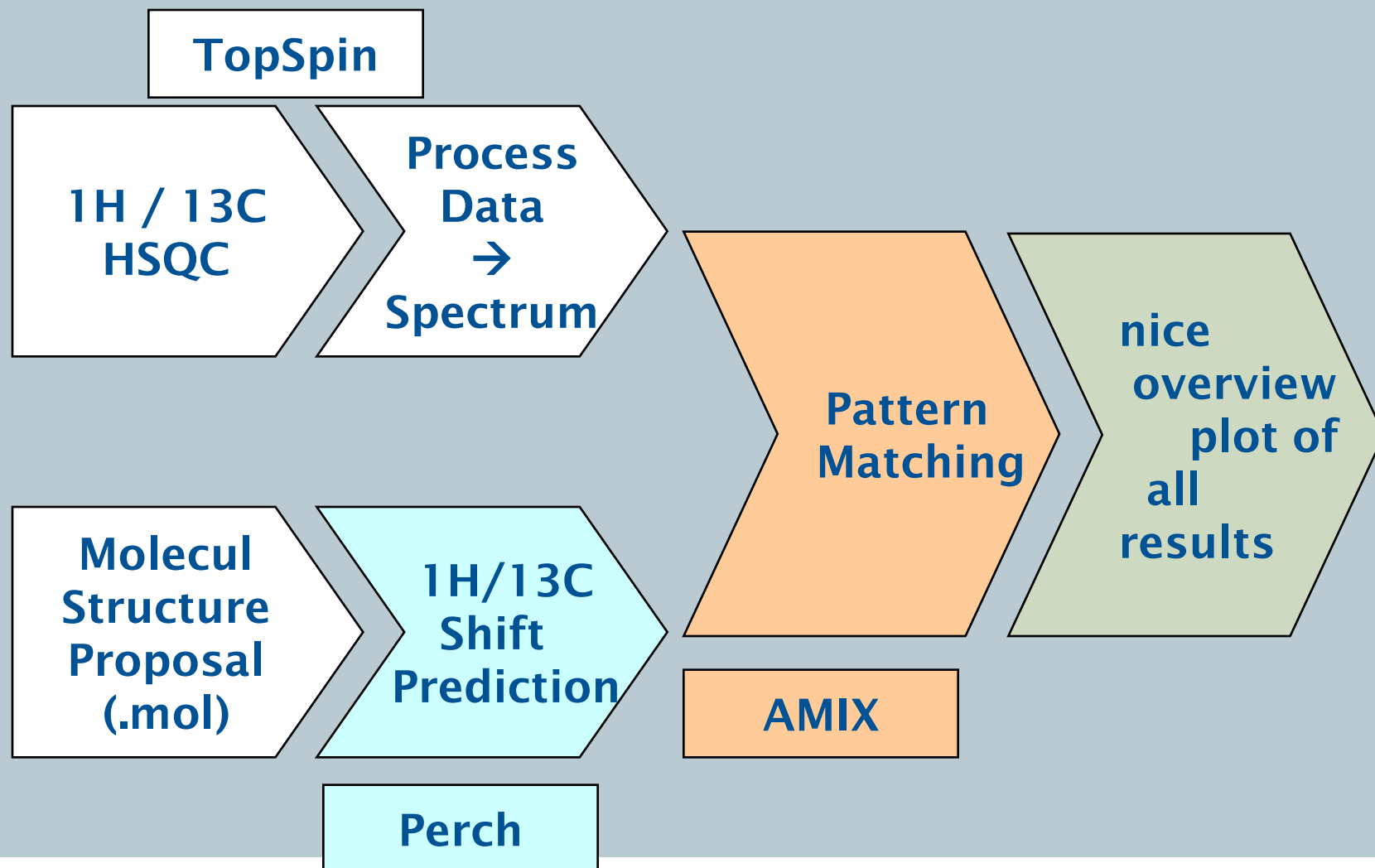
# Teamwork:

## TopSpin/Perch\*/AMIX/TS Plot Editor



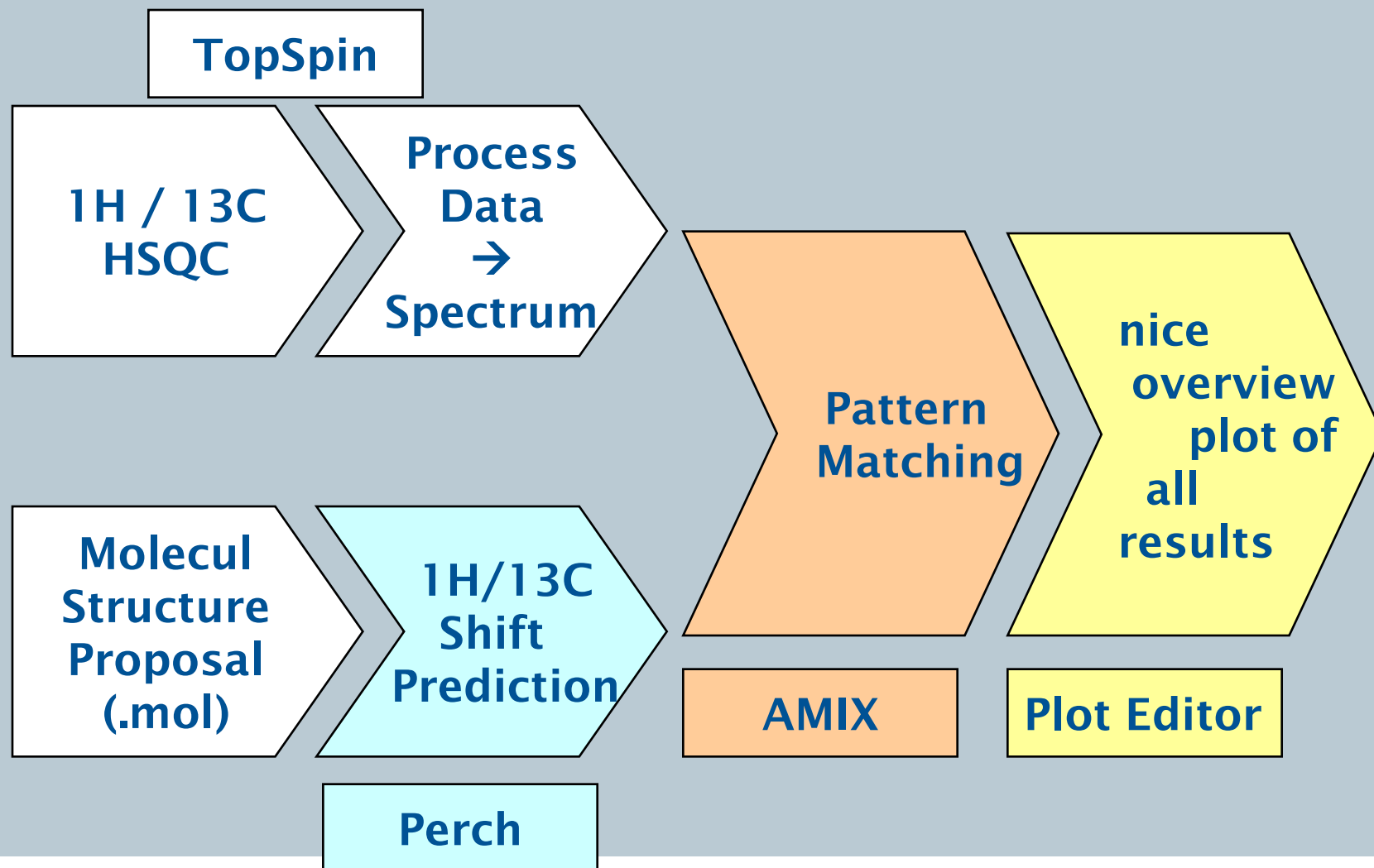
# Teamwork:

## TopSpin/Perch\*/AMIX/TS Plot Editor



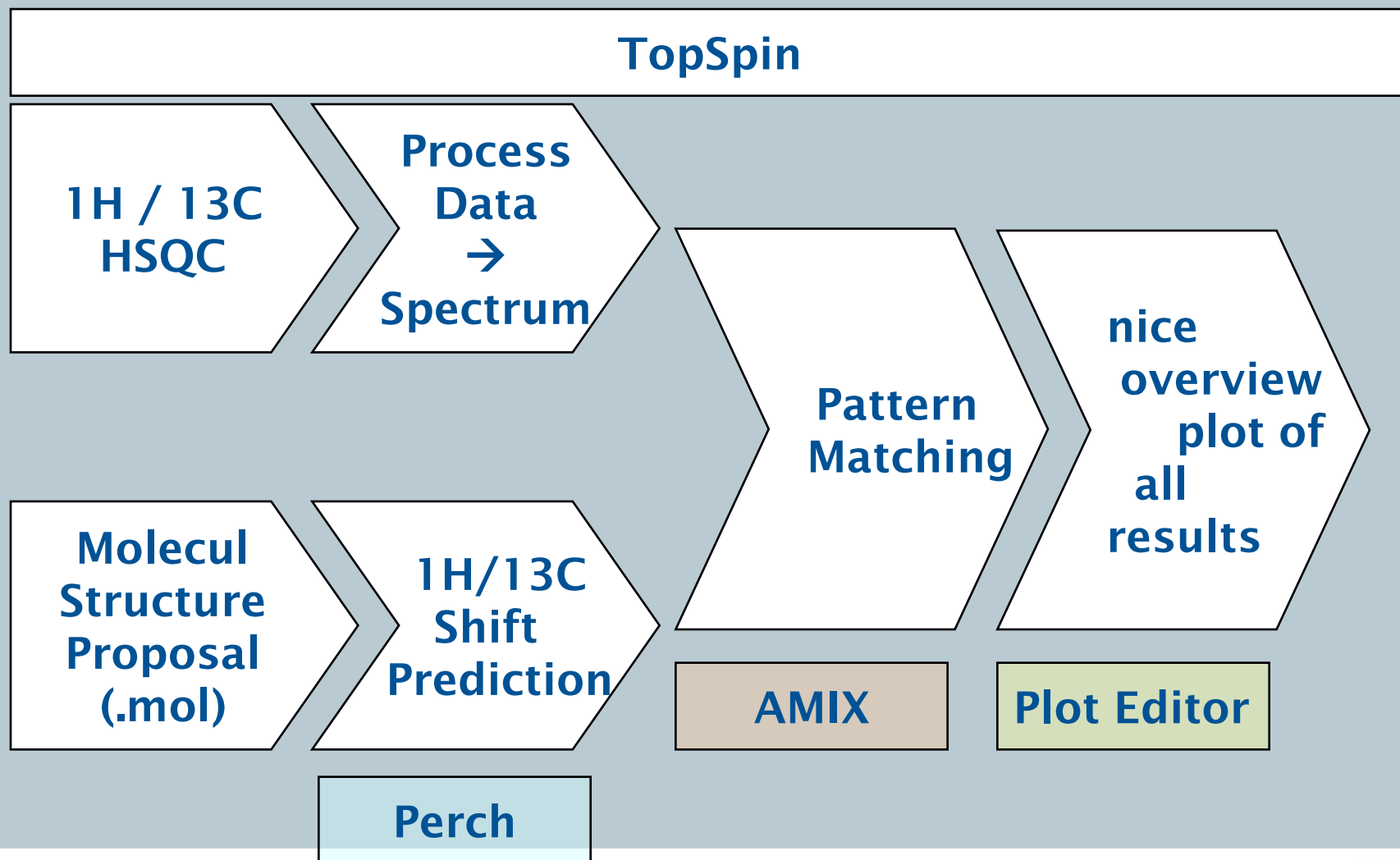
# Teamwork:

## TopSpin/Perch\*/AMIX/TS Plot Editor



# Teamwork:

## TopSpin/Perch\*/AMIX/TS Plot Editor





# Structure Verification Aid



Bruker TopSpin on merlin as svcu

File Edit View Processing Analysis Options Window Help

1d 3d

\*2 /2 \*8 /8 \*X +/-

Browser Last50 Groups Alias

- Wserverhome
- C:\NMR data
- F:\Bruker\TopSpin
- F:\Bruker\topspin1.3pl6
- F:\Bruker\topspin1.3pl8
- F:\Bruker\topspin2.0

Axis Calibration... [cal]

Peak Picking... [pp]

Integration... [int]

Multiple Spectrum Display...

T1/T2 Relaxation

Line Shape Fitting

Simulation

Small Molecules

Structure Edit/View

Dosy

Proteins

Start Amix Viewer

test now

uPars Title PulseProg Peaks Integrals Sample Structure Fid

Perch Shift Prediction [predict]

Verification Aid Using HSQC+Prediction [vyhsqc]

F2 [ppm]	F1 [ppm]
8.5	140
7.5	120
4.5	40
3.5	50
2.5	30
1.5	20

# Structure Verification Aid



The screenshot shows the Bruker TopSpin software interface. The 'Analysis' menu is open, and the 'Small Molecules' option is selected, which has opened a sub-menu. In this sub-menu, 'Perch Shift Prediction [predict]' and 'Verification Aid Using HSQC+Prediction [vyhsqc]' are visible. The 'vyhsqc' dialog box is open in the foreground, displaying the following text:

Structure verification aid based on <sup>1</sup>H/<sup>13</sup>C shift prediction:  
Comparison with the HSQC spectrum contained in the current dataset.  
If the .mol structure file is not given as an absolute path,  
it is taken from the current EXPNO.

Mol file = structure.mol

Use existing shift prediction

Use existing shift prediction

Make new shift prediction

The dialog box also shows a file browser with 'structure.mol' selected. The background shows an HSQC spectrum plot with F2 [ppm] on the x-axis (ranging from 8 to 0) and F1 [ppm] on the y-axis (ranging from 0 to 140).

# Structure Verification Aid



The screenshot shows the Bruker TopSpin software interface. The 'Analysis' menu is open, and the 'Small Molecules' option is selected, leading to a sub-menu where 'Verification Aid Using HSQC+Prediction [vyhsqc]' is highlighted. In the foreground, the 'vyhsqc' dialog box is open, displaying the following text:

Structure verification aid based on <sup>1</sup>H/<sup>13</sup>C shift prediction:  
Comparison with the HSQC spectrum contained in the current dataset.  
If the .mol structure file is not given as an absolute path,  
it is taken from the current EXPNO.

Mol file = F:\Bruker\topspin2.2-alpha\exp\stan\nmr\lists\structure  
Make new shift prediction

Buttons: Execute, Browse (highlighted with a red box), Cancel

The background shows an HSQC spectrum plot with F2 [ppm] on the x-axis (ranging from 8 to 0) and F1 [ppm] on the y-axis (ranging from 0 to 140). The plot displays several cross-peaks, with a prominent one at approximately (2.5 ppm, 40 ppm).

# Structure Verification Aid



Bruker TopSpin on merlin as svcu

File Edit View Processing Analysis Options Window Help

Axis Calibration... [cal] Peak Picking... [pp] Integration... [int]

test now

Browser Last50 Groups Alias

PERCH NMR Software Tools - PERCH Script Executor

C:\Documents and Settings\svcu\AU\_SESSION\perch\_command.txt

```
Group "#21" renamed to "H9"  
Group "#22" renamed to "H11"  
Group "#23" renamed to "H12"  
Group "#24" renamed to "H13"  
Group "#25" renamed to "H14_15"  
WARNING: GENERATED NAME "H14_15" IS NOT A VALID GROUP NAME. UNABL  
Group "#27" renamed to "H16"  
Group "#28" renamed to "H17_18"  
WARNING: GENERATED NAME "H17_18" IS NOT A VALID GROUP NAME. UNABL  
Group "#30" renamed to "H19"  
---NMR GROUP NAMES GENERATED FROM BRUKER FORMAT ATOM NAMES---
```

Predicting NMR-parameters, please wait...

CANCEL

Structure F1d

in [vyhsqc]

F1 [ppm]

F2 [ppm]

# Structure Verification Aid



TOPSPIN Plot Editor - [verification\_report.xwp]

File Edit IOPSPIN Options Window Help

Data Attributes Zoom in Zoom out Full Delete Group Ungroup Rotate Edit 1D/2D-Edit Undo

Expand Zoom

Standard NMR

Title

NMR Text

T<sub>1</sub>T<sub>2</sub>

Mode:

ps-hsqc-5m DMSO /u ps-ddms0 1

NAME 10059  
EXPNO 5  
PROCNO 1  
Date\_ 20041105  
Time 17.36  
INSTRUM av400  
PROBHD 5 mm CPDUL 13C  
PULPROG hsqcetgps1

TOPSPIN 2.1 - vyhsqc 1.1 \$  
AURELIA/AMX : 3.7.5  
F:/Bruker/topspin2.2-alpha\data/guest/nmr/10059/5/structure.mol  
13 of 15 patterns verified (2 empty)  
13 of 16 peaks inside patterns (3 outside)

signal in predicted area no signal matched

ppm

ppm

**BRUKER** HSQC Verification Aid  
TOPSPIN 2.1 - vyhsqc 1.1 \$  
AURELIA/AMX : 3.7.5

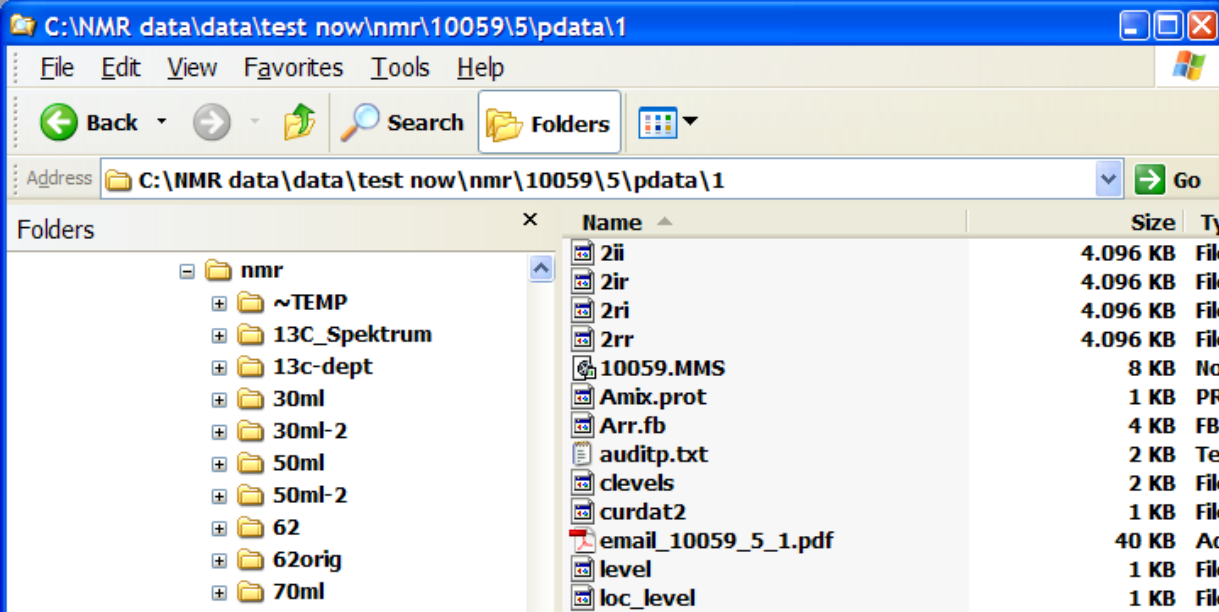
Structure

C:\1001010\_179.04.gmol

Score **0.70**

Patterns hit 13 / 15 (2 empty)  
Peaks covered 13 / 16 (3 outside)

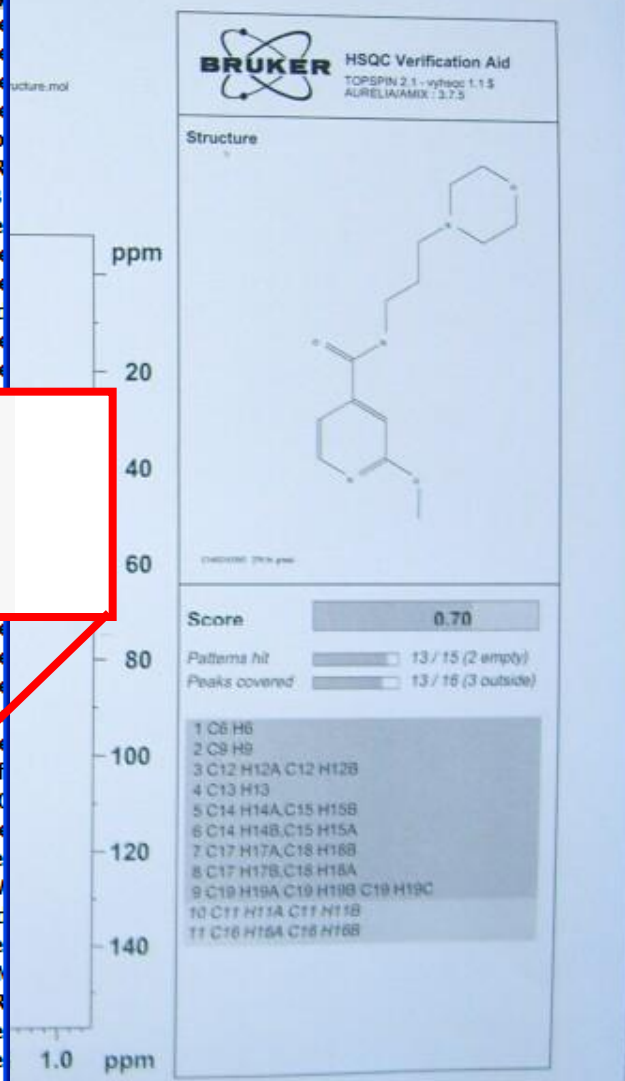
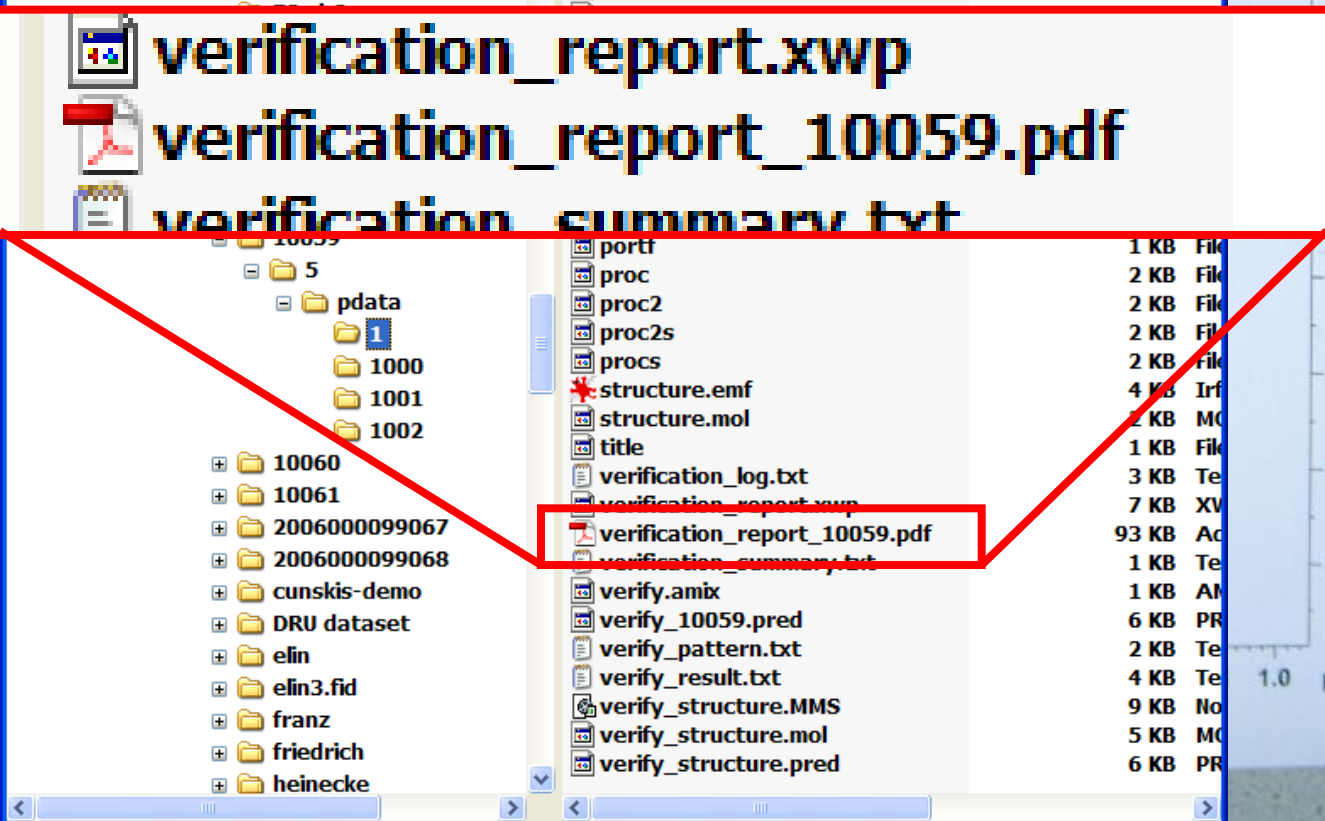
- 1 C6 H6
- 2 C9 H9
- 3 C12 H12A C12 H12B
- 4 C13 H13
- 5 C14 H14A, C15 H15B
- 6 C14 H14B, C15 H15A
- 7 C17 H17A, C18 H18B
- 8 C17 H17B, C18 H18A
- 9 C19 H19A, C19 H19B, C19 H19C
- 10 C11 H11A, C11 H11B
- 11 C16 H16A, C16 H16B



print out



and as PDF

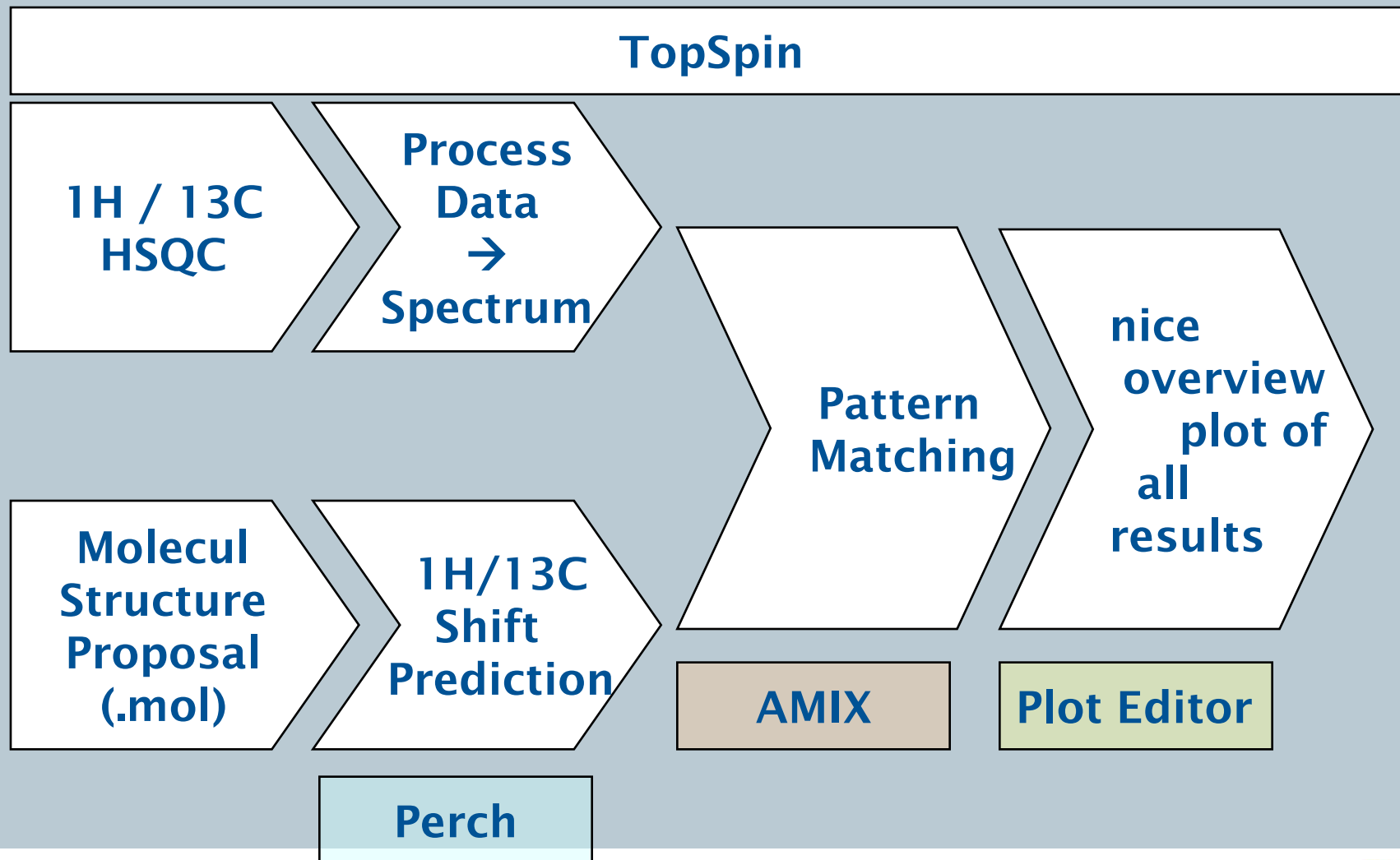


# Teamwork:

## TopSpin/Perch\*/AMIX/TS Plot Editor



### ICON-NMR



# Structure Verification Aid



ICON-NMR: 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
- ToolBox Setup
- Accounting

**Run Control**

Default Automation Mode: Manual Inject/Eject

- Eject last sample in queue
- Never Rotate the Sample
- Start run at user login

**Processing Control**

- Generate a Spectrum Printout
- Process Data Sets after Acquisition: Ask on Startup
- Generate Spectrum Print-Out file in data set for possible dispatch to e-mail recipient: Off
- Perform Structure Consistency Check

**DataSet Management**

- Ignore the TopSpin Prosol Parameters
- Delete temporary datasets after experiment end
- Allow Overwrite of existing Acquisition Data

**BEST Mode Settings**

- Enable BEST-NMR
- BEST-NMR Automation Mode: Standard (No Barcodes)
- Force Solvent Change after (Number of Hours - Day Time only): 0
- BEST Administration Tool: 'bestadm'



# Structure Verification Aid



ICON-NMR: Automation May03-2007-1433-BRUKER-svcu

File Run Holder View Find Parameters Options Help

Available 2 Available

Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Structure/Processing	Par	Title / Orig	Pri	Time	User
1		Available	F:\	03052007-BRUKERsvc	10	CDCI3	PROTON						BRUKER\svc_u
		Available	F:\	03052007-BRUKERsvc	11	CDCI3	HSQCEDETGP	+	bru10059.mol				BRUKER\svc_u
	F2		F:\	03052007-BRUKERsvc	10								BRUKER\svc_u
2		Available											
3		Available											
4		Available											
5		Available											
6		Available											
7		Available											
8		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	Remarks
---	------	--------	------	-----	------------	------	-----	----------	------	------	-----	------	------	------	--------------	---------

Search   search previous runs

Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: BRUKER\svc\_u

# Structure Verification Aid



TOPSPIN Plot Editor - [verification\_report.xwp]

File Edit IOPSPIN Options Window Help

Data Attributes Zoom in Zoom out Full Delete Group Ungroup Rotate Edit 1D/2D-Edit Undo

ps-hsqc-5m DMSO /u ps-ddmsd 1

NAME 10059  
EXPNO 5  
PROCNO 1  
Date\_ 20041105  
Time\_ 17.36  
INSTRUM av400  
PROBHD 5 mm CPDUL 13C  
PULPROG hsqcetgps1

TOPSPIN 2.1 - vyhsqc 1.1 S  
AURELIA/AMIX : 3.7.5  
F:/Bruker/topspin2.2-alpha\data\guest\nmr\10059\5\structure.mol  
6 of 8 patterns verified (2 empty)  
7 of 11 peaks inside patterns (4 outside)

Standard  
NMR

Title

ICON-NMR:  
File Run Ho

Hol... Type

1 2

Mode:

2 3 4 5 6 7 8

Sut

Preceding Exper

# Date

For Help, press F1

Position: 28.30,20.20

Mark object

Zoom: 100.9

signal in predicted area  
no signal matched

ppm

ppm

BRUKER HSQC Verification Aid

TOPSPIN 2.1 - vyhsqc 1.1 S  
AURELIA/AMIX : 3.7.5

Structure

CCCCC(=O)c1ccc(C)cc1

Score 0.48

Patterns hit 6 / 8 (2 empty)

Peaks covered 7 / 11 (4 outside)

- 1 C7 H7
- 2 C9 H9A C9 H9B
- 3 C10 H10
- 4 C12 H12A C12 H12B
- 5 C14 H14A C14 H14B C14 H14C
- 6 C15 H15A C15 H15B C15 H15C
- 7 C5 H5
- 8 C13 H13A C13 H13B

Change User

# Other Perch\* features within TopSpin



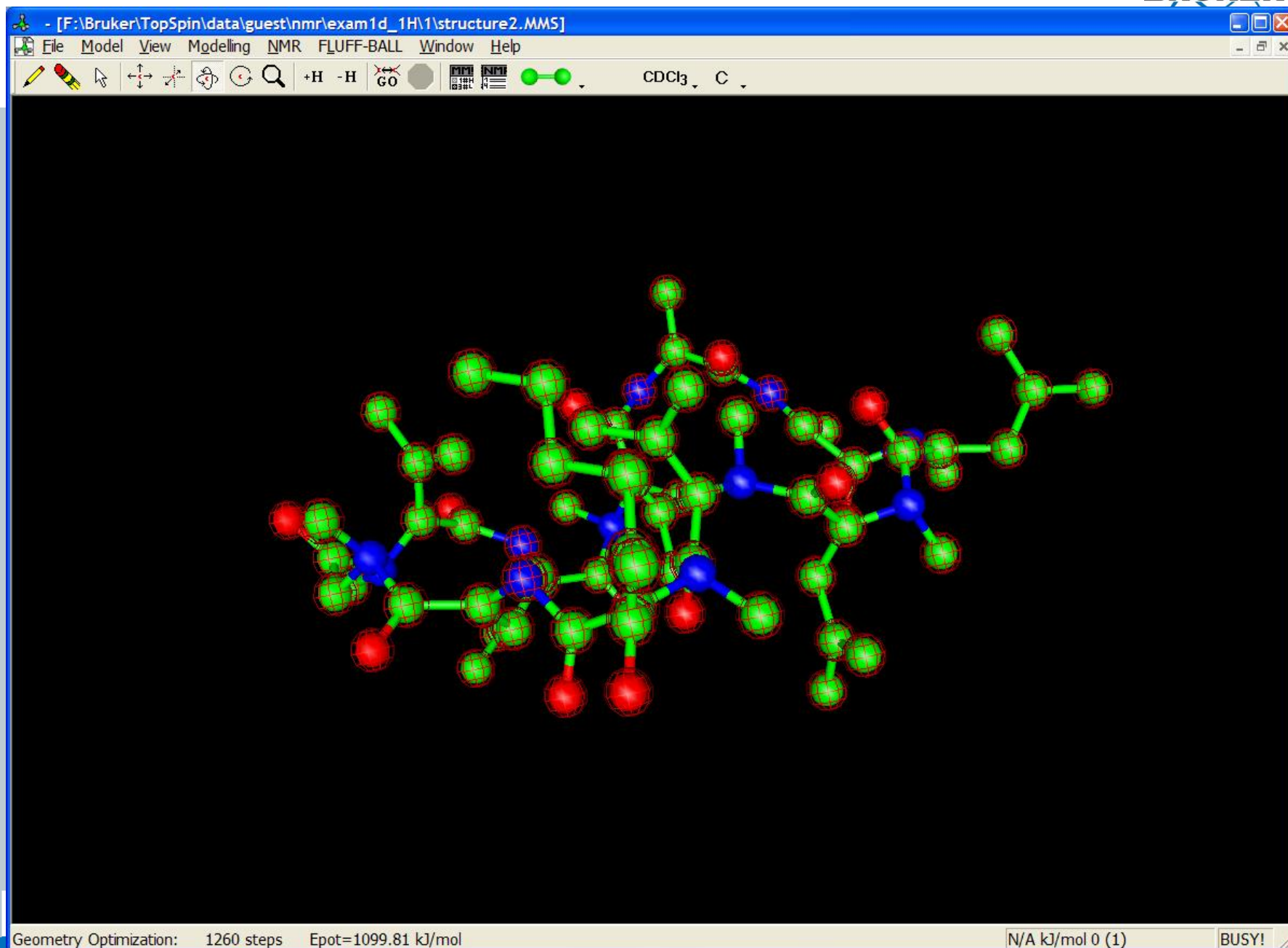
The screenshot shows the Bruker TopSpin software interface. The 'Analysis' menu is open, and 'Perch Shift Prediction [predict]' is highlighted. Other visible options include 'Verification Aid Using HSQC+Prediction [vyhsqc]'. The background shows an NMR spectrum with several peaks and a table of chemical shifts.

Chemical Shift (ppm)
12.15
11.98
11.07
10.57
10.43
10.33
10.20
9.84
9.62
9.59
9.56
9.15
9.13
9.10
9.09
9.03
8.91
8.81
8.60
8.59
8.51
8.50
8.49
8.41
8.40
8.39
8.33
8.31
8.20
8.16
8.15
8.14
8.12
8.11
8.09
8.08
8.07
8.06
8.05
8.04
8.03
8.02
8.01
8.00
7.99
7.98
7.97
7.96
7.95
7.94
7.93
7.92
7.91
7.90
7.89
7.88
7.87
7.86
7.85
7.84
7.83
7.82
7.81
7.80
7.79
7.78
7.77
7.76
7.75
7.74
7.73
7.72
7.71
7.70
7.69
7.68
7.67
7.66
7.65
7.64
7.63
7.62
7.61
7.60
7.59
7.58
7.57
7.56
7.55
7.54
7.53
7.52
7.51
7.50
7.49
7.48
7.47
7.46
7.45
7.44
7.43
7.42
7.41
7.40
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.30
7.29
7.28
7.27
7.26
7.25
7.24
7.23
7.22
7.21
7.20
7.19
7.18

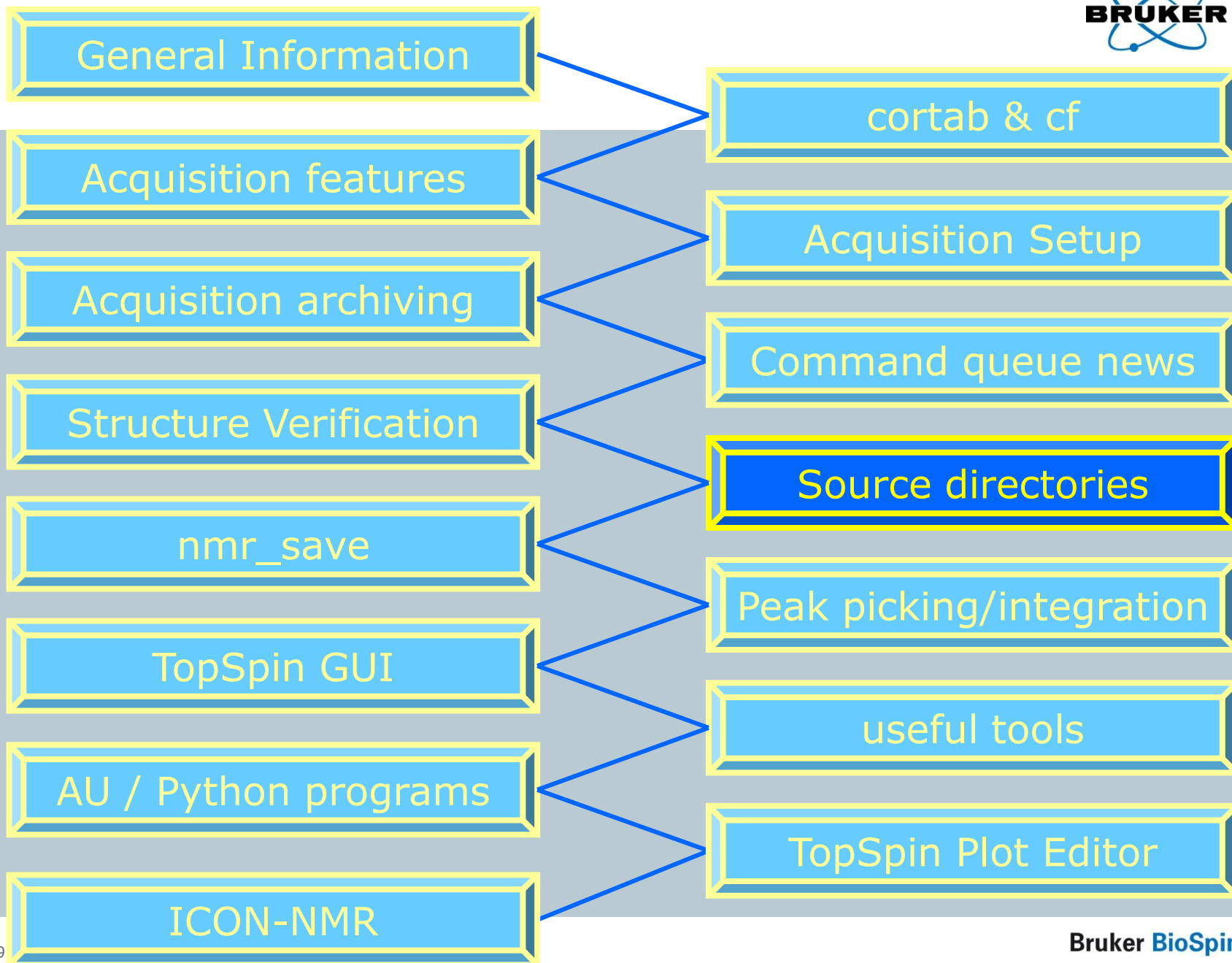
A red-bordered callout box highlights the 'Run Molecule Modeling' button in the software toolbar. The button is represented by a molecular structure icon. A text box with the label 'Run Molecule Modeling' is positioned below the button, with a line pointing to it.

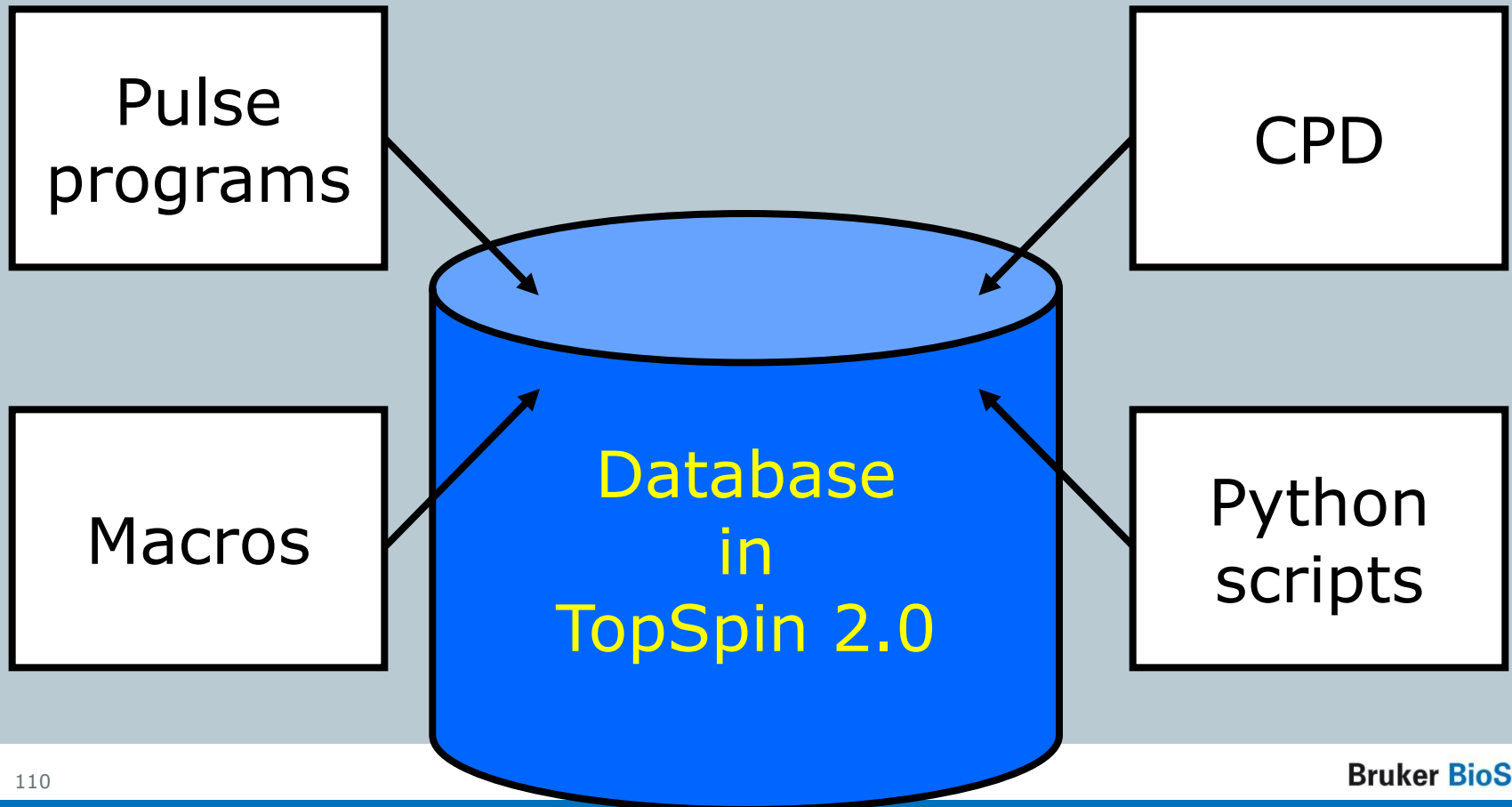
The screenshot shows the Bruker TopSpin software interface with a 3D ball-and-stick model of a complex organic molecule. The molecule features a central ring system with various substituents, including methyl groups, hydroxyl groups, and nitrogen atoms. The interface includes a toolbar with various icons and a 'Run Molecule Modeling' button. The file name 'structure2.mol' is visible at the bottom.

# Perch\*: e.g. geometry optimization



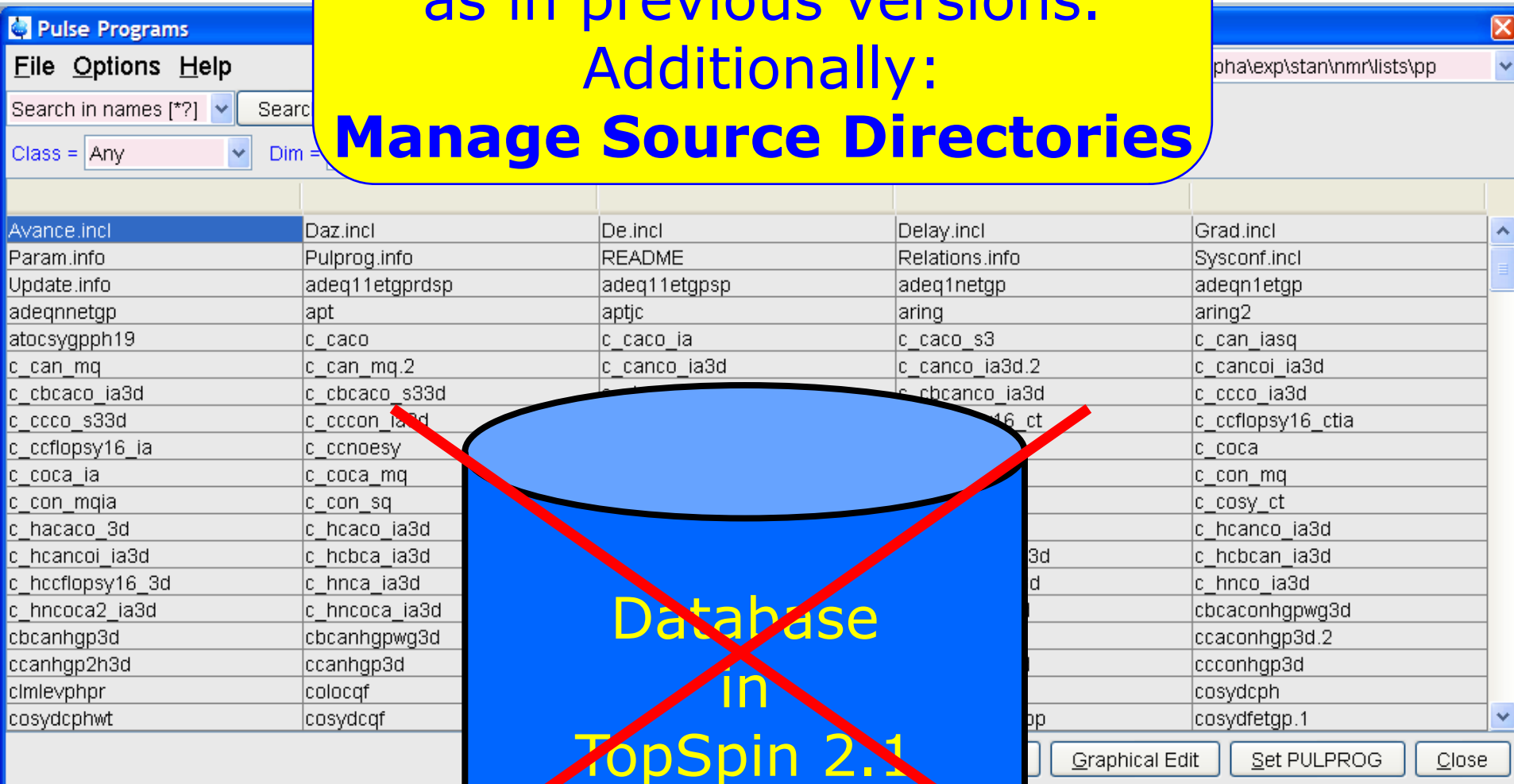
# Content





No database anymore in 2.1!  
Again directory/file structure  
as in previous versions.

Additionally:  
**Manage Source Directories**



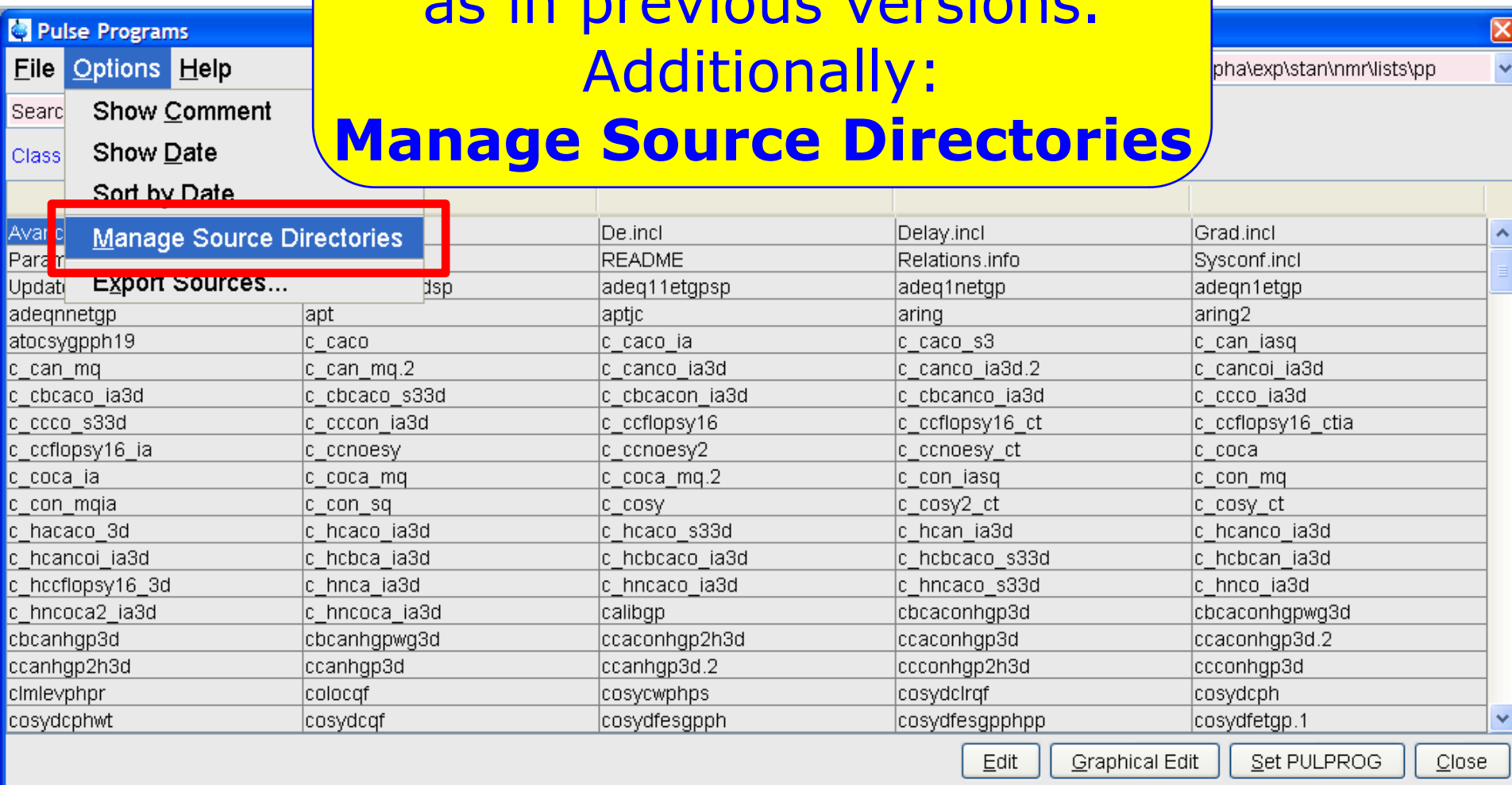
The screenshot shows the 'Pulse Programs' window with a search bar and a list of files. A blue cylinder icon with a red 'X' over it is overlaid on the list, with the text 'Database in TopSpin 2.1' written inside it.

Avance.incl	Daz.incl	De.incl	Delay.incl	Grad.incl
Param.info	Pulprog.info	README	Relations.info	Sysconf.incl
Update.info	adeq11etgprdsp	adeq11etgppsp	adeq1netgp	adeqn1etgp
adeqnnetgp	apt	aptjc	aring	aring2
atocsygpph19	c_caco	c_caco_ia	c_caco_s3	c_can_iasq
c_can_mq	c_can_mq.2	c_canco_ia3d	c_canco_ia3d.2	c_cancoi_ia3d
c_cbcaco_ia3d	c_cbcaco_s33d		c_cbcanco_ia3d	c_ccco_ia3d
c_ccco_s33d	c_cccon_ia3d		c_ccco_ia3d.16.ct	c_ccflopsy16_ctia
c_ccflopsy16_ia	c_ccnoesy			c_coca
c_coca_ia	c_coca_mq			c_con_mq
c_con_mqia	c_con_sq			c_cosy_ct
c_hacaco_3d	c_hcaco_ia3d			c_hcanco_ia3d
c_hcancoi_ia3d	c_hcbca_ia3d			c_hcbcan_ia3d
c_hccflopsy16_3d	c_hnca_ia3d			c_hnco_ia3d
c_hncoca2_ia3d	c_hncoca_ia3d			cbcaconhgpwg3d
cbcanhgp3d	cbcanhgpwg3d			ccaconhgp3d.2
ccanhgp2h3d	ccanhgp3d			ccconhgp3d
clmlevphpr	colocqf			cosydcph
cosydcphwt	cosydcqf			cosydfetgp.1

No database anymore in 2.1!  
Again directory/file structure  
as in previous versions.

Additionally:

**Manage Source Directories**



The screenshot shows the 'Pulse Programs' window with a menu bar (File, Options, Help) and a search bar. A red box highlights the 'Manage Source Directories' button in the 'Options' menu. Below the menu is a table listing various source directories and their corresponding files.

Program Name	Source Directory	File 1	File 2	File 3
Avarc		De.incl	Delay.incl	Grad.incl
Param		README	Relations.info	Sysconf.incl
Update		adeq11etgpp	adeq1netgp	adeqn1etgp
adeqnnetgp	apt	aptjc	aring	aring2
atocsygpph19	c_caco	c_caco_ia	c_caco_s3	c_can_iasq
c_can_mq	c_can_mq.2	c_canco_ia3d	c_canco_ia3d.2	c_cancoi_ia3d
c_cbcaco_ia3d	c_cbcaco_s33d	c_cbcaco_ia3d	c_cbcaco_ia3d	c_ccco_ia3d
c_ccco_s33d	c_cccon_ia3d	c_ccflopsy16	c_ccflopsy16_ct	c_ccflopsy16_ctia
c_ccflopsy16_ia	c_ccnoesy	c_ccnoesy2	c_ccnoesy_ct	c_coca
c_coca_ia	c_coca_mq	c_coca_mq.2	c_con_iasq	c_con_mq
c_con_mqia	c_con_sq	c_cosy	c_cosy2_ct	c_cosy_ct
c_hacaco_3d	c_hcaco_ia3d	c_hcaco_s33d	c_hcan_ia3d	c_hcanco_ia3d
c_hcancoi_ia3d	c_hcbca_ia3d	c_hcbca_ia3d	c_hcbca_ia3d	c_hcbcan_ia3d
c_hccflopsy16_3d	c_hnca_ia3d	c_hncaco_ia3d	c_hncaco_s33d	c_hnco_ia3d
c_hncoca2_ia3d	c_hncoca_ia3d	calibgp	cbcaconhgp3d	cbcaconhgp3d
cbcanhgp3d	cbcanhgp3d	ccaconhgp2h3d	ccaconhgp3d	ccaconhgp3d.2
ccanhgp2h3d	ccanhgp3d	ccanhgp3d.2	ccconhgp2h3d	ccconhgp3d
clmlevphpr	colocqf	cosycwphps	cosydclrqf	cosydcph
cosydcphwt	cosydcqf	cosydfesgpph	cosydfesgpph	cosydfetgp.1

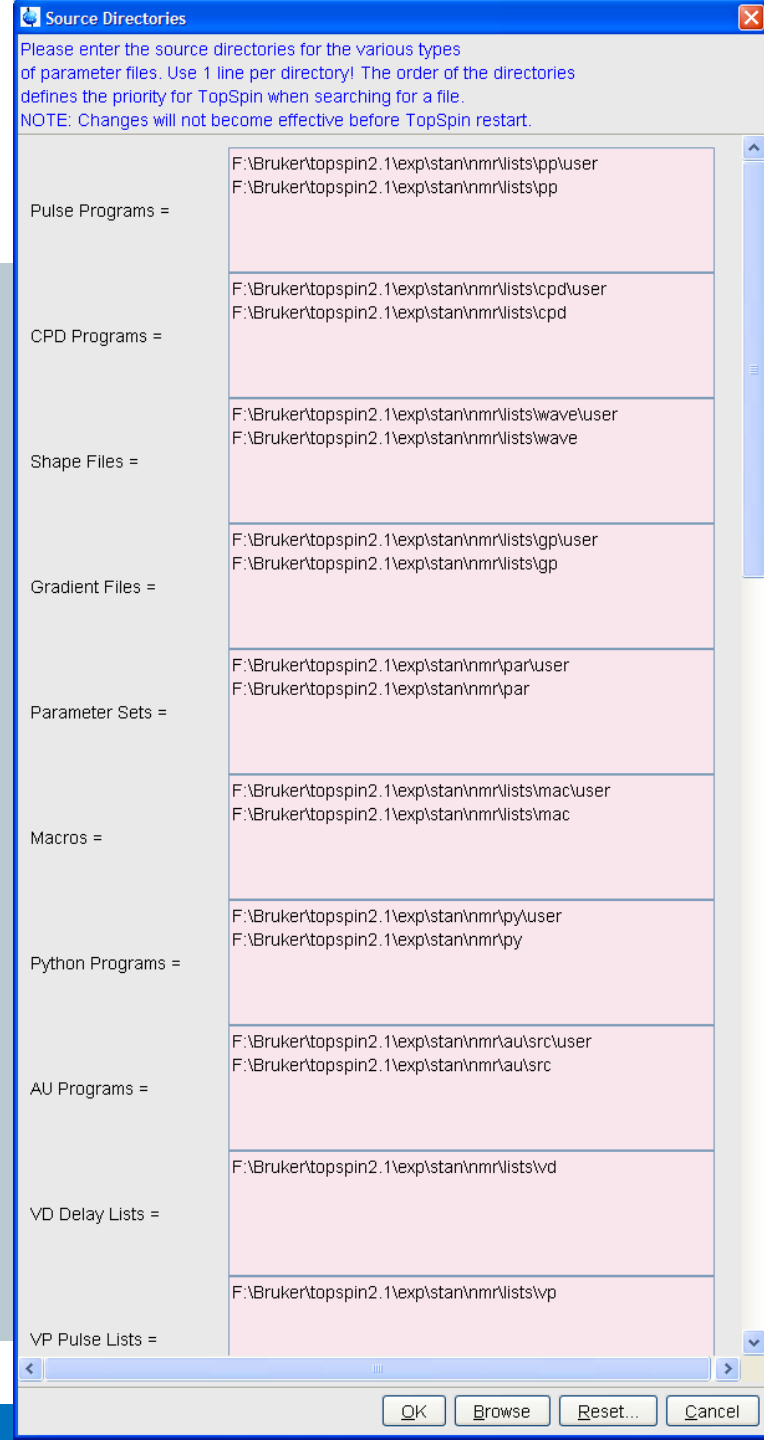
Buttons at the bottom: Edit, Graphical Edit, Set PULPROG, Close



# Source directories

User can specify individual directories for:

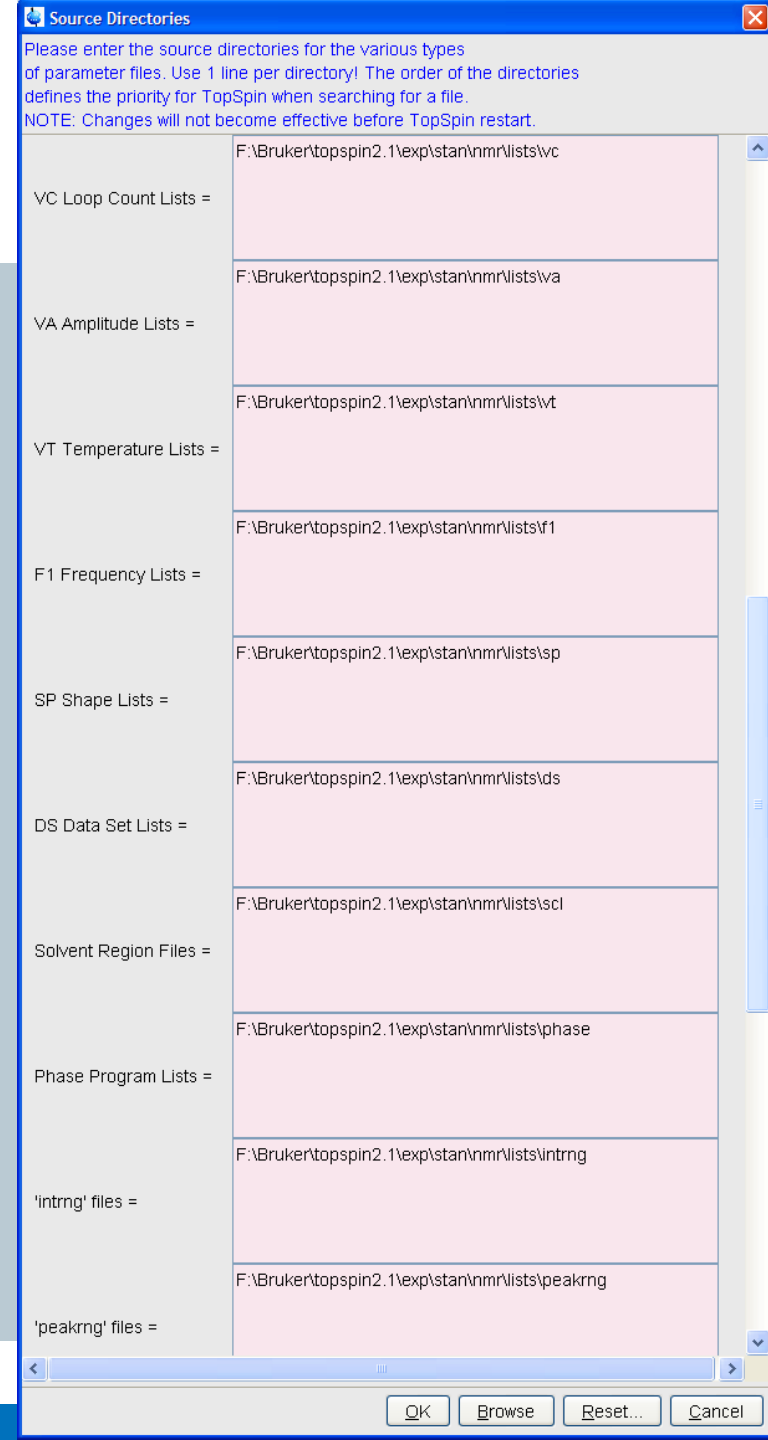
- Pulse programs
- CPD programs
- Shape Files
- Gradient Files
- Parameter Sets
- Macros
- Python programs
- AU programs
- VD lists
- VP lists ...



# Source directories

User can specify individual directories for:

- ...
- VC lists
- VA lists
- VT lists
- F1 lists
- SP lists
- DS lists
- Solvent Region Files
- Phase lists
- intrng files ...

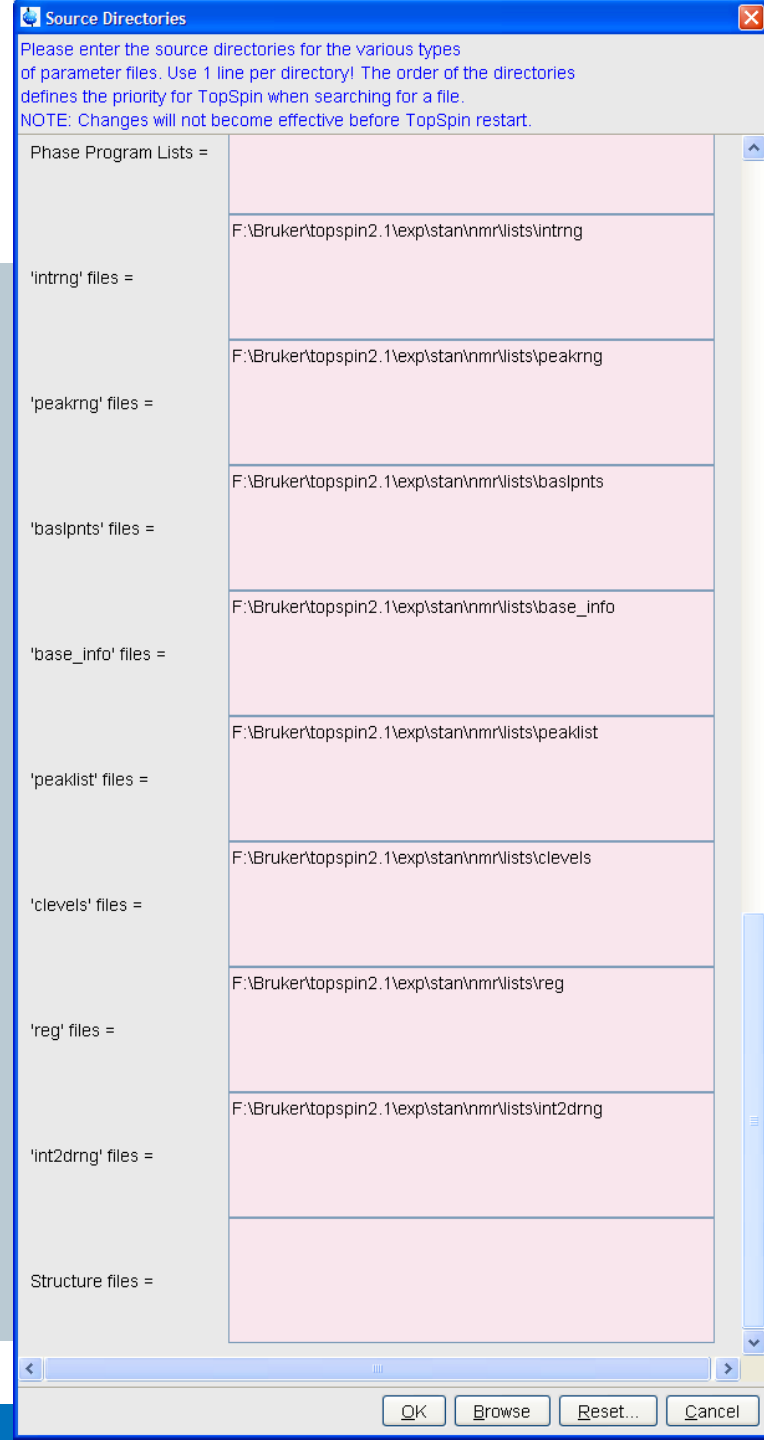


# Source directories

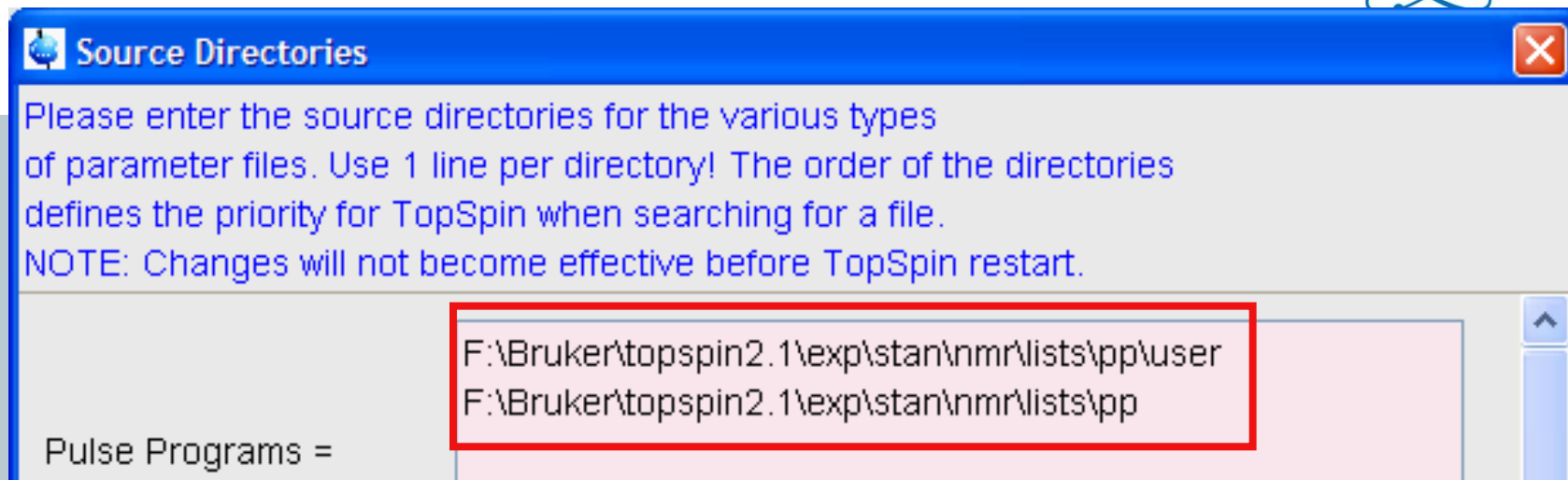
User can specify individual directories for:

...

- peakrng files
- baslpnts files
- base\_info files
- peaklist files
- clevels files
- reg files
- int2drng files
- structure files



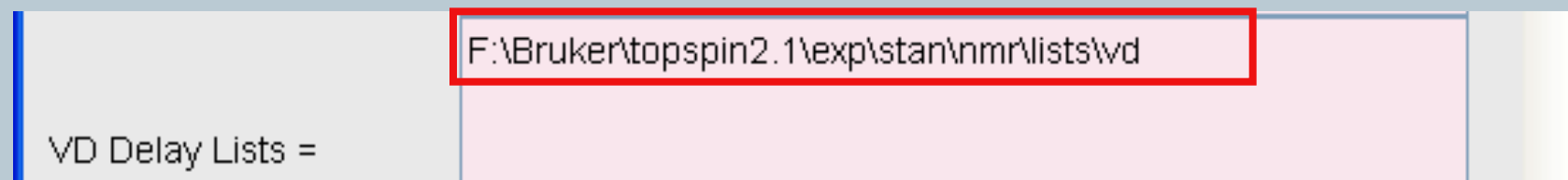
# Default directories



Default path for e.g. pulse programs:

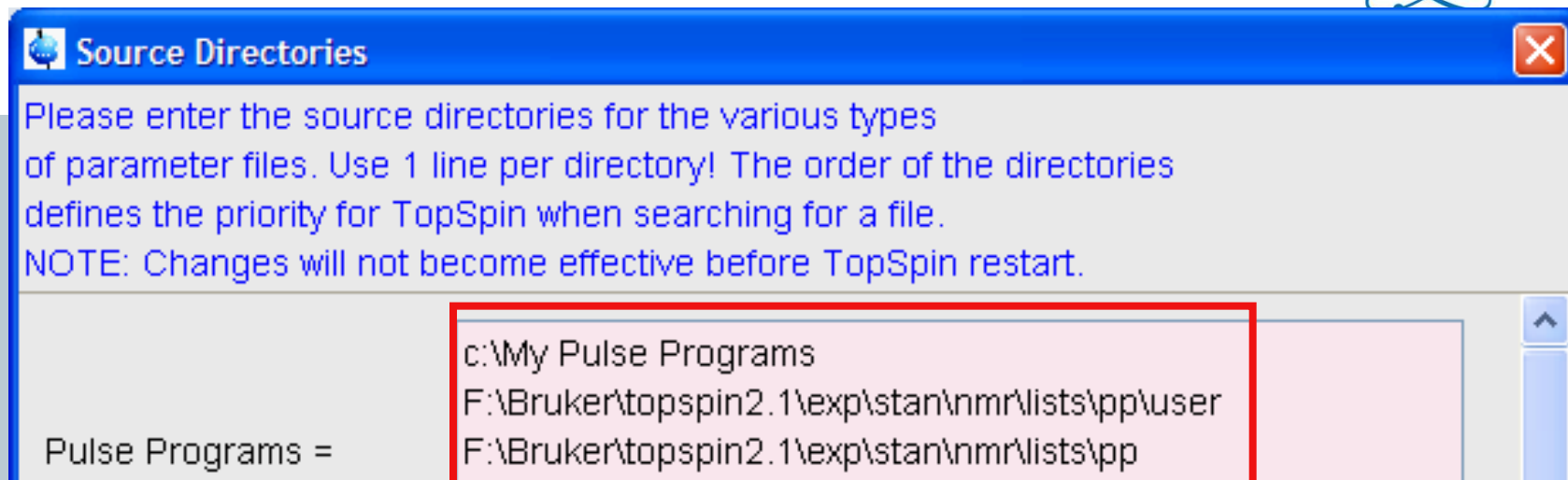
Bruker files in: *.../exp/stan/nmr/lists/pp*

User files in: *.../exp/stan/nmr/lists/pp/user*



Default path for e.g. VD lists:

Bruker/User files in: *.../exp/stan/nmr/lists/vd*



Default path for pulse programs:

Bruker files in: *.../exp/stan/nmr/lists/pp*

User files in: *.../exp/stan/nmr/lists/pp/user*

Each user can define his own directories  
(in an unlimited number)

# Definition of the content of e.g.: edpul



**Pulse Programs** [X]

File Options Help

Source = F:\Bruker\topspin2.1\exp\stan\nmr\lists\pp

Search in names [\*?] [v] Search [input]

Class = Any [v] Dim = Any [v] All

Avance.incl	Daz.incl	De.incl	Delay.incl	Grad.incl
Param.info	Pulprog.info	README	Relations.info	Sysconf.incl
Update.info	adeq11etgprdsp	adeq11etgprdsp.2	adeq11etgpsp	adeq1netgp
adeqn1etgp	adeqnnetgp	apt	aptjc	aring
aring2	atocsygp19	c_caco	c_caco_ia	c_caco_s3
c_can_iasq	c_can_mq	c_can_mq.2	c_canco_ia3d	c_canco_ia3d.2
c_cancoi_ia3d	c_cbcaco_ia3d	c_cbcaco_s33d	c_cbcaco_ia3d	c_cbcanco_ia3d
c_ccco_ia3d	c_ccco_s33d	c_cccon_ia3d	c_ccflopsy16	c_ccflopsy16_ct
c_ccflopsy16_ctia	c_ccflopsy16_ia	c_ccnoesy	c_ccnoesy2	c_ccnoesy_ct
c_coca	c_coca_ia	c_coca_mq	c_coca_mq.2	c_con_iasq
c_con_mq	c_con_mqia	c_con_sq	c_cosy	c_cosy2_ct
c_cosy_ct	c_hacaco_3d	c_hcaco_ia3d	c_hcaco_s33d	c_hcan_ia3d
c_hcaco_ia3d	c_hcaco_ia3d	c_hcaco_ia3d	c_hcaco_ia3d	c_hcaco_ia3d

Edit Graphical Edit Set PULPROG Close

# Definition of the content of e.g.: **edpul**



**Pulse Programs** [X]

**File Options Help**

Source = F:\Bruker\topspin2.1\exp\stan\nmr\lists\pp  
 c:\My Pulse Programs  
 F:\Bruker\topspin2.1\exp\stan\nmr\lists\pp\user  
 F:\Bruker\topspin2.1\exp\stan\nmr\lists\pp

Search in names [\*?] [v] Search [ ]

Class = Any [v] Dim = Any [v] All [ ]

Avance.incl	Daz.incl	De.incl	Delay.incl	Grad.incl
Param.info	Pulprog.info	README	Relations.info	Sysconf.incl
Update.info	adeq11etgprdsp	adeq11etgprdsp.2	adeq11etgpsp	adeq1netgp
adeqn1etgp	adeqnnetgp	apt	aptjc	aring
aring2	atocsygp19	c_caco	c_caco_ia	c_caco_s3
c_can_iasq	c_can_mq	c_can_mq.2	c_canco_ia3d	c_canco_ia3d.2
c_cancoi_ia3d	c_cbcaco_ia3d	c_cbcaco_s33d	c_cbcaco_ia3d	c_cbcanco_ia3d
c_ccco_ia3d	c_ccco_s33d	c_cccon_ia3d	c_ccflopsy16	c_ccflopsy16_ct
c_ccflopsy16_ctia	c_ccflopsy16_ia	c_ccnoesy	c_ccnoesy2	c_ccnoesy_ct
c_coca	c_coca_ia	c_coca_mq	c_coca_mq.2	c_con_iasq
c_con_mq	c_con_mqia	c_con_sq	c_cosy	c_cosy2_ct
c_cosy_ct	c_hacaco_3d	c_hcaco_ia3d	c_hcaco_s33d	c_hcan_ia3d
c_hcaco_ia3d	c_hcaco_ia3d	c_hcaco_ia3d	c_hcaco_ia3d	c_hcaco_ia3d

Edit Graphical Edit Set PULPROG Close

# Definition of the content of e.g.: edpul



Pulse Programs

File Options Help

Source = c:\My Pulse Programs

Search in names [\*?] Search

Class = Any Dim = Any All

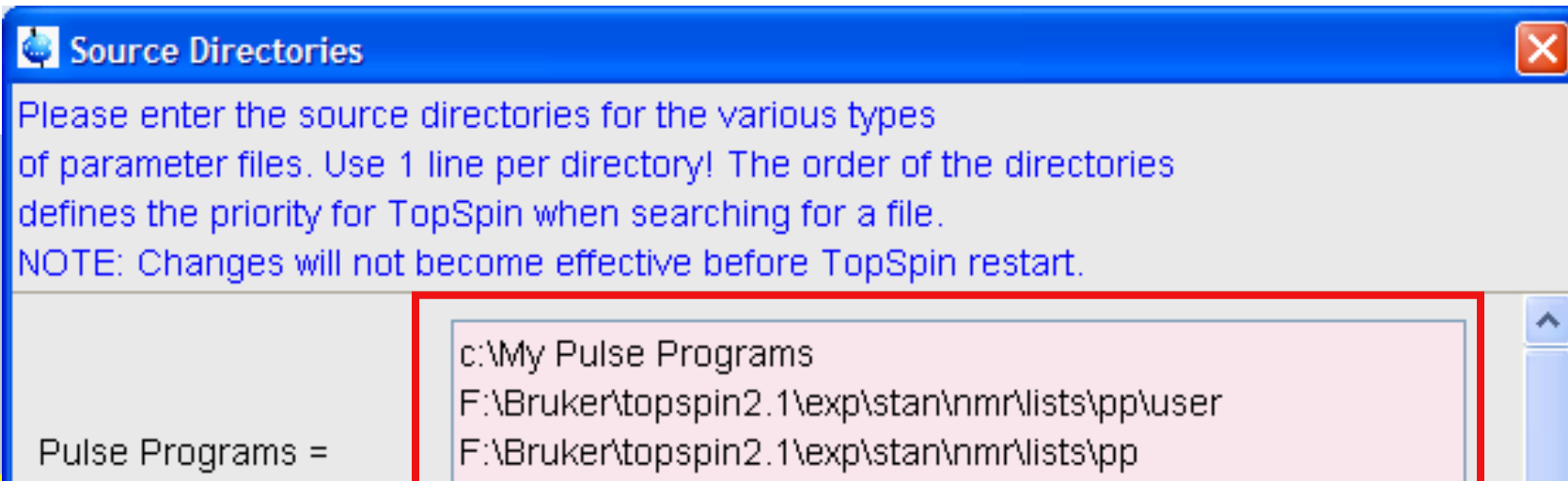
zg	zg30		
----	------	--	--

Last displayed source directory will automatically be displayed next time this window is opened.

Edit Graphical Edit Set PULPROG Close



# User-specific directory



The order of the directories defines the priority for searching a file.

Example above:

- 1) Pulse program **zg** can be available in all three directories
- 2) e.g. **zg** should be used for acquisition,
  - TopSpin (and/or ICON-NMR) searches for **zg**
  - if the first directory *C:\My Pulse Programs* contains a **zg**
  - this one will be used for acquisition ('first come, first served')

# Create a new file in *pp/user* !



**Pulse Programs**

File Options Help

Source = F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp

New... Save As... Delete... Rename... Export... Import... Close

Daz.incl	De.incl	Delay.incl	Grad.incl
Pulprog.info	README	Relations.info	Sysconf.incl
adeq11etgprdsp	adeq11etgpsp	adeq1netgp	adeqn1etgp
apt	aptjc	aring	aring2
c_caco	c_caco_ia	c_caco_s3	c_can_iasq
c_can_mq.2	c_canco_ia3d	c_canco_ia3d.2	c_cancoi_ia3d
c_cbcaco_ia3d	c_cbcaco_s33d	c_cbcanco_ia3d	c_ccco_ia3d
c_ccco_s33d	c_cccon_ia3d	c_ccflopsy16	c_ccflopsy16_ctia
c_ccflopsy16_ia			c_coca
c_coca_ia			c_con_mq
c_con_mqia			c_cosy_ct
c_hacaco_3d			c_hcanco_ia3d
c_hcancoi_ia3d			c_hcbcan_ia3d
c_hccflopsy16_3d			c_hnco_ia3d
c_hncoca2_ia3d			cbcaonhgpwg3d
cbcanhgp3d			ccaonhgp3d.2
ccanhgp2h3d			ccconhgp3d
ccanhgpsd	ccanhgpsd.2	ccconhgpznsd	ccosydcph
colocqf	cosycwphps	cosydcrlrqf	cosydcph
cosydcqf	cosydfesgpph	cosydfesgpph	cosydfetgp.1

New...  
Destination Dir. = F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp\user  
New Name =  
OK Cancel

Edit Graphical Edit Set PULPROG Close

# Create a new file in *pp/user* !

Two overlapping Notepad++ windows are shown. The top window is titled "pp-test (F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp\user) \*". The bottom window is also titled "pp-test (F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp\user) \*". The bottom window has a context menu open with the following options: "New [Ctrl N]", "Open... [Ctrl O]", and "Save [Ctrl S]". The "Save" option is highlighted. The text in the background window includes:

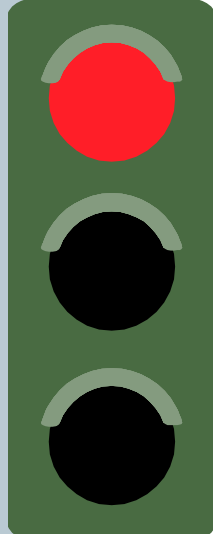
```
1 ;zg-test
2 ;avance-vers
3 ;1D sequence
4 ;
5 ;$CLASS=High
6 ;$DIM=1D
7 ;$PULPRG=
```

The "Pulse Programs" dialog box is displayed. It has a title bar "Pulse Programs" and a menu bar "File Options Help". The "Source" field is set to "F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp\user". Below the source field, there are search filters: "Search in names [\*\*?]" with a dropdown arrow, a "Search" button, and an empty text input field. Below that, there are "Class = Any" and "Dim = Any" dropdown menus, and an "All" button. A table below these filters shows a list of programs. The first row is highlighted in blue and contains the text "pp-test".

Program Name	Class	Dim
pp-test	Any	Any

At the bottom of the dialog, there are four buttons: "Edit", "Graphical Edit", "Set PULPROG", and "Close".

# Create a new file in *pp* ?



```
test-pp (F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp) *  
File Edit Search  
Graphical Edit  
1
```

```
test-pp (F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp) *  
File Edit Search  
Graphical Edit  
1 ;zg-test  
2 ;avance-vers... (06/11/09)  
3 ;1D sequence  
4 ;  
5 ;$CLASS=High  
6 ;$DIM=1D  
7 ;$TYPE=  
8 ;$SUBTYPE=  
9 ;$COMMENT=  
10  
11  
12 #include <Av  
13  
14  
15 "acqt0=-p1*2  
16  
17  
18 1 ze  
19 2 30m  
20 d1  
21 p1 ph1  
22 go=2 ph31  
23 30m mc #0  
24 exit
```

```
test-pp (F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp)
```

- File Edit Search
- New [Ctrl N]
- Open... [Ctrl O]
- Save [Ctrl S]
- Save as...
- Print [Ctrl P]
- Close

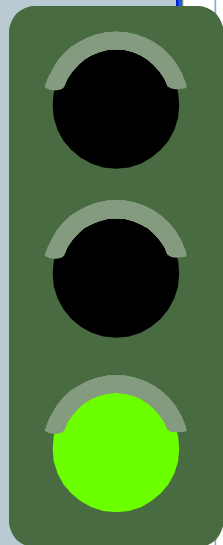
(06/11/09)

```
9 ;$COMMENT=  
10  
11  
12 #include <Avance.incl>  
13  
14  
15 "acqt0=-p1*2/3.1416"  
16  
17  
18 1 ze  
19 2 30m  
20 d1  
21 p1 ph1  
22 go=2 ph31  
23 30m mc #0 to 2 F0(zd)  
24 exit
```

TopSpin does NOT support changing or storing files in the Bruker standard directory:  
F:/Bruker/TOPSPIN2.1-alpha/exp/stan/nmr/lists/pp

Close Details...

# Create a new file in *pp/user* !



```
test-pp (F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp) *
File Edit Search
Graphical Edit
1
```

```
test-pp (F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp) *
File Edit Search
Graphical Edit
1 ;zg-test
2 ;avance-vers... (06/11/09)
3 ;1D sequence
4 ;
5 ;$CLASS=High
6 ;$DIM=1D
7 ;$TYPE=
8 ;$SUBTYPE= (06/11/09)
9 ;$COMMENT=
10
11
12 #include <Av
13
14
15 "acqt0=-p1*2
16
17
18 1 ze
19 2 30m
20 dl
```

```
test-pp (F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp)
File Edit Search
New [Ctrl N]
Open... [Ctrl O]
Save [Ctrl S]
Save as...
Print [Ctrl P]
Close
```

```
New...
Destination Dir. = F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp\user
New Name =
```

```
Pulse Programs
File Options Help
Source = F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\pp\user
Search in names [*?] Search
Class = Any Dim = Any All
pp-test
```

1. each user starts with a list of default directories (e.g. *lists/pp* and *lists/pp/user*)
2. only the **user** directory is writable
3. each user can remove one or more default directories from its list
4. each user can specify one or more additional source directories
5. each user can define the order of the directories which defines the search order within TopSpin

# Source directories – advantages

e.g. pulse programs



---

Bruker files in: *.../exp/stan/nmr/lists/pp*

These files are write protected!

→ You can be sure that these files always contain the right content

---

User files in: *.../exp/stan/nmr/lists/pp/user*

By default any user-specific file will be stored here, they are read- and writable

→ You have an easy setup to distribute user-specific files to all users of the spectrometer

# Source directories – advantages

e.g. pulse programs



---

Each user can define his **own source directories**

→ These files will have the permissions you want to!  
If you store them e.g. in your home directory, the files will be only readable by yourself

→ These files can be easily distributed!  
If you want to use e.g. your pulse programs on different spectrometers, just define a network drive as a source directory.



User can specify individual directories for:

- Pulse programs
- CPD programs
- Shape Files
- Parameter Sets
- Macros
- Python programs
- AU programs
- VD,VP,VC,VA,VT,F1,DS,  
solvent region files, phases
- intrng, peakrng, ...

⇒ edpul

⇒ edcpd

⇒ edshape

⇒ rpar

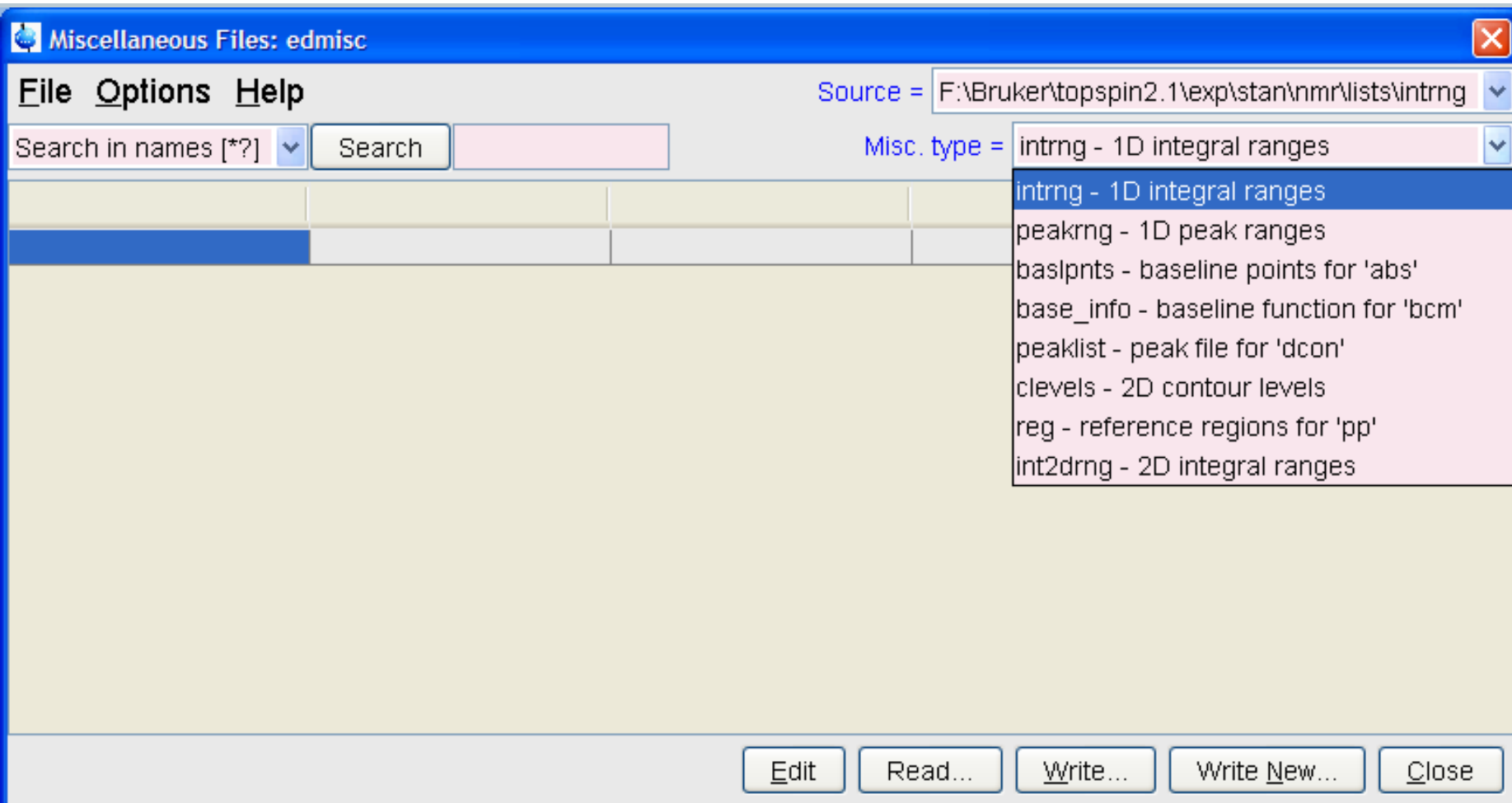
⇒ edmac

⇒ edpy

⇒ edau

⇒ edlist

⇒ edmisc



**Parameter Lists** [X]

**File Options Help** Source = F:\Bruker\topspin2.1\exp\stan\nmr\lists\scl [v]

Search in names [??] [v] Search [ ] List type = scl - solvent regions [v]

13C.Acetic	13C.Acetone	13C.C6D6	13C.CD2Cl2	vd - delays
13C.CDCI3	13C.CH3CN+D2O	13C.CH3OH+D2O	13C.D2O	vp - pulses
13C.DME	13C.DMF	13C.DMSO	13C.Dioxane	vc - loop counts
13C.H2O+D2O	13C.MeOD	13C.Pyr	13C.TFA	va - amplitudes
13C.Tol	1H.Acetic	1H.Acetone	1H.C6D6	vt - temperatures
1H.CD3CN	1H.CDCI3	1H.CH3CN+D2O	1H.CH3OH+D2O	f1 - frequencies
1H.DEE	1H.DME	1H.DMF	1H.DMSO	sp - shapes
1H.EtOD	1H.H2O+D2O	1H.MeOD	1H.Pyr	ds - data sets
1H.THF	1H.Tol	PEG	peg-old	1H.TFA

[Edit] [Close]



**Parameter set conversion**

Parameter set conversion.

Select parameter sets for conversion of the basic frequency (BF) or installed the digitizer from the lists on the right.

Directories containing parameter sets can be added via the "Preferences" menu.

Use the match field to apply wildcards to the list of parameter sets, use the checkbox below to select case sensitive (default) or case insensitive match.

Execute "cf" to set a new basic frequency (BF) or a new digitizer before executing paracon!  
Current basic frequency: 300.13 MHz.

Case insensitive match

Available parameter sets:

F:\Bruker\topspin2.1\exp\stan\nmr\par (Bruker defined)

- AL27ND
- B11ZG
- BESTPROFILE**
- C13APT
- C13CPD**
- C13CPD32
- C13CPDSN
- C13DE45SN

Match:

F:\Bruker\topspin2.1\exp\stan\nmr\par\user

- integ-test**
- opitz-sr-test**

Match:

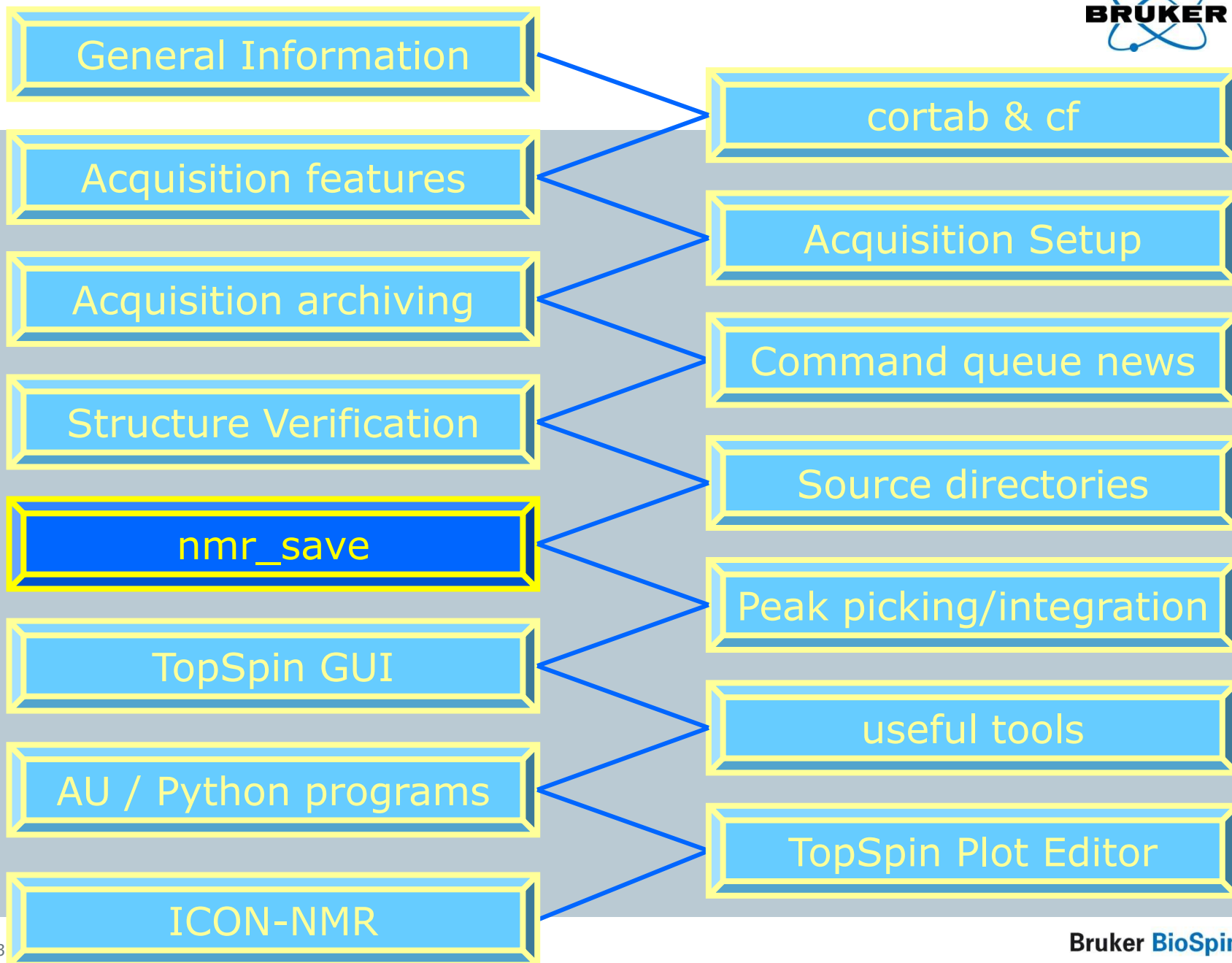
C:\My Parametersets

- C13CPD-test**

Match:

Also **paracon** supports user defined source directories.

# Content



Acquisition finished: es 1

Spectrum ProcPars Ac

[rel]

4

7 6 5 4 3 [ppm]

1

0

Acquisition information: no acquisition running

Fid Flash

Lock

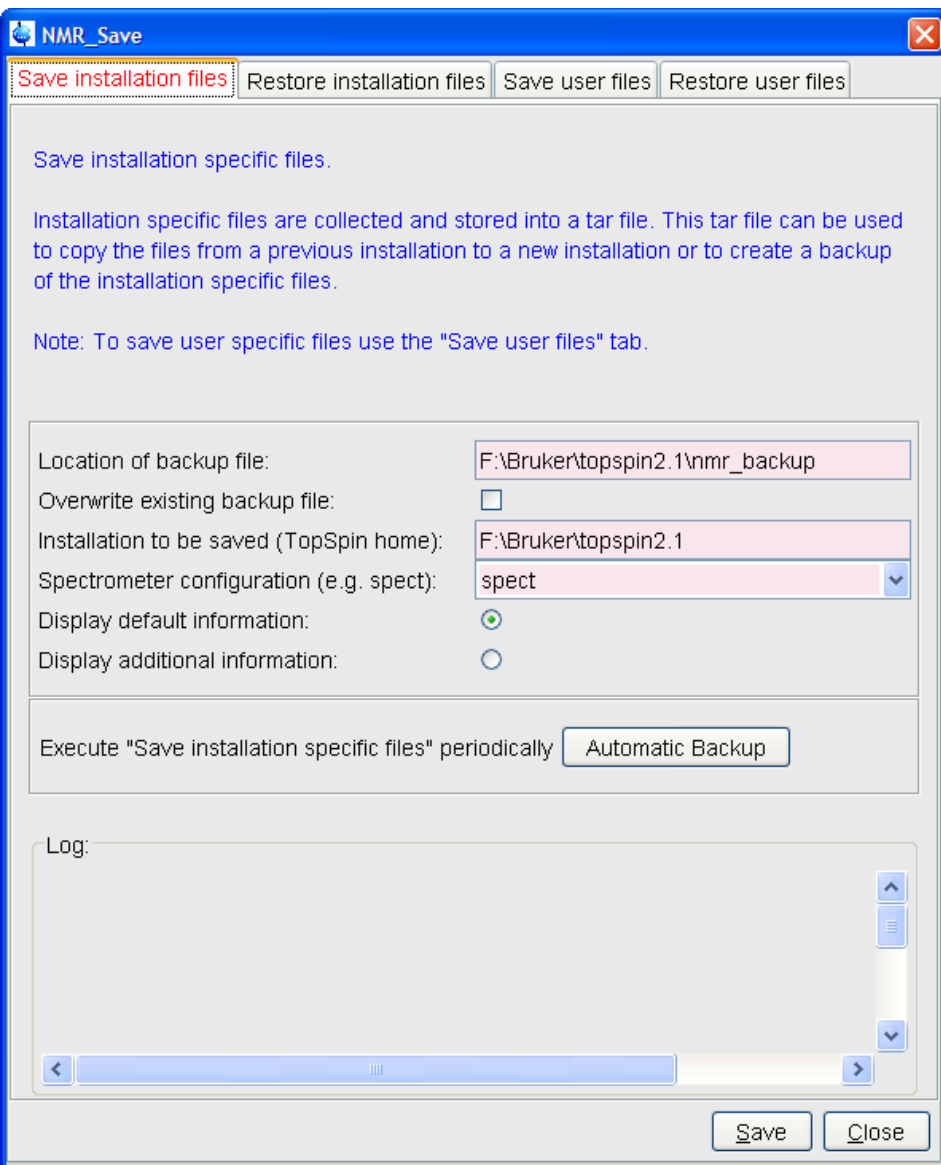
Sample

POWCHK

Spooler: running: 0, queued: 0, delayed: 0

BSMS status message:  $\Delta Z 2$ , Autoshim  Locked  Error

Time: 12:14, Jan 03



**NMR\_Save**

Save installation files | Restore installation files | Save user files | Restore user files

Save installation specific files.

Installation specific files are collected and stored into a tar file. This tar file can be used to copy the files from a previous installation to a new installation or to create a backup of the installation specific files.

Note: To save user specific files use the "Save user files" tab.

Location of backup file: F:\Bruker\topspin2.1\nmr\_backup

Overwrite existing backup file:

Installation to be saved (TopSpin home): F:\Bruker\topspin2.1

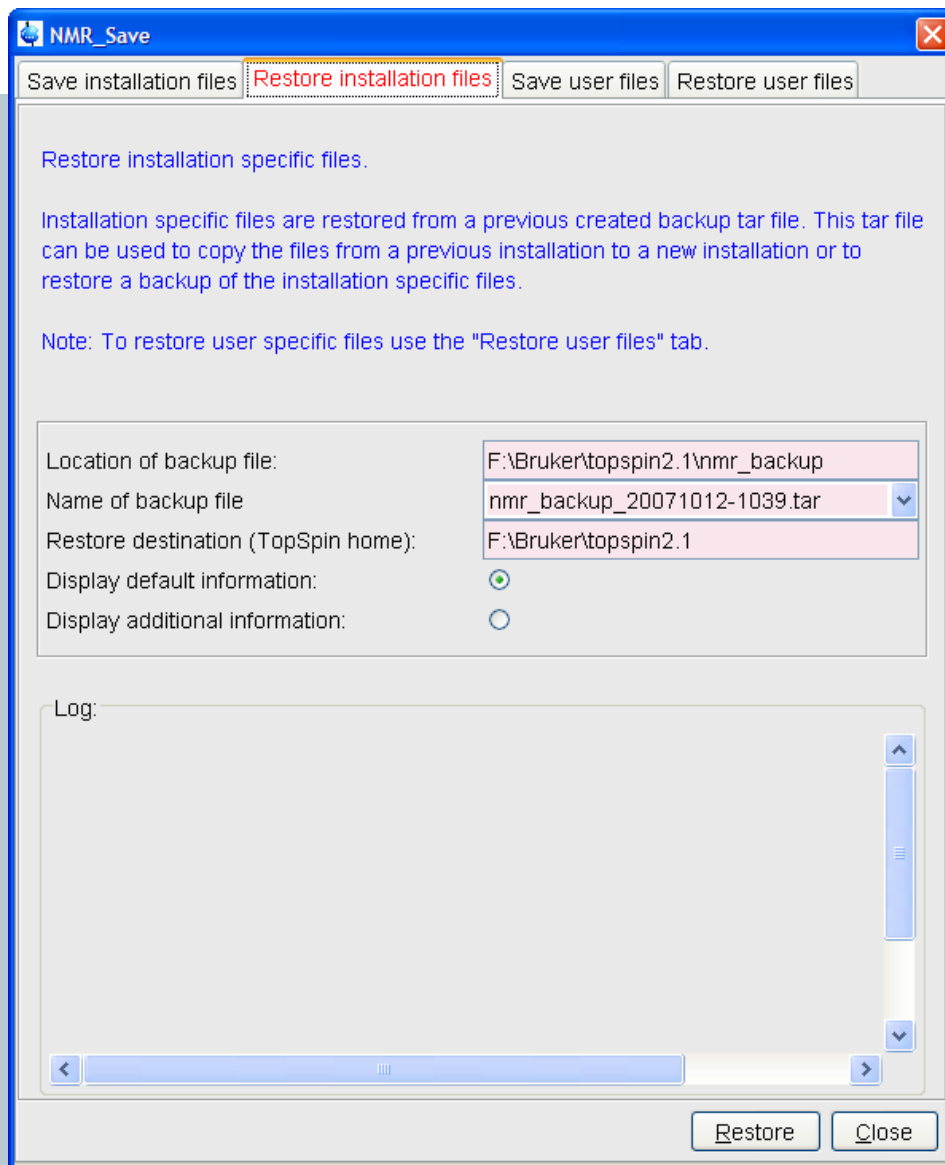
Spectrometer configuration (e.g. spect): spect

Display default information:

Display additional information:

Execute "Save installation specific files" periodically

Log:



**NMR\_Save**

Save installation files | Restore installation files | Save user files | Restore user files

Restore installation specific files.

Installation specific files are restored from a previous created backup tar file. This tar file can be used to copy the files from a previous installation to a new installation or to restore a backup of the installation specific files.

Note: To restore user specific files use the "Restore user files" tab.

Location of backup file: F:\Bruker\topspin2.1\nmr\_backup

Name of backup file: nmr\_backup\_20071012-1039.tar

Restore destination (TopSpin home): F:\Bruker\topspin2.1

Display default information:

Display additional information:

Log:

# nmr\_save/restore



**NMR\_Save**

Save installation files | Restore installation files | Save user files | Restore user files

Save installation specific files.

Installation specific files are collected and stored into a tar file. This tar file can be used to copy the files from a previous installation to a new installation or to create a backup of the installation specific files.

Note: To save user specific files use the "Save user files" tab.

Location of backup file: F:\Bruker\topspin2.1\nmr\_backup

Overwrite existing backup file:

Installation to be saved (TopSpin home): F:\Bruker\topspin2.1

Spectrometer

Display default

Display additional

Execute "Save"

Log:

Source Directories

Please enter the source directories for the various types of parameter files. Use 1 line per directory! The order of the directories define the priority for TopSpin when searching for a file.  
NOTE: Changes will not become effective before TopSpin restart.

Pulse Programs =  
C:\Bruker\alpha\exp\stan\nmr\lists\pp\user  
C:\Bruker\alpha\exp\stan\nmr\lists\pp

CPD Programs =  
C:\Bruker\alpha\exp\stan\nmr\lists\cpd\user  
C:\Bruker\alpha\exp\stan\nmr\lists\cpd

Shape Files =  
C:\Bruker\alpha\exp\stan\nmr\lists\wave\user  
C:\Bruker\alpha\exp\stan\nmr\lists\wave

Save Close

**NMR\_Save**

Save installation files | Restore installation files | Save user files | Restore user files

Restore installation specific files.

Installation specific files are restored from a previous created backup tar file. This tar file can be used to copy the files from a previous installation to a new installation or to restore a backup of the installation specific files.

Note: To restore user specific files use the "Restore user files" tab.

Location

Name of

Restore

by

by

Restore

Close

All global files like spectrometer configuration, license etc. will be saved/restored, also all default directories listed here, e.g. ,pp` and ,pp/user`



# nmr\_save/restore



NMR\_Save

Save installation files | Restore installation files | Save user files | Restore user files

Save installation specific files.

Installation specific files are collected and stored into a tar file. This tar file can be used to copy the files from a previous installation to a new installation or to create a backup of the installation specific files.

Note: To save user specific files use the "Save user files" tab.

Location of backup file: F:\Bruker\topspin2.1\nmr\_backup

Overwrite existing backup file:

Installation to be saved (TopSpin home): F:\Bruker\topspin2.1

Spectrometer configuration (e.g. spect): spect

Display default information:

Display additional information:

Execute "Save installation specific files" periodically

Log:

NMR\_Save

Save installation files | Restore installation files | Save user files | Restore user files

Restore installation specific files.

Installation specific files are restored from a previous created backup tar file. This tar file can be used to copy the files from a previous installation to a new installation or to restore a backup of the installation specific files.

New periodical

Job

Command: .nmrsave -date -path "F:\Bruker\topspin2.1\nmr\_backup" -source "F:\Bruker\

Description: Execute NMR\_SAVE

Execution scope: TopSpin (requires authentication)

Options

Off-schedule execution

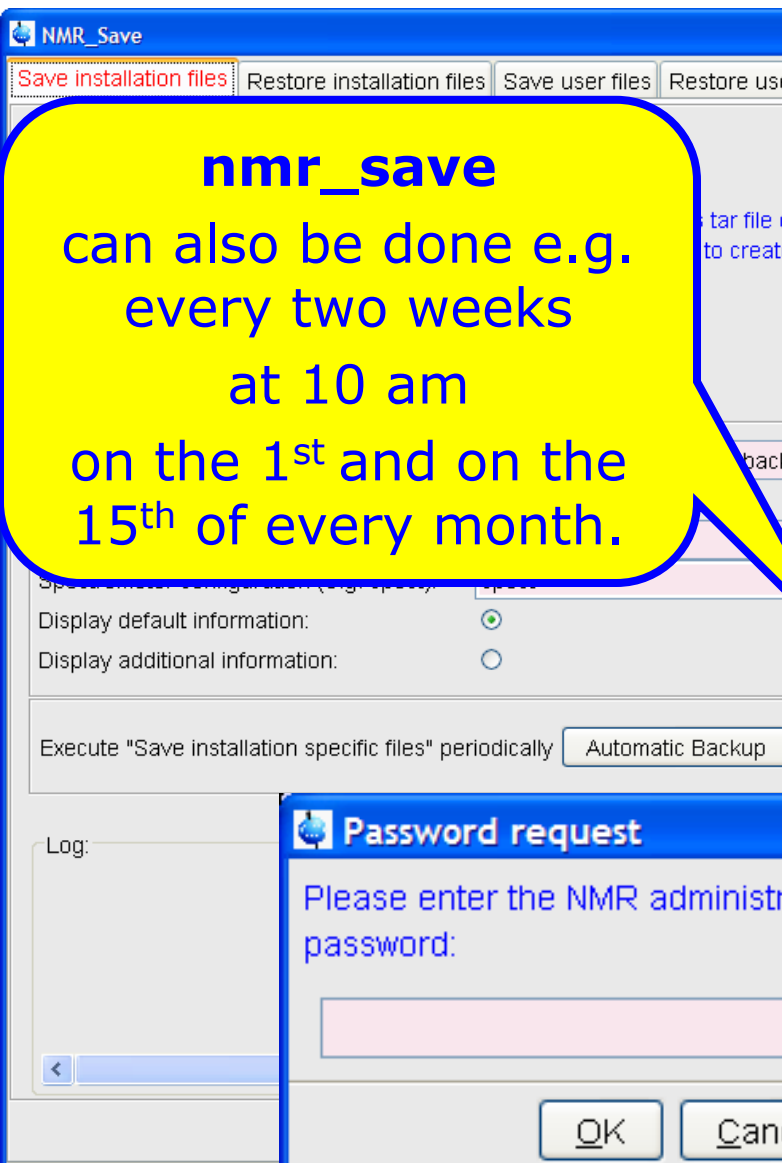
Direct execution

Rules

Minute of the hour	from: 3	to: --- Ignore ---	+ -
Hour of the day	from: 12	to: --- Ignore ---	+ -
Day of the month	from: 4	to: --- Ignore ---	+ -
Month of the year	from: *	to: --- Ignore ---	+ -
Day of the week	from: *	to: --- Ignore ---	+ -

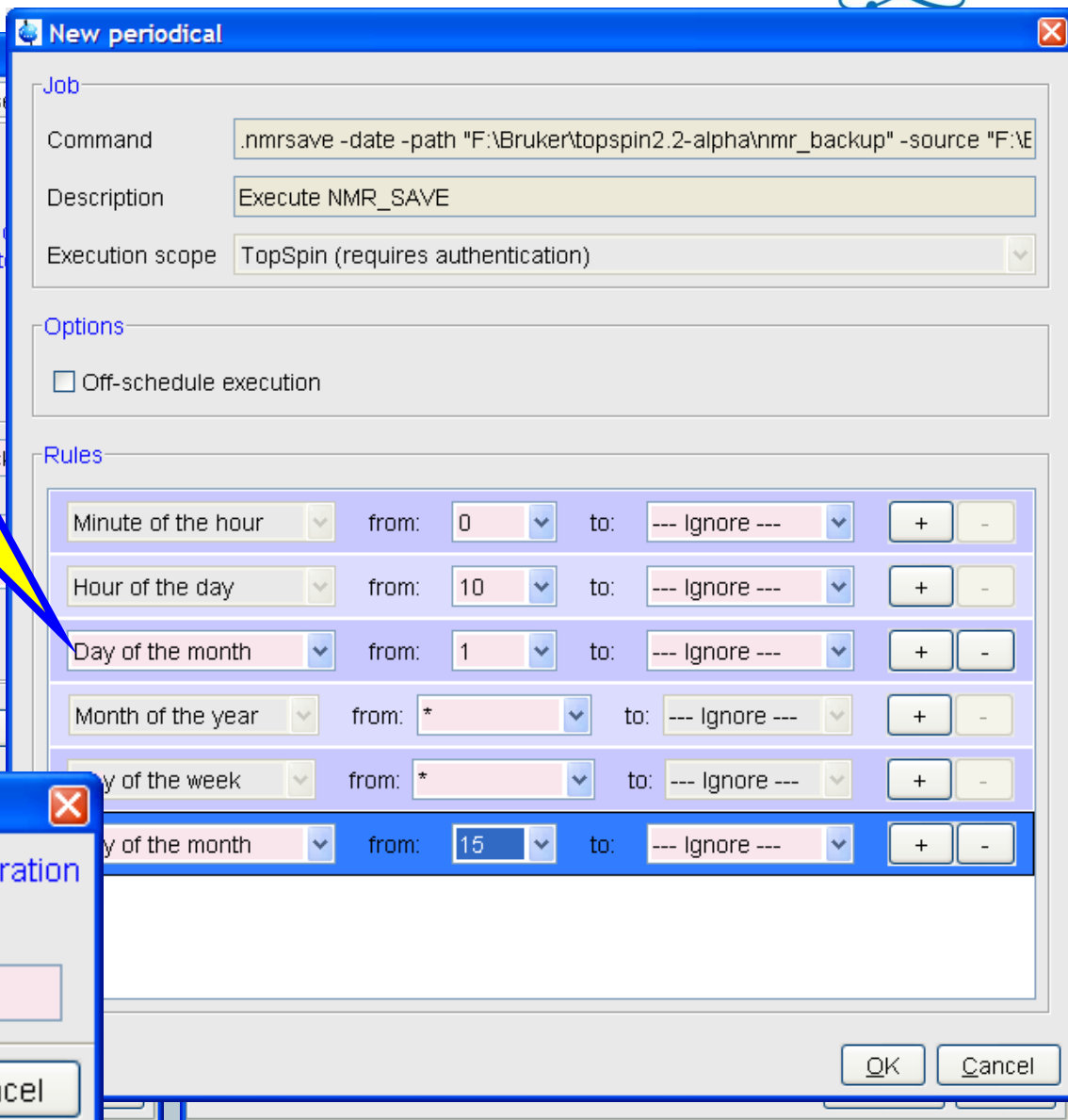
OK Cancel

Current minute, hour and day are preselected. Simply clicking **OK** will define a monthly **nmr\_save**



The screenshot shows the NMR\_Save application window with several tabs: "Save installation files", "Restore installation files", "Save user files", and "Restore user files". The "Save installation files" tab is active. Below the tabs, there are options for "Display default information" (checked) and "Display additional information" (unchecked). At the bottom, there is a checkbox for "Execute 'Save installation specific files' periodically" with an "Automatic Backup" button next to it. A "Log:" section is visible at the bottom left.

**nmr\_save**  
can also be done e.g.  
every two weeks  
at 10 am  
on the 1<sup>st</sup> and on the  
15<sup>th</sup> of every month.

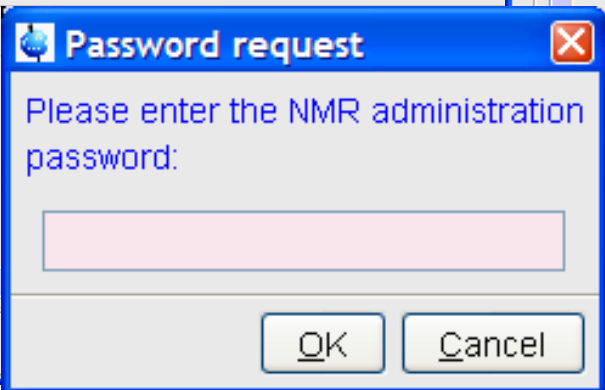


The "New periodical" dialog box is shown with the following settings:

- Job**
  - Command: `.nmrsave -date -path "F:\Bruker\topspin2.2-alpha\nmr_backup" -source "F:\E`
  - Description: Execute NMR\_SAVE
  - Execution scope: TopSpin (requires authentication)
- Options**
  - Off-schedule execution
- Rules**

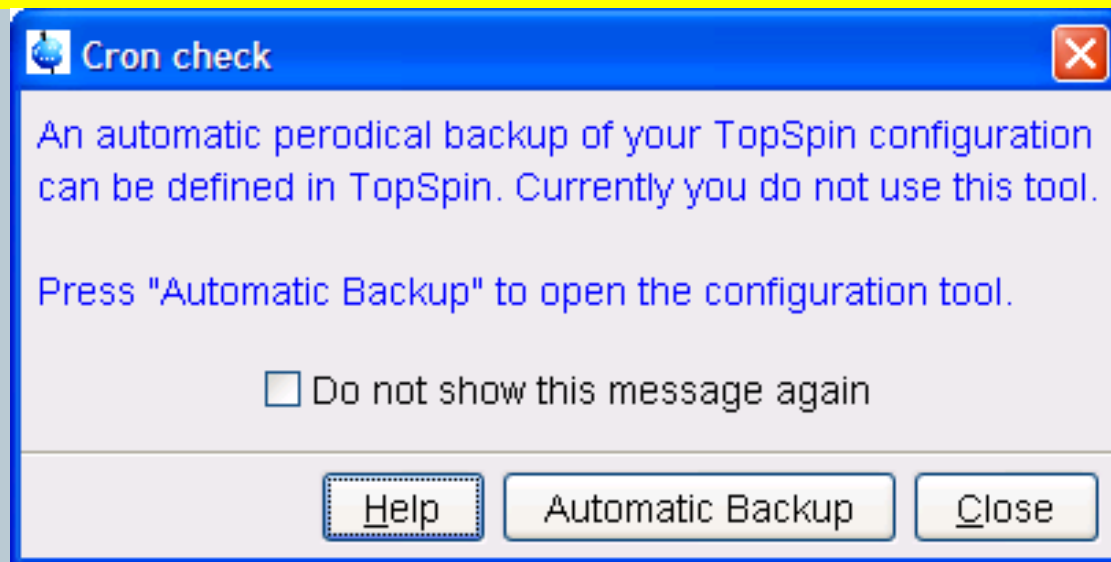
Field	From	To	+	-
Minute of the hour	0	--- Ignore ---	+	-
Hour of the day	10	--- Ignore ---	+	-
Day of the month	1	--- Ignore ---	+	-
Month of the year	*	--- Ignore ---	+	-
Day of the week	*	--- Ignore ---	+	-
Day of the month	15	--- Ignore ---	+	-

Buttons: OK, Cancel

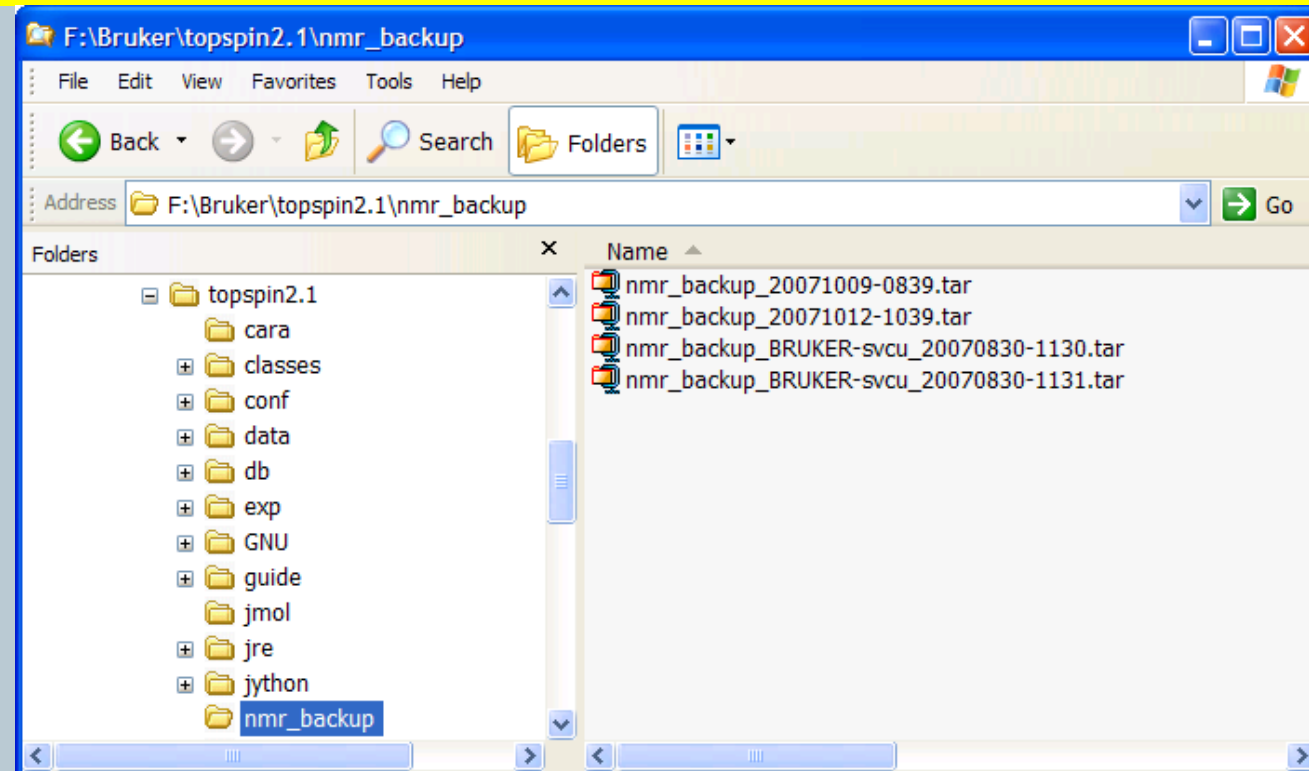


The "Password request" dialog box contains the text: "Please enter the NMR administration password:" followed by a text input field. Buttons: OK, Cancel

When **expinstall** is finished it is checked if an automatic periodic job for **nmr\_save** exists. If not, this message pops up:



The name of the backup files contain now date and time information, so that a periodic backup will not overwrite previous files.



# user\_save/restore



NMR\_Save

Save installation files | Restore installation files | **Save user files** | Restore user files

Save user specific files of user **svcu**.

The user specific files of an installation are collected and stored into a tar file. This tar file can be used to copy user specific files to a different computer or to create a backup of user specific files of an installation.

Note: To save installation specific files use the "Save installation files" tab.

Location of backup file: F:\Bruker\topspin2.1\nmr\_backup

Overwrite existing backup file:

Display default information:

Display additional information:

Execute "Save user files" periodically

Log:

Save Close

NMR\_Save

Save installation files | Restore installation files | Save user files | **Restore user files**

Restore user specific files of user **svcu**.

User specific files are restored from a previous created backup tar file. This can be used to copy user specific files from a different computer to the local installation or to restore a backup of user specific files.

Note: To restore installation specific files use the "Restore installation files" tab.

Location of backup file: F:\Bruker\topspin2.1\nmr\_backup

Name of backup file: nmr\_backup\_BRUKER-svcu\_200708...

Restore destination (TopSpin home): F:\Bruker\topspin2.1

Display default information:

Display additional information:

Log:

Restore Close

# user\_save/restore



Save installation files | Restore installation files | **Save user files** | Restore user files

Only user-specific files in the directories listed here will be saved/restored. The default directories e.g. `.pp` and `.pp/user` are not stored with the **user\_save** but with **nmr\_save**

Execute "Save user files" periodically  Automatic Backup

Log:

Save installation files | Restore installation files | Save user files | **Restore user files**

Restore user specific files of user **svcu**.

User specific files are restored from a previous created backup tar file. This can be used to copy user specific files from a different computer to the local installation or to restore a backup of user specific files.

Note: To restore installation specific files use the "Restore installation files" tab.

**Source Directories**

Please enter the source directories for the various types of parameter files. Use 1 line per directory! The order of the directories define the priority for TopSpin when searching for a file.  
NOTE: Changes will not become effective before TopSpin restart.

Pulse Programs =

- ~~C:\Bruker\alpha\exp\stan\nmr\lists\pp\user~~
- ~~C:\Bruker\alpha\exp\stan\nmr\lists\pp~~
- C:\users\chjo\pp

CPD Programs =

- ~~C:\Bruker\alpha\exp\stan\nmr\lists\cpd\user~~
- ~~C:\Bruker\alpha\exp\stan\nmr\lists\cpd~~
- ~~C:\Bruker\alpha\exp\stan\nmr\lists\wave\user~~
- ~~C:\Bruker\alpha\exp\stan\nmr\lists\wave~~

Restore | Close

The directory:  
`<USER_home>/.<topspin>-<PC_NAME>`  
with all user-specific TopSpin configurations is also stored with **user\_save**

# user\_save/restore



Note that each user has to take care about a backup of his own user-specific files defined here.

**user\_save** must be executed by each user himself!

The screenshot shows the NMR\_Save application with the 'Restore user files' tab selected. The dialog box 'Source Directories' is open, showing the following paths:

- Pulse Programs =
  - ~~C:\Bruker\alpha\exp\stan\nmr\lists\pp\user~~
  - ~~C:\Bruker\alpha\exp\stan\nmr\lists\pp~~
  - C:\users\chjo\pp
- CPD Programs =
  - ~~C:\Bruker\alpha\exp\stan\nmr\lists\cpd\user~~
  - ~~C:\Bruker\alpha\exp\stan\nmr\lists\cpd~~
- Shape Files =
  - ~~C:\Bruker\alpha\exp\stan\nmr\lists\wave\user~~
  - ~~C:\Bruker\alpha\exp\stan\nmr\lists\wave~~

# nmr\_save

**NMR\_Save**

Save installation files | Restore installation files | Save user files

Save installation specific files.

Installation specific files are collected and stored into a tar file. This tar file can be used to copy the files from a previous installation to a new installation or to create a backup of the installation specific files.

Note: To save user specific files use the "Save user files" tab.

Location of backup file: F:\Bruker\topspin2.1\nmr\_backup

Overwrite existing backup file:

Installation to be saved (TopSpin home): F:\Bruker\topspin2.1

Spectrometer configuration (e.g. spect): spect

Display default information:

Display additional information:

Execute "Save installation specific files" periodically

Log:

```
#####  
Backing up of NMR data was successful!  
The tar-file  
  
F:\Bruker\topspin2.1\nmr_backup\nmr_backup_20071012-0727.tar  
  
has been generated!  
  
#####
```

**Password request**

Please enter the NMR administration password:

**NMR\_Save**

Save installation files | **Restore installation files** | Save user files

Restore installation specific files.

Installation specific files are restored from a previous created backup tar file. This tar file can be used to copy the files from a previous installation to a new installation or to restore a backup of the installation specific files.

Note: To restore user specific files use the "Restore user files" tab.

Location of backup file: F:\Bruker\topspin2.1\nmr\_backup

Name of backup file: nmr\_backup\_20071012-0727.tar

Restore destination (TopSpin home): F:\Bruker\topspin2.1

Display default information:

Display additional information:

Log:

```
#####  
All data have successfully been restored!  
#####
```

**Password request**

Please enter the NMR administration password:



# user\_save



NMR\_Save

Save installation files | Restore installation files | **Save user files** | Restore user files

Save user specific files of user **svcu**.

The user specific files of an installation are collected and saved into a tar file. This tar file can be used to copy user specific files to a different installation or to create a backup of user specific files of an installation.

Note: To save installation specific files use the "Save installation files" tab.

Location of backup file:

Overwrite existing backup file:

Display default information:

Display additional information:

Execute "Save user files" periodically

Log:

```
#####  
Backing up of NMR data was successful!  
The tar-file  
  
F:\Bruker\topspin2.1\nmr_backup\nmr_backup_BRUKER-svcu_20071012-0728.tar  
  
has been generated!  
  
#####
```

NMR\_Save

Save installation files | Restore installation files | Save user files | **Restore user files**

Restore user specific files of user **svcu**.

User specific files are restored from a previous created backup. This can be used to copy user specific files from a different local installation or to restore a backup of user specific files of an installation.

Note: To restore installation specific files use the "Restore installation files" tab.

Location of backup file:

Name of backup file:

Restore destination (TopSpin home):

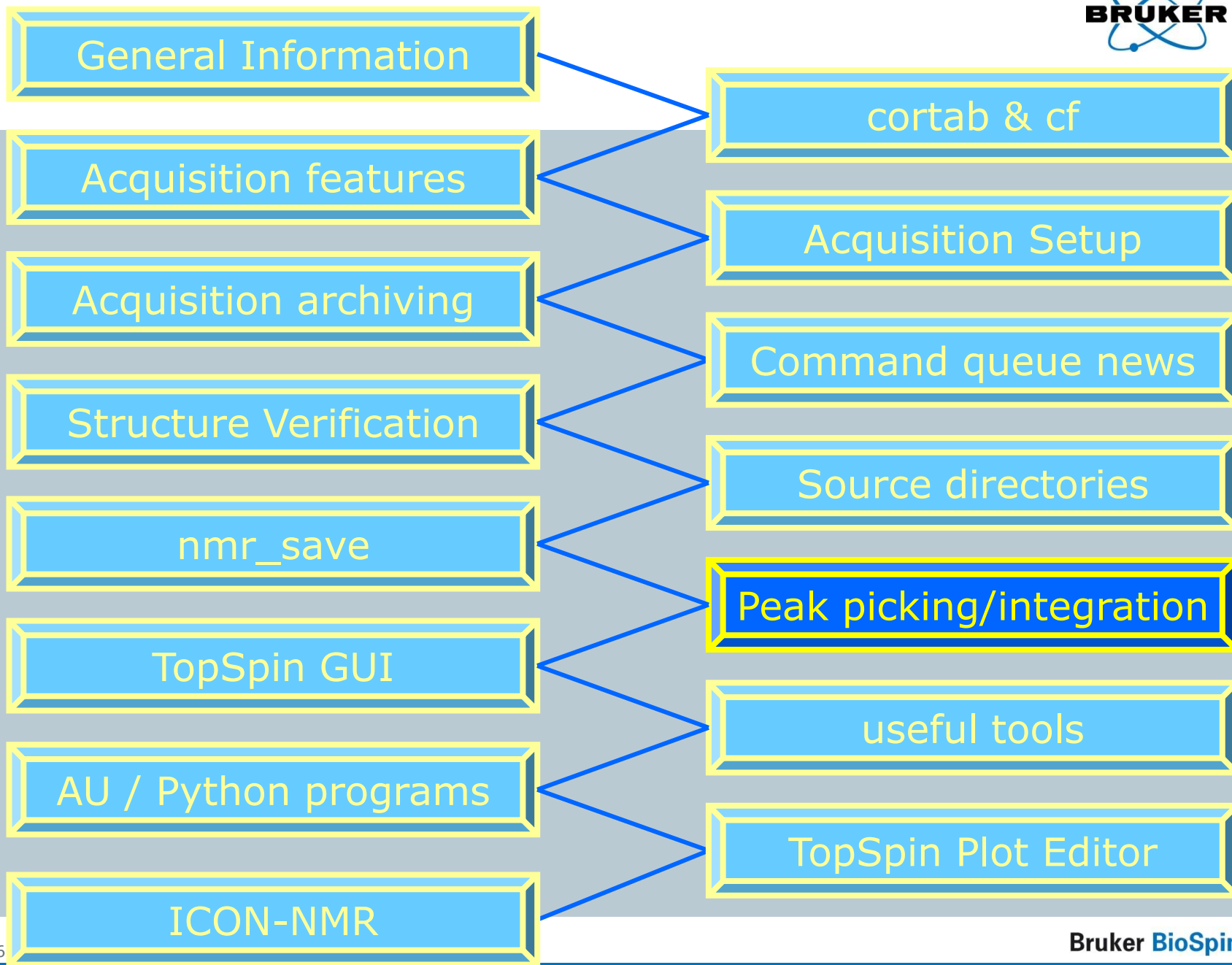
Display default information:

Display additional information:

Log:

```
#####  
All data have successfully been restored!  
#####
```

# Content



TopSpin < 2.1

TopSpin stores peaks as text file

TopSpin 2.1

TopSpin stores peaks as XML file

TopSpin 2.1 stores peaks in the XML file  
peaklist.xml

- New features are possible (see following)
- but if AU/third party programs are used to parse the old file (peak.txt) a conversion has to be done
- for this the command **convertpeaklist txt** is implemented

# Peak picking 1D



Brucker TopSpin on merlin as svcu

File Edit View Spectrometer Processing Analysis Options Window Help

\*2 /2 \*8 /8

exam1d\_1H 1 1 F:\Bruker\topspin2.1-alpha guest

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Fid

14 [rel]  
12  
10  
8  
6  
4  
2  
0

H1 H23 H14a H14b

F:\Bruker\topspin2.1-alpha\data\guest\nmr\exam1d\_1H\1\pdata\1

File Edit View Favorites Tools Help

Back Search Folders

Address F:\Bruker\topspin2.1-alpha\data\guest\nmr\exam1d\_1H\1\pdata\1 Go

Name	Size	Type	Date Modified
1i	128 KB	File	30.12.2006 07:55
1r	128 KB	File	30.12.2006 07:55
auditp.txt	1 KB	Text Document	30.12.2006 07:55
outd	1 KB	File	30.12.2006 07:56
parm.txt	2 KB	Text Document	30.12.2006 07:56
peaklist.xml	1 KB	XML Document	30.12.2006 07:56
peakrng	1 KB	File	30.12.2006 07:56
peaks	3 KB	File	30.12.2006 07:56
proc	2 KB	File	30.12.2006 07:56
procs	2 KB	File	30.12.2006 07:56
title	1 KB	File	16.03.2004 09:43

File and Folder Tasks

- Rename this file
- Move this file
- Copy this file
- Publish this file to the Web
- E-mail this file
- Delete this file

Other Places

- pdata
- My Documents
- My Computer
- My Network Places

Details

next page →

# Peak picking 1D



Brucker TopSpin on merlin as svcu

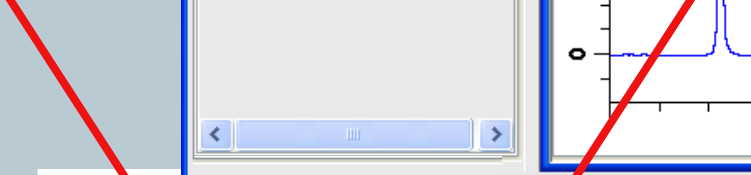
```
peak.txt - Notepad
File Edit Format View Help
DU=F:/Bruker/topspin2.1-alpha, USER=guest, NAME=exam1d_1H, EXPNO=1, PROCNO=1
F1=5.880ppm, F2=5.781ppm, MI=1.12cm, MAXI=2.17cm, PC=1.000
# ADDRESS FREQUENCY INTENSITY
# [Hz] [PPM]
1 14138.1 ? 5.8234 1.56
2 14179.3 ? 5.8083 1.59
-----
DU=F:/Bruker/topspin2.1-alpha, USER=merlin, NAME=exam1d_1H, EXPNO=1, PROCNO=1
Manually picked peaks
# ADDRESS FREQUENCY INTENSITY
# [Hz] [PPM]
3 10177.1 ? 7.2759 7.04
4 10615.6 ? 7.1151 0.01
```

Sample Structure Fid

exam1d\_1H\1\pdata\1

Size	Type	Date Modified
128 KB	File	30.12.2006 07:55
128 KB	File	30.12.2006 07:55
1 KB	Text Document	30.12.2006 07:55
1 KB	File	30.12.2006 07:56
2 KB	Text Document	30.12.2006 07:56
1 KB	XML Document	30.12.2006 07:56
1 KB	File	30.12.2006 07:56
3 KB	File	30.12.2006 07:56
2 KB	File	30.12.2006 07:56
2 KB	File	30.12.2006 07:56
1 KB	File	16.03.2004 09:43
1 KB	Text Document	30.12.2006 08:17

convertpeaklist.txt



convertpeaklist.txt

- Rename this file
- Move this file
- Copy this file
- Publish this file to the Web
- E-mail this file
- Print this file
- Delete this file

- Other Places
- pdata
  - My Documents
  - My Computer
  - My Network Places

Details

- 1r
- auditp.txt
- outd
- parm.txt
- peaklist.xml
- peakrng
- peaks
- proc
- procs
- title
- peak.txt

next page

# Peak picking 1D

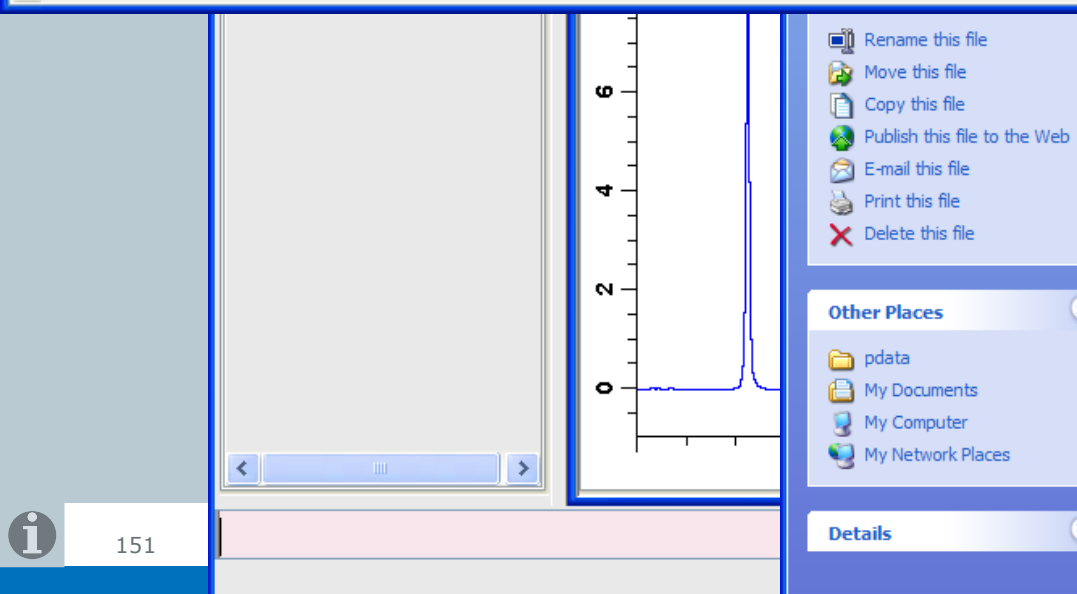


```
Brucker TopSpin on merlin as svcu
peak.txt - Notepad
File Edit Format View Help
DU=F:/Bruker/topspin2.1-alpha, USER=guest, NAME=exam1d_1H, EXPNO=1,
F1=5.880ppm, F2=5.781ppm, MI=1.12cm, MAXI=2.17cm, PC=1.000
# ADDRESS FREQUENCY INTENSITY
# [Hz] [PPM]
1 14138.1 ? 5.8234 1.56
2 14179.3 ? 5.8083 1.59
-----
DU=F:/Bruker/topspin2.1-alpha, USER=merlin, NAME=exam1d_1H, EXPNO=1,
Manually picked peaks
# ADDRESS FREQUENCY INTENSITY
# [Hz] [PPM]
3 10177.1 ? 7.2759 7.04
4 10615.6 ? 7.1151 0.01
```

Note:  
Because peak.txt  
is created manually  
it could be outdated!

→

Whenever TopSpin  
modify the peaklist  
it will move the  
textfile peak.txt  
to peak.txt.bak



next page →

What about datasets/peak lists created with TopSpin < 2.1?

When these datasets are opened with TopSpin 2.1 the file `peak.txt` is automatically converted in:  
`peaklist.xml`  
and the original file `peak.txt` is renamed into `peak.txt.bak`

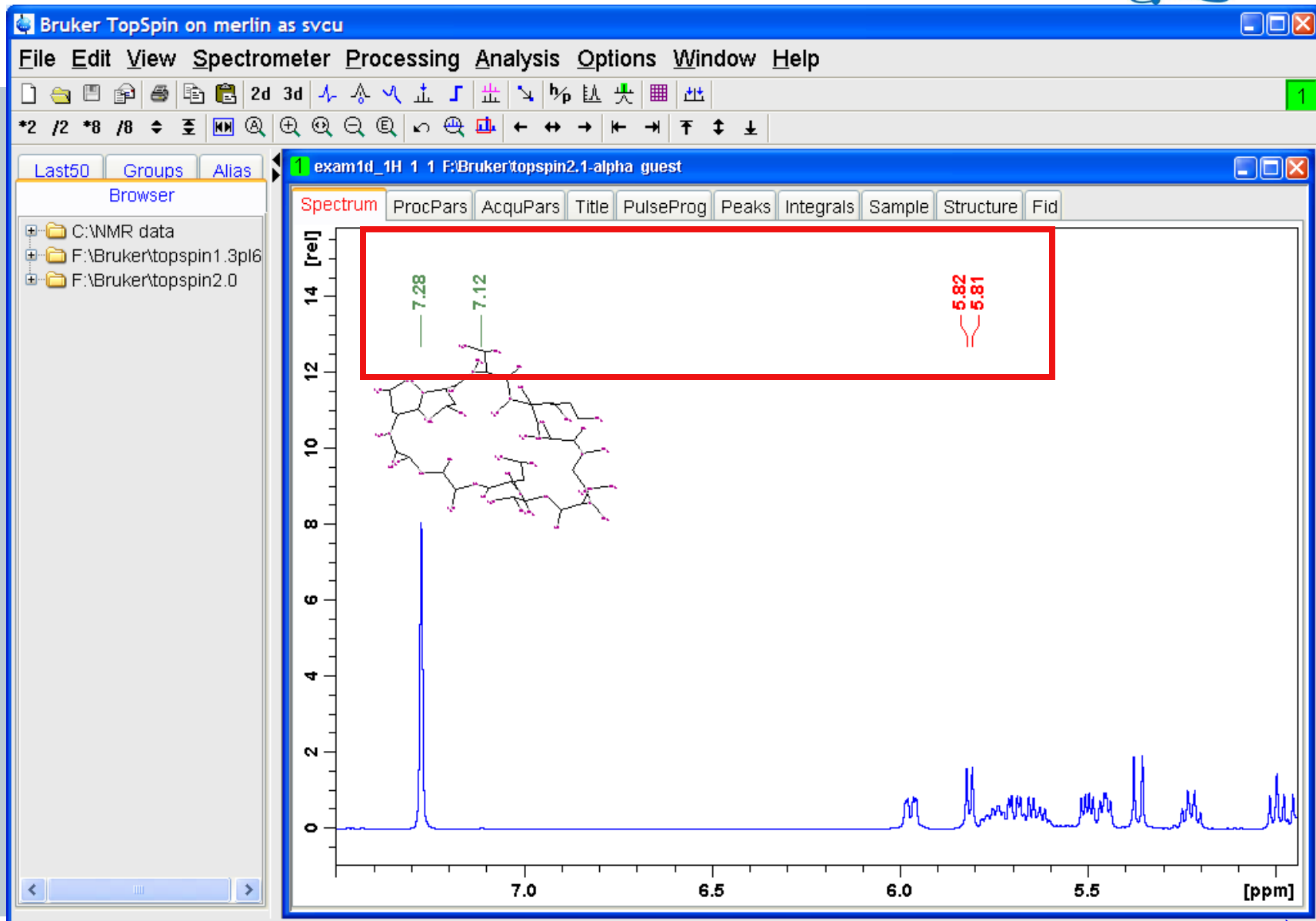


Please note that if you have user-specific AU programs with peak picking AND if the peak file is used for any further procedures you have to modify your setup.

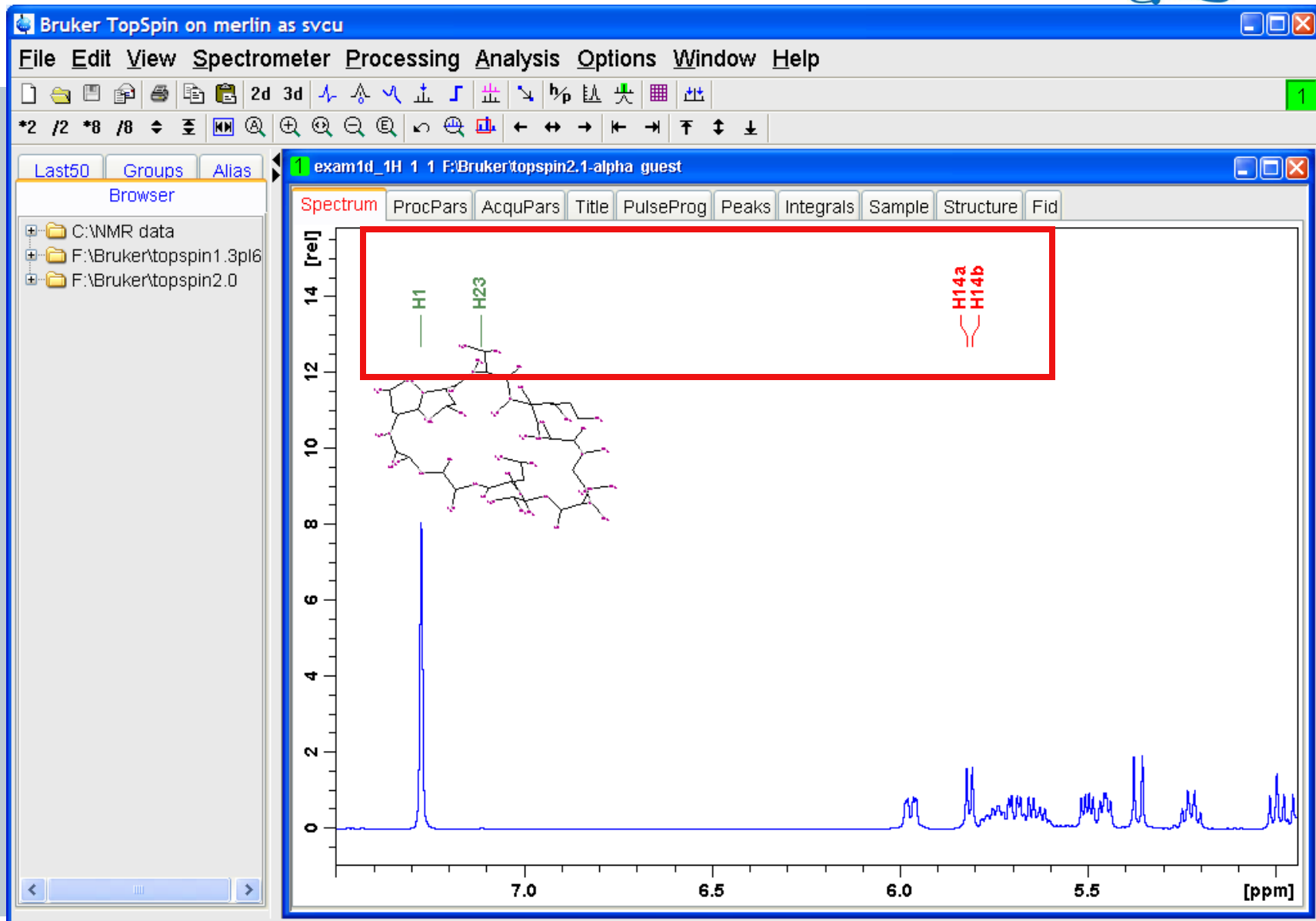
For more details check the Release Letter of TopSpin 2.1.

Because of the new format  
peaklist created with TopSpin 2.1  
can not be displayed with  
XWIN-NMR / TopSpin < 2.1.

# Peak picking 1D



# Peak picking 1D: annotations



# Peak picking 1D: absolute values



Bruker TopSpin on merlin as svcu

File Edit View Spectrometer Processing Analysis Options Window Help

Browser Last50 Groups Alias

1 svcu-test2 1 1 "C:\NMR data" guest mit leerzeichen

Spectrum	ProcPars	AcquPars	Title	PulseProg	Peaks	Integrals	Sample	Structure	Fid	Acqu
Peak	v(F1) [ppm]	Intensity [abs]	Intensity [rel]	Annotation						
1	7.2816	69584.79	0.07							
2	3.4706	36196.65	0.03							
3	3.4563	43161.21	0.04							
4	3.4360	70267.98	0.07							
5	3.4221	76298.28	0.07							
6	3.4019	44391.56	0.04							
7	3.3878	42084.62	0.04							
8	2.2075	45838.90	0.04							
9	2.1916	61833.86	0.06							
10	2.1693	50082.57	0.05							
11	2.0022	59365.59	0.06							
12	1.9624	64642.04	0.06							
13	1.7017	62025.32	0.06							
14	1.6545	127560.61	0.12							
15	1.6127	72593.04	0.07							
16	1.6029	72116.19	0.07							
17	1.4327	116256.38	0.11							
18	1.1668	36323.79	0.03							
19	1.1273	73169.87	0.07							
20	1.0942	58302.92	0.06							
21	1.0488	38541.25	0.04							
22	1.0268	62278.79	0.06							
23	1.0170	81787.62	0.08							
24	1.0070	76020.12	0.07							
25	0.9886	134484.58	0.13							
26	0.9590	520243.62	0.50							
27	0.9416	671913.34	0.64							

# Peak picking 1D: print preview available



Print preview window showing a table of peak data:

Peak	ν(F1) [ppm]	Intensity [abs]	Intensity [rel]	Annotation
1	15.6322	1290584.72	1.21	
2	15.6128	1329574.59	1.25	
3	15.3899	1444536.53	1.37	
4	15.3754	1488207.47	1.40	
5	14.9914	1501603.22	1.41	
6	14.9759	1551324.41	1.47	
7	14.8271	1524911.38	1.44	
8	14.8098	1566904.62	1.49	
9	14.5145	8522929.72	8.00	

Processing Analysis Options Window Help

exam1d\_1H 1 1 F:\Bruker\TopSpin guest

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Fid

Peak	ν(F1) [ppm]	Intensity [abs]	Intensity [rel]	Annotation
1	15.6322	1290584.72	1.21	

Print preview window showing a table of peak data:

Peak	ν(F1) [ppm]	Intensity [abs]	Intensity [rel]	Annotation
1	15.6322	1290584.72	1.21	
2	15.6128	1329574.59	1.25	
3	15.3899	1444536.53	1.37	
4	15.3754	1488207.47	1.40	
5	14.9914	1501603.22	1.41	
6	14.9759	1551324.41	1.47	
7	14.8271	1524911.38	1.44	
8	14.8098	1566904.62	1.49	

Context menu for peak 1:

- Show spectrum
- Expand spectrum
- Delete
- Edit annotation
- Remove
- Define as reference
- Annotate by reference...
- Shift peaks...
- Show detailed information...
- Copy
- Export...
- Import...
- Print...
- Print preview...**
- Table properties...

Main window showing a table of peak data:

22	10.4300	13382252.19	12.65	
23	10.3262	12676161.09	12.03	
24	10.2883	12762428.41	12.35	
25	10.2002	13736860.97	12.92	
26	9.9394	13255537.78	12.46	
27	9.6355	1265973.50	1.19	
28	9.6217	1741186.75	1.64	

Print preview window showing a table of peak data:

Peak	ν(F1) [ppm]	Intensity [abs]	Intensity [rel]	Annotation
46	8.5900	1606999.09	1.51	
47	8.5254	6908794.78	5.94	
48	8.5145	8972199.72	8.42	
49	8.5035	15929740.91	15.00	
50	8.4894	13781475.06	12.94	
51	8.4778	6935130.56	6.52	
52	8.4066	658670.81	6.07	
53	8.3988	8191796.59	7.71	
54	8.3960	8249641.12	7.75	
55	8.3854	6528555.72	6.14	
56	8.3286	6362972.81	6.02	

# Peak picking 1D: print preview available



available for many tables in TopSpin 2.1

Print preview

May 2, 2007 (2:24:09 PM) exam1d\_1H 1 1 F:\Bruker\TopSpin ... Page 1/1

Peak	$\nu(F1)$ [ppm]	Intensity [abs]	Intensity [rel]	Annotation
1	15.6322	1290584.72	1.21	
2	15.6128	1329574.59	1.25	
3	15.3899	1444536.53	1.37	
4	15.3754	1488207.47	1.40	
5	14.9914	1501603.22	1.41	
6	14.9759	1551324.41	1.47	
7	14.8271	1524911.38	1.44	
8	14.8098	1566904.62	1.49	
9	14.5145	8522929.72	8.00	

Print preview

May 2, 2007 (2:24:09 PM) exam1d\_1H 1 1 F:\Bruker\TopSpin ... Page 1/16

Peak	$\nu(F1)$ [ppm]	Intensity [abs]	Intensity [rel]	Annotation
1	15.6322	1290584.72	1.21	
2	15.6128	1329574.59	1.25	
3	15.3899	1444536.53	1.37	
4	15.3754	1488207.47	1.40	
5	14.9914	1501603.22	1.41	
6	14.9759	1551324.41	1.47	
7	14.8271	1524911.38	1.44	
8	14.8098	1566904.62	1.49	

May 2, 2007 (2:24:09 PM) exam1d\_1H 1 1 F:\Bruker\TopSpin ... Page 2/2

Peak	$\nu(F1)$ [ppm]	Intensity [abs]	Intensity [rel]	Annotation
46	8.5900	1606999.09	1.51	
47	8.5254	6908794.78	5.94	
48	8.5145	8972199.72	8.42	
49	8.5035	15929710.91	15.00	
50	8.4894	19781475.06	12.94	
51	8.4778	6935130.56	6.52	
52	8.4086	6288670.51	6.07	
53	8.3988	8191796.59	7.71	
54	8.3960	8249641.12	7.75	
55	8.3854	6528555.72	6.14	
56	8.3286	6262972.81	6.02	

Processing Analysis Options Window Help

exam1d\_1H 1 1 F:\Bruker\TopSpin ...

Spectrum

Annotation

- Show spectrum
- Export spectrum
- Delete
- Edit annotation
- Define as reference
- Annotate by reference...
- Shift peaks...
- Show detailed information...
- Copy
- Export...
- Import...
- Print...
- Print preview...**
- Table properties...

22	10.4300	13382252.19	12.65	
23	10.3262	12676161.09	12.03	
24	10.2883	12762428.41	12.35	
25	10.2002	13736860.97	12.92	
26	9.9394	13255537.78	12.46	
27	9.6355	1265973.50	1.19	
28	9.6217	1741186.75	1.64	

# Peak picking 1D: transfer annotations



Bruker TopSpin on merlin as svcu

File Edit View Spectrometer Processing Analysis Options Window Help

\*2 /2 \*8 /8

Browser Last50 Groups Alias

- \\server\home
- C:\NMR data
- F:\Bruker\TopSpin
- F:\Bruker\topspin1.3pl6
- F:\Bruker\topspin1.3pl8
- F:\Bruker\topspin2.0

exam1d\_1H 1 1 F:\Bruker\TopSpin guest

Peak	v(F1) [ppm]	Intensity [abs]	Intensity [rel]	Annotation
1	15.6322	1290584.72	1.21	H1
2	15.6128	1329574.59	1.25	H2
3	15.3899	1444536.53	1.37	hello world
4	15.3899	1444536.53	1.40	??
5	15.3899	1444536.53	1.41	
6	15.3899	1444536.53	1.47	H12
7	15.3899	1444536.53	1.44	
8	15.3899	1444536.53	1.49	
9	15.3899	1444536.53	8.00	

Annotations will be matched against 'exam1d\_1H 1 1 F:\Bruker\TopSpin guest'

Allow variations of  ppm

Overwrite existing annotations

OK Cancel

- Show spectrum
- Expand spectrum
- Delete
- Edit annotation
- Remove
- Define as reference
- Annotate by reference...
- Shift peaks...
- Show detailed information...
- Copy
- Export...
- Import...
- Print...
- Print preview...
- Table properties...



# Auto-resize all columns



Bruker TopSpin on merlin as svcu

File Edit View Processing Analysis Options Window Help

\*2 /2 \*8 /8

Browser Last50 Groups Alias

1 exam1d\_1H 1 1 F:\Bruker\TopSpin guest

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Fid

Object	Integral [abs]	Integral [rel]	Peaks	v(F1) [ppm]
Integral 1	0.875		4	3.7042
Integral 2	0.1421		1	3.5872
Integral 3	0.0136		0	5.365
Integral 4	0.0419		1	3.871

Object  
Integral [abs]  
Integral [rel]  
Peaks  
Range (F1) from  
Range (F1) to  
v(F1) [ppm]  
Intensity [abs]  
**Auto-resize all columns**  
More...

# More table properties



The image shows three overlapping 'Table properties' dialog boxes in a Bruker software interface. The top-left dialog has the 'Column' tab selected. The middle dialog has the 'Colours' tab selected. The bottom dialog has the 'Spacings' tab selected, and a red box highlights the 'More...' button. A red arrow points from this button to the 'v(F1) [ppm]' column header in the background table. The background table has columns for 'Integral [abs]', 'Integral [rel]', 'Peaks', and 'v(F1) [ppm]'. The 'v(F1) [ppm]' column contains the value '49045084.44'. The 'More...' button is highlighted with a red box.

# An example for different table colours



Bruker TopSpin on merlin as svcu

File Edit View Spectrometer Processing Analysis Options Window Help

\*2 /2 \*8 /8

exam1d\_1H 11 1 F:\Bruker\TopSpin guest

Peak	Type	$\nu(F1)$ [ppm]	Intensity	Half width [Hz]	Annotation
33	Manual	4.6884E0	0.00	0.1834	
34	Manual	4.1501E0	0.17	1.1004	
35	Manual	3.4208E0	0.03	0.3668	
36	Manual	2.3963E0	1.14	2.5676	
37	Manual	2.2572E0	0.69	1.2838	
38	Manual	1.2378E0	6.62	3.1178	
1	Automatic	8.3921E0	1.22	3.4846	
2	Automatic	8.3727E0	1.25	3.3012	
3	Automatic	8.1498E0	1.38	3.1178	
4	Automatic	8.1353E0	1.41	3.1178	
5	Automatic	7.7514E0	1.42	2.9344	
6	Automatic	7.7359E0	1.47	2.7510	
7	Automatic	7.5870E0	1.45	2.9344	
8	Automatic	7.5697E0	1.49	2.7510	
9	Automatic	7.2745E0	8.02	3.8514	
10	Automatic	5.9798E0	0.77	3.6680	
11	Automatic	5.9652E0	0.83	3.8514	
12	Automatic	5.9582E0	0.78	3.3012	
13	Automatic	5.8234E0	1.56	2.7510	
14	Automatic	5.8083E0	1.59	2.5676	
15	Automatic	5.7119E0	0.79	3.6680	
16	Automatic	5.7044E0	0.84	3.6680	

# Scientific notation



**Table properties**

Column Colours Spacings

- Peak
- Region
- Type
- Index (F1)
- $\nu(F1)$  [ppm]
- $\nu(F1)$  [Hz]
- Intensity [abs]
- Intensity [rel]

**Column properties**

Column width: 131

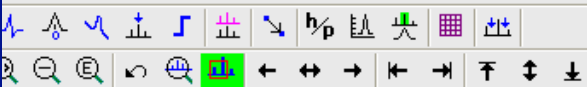
Fraction digits: 2

**Scientific notation**

OK Cancel Apply

	$\nu(F1)$ [ppm]	Intensity [abs]	$\Delta$ Intensity [rel]	Annotation
atic	21.1484	1068523000.00	15.34	
atic	39.4959	1015885868.00	15.43	
atic	31.8216	993662032.00	15.70	
atic	18.6931	980767120.00	18.00	
atic	11.7985	1035075668.00	18.65	
atic	19.2154	1418837464.00	20.10	
atic	42.2502	994824408.00	21.32	

## Analysis Options Window Help



1 exam1d\_13C 1 1 F:\Bruker\TopSpin guest

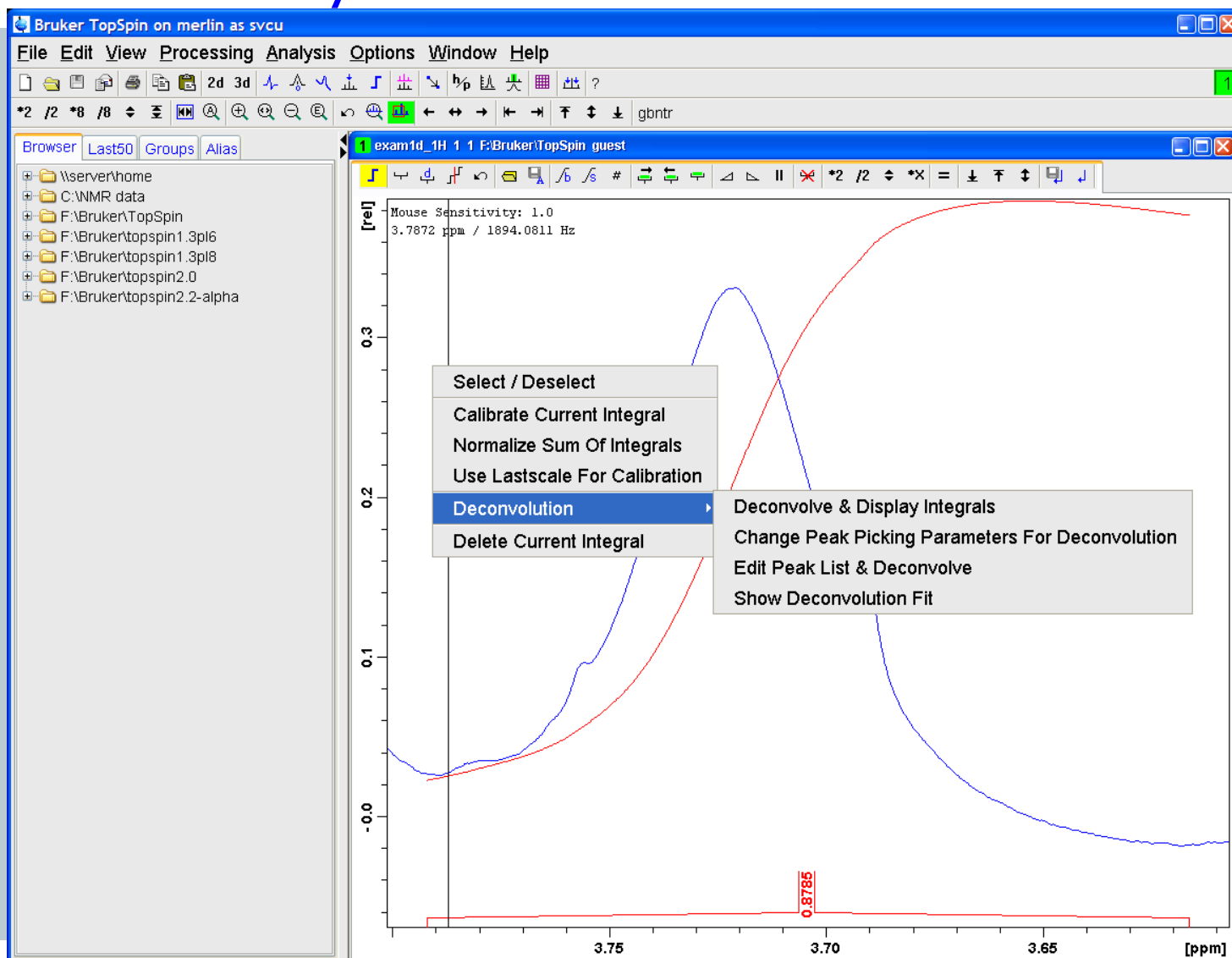
Peak	Type	$\nu(F1)$ [ppm]	Intensity [abs]	$\Delta$ Intensity [rel]
8	Automatic	21.1484	1.07E9	15.34
2	Automatic	39.4959	1.02E9	15.43
4	Automatic	31.8216	9.94E8	15.70
10	Automatic	18.6931	9.81E8	18.00
11	Automatic	11.7985	1.04E9	18.65
9	Automatic	19.2154	1.42E9	20.10
1	Automatic	42.2502	9.95E8	21.32
3	Automatic	36.4876	1.72E9	24.53
7	Automatic	22.5237	1.92E9	27.24
6	Automatic	22.7571	1.97E9	27.84
5	Automatic	27.9136	2.04E9	28.90

- 5 - dept90
- 6 - zgig30
- 11 - zgpg30
- 99 - zgpg30
- exam1d\_1H
- exam2d\_CH
- exam2d\_HC

# Integration of peak shoulders



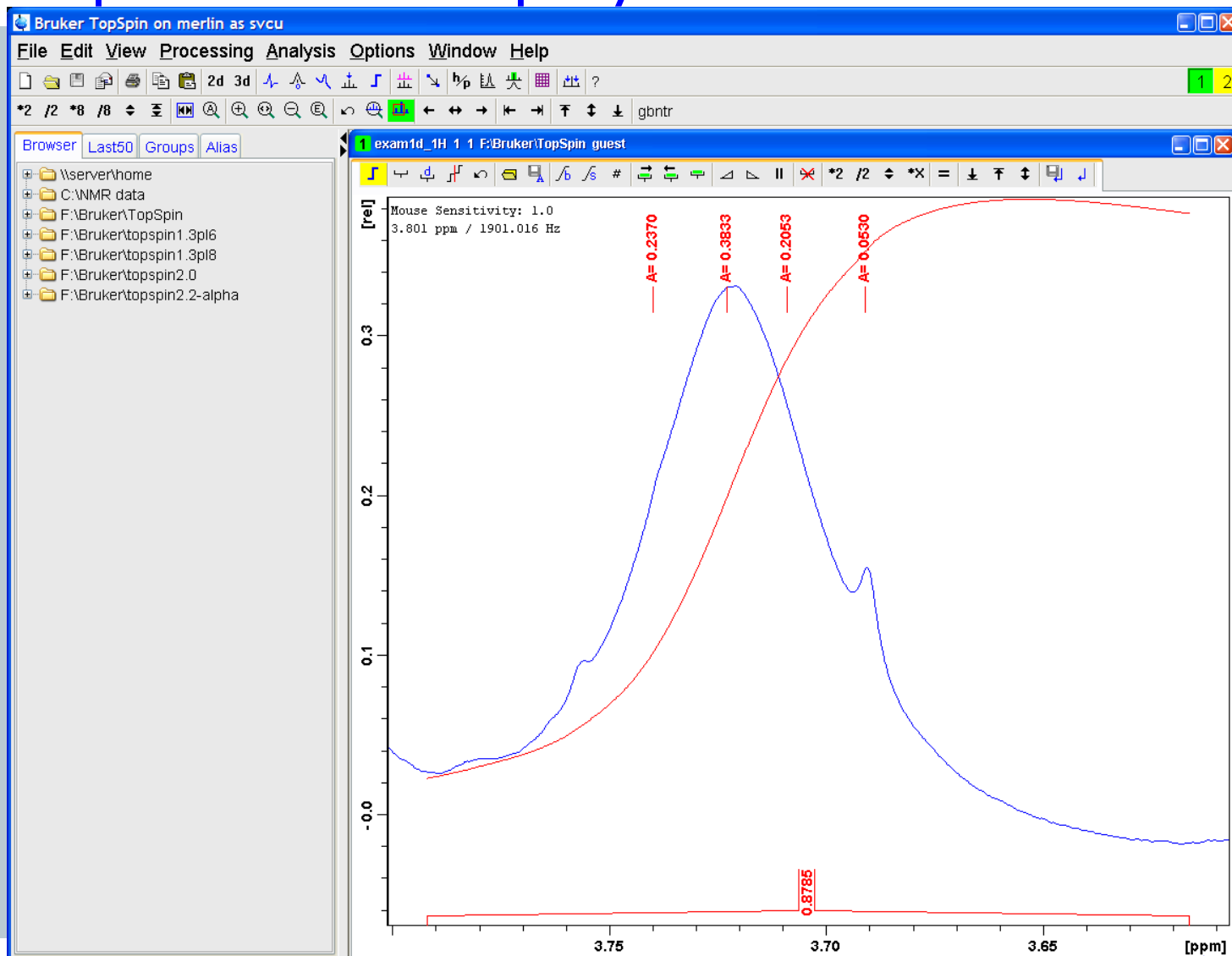
## Integration offers easy access to deconvolution



# Integration of peak shoulders



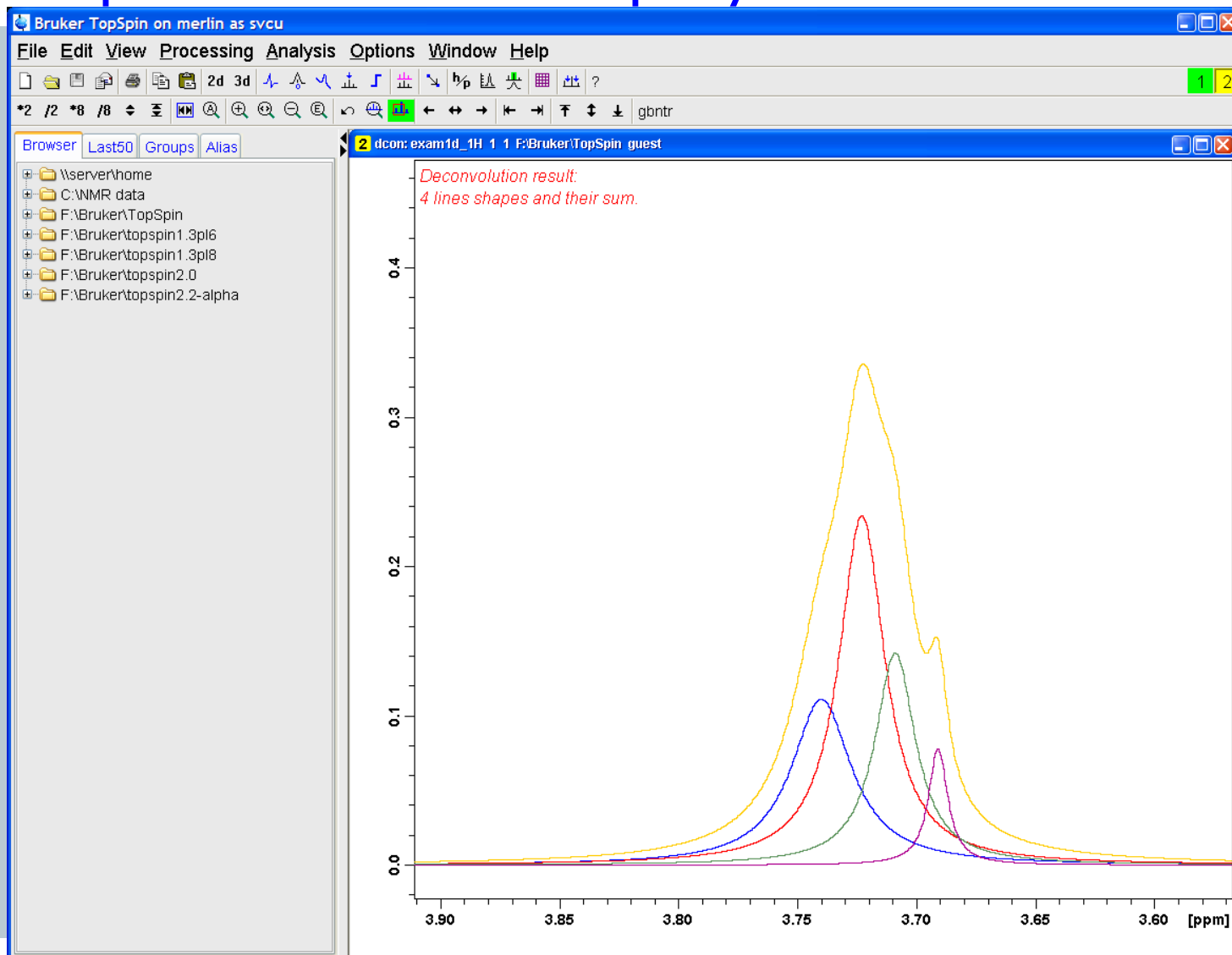
## Deconvoluted peaks are displayed



# Integration of peak shoulders



## Shapes of the peaks can be displayed



# Integration of peak shoulders



## Peak list contains also deconvoluted peaks

The screenshot shows the Bruker TopSpin software interface. The main window displays a peak list table with the following data:

Peak	Type	$\nu(F1)$ [ppm]	Intensity [abs]	$\Delta$ Intensity [rel]	Annotation
4	Deconvolution	3.6910	161157.56	0.05	
3	Deconvolution	3.7090	267492.25	0.21	
1	Deconvolution	3.7400	208758.09	0.24	
<b>2</b>	<b>Deconvolution</b>	<b>3.7230</b>	<b>343990.19</b>	<b>0.38</b>	



# Integration of peak shoulders

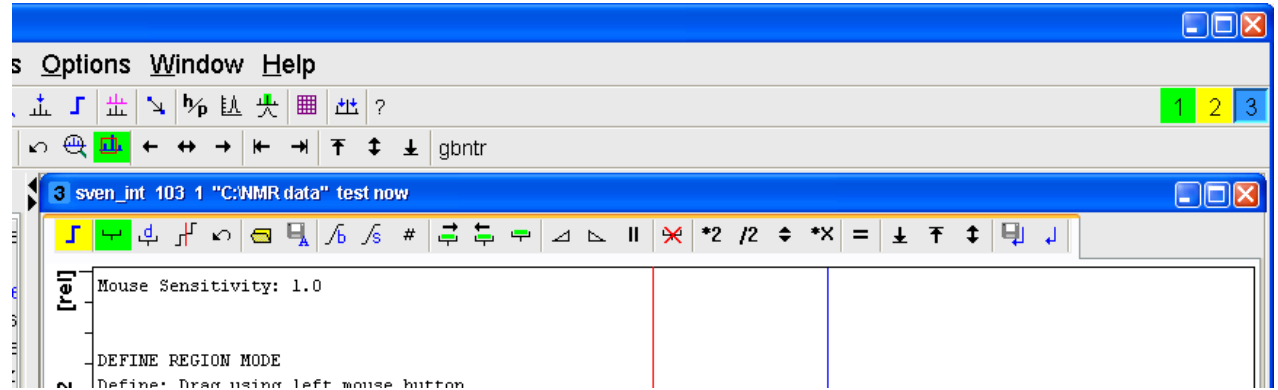


Integration list contains also intensities of deconv. peaks

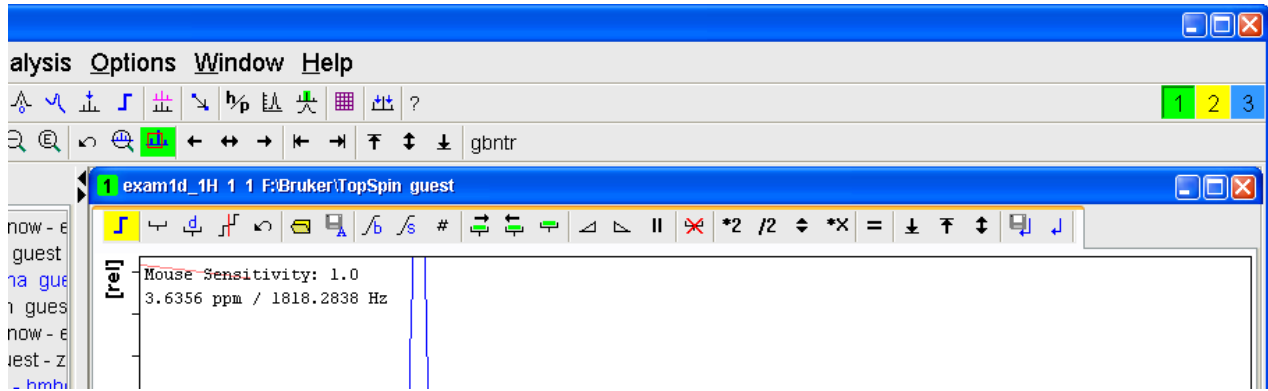
The screenshot shows the Bruker TopSpin software interface. The main window displays a table of integration results for a spectrum named 'exam1d\_1H'. The table includes columns for Object, Integral [abs], Integral [rel], Peaks,  $\nu(F1)$  [ppm], and Intensity [abs]. The 'Integral 1' row is expanded to show four deconvoluted peaks.

Object	Integral [abs]	Integral [rel]	Peaks	$\nu(F1)$ [ppm]	Intensity [abs]
Integral 1	49045084.44	0.8785	4	3.7042	
Deconvoluted peak 1				3.7400	0.24
Deconvoluted peak 2				3.7230	0.38
Deconvoluted peak 3				3.7090	0.21
Deconvoluted peak 4				3.6910	0.05

# Behaviour of integration submenu



No integrals exist → creating integrals is enabled when entering



integrals exist → creating integrals is disabled when entering

nD peak lists can be displayed  
in TopSpin.


TopSpin < 2.1

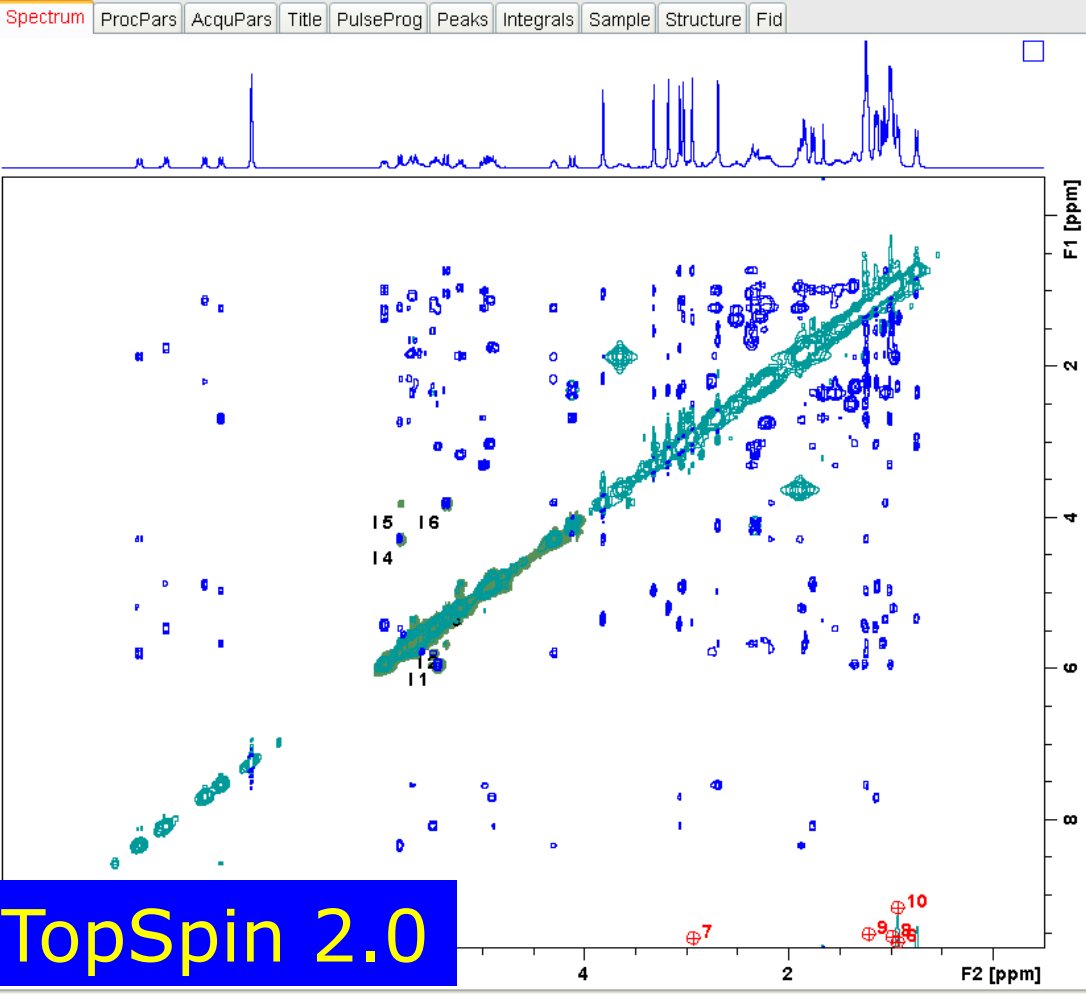
TopSpin picks as many peaks  
as defined in **PPMPNUM**

TopSpin 2.1

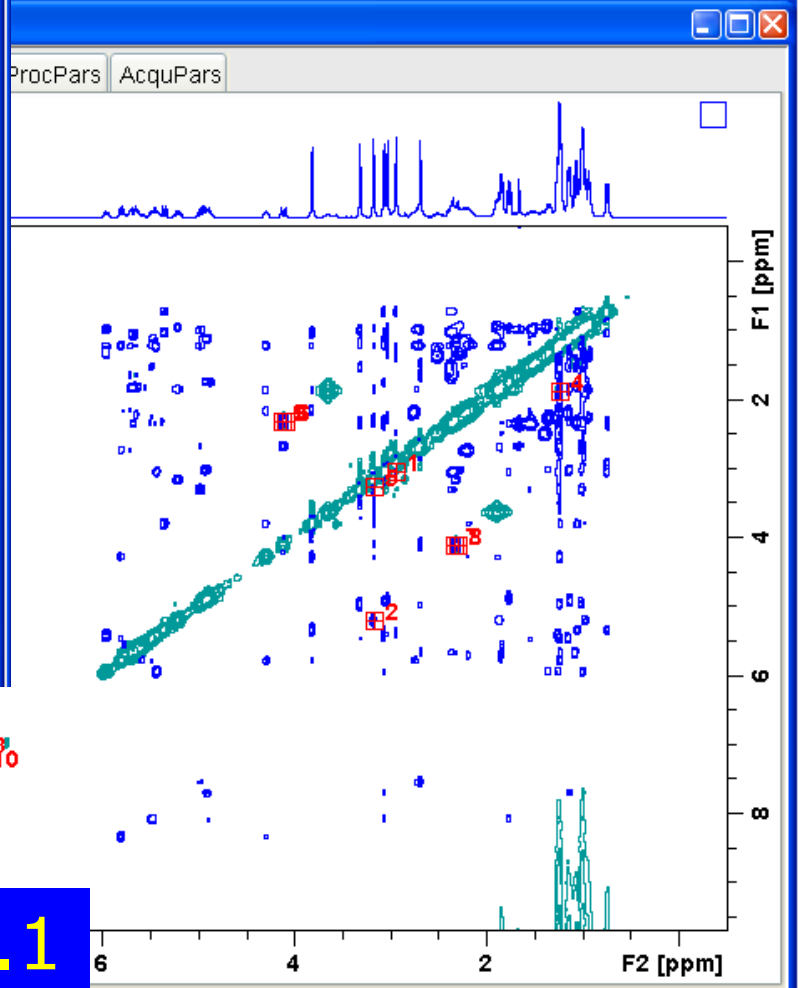
TopSpin picks all peaks

- the most intensive ones will be displayed
- as many as defined in **PPMPNUM**

next page 



Navigation controls: 1

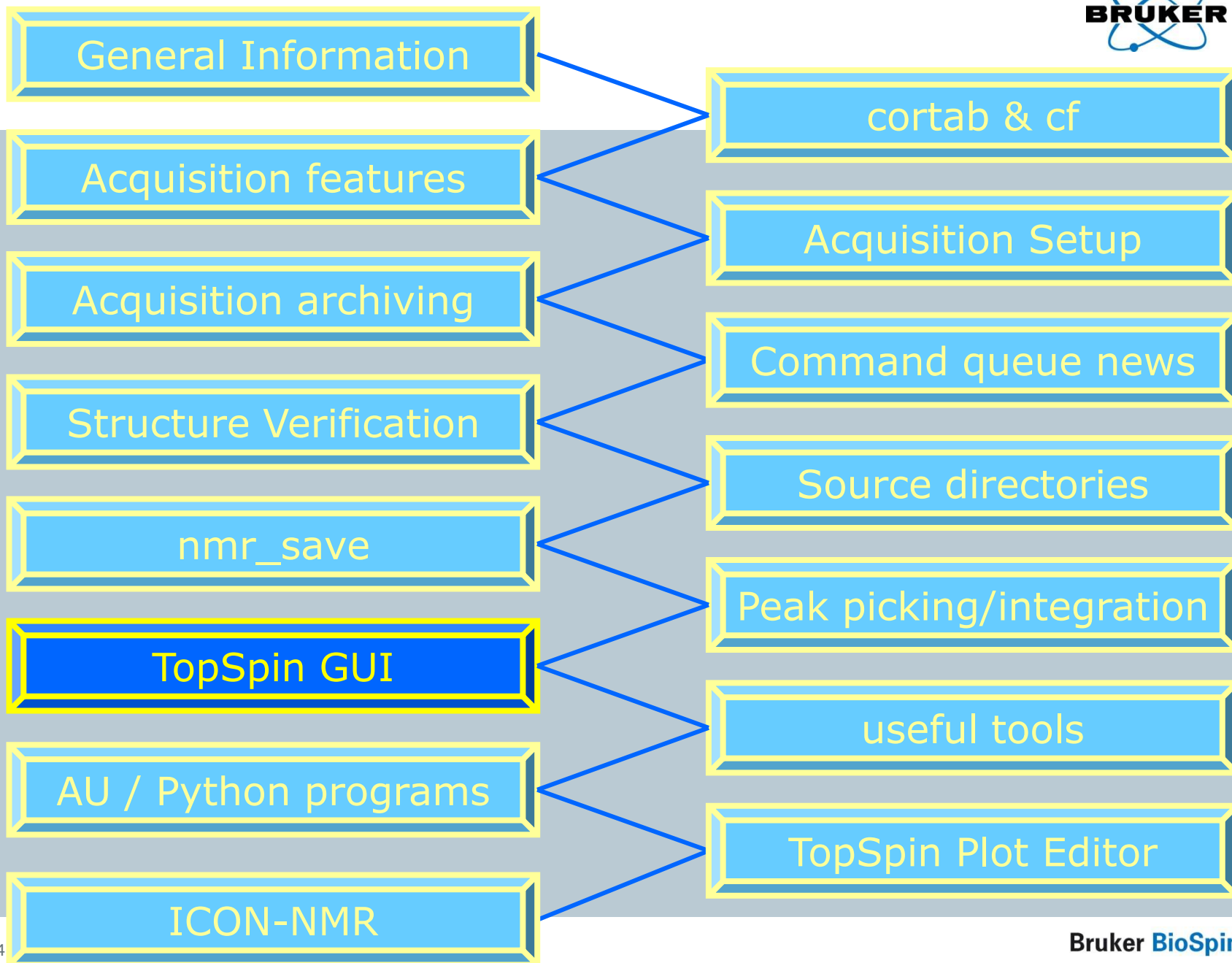


TopSpin 2.0

TopSpin 2.1



# Content



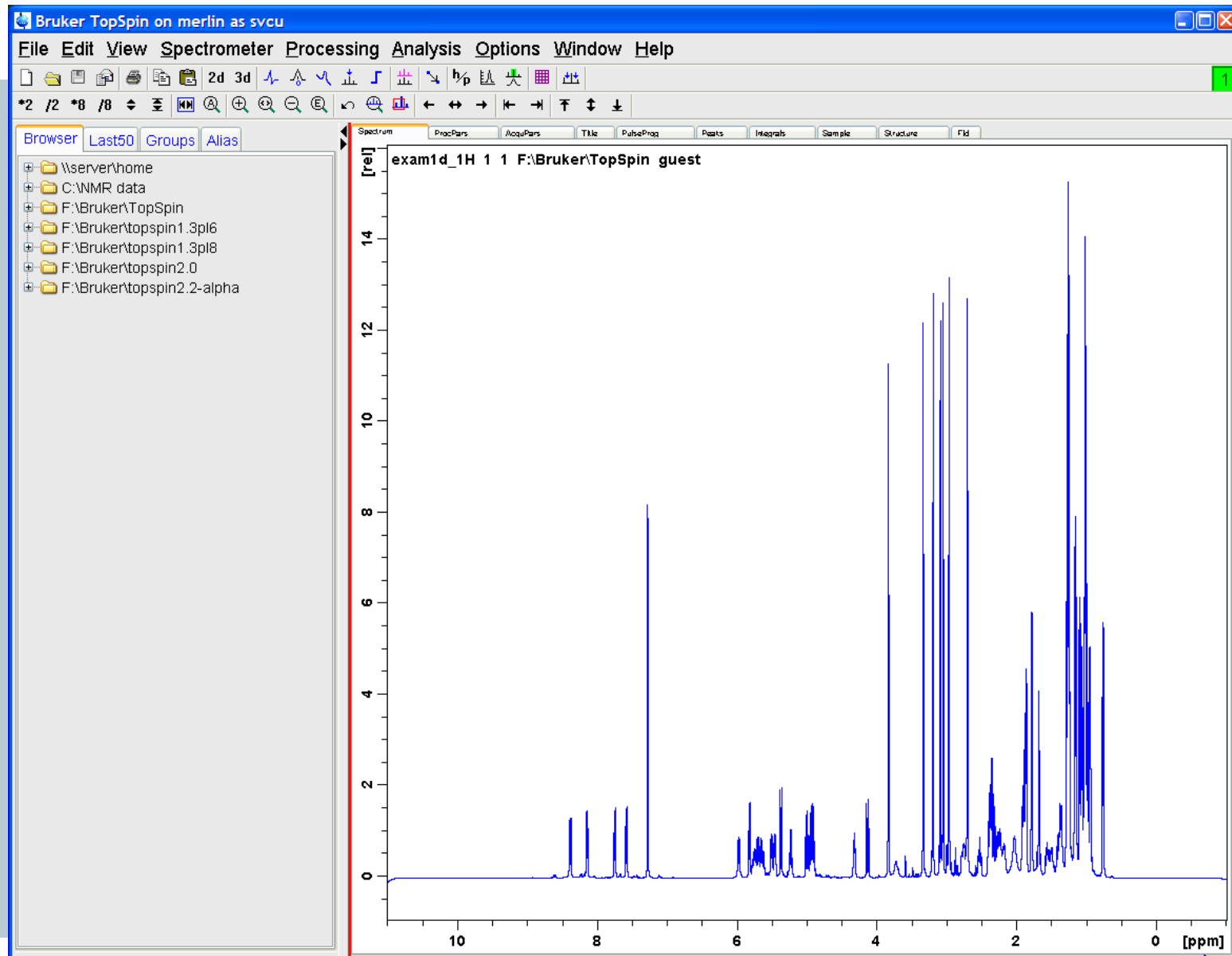
# New design of the TopSpin start window



The advertisement banner for TopSpin software features the following elements:

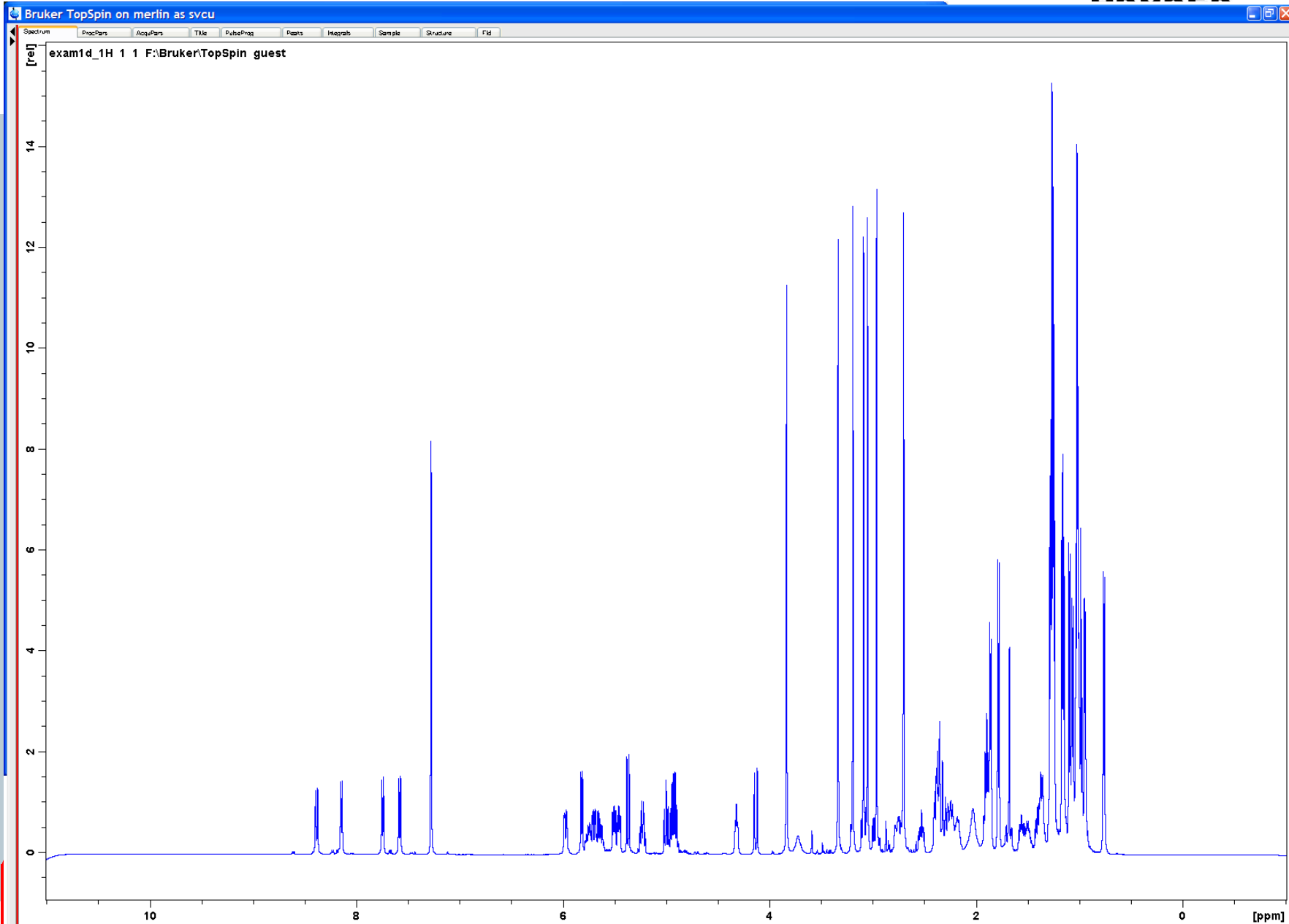
- topspin**: The product name in a large, lowercase, black, rounded font with blue dots for the 'o's.
- BRUKER**: The Bruker logo in the top right corner.
- NMR With Ease**: A central headline in white text.
- Visuals**: A composite image showing a woman in a white lab coat sitting at a computer workstation, with a large, stylized blue and green molecular structure on the left and a computer monitor displaying data on the right.
- Data service is up.**: A red headline at the bottom left.
- The Next Generation in NMR Software**: A blue headline at the bottom right.
- © 2007 Bruker BioSpin**: Copyright information at the bottom left.

# New feature: Toggle Window decoration





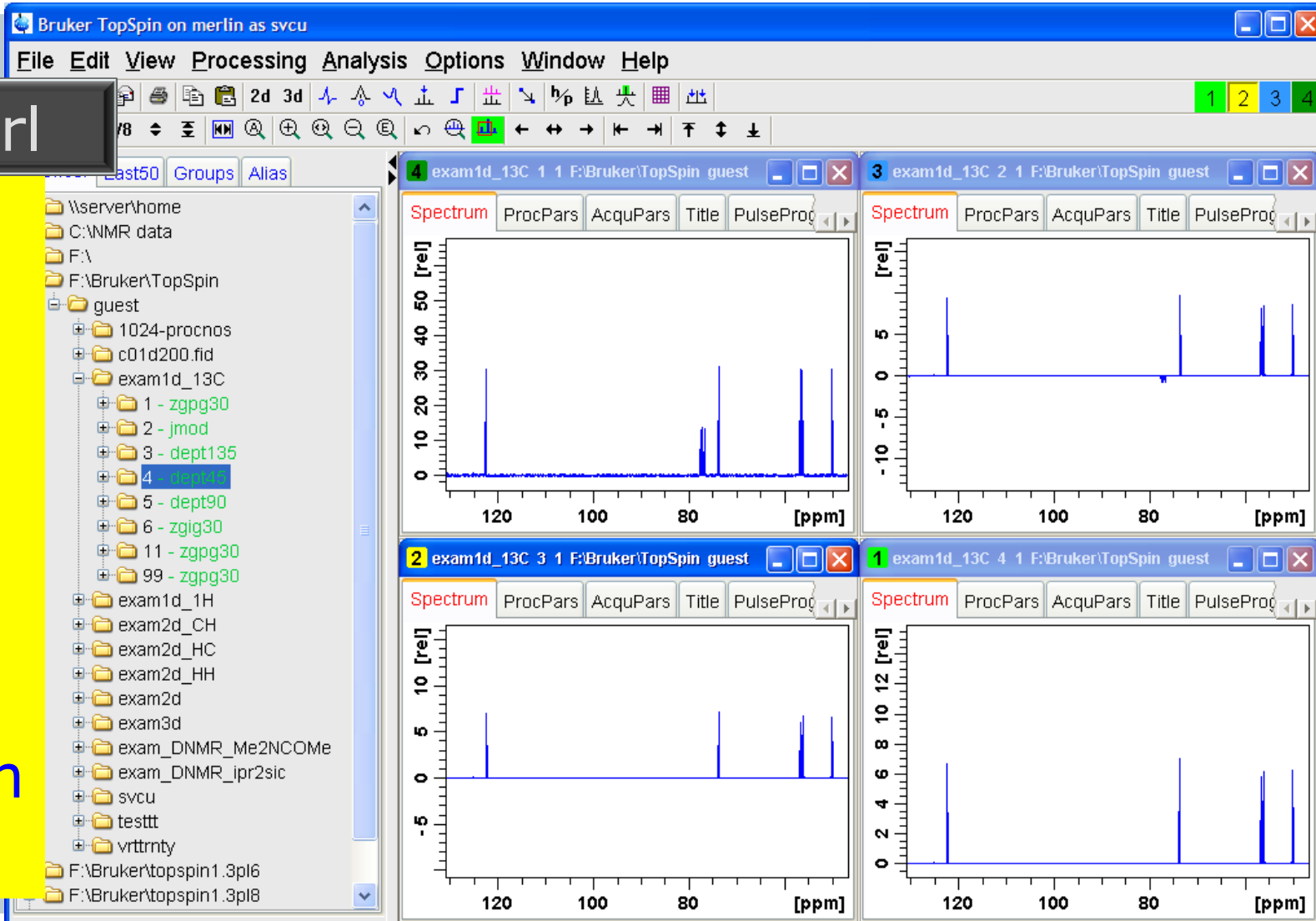
# Even in Full screen mode available



# Zoom behaviour with multiple windows in TopSpin 2.1



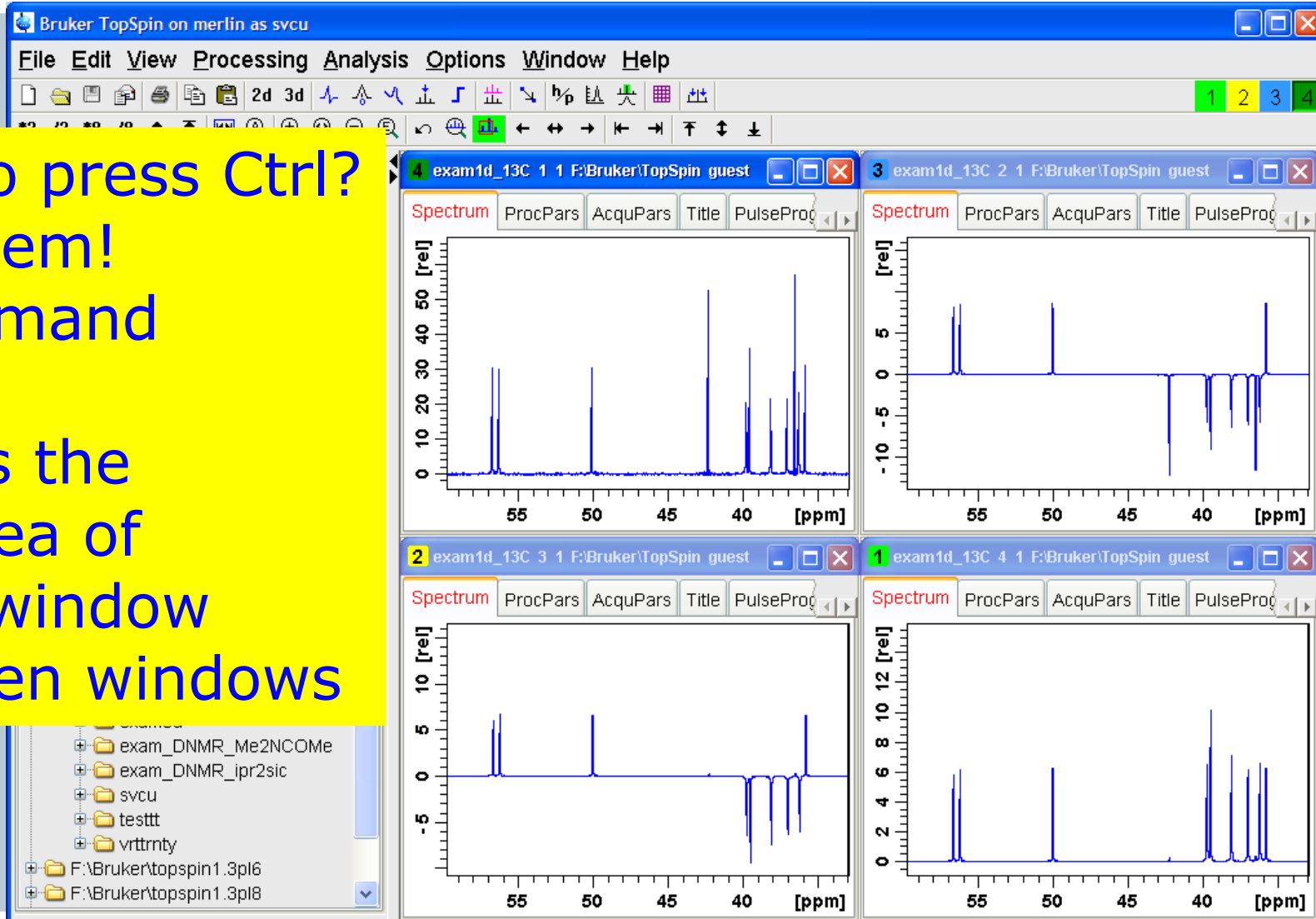
press **Ctrl** key and keep it pressed → all open datasets display same spectrum range



# Zoom behaviour with multiple windows TopSpin 2.1 – new command **.sync**

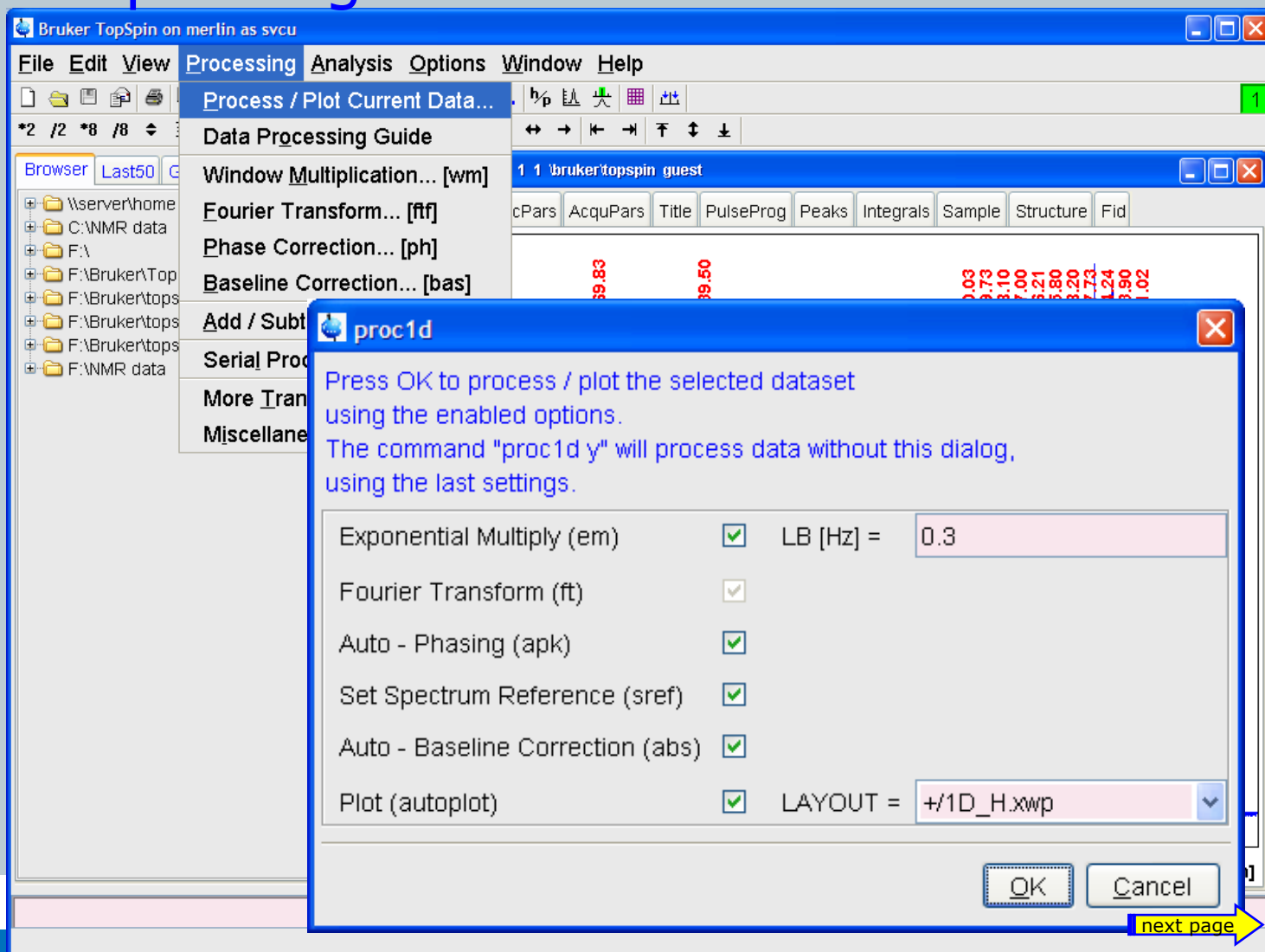


Forgot to press Ctrl?  
No problem!  
the command  
**.sync**  
transfers the  
zoom area of  
current window  
to all open windows



# New command **proc1d**

**proc1d** offers a push-button solution for 1D processing and plotting



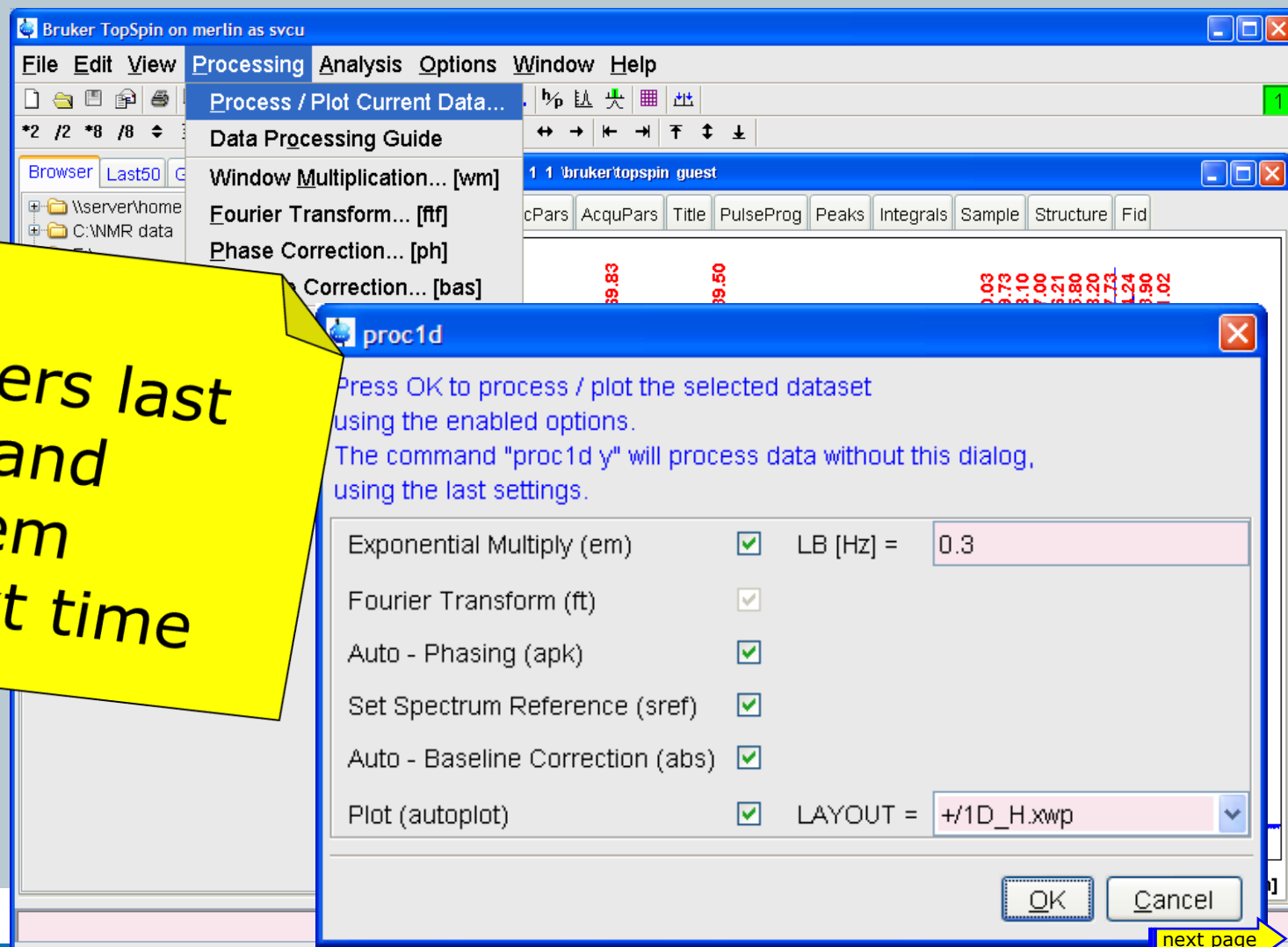
The screenshot shows the Bruker TopSpin interface with the 'proc1d' dialog box open. The background displays a 1D NMR spectrum with several peaks labeled with their chemical shifts: 99.83, 99.50, 0.03, 0.73, 1.10, 1.21, 1.80, 3.20, 7.73, 1.24, and 3.90. The 'proc1d' dialog box contains the following options:

- Exponential Multiply (em)  LB [Hz] = 0.3
- Fourier Transform (ft)
- Auto - Phasing (apk)
- Set Spectrum Reference (sref)
- Auto - Baseline Correction (abs)
- Plot (autoplot)  LAYOUT = +/1D\_H.xwp

The dialog box also includes instructions: "Press OK to process / plot the selected dataset using the enabled options. The command 'proc1d y' will process data without this dialog, using the last settings." and buttons for 'OK' and 'Cancel'.

# New command **proc1d**

**proc1d** offers a push-button solution for 1D processing



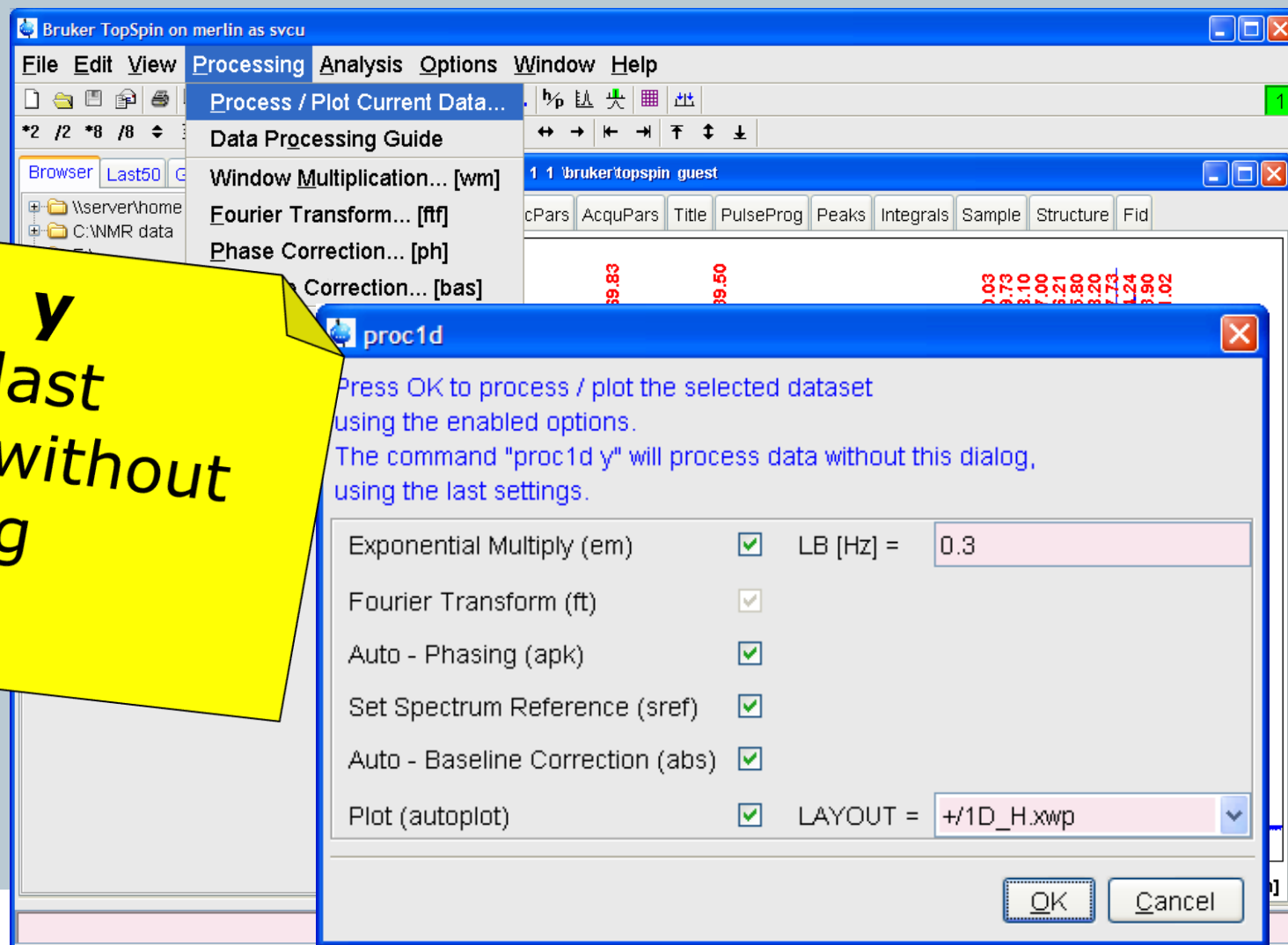
Press OK to process / plot the selected dataset using the enabled options.  
The command "proc1d y" will process data without this dialog, using the last settings.

Exponential Multiply (em)	<input checked="" type="checkbox"/>	LB [Hz] =	0.3
Fourier Transform (ft)	<input checked="" type="checkbox"/>		
Auto - Phasing (apk)	<input checked="" type="checkbox"/>		
Set Spectrum Reference (sref)	<input checked="" type="checkbox"/>		
Auto - Baseline Correction (abs)	<input checked="" type="checkbox"/>		
Plot (autoplot)	<input checked="" type="checkbox"/>	LAYOUT =	+/1D_H.xwp

*TopSpin remembers last settings and offers them again next time*

# New command **proc1d**

**proc1d** offers a push-button solution for 1D processing



Press OK to process / plot the selected dataset using the enabled options.  
The command "proc1d y" will process data without this dialog, using the last settings.

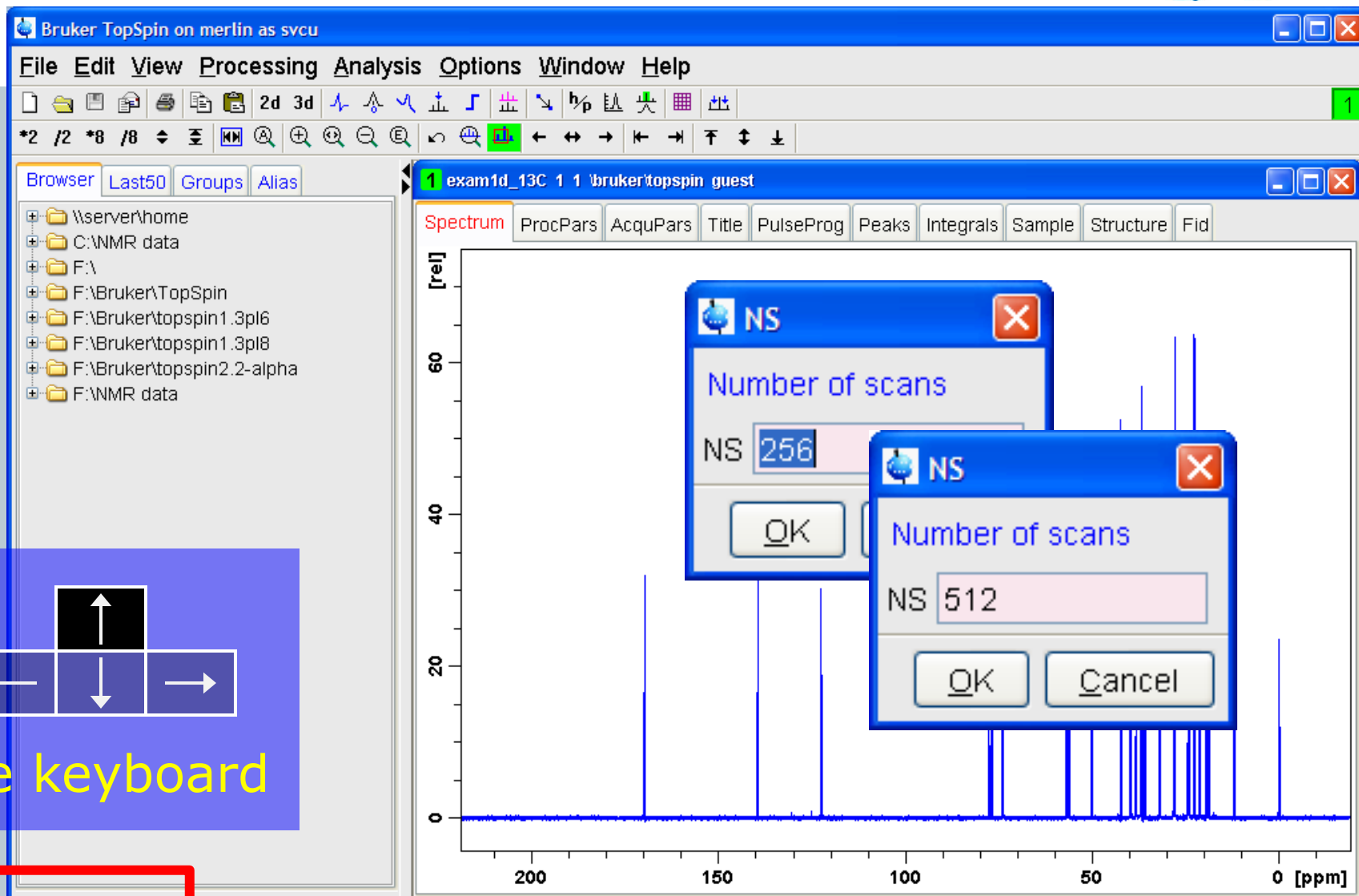
Exponential Multiply (em)	<input checked="" type="checkbox"/>	LB [Hz] =	0.3
Fourier Transform (ft)	<input checked="" type="checkbox"/>		
Auto - Phasing (apk)	<input checked="" type="checkbox"/>		
Set Spectrum Reference (sref)	<input checked="" type="checkbox"/>		
Auto - Baseline Correction (abs)	<input checked="" type="checkbox"/>		
Plot (autoplot)	<input checked="" type="checkbox"/>	LAYOUT =	+1D_H.xwp

OK Cancel

**proc1d y**  
will use last  
settings without  
this dialog

TopSpin command history offers now the parameter and its modified value, even if it was not modified in the command line but in the parameter window.

# Command history



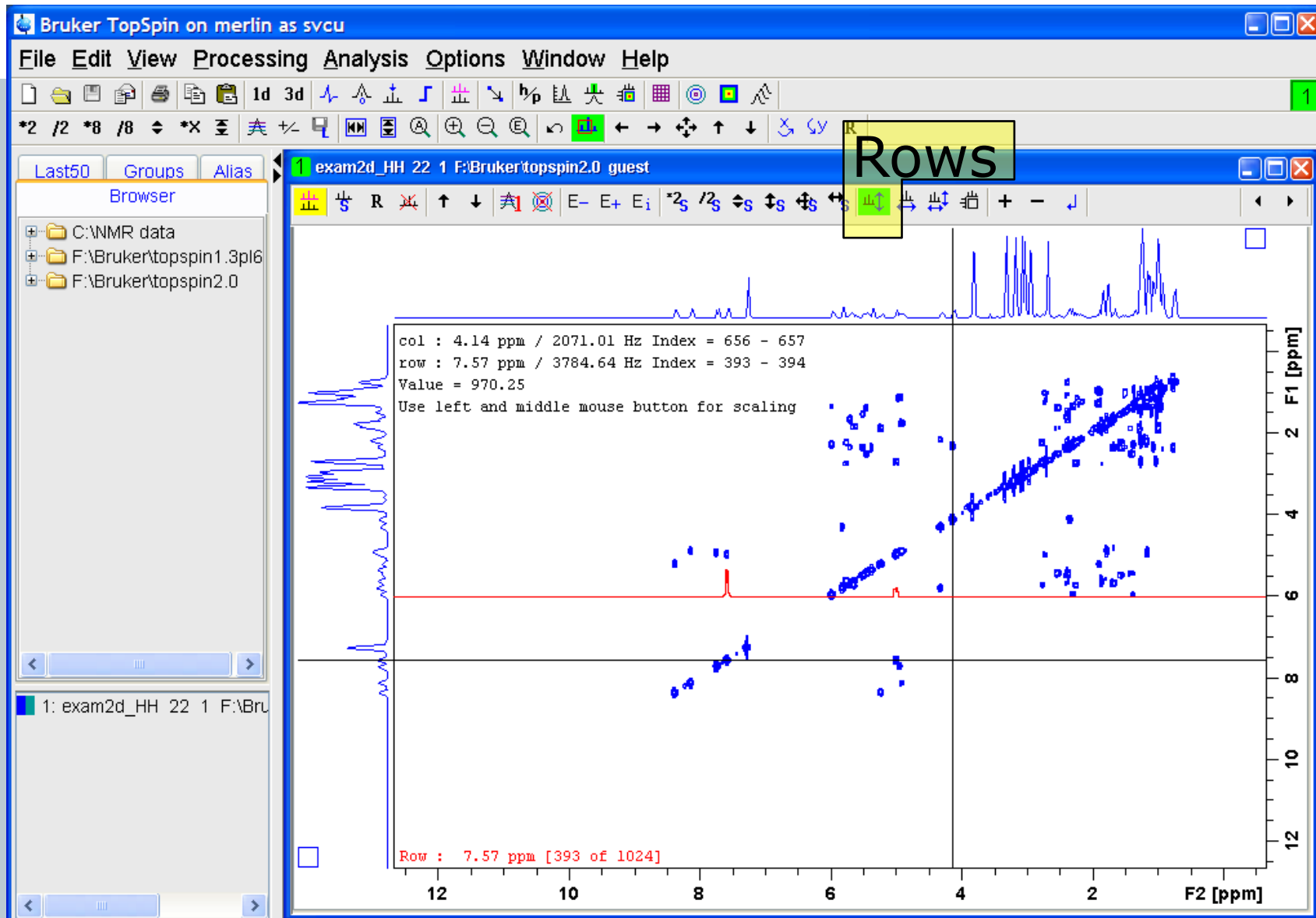
↑  
← ↓ →  
use keyboard

ns  
1 NS 512

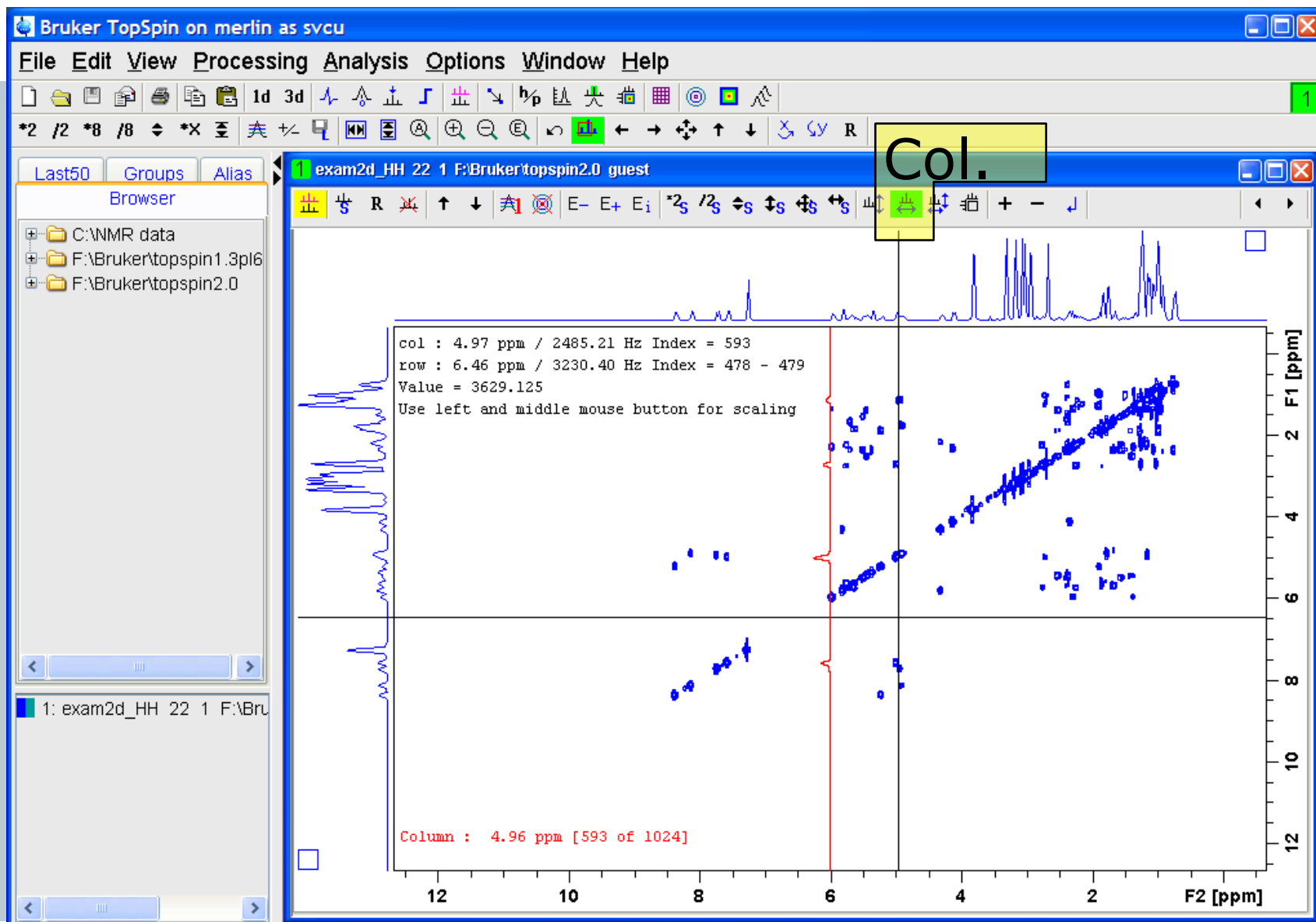


Now 2D multiple display allows scanning rows and columns simultaneously.

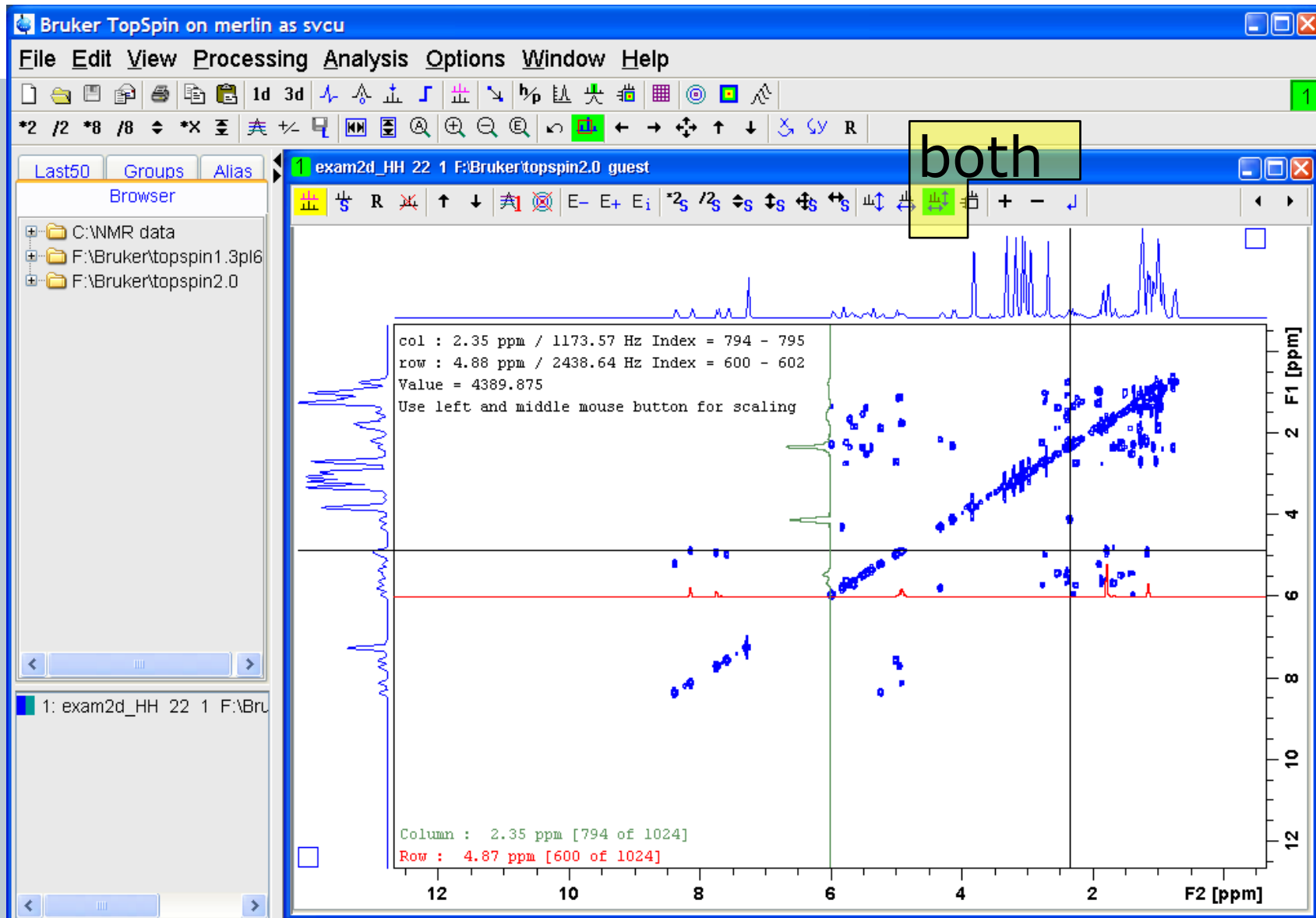
# row/column scan



# row/column scan



# row/column scan



# Browser: Fully Expand Selection



The screenshot shows the Bruker TopSpin software interface. The window title is "Bruker TopSpin on merlin as svcu". The menu bar includes "File", "Edit", "View", "Spectrometer", "Processing", "Analysis", "Options", "Window", and "Help". The toolbar contains various icons for file operations and processing. The main area is a file browser showing a tree structure of folders and files. The "Fully Expand Selection" option is highlighted in the left-hand menu. The file browser shows a tree structure starting with "F:\Bruker\TopSpin" and "exam1d\_13C".

- Browser: Last50 Groups Alias
- \server\home
- C:\NMR data
- F:\Bruker\TopSpin
  - guest
    - 1024-procnos
    - c01d200.fid
    - exam1d\_13C
      - 1
        - 1
        - 2
        - 8
      - 2
        - 1
      - 3
        - 1
      - 4
        - 1
      - 5
        - 1
      - 6
        - 1
      - 11
        - 1
    - exam1d\_1H
    - exam2d\_CH
    - exam2d\_HC
    - exam2d\_HH
    - exam2d
    - exam3d
    - exam\_DNMR\_Me2NCOMe
    - exam\_DNMR\_ipr2sic
    - svcu
    - vrtrnty
  - F:\Bruker\topspin1.3pl6
  - F:\Bruker\topspin1.3pl8
  - F:\Bruker\topspin2.0

- Display
- Display In New Window
- Display As 2D Projection
- Scroll to active dataset
- Fully Expand Selection**
- Show PULPROG/Title
- Show Date
- Sort by Date
- Copy
- File Properties
- Delete...
- Files
- Add New Data Dir...
- Remove Selected Data Dirs...

# Browser: Show Date



The screenshot shows the Bruker TopSpin software interface. The 'Browser' window displays a file tree with folders and files, each followed by a date and time. A menu on the left has 'Show Date' selected. Two callout boxes explain the naming convention: 'Date of dataset name: date of last modification' and 'Date of expno: date of acquisition'.

Folder Name	Date and Time
quest	
1024-procnos	2007-03-20 13:01:07
c01d200.fid	2007-03-13 16:27:58
exam1d_13C	2007-01-16 06:21:09
1	2004-03-30 11:43:33
2	2004-03-30 12:01:05
3	2004-03-30 12:18:36
4	2004-03-30 12:53:06
5	2004-03-30 13:27:39
6	2004-03-30 14:35:54
11	2004-03-30 11:43:33
exam1d_1H	2007-03-09 16:27:03
exam2d_CH	2007-01-16 06:21:02
exam2d_HC	2007-01-16 06:21:00
exam2d_HH	2007-01-16 06:20:55
exam2d	2007-01-21 06:57:40
exam3d	2007-01-16 06:20:44
exam_DNMR_Me2NCOme	2007-01-16 06:20:42
exam_DNMR_lpr2sic	2007-01-16 06:20:44
svcu	2007-01-16 06:20:36
vrrtrnty	2007-02-15 16:12:19

- Display
- Display In New Window
- Display As 2D Projection
- Scroll to active dataset
- Fully Expand Selection
- Show PULPROG/Title
- Show Date
- Sort by Date
- Copy
- File Properties
- Delete...
- Files
- Add New Data Dir...
- Remove Selected Data Dirs...

Date of dataset name:  
date of last modification

Date of expno:  
date of acquisition

# Browser: Date / Pulprog / Title



Bruker TopSpin on merlin as svcu

File Edit View Spectrometer Processing Analysis Options Window Help

\*2 /2 \*8 /8

Browser Last50 Groups Alias

- Wserver\home
- C:\NMR data
- F:\Bruker\TopSpin
  - guest
    - 1024-procnos - 2007-03-20 13:01:07
    - c01d200.fid - 2007-03-13 16:27:58
    - exam1d\_1H - 2007-03-09 16:27:03
    - vrtrnty - 2007-02-15 16:12:19
    - exam2d - 2007-01-21 06:57:40
    - exam1d\_13C - 2007-01-16 06:21:09
      - 1 - zgpg30, 2004-03-30 11:43:33
        - 1 - 13C(1H) AV 300 Automation Cholesterylacetate
        - 2 - 13C(1H) AV 300 Automation Cholesterylacetate
        - 8 - 13C(1H) AV 300 Automation Cholesterylacetate
      - 2 - jmod, 2004-03-30 12:01:05
        - 1 - 13C APT AV 300 Automation Cholesterylacetate
      - 3 - dept135, 2004-03-30 12:18:36
        - 1 - 13C DEPT135 AV 300 Automation Cholesterylacetate
      - 4 - dept45, 2004-03-30 12:53:06
        - 1 - 13C DEPT45 AV 300 Automation Cholesterylacetate
      - 5 - dept90, 2004-03-30 13:27:39
        - 1 - 13C DEPT90 AV 300 Automation Cholesterylacetate
      - 6 - zgig30, 2004-03-30 14:35:54
        - 1 - 13C IG AV 300 Automation Cholesterylacetate
      - 11 - zgpg30, 2004-03-30 11:43:33
        - 1 - 13C(1H) AV 300 Automation Cholesterylacetate
    - exam2d\_CH - 2007-01-16 06:21:02
    - exam2d\_HC - 2007-01-16 06:21:00
    - exam2d\_HH - 2007-01-16 06:20:55
    - exam\_DNMR\_ipr2sic - 2007-01-16 06:20:44
    - exam3d - 2007-01-16 06:20:44
    - exam\_DNMR\_Me2NCOMe - 2007-01-16 06:20:42
    - svcu - 2007-01-16 06:20:36
  - F:\Bruker\topspin1.3pl6
  - F:\Bruker\topspin1.3pl8
  - F:\Bruker\topspin2.0

- Display
  - Display In New Window
  - Display As 2D Projection
- Scroll to active dataset
- Fully Expand Selection
- ✓ Show PULPROG/Title
- ✓ Show Date
- ✓ Sort by Date
- Copy
- File Properties
- Delete...
- Files
  - Add New Data Dir...
  - Remove Selected Data Dirs...

# Sort by Date – e.g. edpul



**Pulse Programs** Source = F:\Bruker\topspin2.1-alpha\exp\stan\nmr\lists\pp

File Options Help

Search Show Comment

Class  Show Date All

Sort by Date

Avanc Manage Source Directories 0:31:43

Daz.in 0:31:43

De.inc Export Sources... 0:31:43

Delay.incl	2007-03-27 10:31:43
Grad.incl	2007-03-27 10:31:43
Param.info	2007-03-27 10:31:43
Pulprog.info	2007-03-27 10:31:43
README	2007-03-27 10:31:43
Relations.info	2007-03-27 10:31:43
Sysconf.incl	2007-03-27 10:31:43
Update.info	2007-03-27 10:31:43
adeq11etgprdsp	2007-03-27 10:31:43
adeq11etgsp	2007-03-27 10:31:43
adeq1netgp	2007-03-27 10:31:43
adeqn1etgp	2007-03-27 10:31:43
adeqnnetgp	2007-03-27 10:31:43
apt	2007-03-27 10:31:43
aptjc	2007-03-27 10:31:43
aring	2007-03-27 10:31:43

Edit Graphical Edit Set PULPROG Close



# Search results



Found: 21 Data  
Please right-click

Dataset ID	Dataset Name	Date
svcu-ns_test	zg30	2003-10-15 07:56:15
svcu-ns_test 2	zg30	2003-10-15 07:56:50
svcu-ns_test 3	zg30	2003-10-15 07:58:17
svcu-ns_test 4	zg30	2003-10-15 08:16:32
svcu-ns_test 5	zg30	2003-10-15 08:21:21
svcu-test 1 1	zgpg30	1970-01-01 01:00:00
svcu-test2 1	zg30	2003-05-20 08:52:16
svcu-test2 2	zg30	2003-05-20 08:52:40
svcu-test2 3	zg30	2001-04-05 09:33:36
svcu-test2 4	zg30	2001-04-05 09:33:36
svcu 1 1 "C:\	zg30	2001-04-05 09:33:36
svcu 1 777 "	zg30	2001-04-05 09:33:36
svcu 1 888 "	zg30	2001-04-05 09:33:36
svcu 1 999 "C:\NMR data" guest mit leerzeichen	zg30	2001-04-05 09:33:36
		1970-01-01 01:00:00
		2006-04-26 12:22:47
		1970-01-01 01:00:00
		2006-04-26 12:35:54
		2006-04-26 11:51:00
		2004-03-30 16:00:44
		2004-03-30 12:28:01

Buttons: Display, Close

Find results can display date information and can be sorted by date.

Furthermore selected datasets can be defined as dataset group.

# Colours of additional information are configurable



Administration items

Spectrum

Contour plot

Spectrum title

Spectrum cursor

Spectrum parameters

Printer

Fonts / Dialogs / Icons

Window settings

Miscellaneous

Directories

Acquisition status bar

Acquisition

BSMS display

Lock display

Window settings

Open new internal windows "cascaded" rather than "maximized"

Configure cascaded windows  Change

Display data set browser in a separate window (restart required)

Arrange internal windows is only applied to dataset windows

Color of date display (of NAMEs) in data browser  Change

Color of pulseprog display in data browser  Change

Color of title display in data browser  Change

Color of 1D datasets in data browser  Change

Color of 2D datasets in data browser  Change

Color of 3D datasets in data browser  Change

Color of 4D+ datasets in data browser  Change

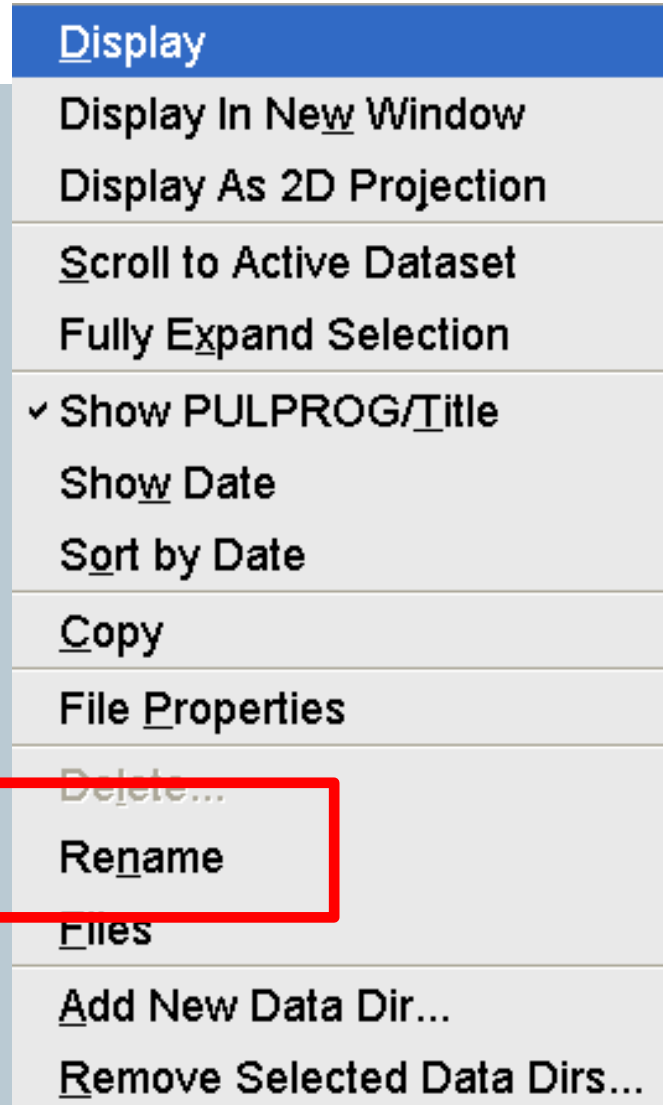
Miscellaneous

Show "ased" parameter selection with "eda"

# TopSpin databrowser offers 'Rename'



TopSpin data browser allows renaming of Names, Expnos or Procnos.



# Drag&Drop from TopSpin databrowser can be turned off



Drag&Drop of datasets into TopSpin main window can now be disabled.

This is useful if this functionality leads to any problems like a graphics hangup.

For details see respective FAQ in the Bruker Knowledge Base, item #7222:

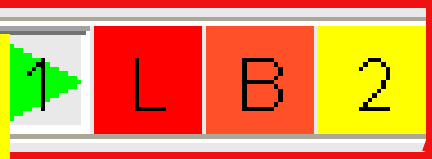
[http://www.bruker-biospin.com/shell/bkb/show\\_bug.cgi?id=7222](http://www.bruker-biospin.com/shell/bkb/show_bug.cgi?id=7222)

# Window numbering



The screenshot shows the Bruker TOPSPIN 2.1.a software interface. The main window displays acquisition parameters for 'es1'. A red box highlights a toolbar icon with a green play button and the number '1', and another red box highlights an inframe icon with a green play button and the number '1'. A yellow box at the bottom left contains the text: 'L = Lock display', 'B = BSMS display', '<number> appears now in toolbar and inframe icon'. The status bar at the bottom shows 'no acquisition running', 'Lock' status, 'Sample' status, 'POWCHK' status, 'Spooler' status, 'BSMS status message' (Δ Z3 -5), and 'Time' (12:23 Jan 03).

L = Lock display  
B = BSMS display  
<number> appears now  
in toolbar and inframe icon



# User-specific icons can now be edited



The screenshot shows the Bruker TopSpin software interface. The title bar reads "Bruker TopSpin on merlin as svcu". The menu bar includes "File", "Edit", "View", "Processing", "Analysis", "Options", "Window", and "Help". The toolbar contains various icons for file operations and processing. A context menu is open over a toolbar button, with the "Edit button properties" option highlighted by a red box. The menu items are:

- Edit button properties
- Add User-Defined Button
- Remove This User-Defined Button...
- Shift left
- Shift right
- Make Button Invisible...
- Make Button Inactive
- Reactivate All Invisible/Inactive Buttons
- Change Icon Size
- Change Toolbar Offset
- Hide Toolbars (type SHIFT ESC to reset)
- Print Associated Command

The background shows a file browser on the left with folders like "F:\Bruker\topspin1.3pl6" and "F:\Bruker\topspin2.2-alpha". The main window displays a spectrum plot titled "exam1d\_13C 1 1 \bruker\topspin guest" with peaks labeled at 169.83, 139.50, and 130.43 ppm. The y-axis is labeled "[rel]" and ranges from 20 to 25. The plot is labeled "Unsigned".

next page

# User-specific icons can now be edited and shifted to another position



The screenshot displays the Bruker TopSpin software interface. The main window shows a spectrum plot with peaks labeled at 169.83, 139.50, and 130.43 ppm. A context menu is open over the toolbar, listing various options for editing user-defined buttons. The 'Shift left' and 'Shift right' options are highlighted with a red box.

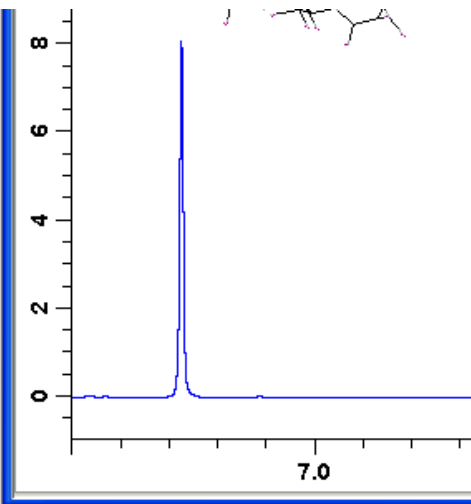
**Edit button properties**

- Add User-Defined Button
- Remove This User-Defined Button...
- Shift left**
- Shift right**
- Make Button Invisible...
- Make Button Inactive
- Reactivate All Invisible/Inactive Buttons
- Change Icon Size
- Change Toolbar Offset
- Hide Toolbars (type SHIFT ESC to reset)
- Print Associated Command

# Thick spectra lines

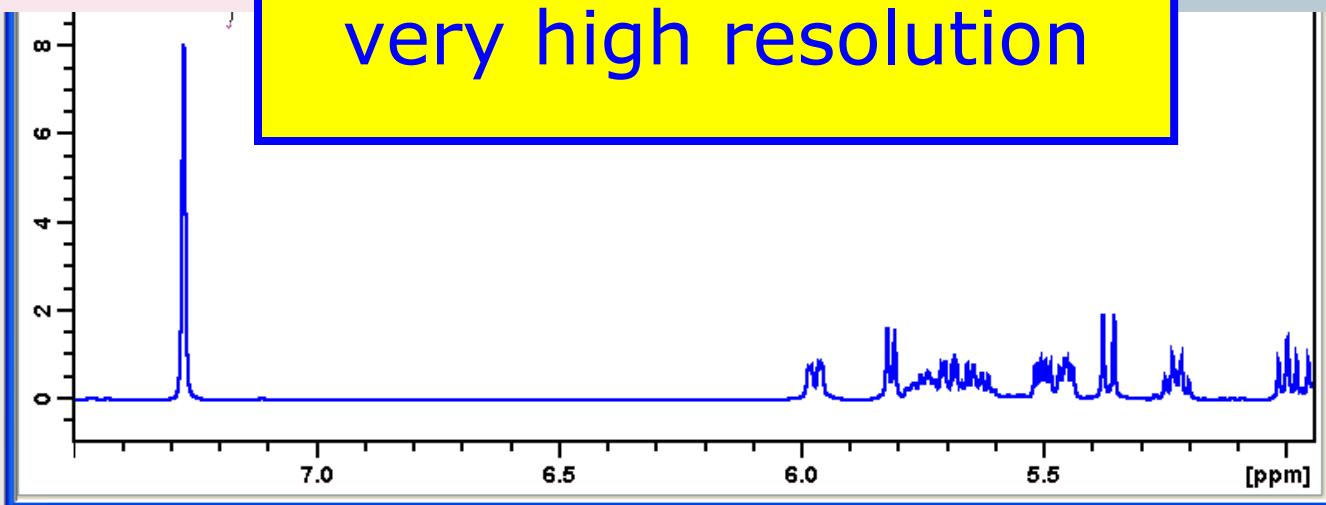


- 6 - zgig30
- exam1d\_1H
- exam2d\_CH
- exam2d\_HC
- exam2d\_HH
- 1 - cosygpqf
- 2 - cosygpmfq
- 3 - mlevph
- 22 - cosygpqf
- exam3d
- exam\_DNMR\_Me
- exam\_DNMR\_ipr
- svcu



Useful for screens with very high resolution

- 6 - zgig30
- exam1d\_1H
- exam2d\_CH
- exam2d\_HC
- exam2d\_HH
- 1 - cosygpqf
- 2 - cosygpmfq
- 3 - mlevph
- 22 - cosygpqf
- exam3d
- exam\_DNMR\_Me
- exam\_DNMR\_ipr
- svcu



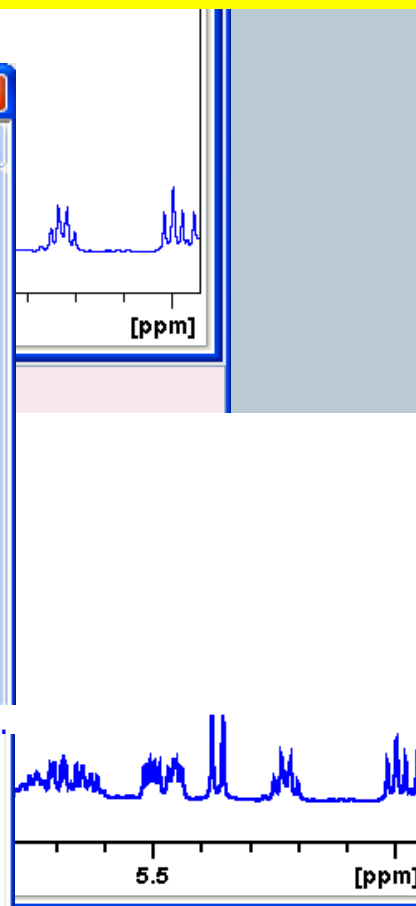
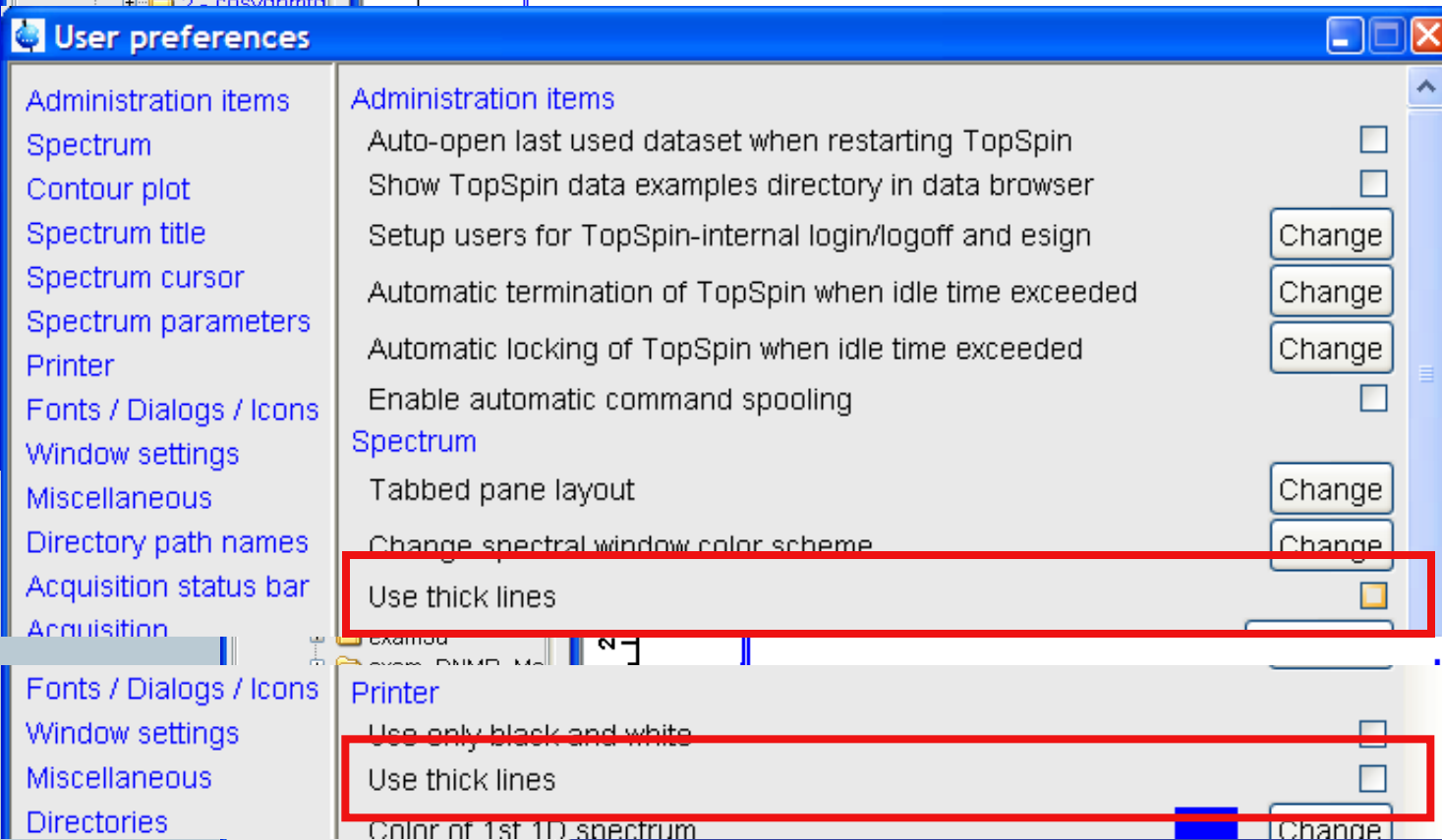
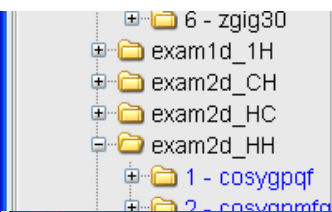
next page



# Thick spectra lines



Configuration is available with:  
**set** or *Options* → *User Preferences*



next page

# Thick spectra lines



Useful for printing or creating PDF via TopSpin

**User preferences**

Administration items

Spectrum

Contour plot

Spectrum title

Spectrum cursor

Spectrum parameters

Printer

Fonts / Dialogs / Icons

Window settings

Miscellaneous

Directory path names

Acquisition status bar

Acquisition

Fonts / Dialogs / Icons

Window settings

Miscellaneous

Directories

Administration items

Auto-open last used dataset when restarting TopSpin

Show TopSpin data examples directory in data browser

Setup users for TopSpin-internal login/logoff and esign

Automatic termination of TopSpin when idle time exceeded

Automatic locking of TopSpin when idle time exceeded

Enable automatic command spooling

**Spectrum**

Tabbed pane layout

Change spectral window color scheme

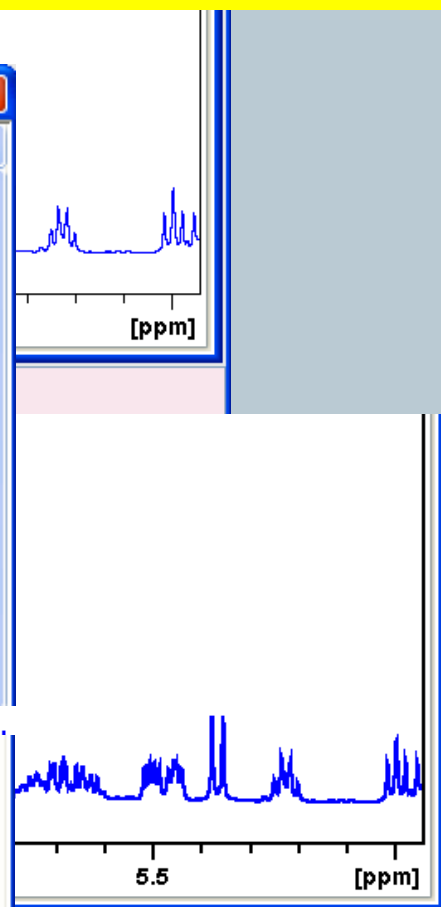
**Use thick lines**

**Printer**

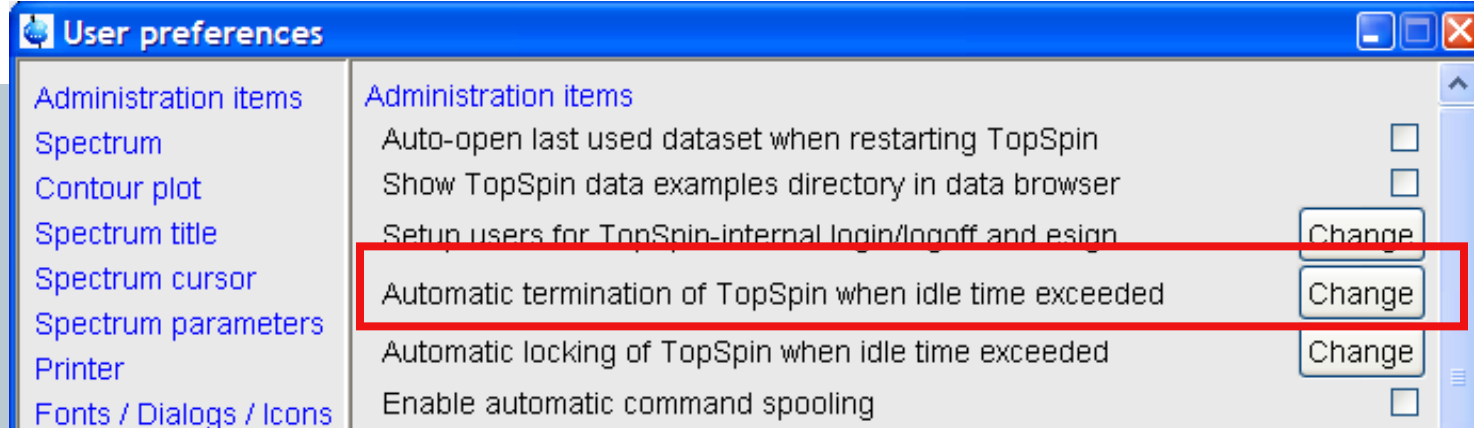
Use only black and white

**Use thick lines**

Color of 1st 1D spectrum



# Thick spectra lines



Idle time for automatic termination of TopSpin can be configured globally for all users.

More details can be found in the Bruker Knowledge Base item

[http://www.bruker-biospin.com/shell/bkb/show\\_bug.cgi?id=7236](http://www.bruker-biospin.com/shell/bkb/show_bug.cgi?id=7236)

The desired font for the tabs can now be configured within *User* → *Preferences*

The height of the tabs corresponds to the height of the icon size, which can also be configured within *User* → *Preferences*

# TopSpin Panorama Tour



A short overview about some special TopSpin topics:

The screenshot displays the Bruker TopSpin software interface. The main window is titled "Bruker TopSpin on merlin as svcu" and features a menu bar with "File", "Edit", "View", "Processing", "Analysis", "Options", "Window", and "Help". Below the menu bar is a toolbar with various icons for file operations and data processing. The "Help" menu is open, showing options such as "Manuals [docs]", "Command Index", "Parameter Index", "Function Keys", "Panorama Tour", "Advanced Search...", "Start NMR Guide", "Version Info", and "License Info".

In the foreground, a window titled "TopSpin, Amix, Auremol Panorama Tour" is open. It contains a list of "Panorama Topics" with descriptions:

Topic	Description
User Interface Concepts	How TopSpin complies with PC standards
Acquisition	Guided & parameter driven, automation, BioTools, spectrometer subsystems, remote control
Display & Processing	Display modes, processing functions, serial processing
Analysis	Integration, deconvolution, relaxation, multiplets, DNMR, solids, shift prediction
Printing & Plotting	Fast data plots, layout creation, plot automation
NmrGuide	Pulse program diagrams, experiment descriptions, representative spectra, literature references
Method Development	Develop Pulse-, AU-, Python programs, shapes, simulate experiments
Documentation	Manuals, command & parameter index
Regulatory Compliance	Audit trails, electronic signatures, 21CFR11
Licensing	Available TopSpin licenses
Service & Support	How Bruker can help you with your problems
AMIX	Drug Discovery, Quality Control, Hyphenation, Metabolomics, Spectra bases
AUREMOL	Automated protein structure determination and related tasks

Below the list is a "Close" button. In the background, a 2D NMR spectrum is visible, showing a diagonal line of peaks and several off-diagonal cross-peaks. The x-axis is labeled "F2 [ppm]" and the y-axis is labeled "F1 [ppm]". A "next page" button is located at the bottom right of the interface.

# TopSpin Panorama Tour



**Basic User Interface Principles**

**Right-click context menus everywhere!**

- User-Defined Menus
- Change Menu Font
- Define Right-Click Action
- Hide Menubar (type SHIFT ESC to reset)
- Reactivate All Invisible/Inactive Buttons
- Add User-Defined Button
- Change Icon Size
- Change Toolbar Offset
- Hide Toolbars (type SHIFT ESC to reset)
- Display Properties...
- Save Display Region To...
- Restore Display Region From Params. F1/2
- Set plot height for current position
- File Properties...
- Files
- Command Line History
- Resize Command Line
- Save As A Macro...
- Acquisition Status Bar On/Off

206

6

# Filename of exported picture available in clipboard

1) file on the disk

and

2) filename into clipboard  
*C:\Documents and Settings\svcu\spectrum-xyz.png*



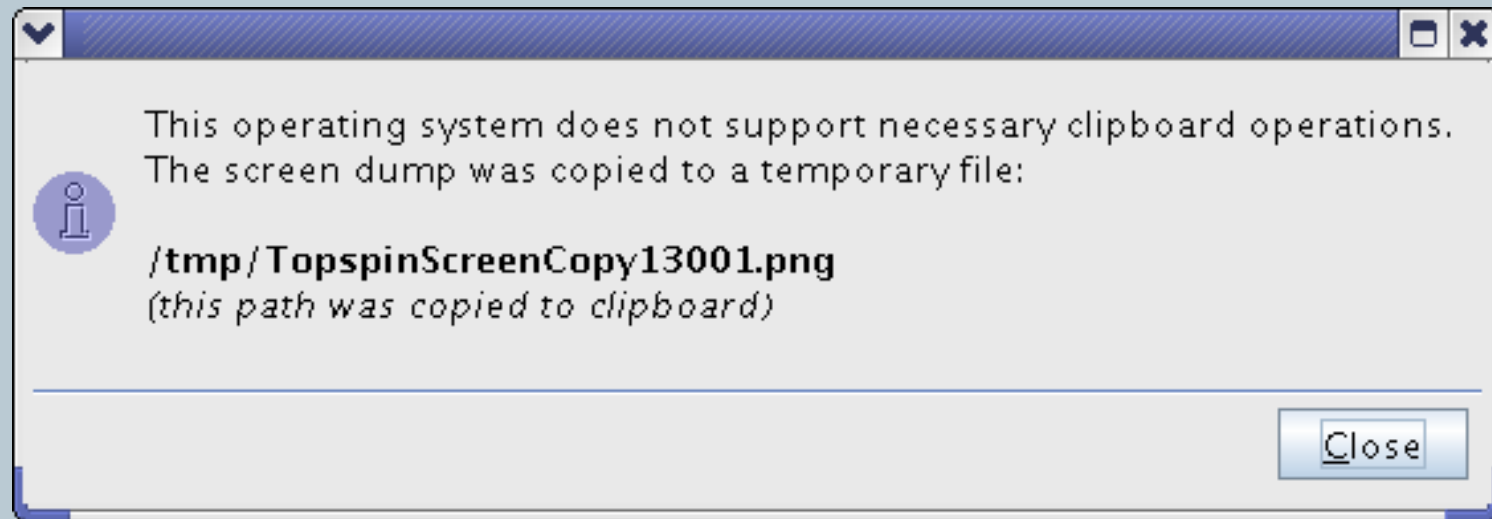
On Windows systems:  
**copy** now stores in bmp format

The new command  
**copy wmf**  
stores wmf format, which was the default  
format in previous TopSpin versions



On Linux **systems**:

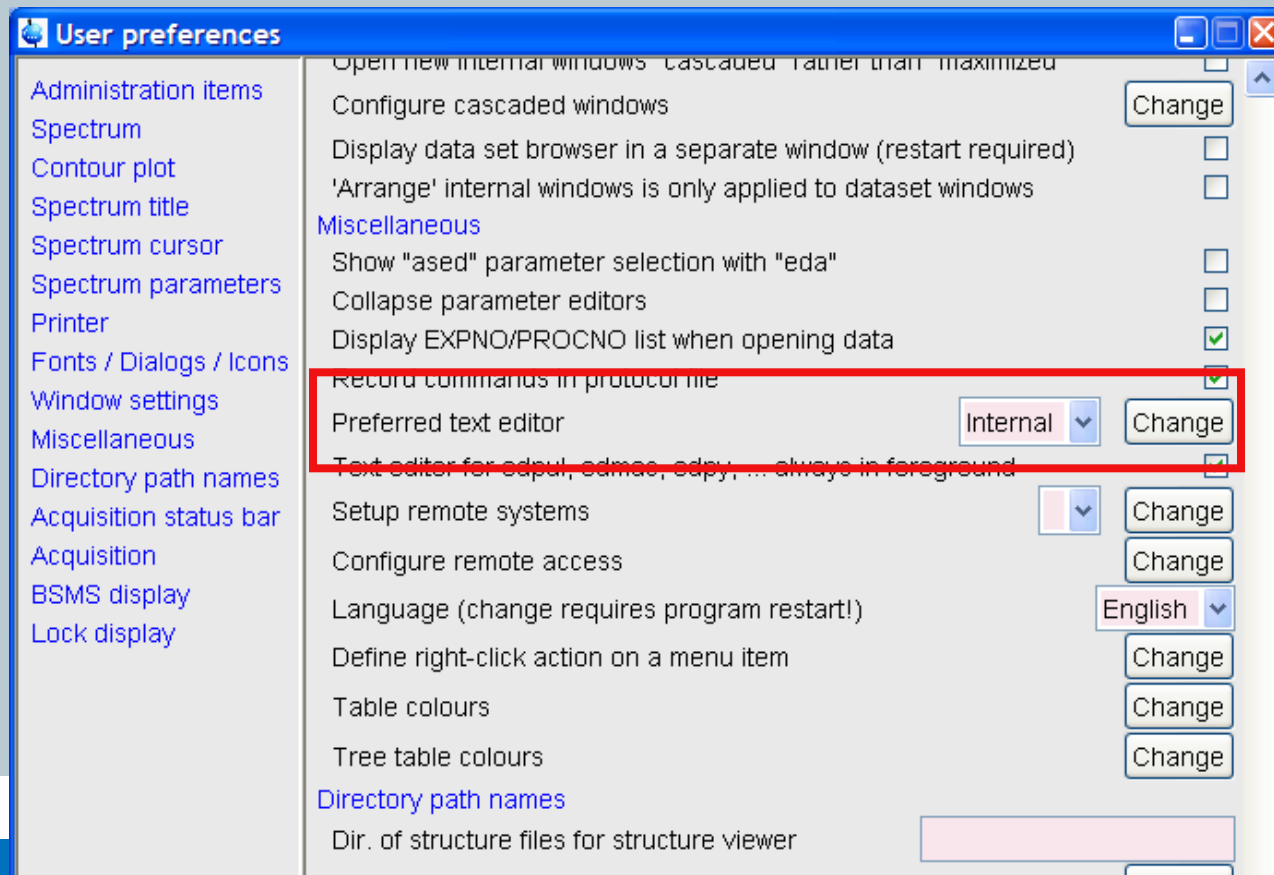
**Copy** stores png format into a temporary file,  
the pathname of this file is copied to clipboard



# External editor



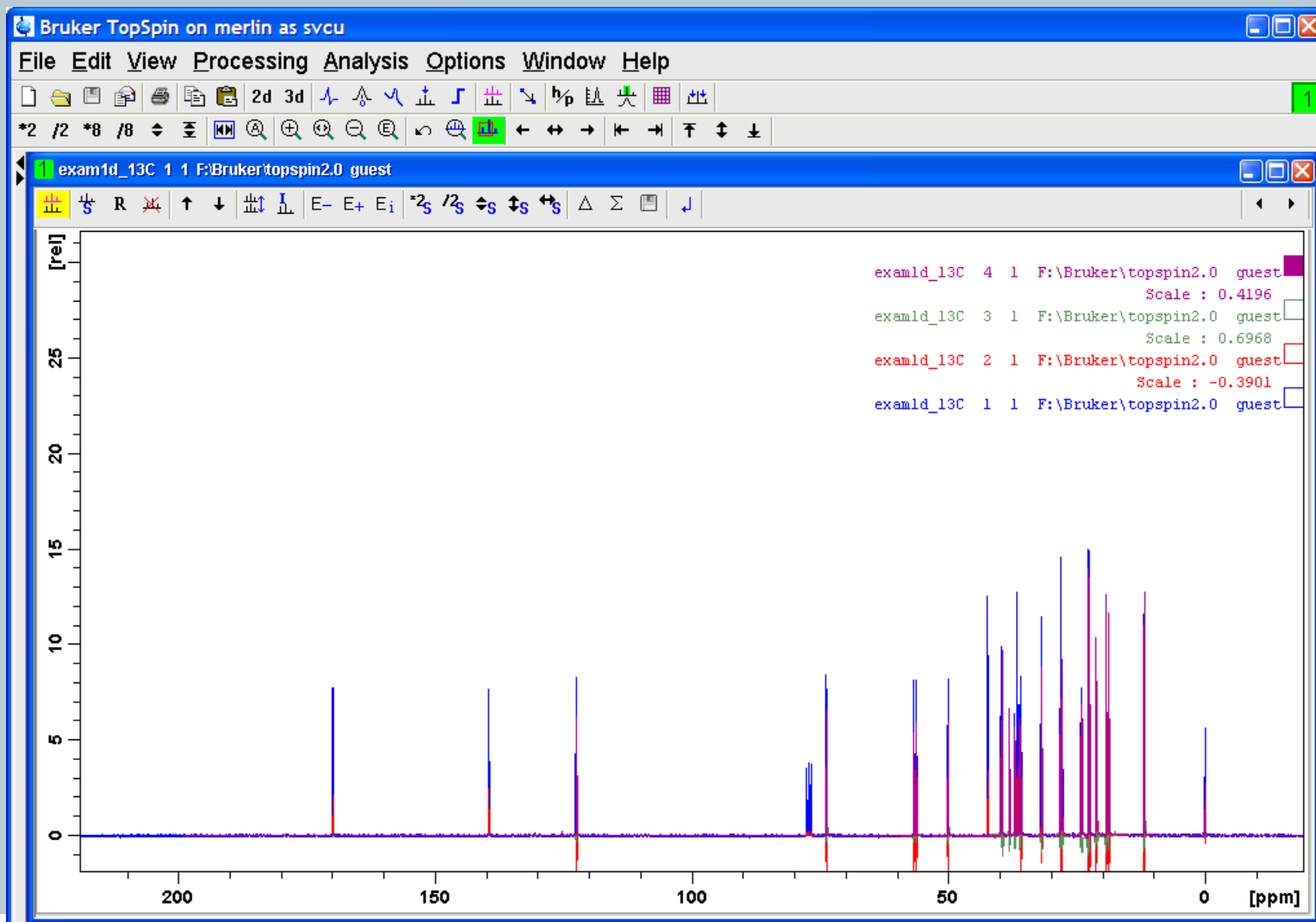
The preferred external editor as defined in Options → Preferences will always be used. For read-only files the internal editor will be taken.



# 1D multiple display



Dataset rectangles visible also with display on-top



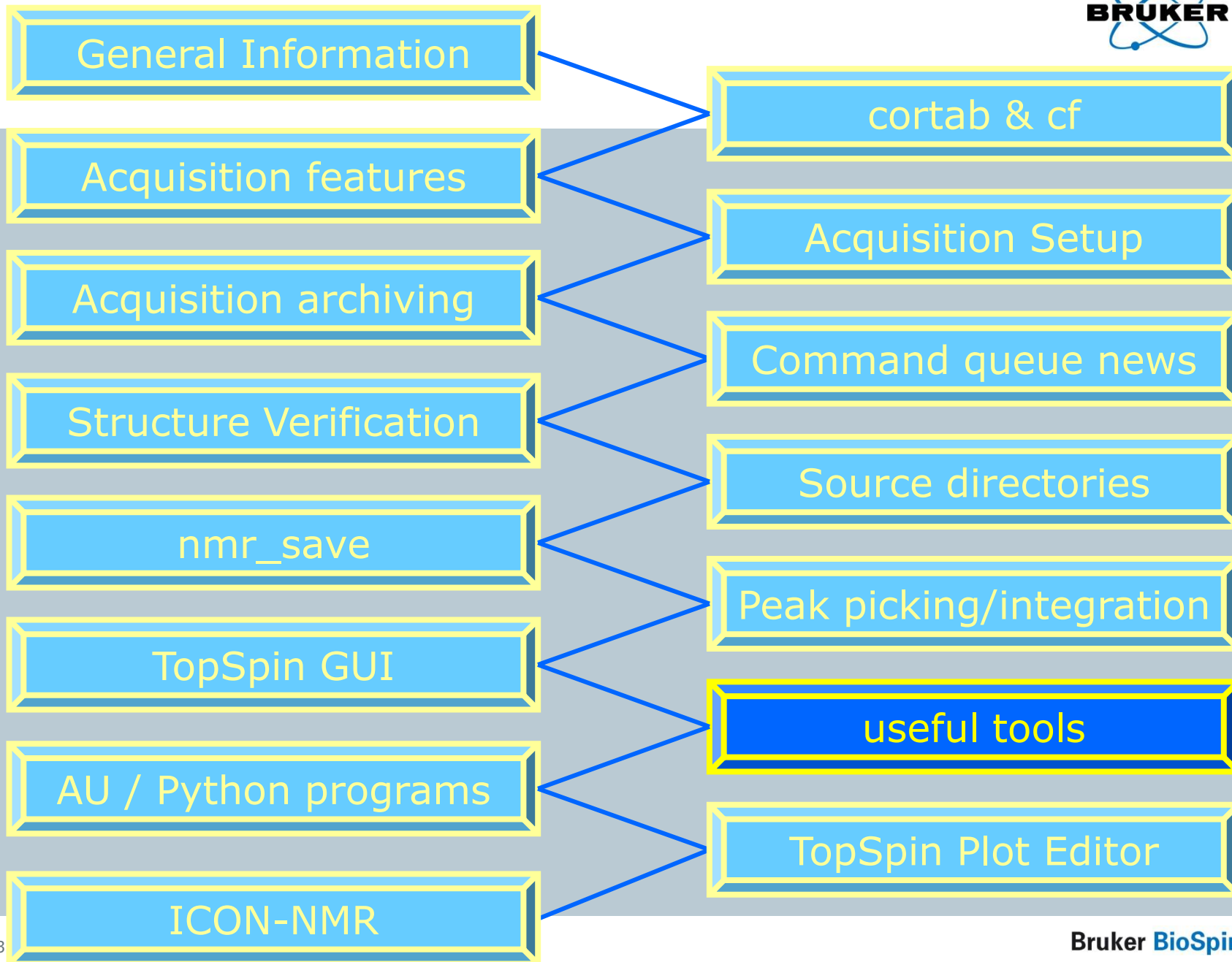
# JMOL comes within a separate window



Executing commands are available on a console

The screenshot displays the Bruker TopSpin software interface. At the top, a window titled "Bruker TopSpin on merlin as svcu" is visible. Below it, a yellow banner contains the text "Executing commands are available on a console". The main interface shows a file browser with "Last50", "Groups", and "Alias" tabs, and a file tree containing "vserver/home" and "C:\NMR data". A window titled "exam1d\_1H 1 1 F:\Bruker\TopSpin guest" contains a menu with "Spectrum", "ProcPars", "AcquPars", "Title", "PulseProg", "Peaks", "Integrals", "Sample", "Structure", and "Fid". A "Jmol" window displays a 3D ball-and-stick model of cyclosporin A, with a menu on the left listing options like "cyclosporina", "model 1/1", "Configurations", "Select (193)", "View", "Style", "Farbe", "Surfaces", "Symmetry", "Vergrößerung", "Spin", "Vibration", "Animation", "Measurement", "Set picking", "Console", "Show", and "Über Jmol". A "Jmol Script Console" window is open in the foreground, showing a prompt "\$" and buttons for "Ausführen", "Stoppen", "Leeren", "History", "State", and "Hilfe". The console window is positioned over a chemical structure diagram of cyclosporin A, which is also visible in the background. The diagram shows the complex ring structure of the molecule with various functional groups like hydroxyl (OH), methyl (CH3), and amide (NH) groups. The Jmol window title bar includes a "Start Jmol" button. At the bottom of the Jmol window, the file name "structure2.mol" is displayed.

# Content



# Serial Processing – revised step-by-step procedure



The screenshot shows the Bruker TopSpin software interface. The main window displays a 1D NMR spectrum with chemical shifts in ppm on the x-axis (ranging from 18 to 8) and intensity on the y-axis (ranging from 0 to 12). A list of chemical shifts is displayed above the spectrum, including 14.51, 11.07, 10.57, 10.43, 10.33, 10.29, 10.20, 9.94, 9.10, 9.09, 9.03, 9.01, 8.91, 8.53, 8.51, 8.50, 8.49, 8.48, 8.41, 8.40, 8.40, 8.39, 8.34, 8.33, 8.31, 8.30, 8.27, 8.26, 8.25, 8.24, 8.22, 8.21, 8.19, 8.18, 8.01, and 7.99. A dialog box titled "Serial Processing - Define Datasets" is open in the foreground, prompting the user to define the full path name of the dataset list to be processed. The dialog box contains the following instructions:

- Click on:
- > Browse For List = locate an existing dataset list
- > Find Datasets = search for datasets and use the selected ones as the list
- > Edit List = edit the current or a new dataset list
- > Next = continue with command definition

The dialog box also features a text input field and five buttons: "Browse For List", "Find Datasets", "Edit List", "Next >", and "Cancel".

# Serial Processing

**Serial Processing - Define Datasets**

Please define the full path name of the dataset list to be processed.  
Click on:

- > Browse For List = locate an existing dataset list
- > Find Datasets = search for datasets and use the selected ones as the list
- > Edit List = edit the current or a new dataset list
- > Next = continue with command definition

**Browse For List** Find Datasets Edit List Next > Cancel

**OK**

Look in: svcu

- My Recent Documents
- Desktop
- My Documents
- My Computer
- My Network Places

- .jmol
- .topspin-merlin
- .ts-bak
- Application Data
- AU\_SESSION
- Bluetooth Software
- Cookies
- Desktop
- Favorites
- Local Settings
- My Documents
- NetHood
- NMRSIM\_SESSION
- Nokia
- Phone Browser
- PrintHood
- My Recent Documents
- SendTo
- Start Menu
- Templates
- topspin-bak
- UserData
- WINDOWS
- 1d-peaks-xwin.txt
- 2d-integral-test\_exam2d\_HH\_1.txt
- expt-list.txt
- list-date.txt
- list1.txt
- list2.txt
- list33.txt
- LuResult.txt

File name:

Files of type: Text file \*.txt

**next page** OK Cancel

# Serial Processing



**Serial Processing - Define Datasets**

Please define the full path name of the data  
Click on:

- > Browse For List = locate an existing data
- > Find Datasets = search for datasets and
- > Edit List = edit the current or a new data
- > Next = continue with command definition

**Find data**

Searching will be performed in all data directories  
marked in the data directories list below!  
The checkboxes at the right will enforce exact matching if enabled.

NAME	13	<input type="checkbox"/>
EXPNO		<input checked="" type="checkbox"/>
PROCNO		<input checked="" type="checkbox"/>
USER		<input checked="" type="checkbox"/>
Title		
Pulse Prog.		
Dimension		
Data type		
Date, from: mm/dd/yy		
Date, till: mm/dd/yy		

**Data directories**

- C:\NMR data
- F:\Bruker\TopSpin
- F:\Bruker\topspin1.3pl6
- F:\Bruker\topspin1.3pl8

**Search result**

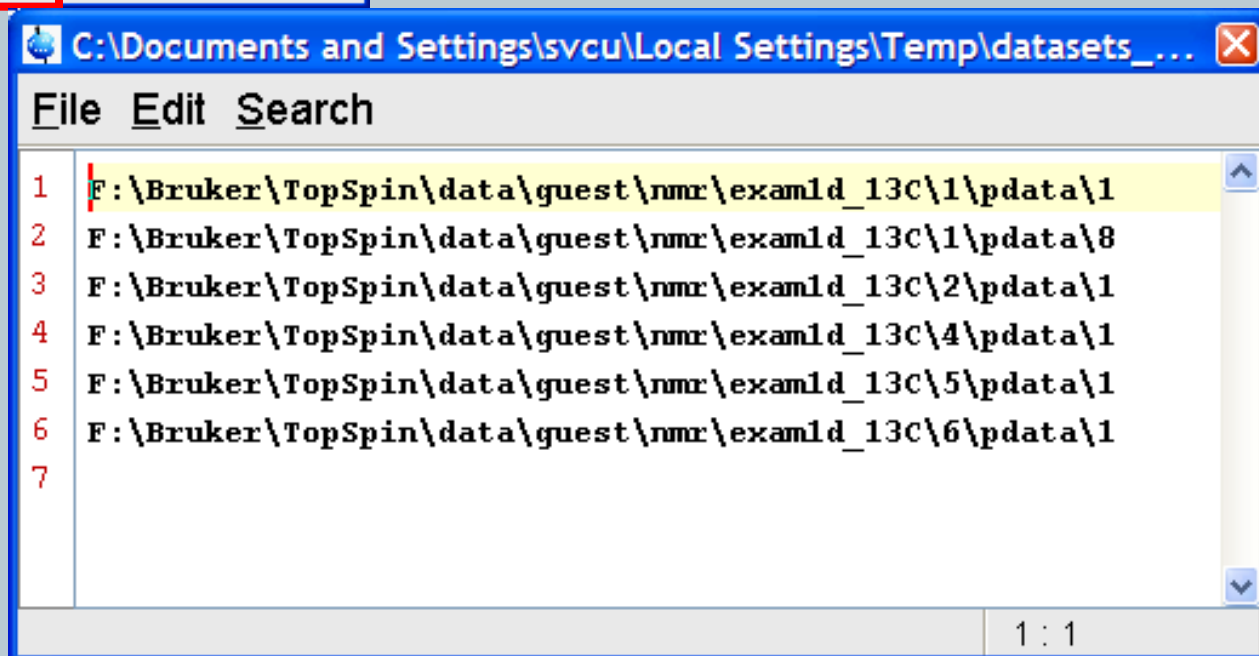
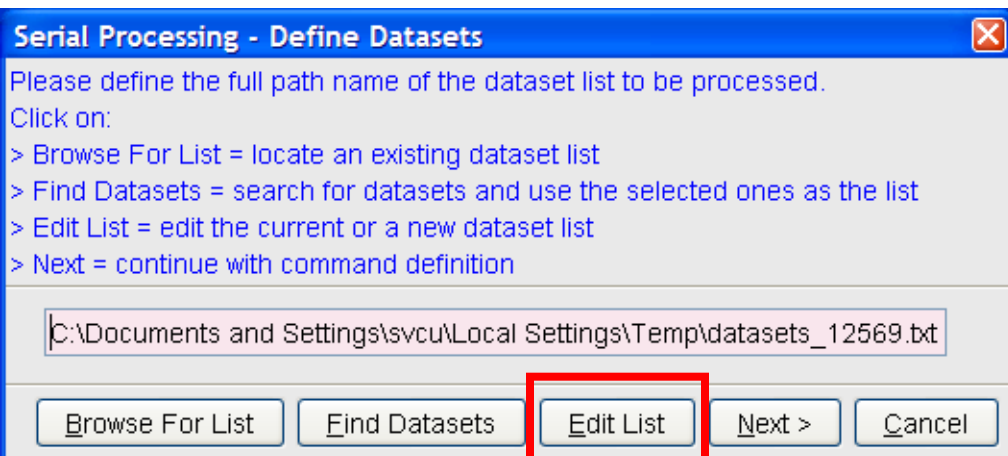
Found: 9 Data Sets.  
Please right-click in a list for more options!

exam1d_13C	1	1	F:\Bruker\TopSpin	guest	1	zgpg30	2004-03-30 11:43:33
exam1d_13C	1	2	F:\Bruker\TopSpin	guest	1	zgpg30	2004-03-30 11:43:33
exam1d_13C	1	8	F:\Bruker\TopSpin	guest	1	zgpg30	2004-03-30 11:43:33
exam1d_13C	11	1	F:\Bruker\TopSpin	guest	1	zgpg30	2004-03-30 11:43:33
exam1d_13C	2	1	F:\Bruker\TopSpin	guest	1	jmod	2004-03-30 12:01:05
exam1d_13C	3	1	F:\Bruker\TopSpin	guest	1	dept135	2004-03-30 12:18:36
exam1d_13C	4	1	F:\Bruker\TopSpin	guest	1	dept45	2004-03-30 12:53:06
exam1d_13C	5	1	F:\Bruker\TopSpin	guest	1	dept90	2004-03-30 13:27:39
exam1d_13C	6	1	F:\Bruker\TopSpin	guest	1	zgif30	2004-03-30 14:35:54





# Serial Processing



# Serial Processing

**Serial Processing - Define Command**

Please define the command to be executed on the datasets.  
Examples:

- (a full path indicates a macro)
- full path with '.py' indicates a Python script)
- locate a TopSpin macro
- locate a TopSpin Python program
- using the dataset list
- definition
- while processing

Show    Browse For Macro    Browse For Python    Execute    < Back    Cancel

**Serial Processing - Define Datasets**

Please define the full path name of the dataset list to be processed.  
Click on:

- > Browse For List = locate an existing dataset list
- > Find Datasets = search for datasets and use the selected ones as the list
- > Edit List = edit the current or a new dataset list
- > Next = continue with command definition

C:\Documents and Settings\svcu\Local Settings\Temp\datasets\_12569.txt

# Serial Processing

### Serial Processing - Define Command

Please define the command to be executed on the datasets.  
Examples:  
1) efp  
2) lb 0.8;em;ft;pk  
3) c:\mymacros\mac-efp (a full path indicates a macro)  
4) c:\mypys\py-efp.py (a full path with '.py' indicates a Python script)

Click on:  
> Browse For Macro = locate a TopSpin macro  
> Browse For Python = locate a TopSpin Python program  
> Execute = start processing the dataset list  
> Back = return to list definition  
> Show = show datasets while processing

Show

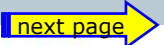
### Macros

File Options Help

Source = F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\lists\mac\user

Search in names [??] Search

exam_efapk	exam_efp	exam_lb_si_efp	exam_lbefp	exam_lbefp2
------------	----------	----------------	------------	-------------

next page 

# Serial Processing

### Serial Processing - Define Command

Please define the command to be executed on the datasets.  
Examples:

- 1) efp
- 2) lb 0.8;em;ft;pk
- 3) c:\mymacros\mac-efp (a full path indicates a macro)
- 4) c:\mypys\py-efp.py (a full path with '.py' indicates a Python script)

Click on:

- > Browse For Macro = locate a TopSpin macro
- > Browse For Python = locate a TopSpin Python program
- > Execute = start processing the dataset list
- > Back = return to list definition
- > Show = show datasets while processing

Show    Browse For Macro    **Browse For Python**    Execute    < Back    Cancel

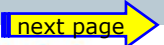
### Python Programs

File Options Help    Source = F:\Bruker\TOPSPIN2.1-alpha\exp\stan\nmr\py

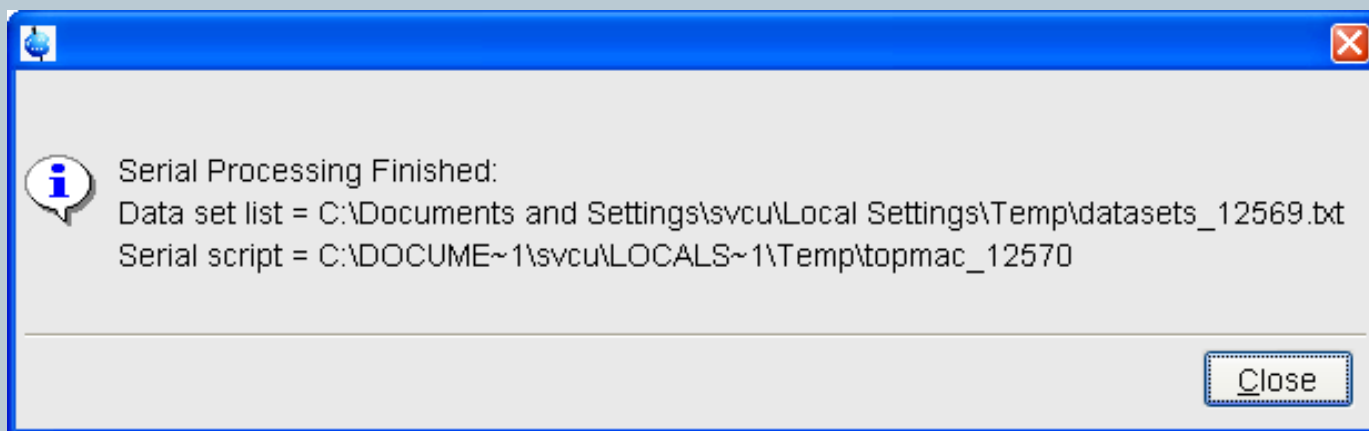
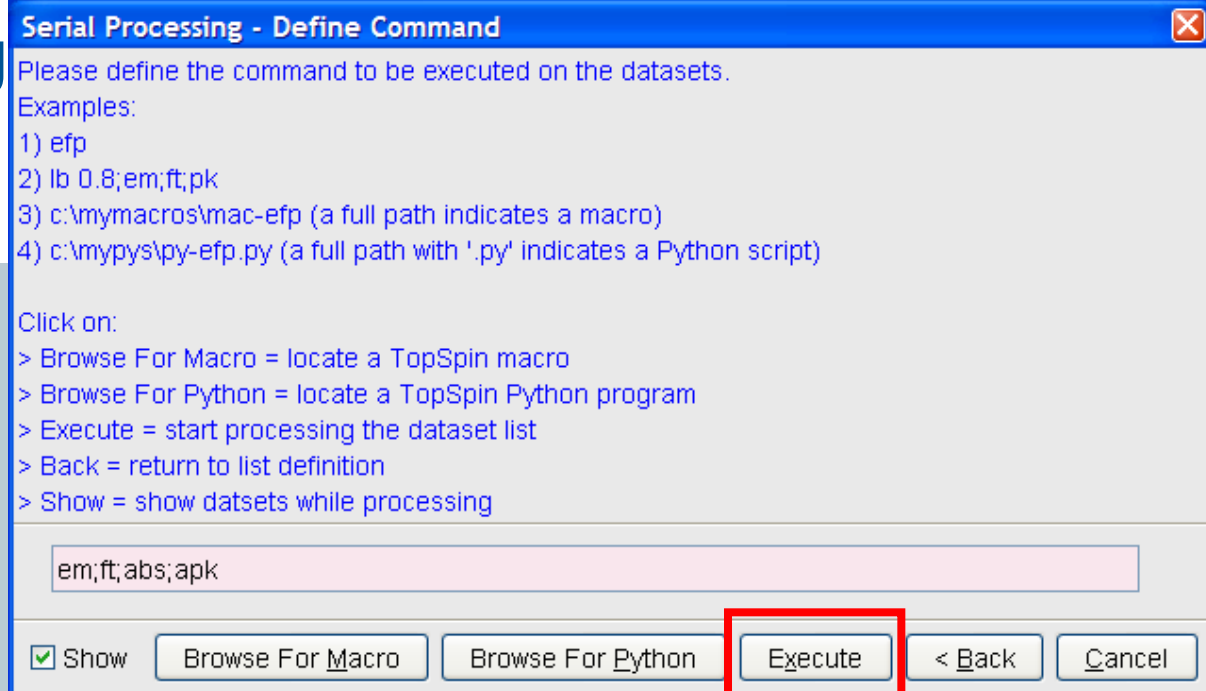
Search in names [??]    Search

Cursor2d.py	exam-em-ft-apk.py	exam-multi-efp.py	exam-pulsprog.py	exam-splitser.py
exam-sum-real.py	inadph.py	inadph2.py	ineptrdsp.py	py-test-suite.py
ser_ef_apk.py	ser_efp.py	t1ir.py		

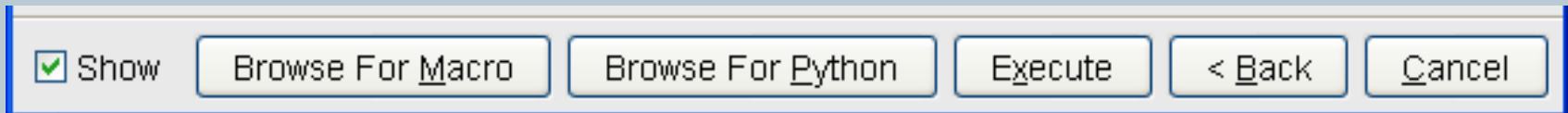
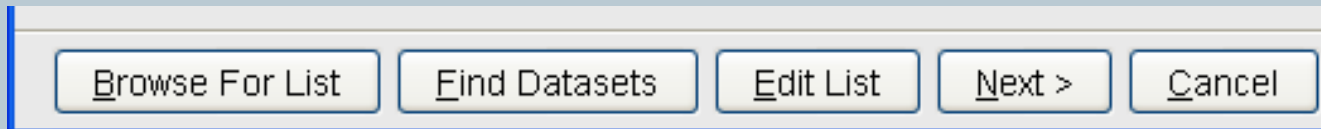
OK    Cancel

next page 

# Serial Processing



# Serial Processing

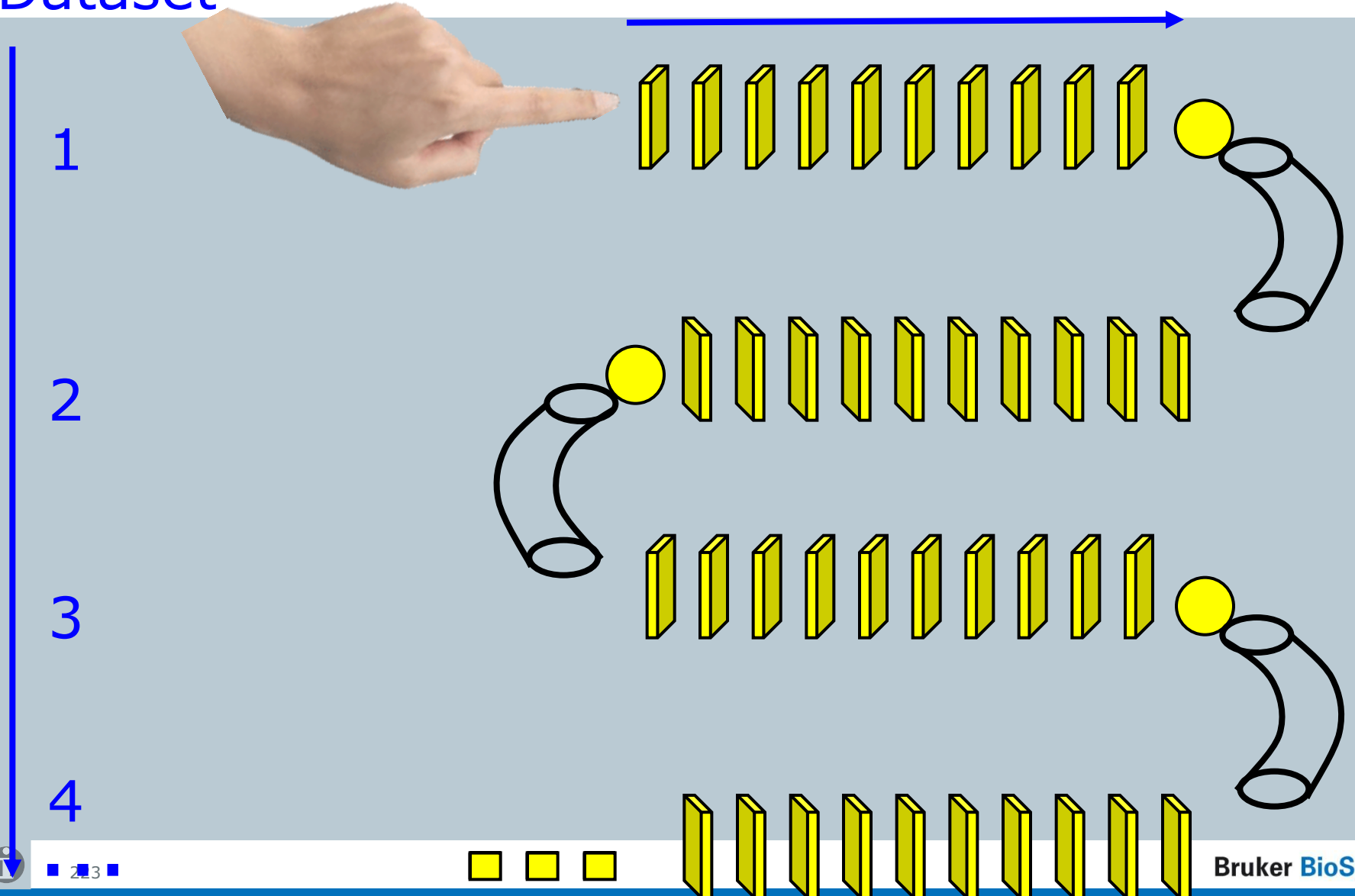


# Serial Processing



Dataset

commands



# Group members meet serial processing



The screenshot shows the Bruker TopSpin software interface. On the left is a file browser with a tree structure containing folders like 'helloworld' and 'test1', and files such as 'exam1d\_13C 1 1 - zgpg30 - 13C(1)'. A context menu is open over the file browser, listing actions like 'Display', 'Display In New Window', 'Display Group', 'Add Selected Data Window', 'Update Window Bounds & Display Limits', 'Remove Selected Datasets From Group...', 'Collapse All Groups', 'Toggle Dim/Pulprog/Title', 'Add new Dataset Group...', 'Close All Group Windows', 'Process Selected Datasets...', 'File Properties', 'Files', and 'Copy'. The 'Process Selected Datasets...' option is highlighted. The main area displays several spectral plots. The top plot is a 2D spectrum with axes 'F1 [ppm]' and 'F2 [ppm]'. Below it are three 1D spectra, each with its own 'Spectrum' tab and 'ProcParams' tab. The bottom-most spectrum has a y-axis labeled '10 30 [rel]' and an x-axis labeled '200 150 100 50 [ppm]'. The interface includes a menu bar (File, Edit, View, Spectrometer, Processing, Analysis, Options, Window, Help) and a toolbar with various icons for file operations and data processing.





# Group members meets **serial processing**



TopSpin adds all selected datasets into a temporary dataset list file.

The screenshot displays the Bruker TopSpin software interface. A dialog box titled "Serial Processing - Define Datasets" is open, prompting the user to define the full path name of the dataset list to be processed. The dialog includes instructions and a list of options: "> Browse For List = locate an existing dataset list", "> Find Datasets = search for datasets and use the selected ones as the dataset list", "> Edit List = edit the current or a new dataset list", and "> Next = continue with command definition". A text field contains the path "C:\DOCUME~1\svcu\LOCALS~1\Temp\datasets\_49199.txt". Below the text field are buttons for "Browse For List", "Find Datasets", "Edit List", "Next >", and "Cancel".

A context menu is open over the "Find Datasets" button, listing the following options: "Update window bounds & Display Limits", "Remove Selected Datasets From Group...", "Collapse All Groups", "Toggle Dim/Pulprog/Title", "Add new Dataset Group...", "Close All Group Windows", "Process Selected Datasets..." (highlighted), "File Properties", "Files", and "Copy".

In the background, several NMR spectra are visible. One window shows a 2D spectrum with axes labeled "F1 [ppm]" and "F2 [ppm]". Another window shows a 1D spectrum with the x-axis labeled "150 100 50 0 [ppm]" and the y-axis labeled "5 [rel]". A third window shows a 1D spectrum with the x-axis labeled "200 150 100 50 [ppm]" and the y-axis labeled "10 30 [rel]".

The **nmrq** command is required to perform reliable quantitative analysis of 1D spectra comprising complex overlapping spectra. The program is able to:

- Perform mole ratio calculations given integral heights and number of protons per signal.
- Perform absolute weight calculations given the information detailed in plus molecular weights of all components and the weight of a reference component.
- Permit analysis of spectra characterised by poor baseline.

- **expl spect**  
opens explorer window in:  
*TOPHOME/conf/instr/<currently configure instrument>*
- **expl prop**  
opens explorer window in:  
*USERHOME/.topspin-<NAME\_OF\_PC>/prop*
- **expl help**  
shows all available options (top, home ...)

# **rpar** behaviour has been improved



The command **rpar** will not delete existing data if there is no change of the dimension.  
This allows e.g. reading in processing parameters for special processing purposes on existing data.

# Script 'savelogs' goes online



The savelogs script has been improved.

If you are asked by Bruker to send debug information you can easily give the results file the dispatch number, the script will place it automatically on the Bruker FTP server.

A screenshot of a Windows command prompt window titled "C:\WINDOWS\system32\cmd.exe". The window has a black background with white text. The text reads: "Welcome to Bruker Software Support!", "This tool will collect support information about your TOPSPIN installation and send it to Bruker. Use this tool only if you have been instructed to do so.", "Press CTRL+C otherwise to quit now.", and "Please enter your support token here: debug-info-xyz". The last line is highlighted with a red rectangular box. The window also shows standard Windows window controls (minimize, maximize, close) in the top right corner and a scrollbar on the right side.

[next page](#)

savelogs can be started under Windows from **Bruker Utilities** → **Miscellaneous** or under Linux just by typing the command in a shell

# Script 'savelogs' goes online



The savelogs script has been improved.

If you are asked by Bruker to send debug information you can easily give the results file the dispatch number, the script will place it automatically on the Bruker FTP server.

A screenshot of a Windows command prompt window. The title bar reads "C:\WINDOWS\system32\cmd.exe". The command prompt shows the execution of the savelogs script, which has archived support information for a TOPSPIN session. The output text is as follows:

```
prog/curdir/BRUKER-svcu/stdout.cprserver.log
prog/curdir/BRUKER-svcu/stdout.dataserver.6100

-----
Files containing support information about your last TOPSPIN session
have been archived in the file

      "C:\DOCUME~1\svcu\LOCALS~1\Temp\TopspinSupportFiles_debug-info-xyz_MERLIN_sv

After the next key press your computer is going to upload this file to
Bruker ftp server for further reference.

If you do not like this automatic upload press Ctrl+C now!

-----
Press any key to continue . . .
```

A red rectangular box highlights the text: "After the next key press your computer is going to upload this file to Bruker ftp server for further reference. If you do not like this automatic upload press Ctrl+C now!".

next page

# Script 'savelogs' goes online



The savelogs script has been improved.

If you are asked by Bruker to send debug information you can easily give the results file the dispatch number, the script will place it automatically on the Bruker FTP server.

A screenshot of a Windows command prompt window titled "C:\WINDOWS\system32\cmd.exe". The window contains the following text:

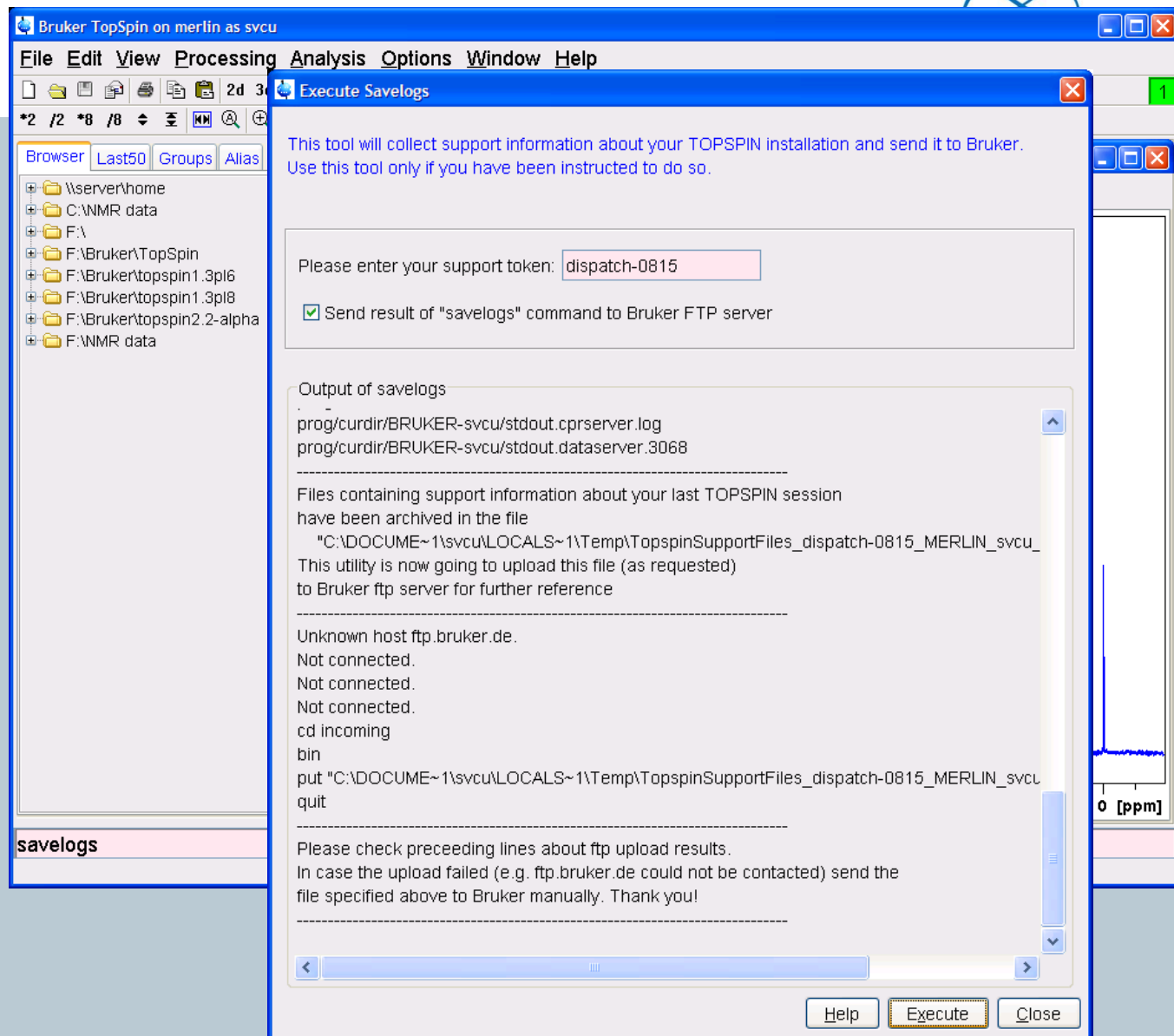
```
-----  
Press any key to continue . . .  
Unknown host ftp.bruker.de.  
ftp> cd incoming  
Not connected.  
ftp> bin  
Not connected.  
ftp> put "C:\DOCUME~1\svcu\LOCALS~1\Temp\TopspinSupportFiles_debug-info-xyz_MERL  
Not connected.  
ftp> quit  
-----  
Please check preceding lines about ftp upload results.  
In case the upload failed (e.g. ftp.bruker.de could not be contacted) send the  
file specified above to Bruker manually. Thank you!  
-----  
Press any key to continue . . .
```

The text "Press any key to continue . . ." at the bottom is highlighted with a red rectangular box.

next page

# savelogs can be started from within TopSpin

TopSpin offers the new command **savelogs** which internally calls the script **savelogs**



Execute Savelogs

This tool will collect support information about your TOPSPIN installation and send it to Bruker. Use this tool only if you have been instructed to do so.

Please enter your support token:

Send result of "savelogs" command to Bruker FTP server

Output of savelogs

```
prog/curdir/BRUKER-svcu/stdout.cprserver.log
prog/curdir/BRUKER-svcu/stdout.dataserver.3068
-----
Files containing support information about your last TOPSPIN session
have been archived in the file
"C:\DOCUME~1\svc\LOCALS~1\Temp\TopspinSupportFiles_dispatch-0815_MERLIN_svcu_
This utility is now going to upload this file (as requested)
to Bruker ftp server for further reference
-----
Unknown host ftp.bruker.de.
Not connected.
Not connected.
Not connected.
cd incoming
bin
put "C:\DOCUME~1\svc\LOCALS~1\Temp\TopspinSupportFiles_dispatch-0815_MERLIN_svcu_
quit
-----
Please check preceeding lines about ftp upload results.
In case the upload failed (e.g. ftp.bruker.de could not be contacted) send the
file specified above to Bruker manually. Thank you!
-----
```


Buttons: Help, Execute, Close





TopSpin includes the AutoLink backbone assignment algorithm.

This software analyses the peak information available on a given set of protein spectra and calculates a backbone assignment.


next page 

Syntax: **autolink** or

*Analysis* → *Proteins* → *Automatic Backbone Assignment*

The Help button in the AutoLink window opens a manual which guides you step-by-step through the setup of an Automatic Backbone Assignment. The molecule Ribonuclease-T1 is used as an example in this manual.

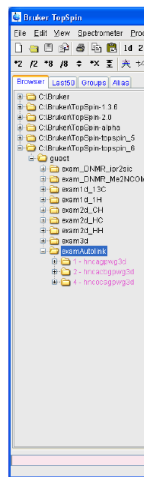
The respective datasets are available with the example datasets of TopSpin 2.1.

next page 

## Step 2: Process data

## Step 6: Review results

The assignment view is organised in a tree, where the outer level contains the residue sequence. Expanding any residue displays the corresponding calculated assignments.



## Step 6: Review results

Once the software has create peak annotations based on the calculated assignments, the results may immediately be reviewed on the Peaks tabulator in the respective dataset windows. The generated information includes the assignment of each frequency component for a given peak.

Residue tree view:

Residue	Residue name
+ SER-96	Serine
+ GLY-97	Glycine
+ ASN-98	Asparagine
+ ASN-99	Asparagine
+ PHE-100	Phenylalanine
+ VAL-101	Valine
C	
CA	
CB	
CG1	
CG2	
H	
HA	
HB	
HG1	
HG2	
N	
O	
+ GLU-102	Glutamate
+ CYS-103	Cysteine
+ THR-104	Threonine

Fig. 2: Process e

Fig. 10: The ass displays the calci

F3 [ppm]	F2 [ppm]	F1 [ppm]	Assignment
9.4560	112.4480	57.0300	H(THR-91)(NTHR-91) CA(LE-80)
9.4580	112.4480	58.7780	H(THR-91)(NTHR-91) CA(THR-81)
9.9260	112.9220	55.1290	H(NAL-101)(NVAL-101) CA(PHE-100)
9.9350	113.9220	57.7580	H(NAL-101)(NVAL-101) CA(AL-101)
9.1300	123.8210	53.5270	H(THR-92)(NTHR-92) CA(HS-100)
9.1580	123.8210	62.4530	H(THR-92)(NTHR-92) CA(THR-81)
9.3110	124.1160	53.5950	H(HS-92)(NHS-92) CA(HS-92)
9.3110	124.1160	58.8650	H(HS-92)(NHS-92) CA(THR-91)
9.1150	133.7200	49.2120	H(ALA-87)(NALA-87) CA(AL-87)
9.1150	133.7200	62.9890	H(ALA-87)(NALA-87) CA(LE-80)
9.0320	114.4520	53.7230	H(PHE-100)(NPE-100) CA(ASN-89)
8.9320	114.4520	55.2410	H(PHE-100)(NPE-100) CA(PHE-100)
8.0500	114.7480	62.4440	H(NLY-94)(NLY-94) CA(THR-81)
8.0500	114.7480	62.3140	H(NLY-94)(NLY-94) CA(LY-94)
8.0770	114.7480	65.8690	H(NLY-94)(NLY-94) CA(AL-101)
8.0000	123.7550	57.6330	H(NLA-102)(NLA-102) CA(AL-101)
8.7800	118.1810	48.8830	H(LEU-90)(NLEU-90) CA(AL-90)
8.7800	118.1810	57.9510	H(LEU-90)(NLEU-90) CA(L-90)
8.0770	122.4750	49.5840	H(ASN-98)(NASN-98) CA(ASN-98)
8.0770	122.4750	44.9110	H(ASN-98)(NASN-98) CA(NLY-97)
8.9800	121.3770	55.7030	H(CYS-103)(NLYS-103) CA(CYS-103)
8.9800	121.3770	61.8750	H(CYS-103)(NLYS-103) CA(ALU-102)
8.9320	118.4520	53.8690	H(PHE-100)(NPE-100) CA(LY-97)
8.9320	118.4520	54.7020	H(PHE-100)(NPE-100) CA(THR-81)
8.4500	124.3140	51.1030	H(LEU-90)(NLEU-90) CA(ALN-55)
8.4500	124.3140	52.8190	H(LEU-90)(NLEU-90) CA(LE-80)

Fig. 12: The annotated peak lists of Ribonuclease-T1. The annotations are generated based on the assignments calculated by AutoLink.

# New command - **auremol**




Syntax: **auremol** or

*Analysis* → *Proteins* → *Auremol*

The Protein Structure Elucidation Tool AUREMOL can now be started easily from within TopSpin.

Auremol requires a separate license, but each new Full und Processing\_only TopSpin license offers automatically a 6-months demo license for Auremol. A separate demo license can be ordered anytime under: [www.bruker-biospin.com](http://www.bruker-biospin.com)

next page 



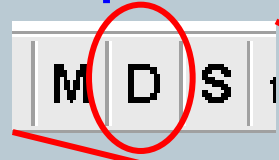
AUREMOL master list files can now be easily imported or exported from within the TopSpin peak list.

# DOSY parameter



DOSY parameters are accessible after **eddosy**

from the processing parameter tab, click on: D



Reference

	F2	F1	Frequency axis
SI	1024	1024	Size of real spectrum
SF [MHz]	500.1300000	500.1300000	Spectrometer frequency
OFFSET [ppm]	12.67713	12.67713	Low field limit of spectrum
SR [Hz]	0.00	0.00	Spectrum reference frequency
HZpPT [Hz]	6.510417	6.510417	Spectral resolution

Window function

WDW	SINE	SINE	Window functions for trf, xfb,...
LB [Hz]	1.00	0.30	Line broadening for em
GB	0	0.1	Gaussian max. position for gm, 0<GB<1
SSB	0	0	Sine bell shift SSB (0,1,2,...)
TM1	0	0.1	Left limit for tm 0<TM1<1
TM2	0	0.9	Right limit for tm 0<TM2<1

Phase correction

PHC0 [degree]	0.000	0.000	0th order correction for pk
PHC1 [degree]	0.000	0.000	1st order correction for pk
PH_mod	no	mc	Phasing modes for trf, xfb, ...

Baseline correction

ABSG	5	5	Degree of polynomial for abs (0..5)
ABSF1 [ppm]	1000.00000	1000.00000	Left limit for absf

next page

Acquisition information: no acquisition running

Fid Flash: [grid]

Lock: [grid]

Sample: [grid]

POWCHK: [X]

Spooler: running: 0, queued: 0, delayed: 0

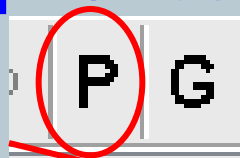
BSMS status message: **Δ Z3 5**

Time: 10:59 Mar 26

# DOSY parameter



To jump back from the DOSY parameter list to the processing parameters click: P



File Edit View Spectrometer Processing Analysis Options Window Help

\*2 /2 \*8 /8

exam2d\_HH 1 1 C:\Bruker\alpha guest

Spectrum ProcParams AcquiParams Title PulseProg Peaks Integrals Sample Structure Fid Acqui

P G

General

▼ General

Method	exponential	Processing method
ExpVar	Gradient	Variable parameter
Xlist	difflist	Variable parameter values file name
Nstart	0	Start of input points
Ndata	256	Number of input points (TD)
Maxiter	100	Maximum number of iterations
EPS	1	Tolerance
Nexpt	1	Number of components to fit
Noise	5565.00	Noise level (S_DEV)
PC	4	Noise sensitivity factor
SpiSup	1	Spike suppression factor
F1mode	Peaks	F1 output data mode
Imode	Integral	Fitted intensity meaning
Scale	Linear	Scaling
LWF	1	Line width factor
DISPmin	1e-010	Lower display limit
DISPmax	1e-008	Upper display limit
Npars	7	Number of parameters
Nvar	2	Number of parameters to fit
Gamma [Hz/G]	4257.64000	Gamma
Grad [G/cm]	0.00000	Diffusion gradient
Gradient [G/cm]	0.00000	Gradient distance, big delta

Acquisition information: no acquisition running

Fid Flash: [grid]

Lock: [grid]

Sample: [grid]

POWCHK: [X]

Spooler: running: 0, queued: 0, delayed: 0

BSMS status message: Δ Z2 4

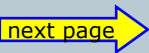
Time: 10:59 Mar 26



MAXENT (maximum entropy), the alternative for deconvolution is available in TopSpin 2.1.

MAXENT requires a separate license.

A demo license can be ordered anytime under: [www.bruker-biospin.com](http://www.bruker-biospin.com)



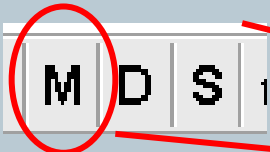


# MAXENT is back

Parameter for MAXENT (maximum entropy)

are available from the Processing Parameters Tab,

click on: M



or use the command:  
**edmax**

next page

Reference	F2	F1	Frequency axis
SI	1024	1024	Size of real spectrum
SF [MHz]	500.1300000	500.1300000	Spectrometer frequency
OFFSET [ppm]	12.67713	12.67713	Low field limit of spectrum
SR [Hz]	0.00	0.00	Spectrum reference frequency
HZpPT [Hz]	6.510417	6.510417	Spectral resolution
Window function			
WDW	SINE	SINE	Window functions for trf, xfb, ...
LB [Hz]	1.00	0.30	Line broadening for em
GB	0	0.1	Gaussian max. position for gm, 0<GB<1
SSB	0	0	Sine bell shift SSB (0,1,2,...)
TM1	0	0.1	Left limit for tm 0<TM1<1
TM2	0	0.9	Right limit for tm 0<TM2<1
Phase correction			
PHC0 [degree]	0.000	0.000	0th order correction for pk
PHC1 [degree]	0.000	0.000	1st order correction for pk
PH_mod	no	mc	Phasing modes for trf, xfb, ...
Baseline correction			
ABSG	5	5	Degree of polynomial for abs (0..5)
ABSF1 [ppm]	1000.00000	1000.00000	Left limit for absf

Acquisition information: no acquisition running

Fid Flash: [grid]

Lock: [grid]

Sample: [grid]

POWCHK: [X]

Spooler: running: 0, queued: 0, delayed: 0

BSMS status message: Δ Z3 5

Time: 10:59 Mar 26

Autoshim ✓ Locked ✓ Error

Export of what is shown in the current dataset can now be stored in PDF format.

Furthermore it can be executed directly from TopSpin command line:

```
exportfile <path>/<filename>.pdf
```

The command **tozip** can be executed on the command line with all arguments:

**tozip -d <path>/<filename>.zip**

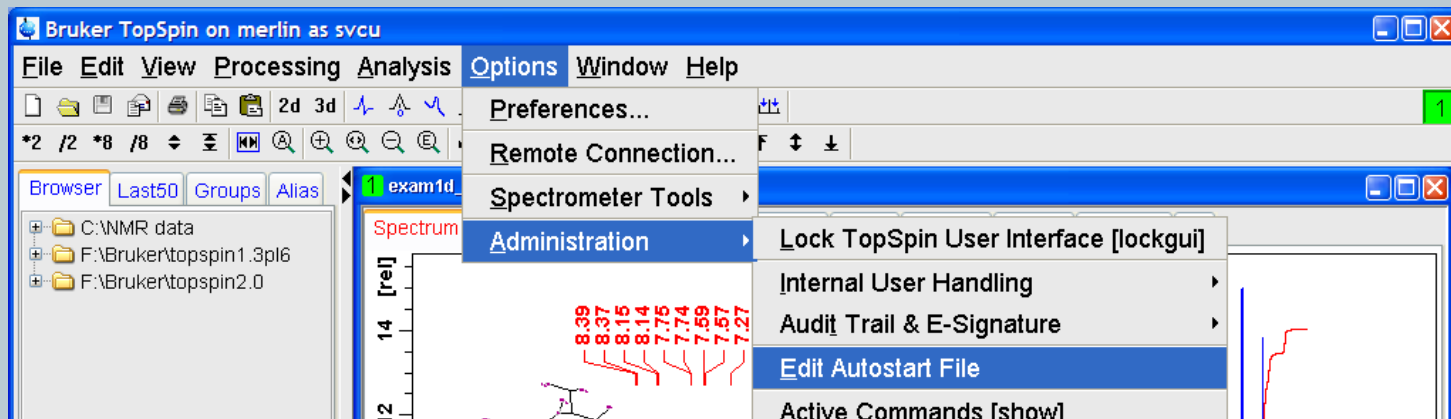
If the graphical user interface should be used, simply use the command **tozip**

# Autostart

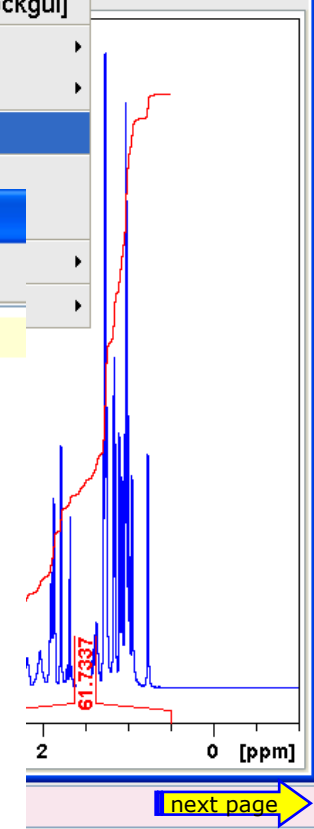


Autostart actions can be configured from the menu:

**Options → Administration → Edit Autostart File**



```
C:\Documents and Settings\svcu\.topspin-merlin\prop\autostart.mac
File Edit Search
1 # The file format of autostart.mac is identical to TopSpin macros. In fact,
2 # autostart.mac is executed as a macro when TopSpin has been started.
3 # Please check the TopSpin Users Guide for details.
4 #
5 # Example:
6 #   re exam1d_13C 1 1 c:/bruker/topspin guest
7 #   em
8 #   ft
9 #   pk
10 #
11 # From here on you may enter your own commands (you may delete or leave this comment text):
12
13
```



# Autostart used already in previous TopSpin versions?

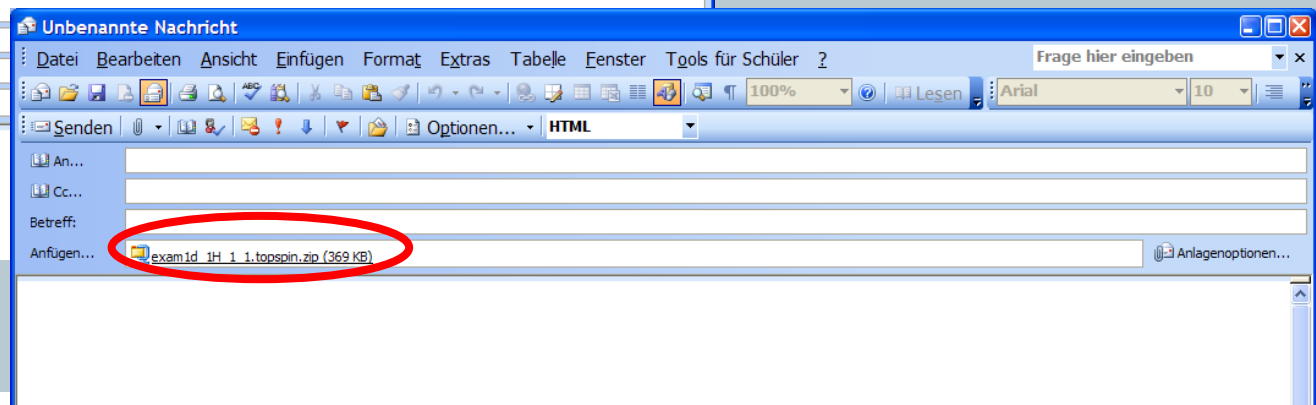
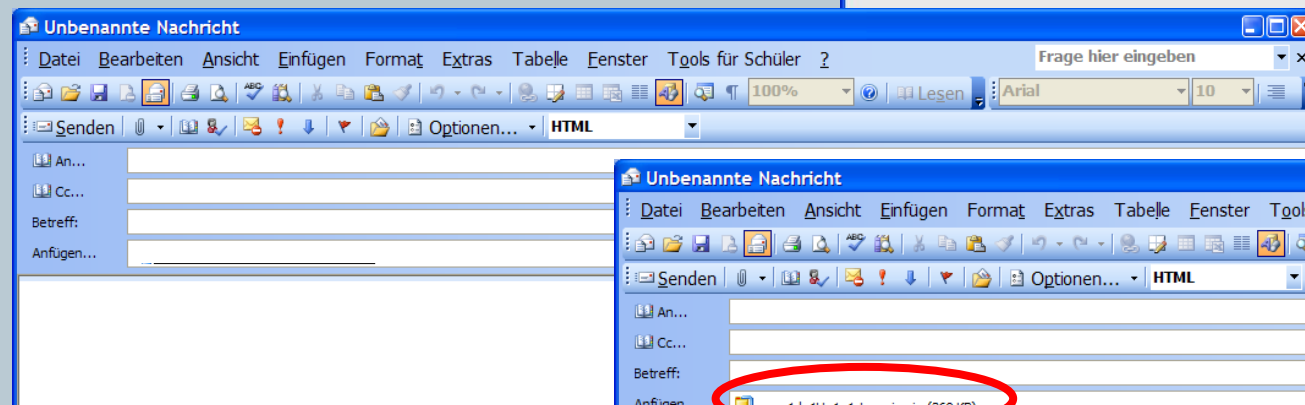
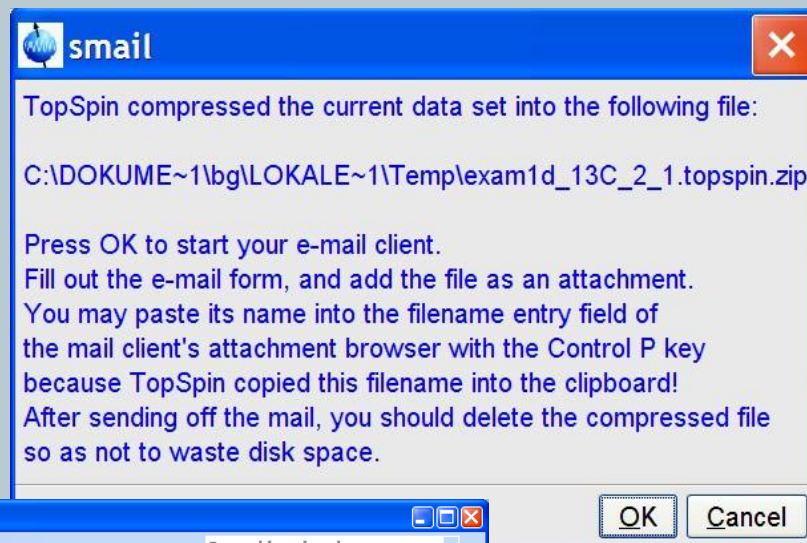
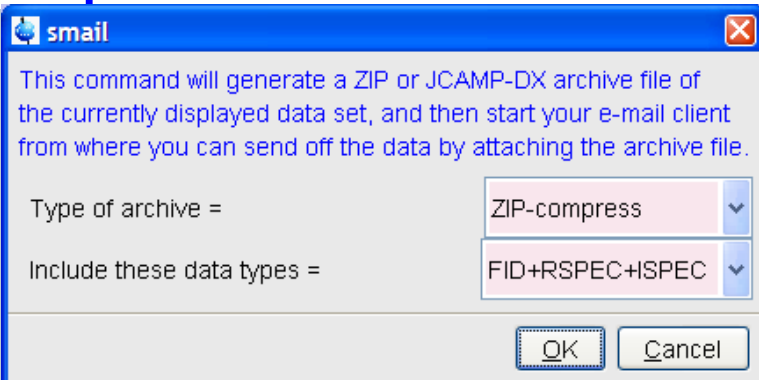


The syntax of the autostart-file has been improved. It is now possible to enter simply any TOPSPIN command that should be executed, one per line.

If an autostart-file of a previous TOPSPIN version is available it will be read with the first start of TOPSPIN 2.1 and the content will be saved in the new format.

From now on only the new file will be used for TopSpin 2.1.

## Opens now user's standard email client



# Restarting the GUI which has been started by CPR



## **restartgui**

Windows: Bruker Utilities → Miscellaneous

Linux: Shell

To restart the CPR-GUI from a second window / remote connection, use TopSpin command:

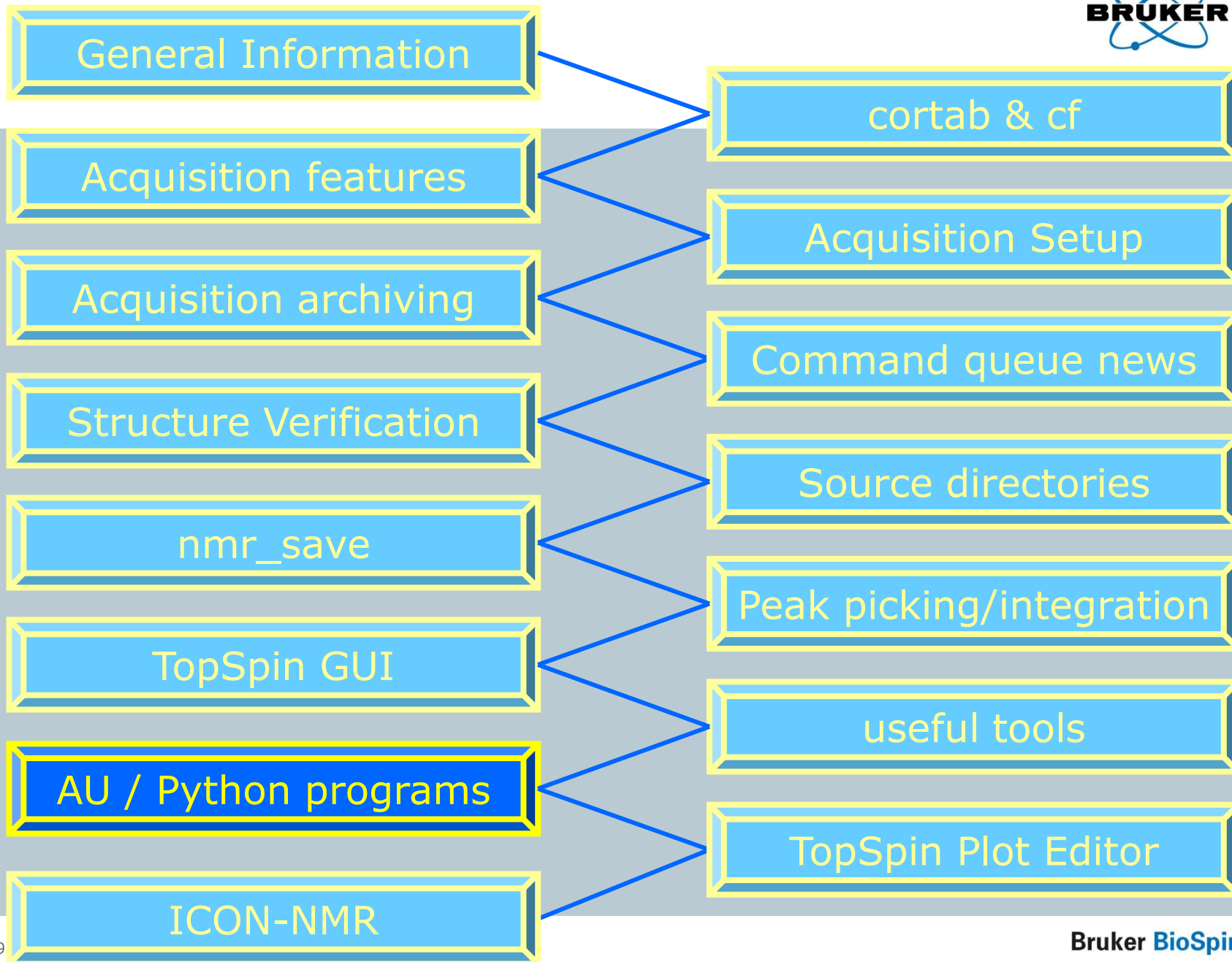
## **restart**



TopSpin can now be installed on directories mounted via NFS.



# Content





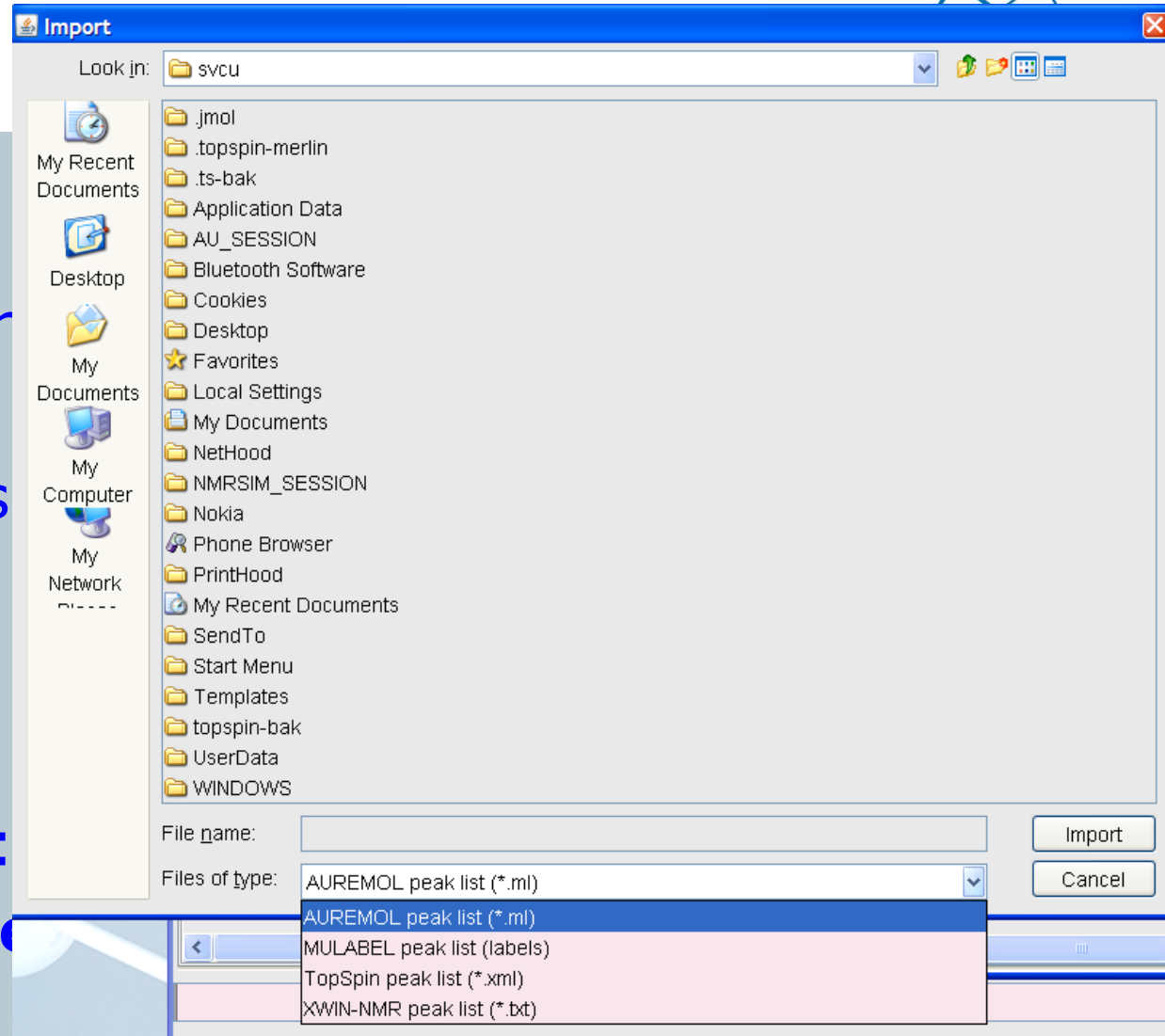
Introduction into python:  
New 60-page overview manual.

# AU program: mulabel



Import command for  
'labels' file as  
annotation for peaks

- Right mouse click  
in peak table
- TopSpin command:  
**peakstransferlabel**



With option to overwrite existing annotations and/or  
value delta for differences in peak shifts



# New handling of AU program macro '**XAU**'



The AU program macro **XAU** is used to start a second AU program from an already running AU program.

The syntax of the **XAU** has been changed. In previous version it has been used like this:

```
XAU("<Name_of_AU_PROGRAM>");
```

In TopSpin 2.1 the new syntax is:

```
XAU("<Name_of_AU_PROGRAM>", "<argument>");
```

Note: Any AU program in TopSpin 2.1 that contains the **XAU** macro must be modified otherwise the compilation of the AU program will fail. All Bruker AU programs have been modified, but user-specific AU programs have to be modified by the customer.

For more details check the Release Letter of TopSpin 2.1.

DELETEPROCDATA(name1,expno1,procno1,disk1,user1)

DELETEIMAGINARYDATA(name1,expno1,procno1,disk1,user1)

DELETERAWDATA(name1,expno1,disk1,user1)

DELETEPROCNO(name1,expno1,procno1,disk1,user1)

DELETEEXPNO(name1,expno1,disk1,user1)

DELETERNAME(name1,disk1,user1)

**getParamDirs()**

**getParfileDirforRead()**

**getParfileDirforWrite()**

For getting the information in AU programs about location of parameter files (pp, mac, AU ...).

For more details check the Release Letter of TopSpin 2.1.

TopSpin 2.0 and previous versions offered different functions to get path information of specific files, e.g.:

**getstan** which offered the path '*<TopSpin\_Home>/exp/stan/nmr/*' and

**PathXWinNMRExpStan** which offered the path '*<TopSpin\_Home>/exp/stan'*

Because with TopSpin 2.1 each user can store these files in any directory it is recommended to use the new AU functions:

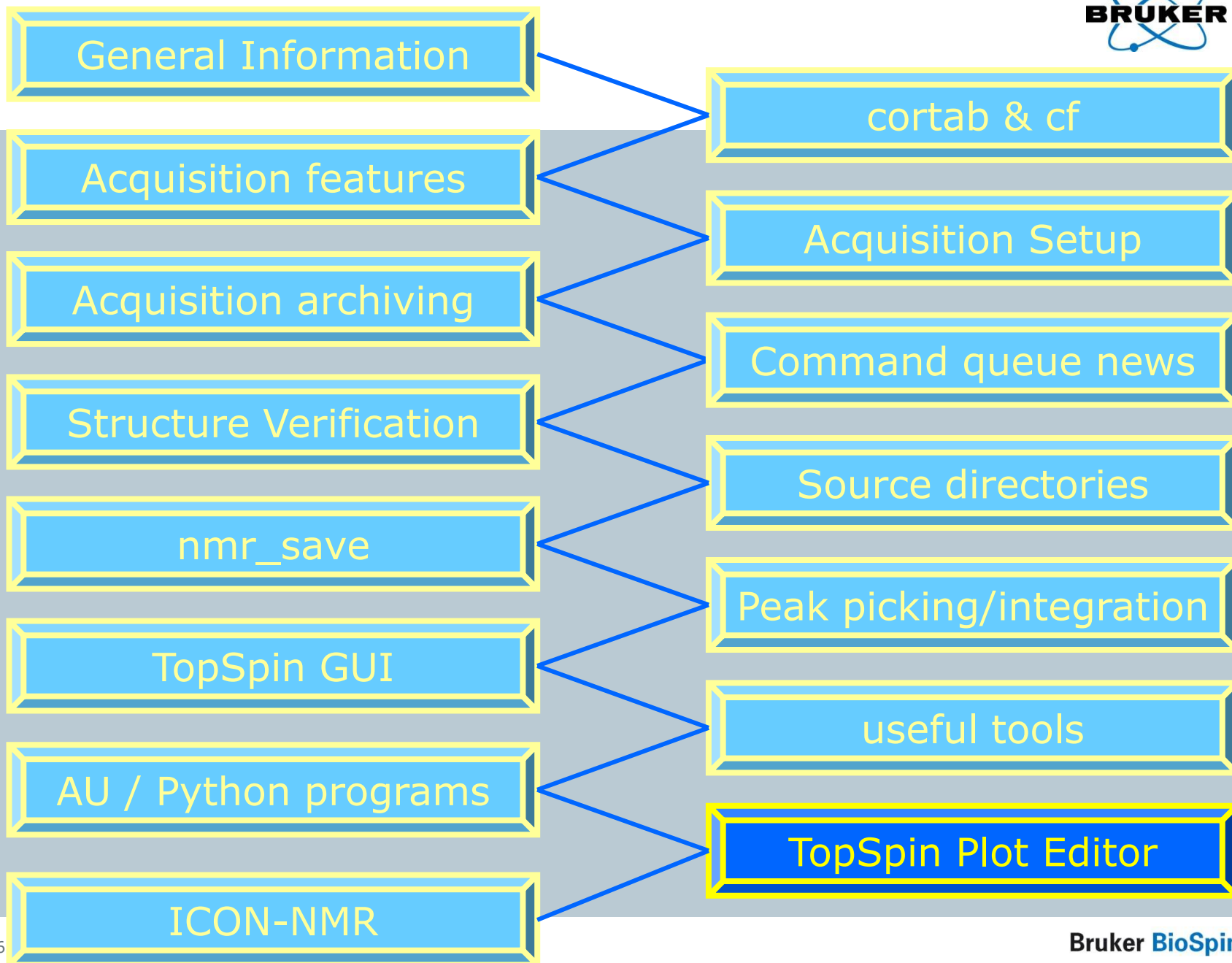
**getParamDirs(<keys>)**

**getParfileDirForRead(<name>,<key>,<var>);**

**getParfileDirForWrite(<name>,<key>,<var>);**

For more details check the  
Release Letter of TopSpin 2.1.

# Content





# Plot Editor warning messages



Plot Editor offers a new menu entry which contains a list off all warnings that have been given by the program. New messages are discrete shown in status line.

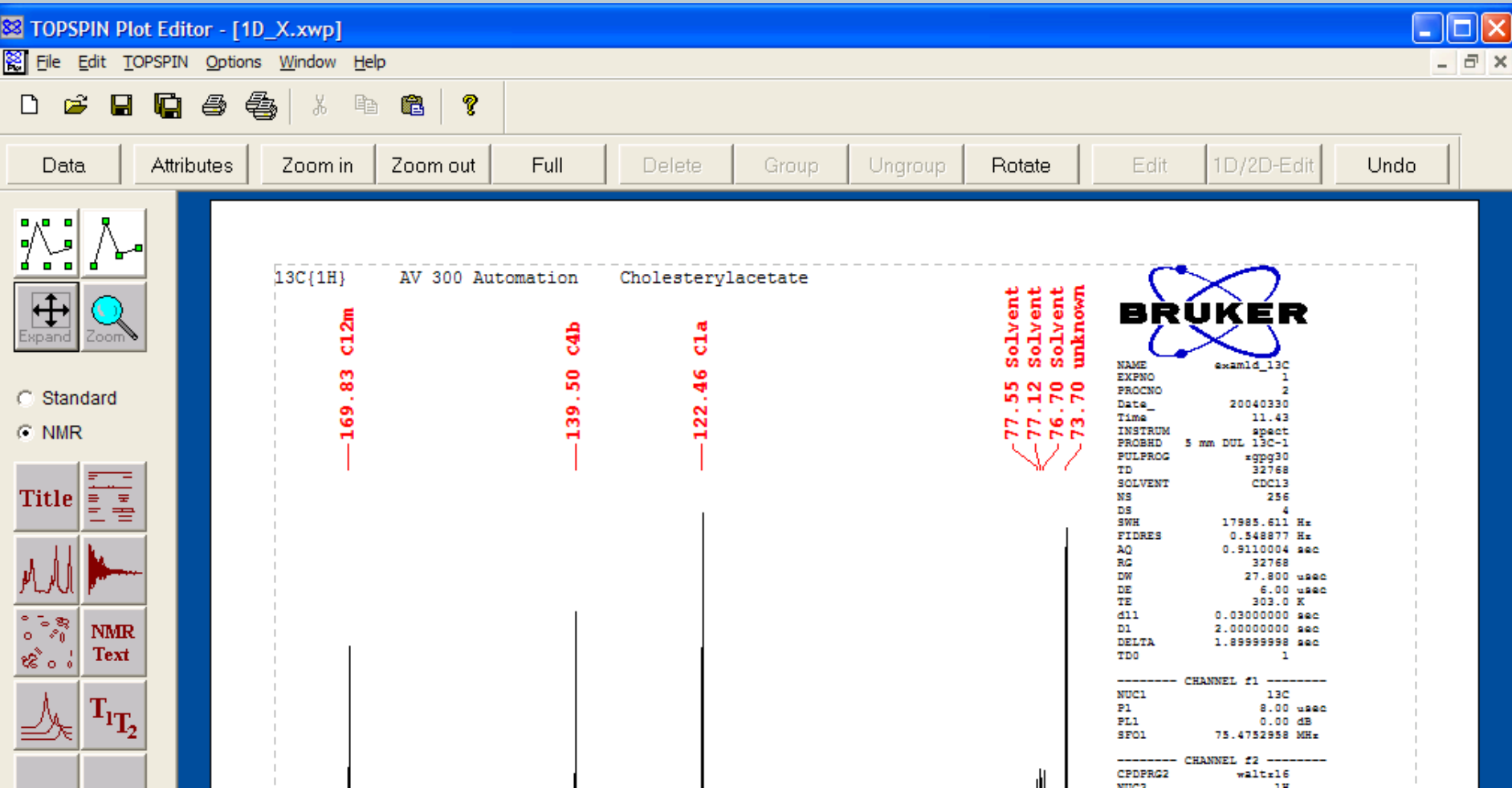
The screenshot shows the TOPSPIN Plot Editor window with the following elements:

- Menu:** File, Edit, TOPSPIN, Options, Window, Help. The TOPSPIN menu is open, showing options like 'Get Current Data Set', 'Update Data from Data Set', and 'View Error Messages ...'.
- Dialog Box:** 'Data Access Error Messages' with the text: 'Data Set Nr. 1: Could not open "F:\Bruker\TopSpin\data/guest/nmr/exam1d\_13C/1/pdata/2/peak.txt" No such file or directory'.
- Plot Area:** Shows a plot with parameters: 13C{1H} AV 300 A.
- Bottom Panel:** Includes 'Standard' and 'NMR' radio buttons, 'Title', 'NMR Text', and 'T<sub>1</sub>T<sub>2</sub>' buttons.
- Bottom Right:** Technical parameters for NUC1, P1, PL1, SFO1, CHANNEL 22, CPDPRG2, and NUC2.

# Plot Editor shows annotations



Plot Editor can now be configured to show position (Hz/ppm) or annotations (if available) or both.



# Plot Editor shows sample info



Plot Editor Layouts can now be configured to show sample info defined in TopSpin.

The screenshot displays the Bruker Plot Editor interface. On the left is a file browser showing a directory tree with folders like 'F:\Bruker\TopSpin' and 'F:\NMR data'. The main window has a title bar 'exam1d\_13C 1 2 \bruker\topspin guest' and a menu bar with tabs: 'Spectrum', 'ProcPars', 'AcquPars', 'Title', 'PulseProg', 'Peaks', 'Integrals', 'Sample', 'Structure', and 'Fid'. The 'Sample' tab is active, showing a 'Sample Description' section with a table of fields:

Sample ID	ABxx1234
Origin	test sample
Concentration	? unknown
Date Prepared	2007/10/01
Buffer	none
Contact	NMR service team
Comment	This is an example

# Plot Editor shows sample info



Plot Editor Layouts can now be configured to show sample info defined in TopSpin.

The screenshot displays the Bruker Plot Editor interface. On the left, the 'Edit' panel is open to the 'Text' tab, showing a text file named '+/./././sample\_info.prop' with a 'Browse...' button. Below this, there are icons for 'Standard' and 'NMR' modes, with 'NMR' selected and highlighted by a red box. The main plot area shows an NMR spectrum for '13C(1H) AV 300 Automation Cholesterylacetate'. The spectrum has several peaks, with chemical shifts marked at 169.43, 139.50, 122.46, 77.55, 76.70, 76.20, and 73.70 ppm. To the right of the spectrum, there is a table of acquisition parameters and a Bruker logo. The parameters include:

NAME	exam1d_13C
EXPNO	1
PROCNO	2
Date_	20040330
Time	11.43
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
FULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	256
DS	4
SWH	17985.611 Hz
FIDRES	0.548977 Hz
AQ	0.9110004 sec
RG	32768
DW	27.800 usec
DE	6.00 usec
TE	303.0 K
d11	0.03000000 sec
D1	2.00000000 sec
DELTA	1.89999998 sec
TDO	1

Below the parameters, there are two channel definitions:

CHANNEL #1	
NUC1	13C
P1	8.00 usec
PL1	0.00 dB
SFO1	75.4752958 MHz
CHANNEL #2	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	0.00 dB
PL12	20.00 dB
PL13	22.00 dB
SFO2	300.1312008 MHz
S1	32768
SF	75.4677480 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

The x-axis of the spectrum is labeled 'ppm' and ranges from 200 to 0. The Bruker logo is also present in the top right corner of the plot area.

Plot Editor now supports customized paper formats on Windows printers.

New formats simply need to be defined using the „Printer → Server Properties“ mechanism as provided by Windows itself.

# Integral reset action



A new reset option for integral height is offered:

After reset size of biggest integral is:  cm

Automation Action

1D Reset Actions

Reset action for Xmin/Xmax

Don't change

Set to minimum/maximum

Set to F1P / F2P

Reset action for Ymin/Ymax

Don't change

Set to minimum/maximum

Set to minimum/maximum between Xmin/Xmax

Use region file on reset:

reg  intmg  defined by SREGLST

After reset, size of biggest peak is

100.00 % of plot size  10.00 cm

defined by parameter CY (in cm)

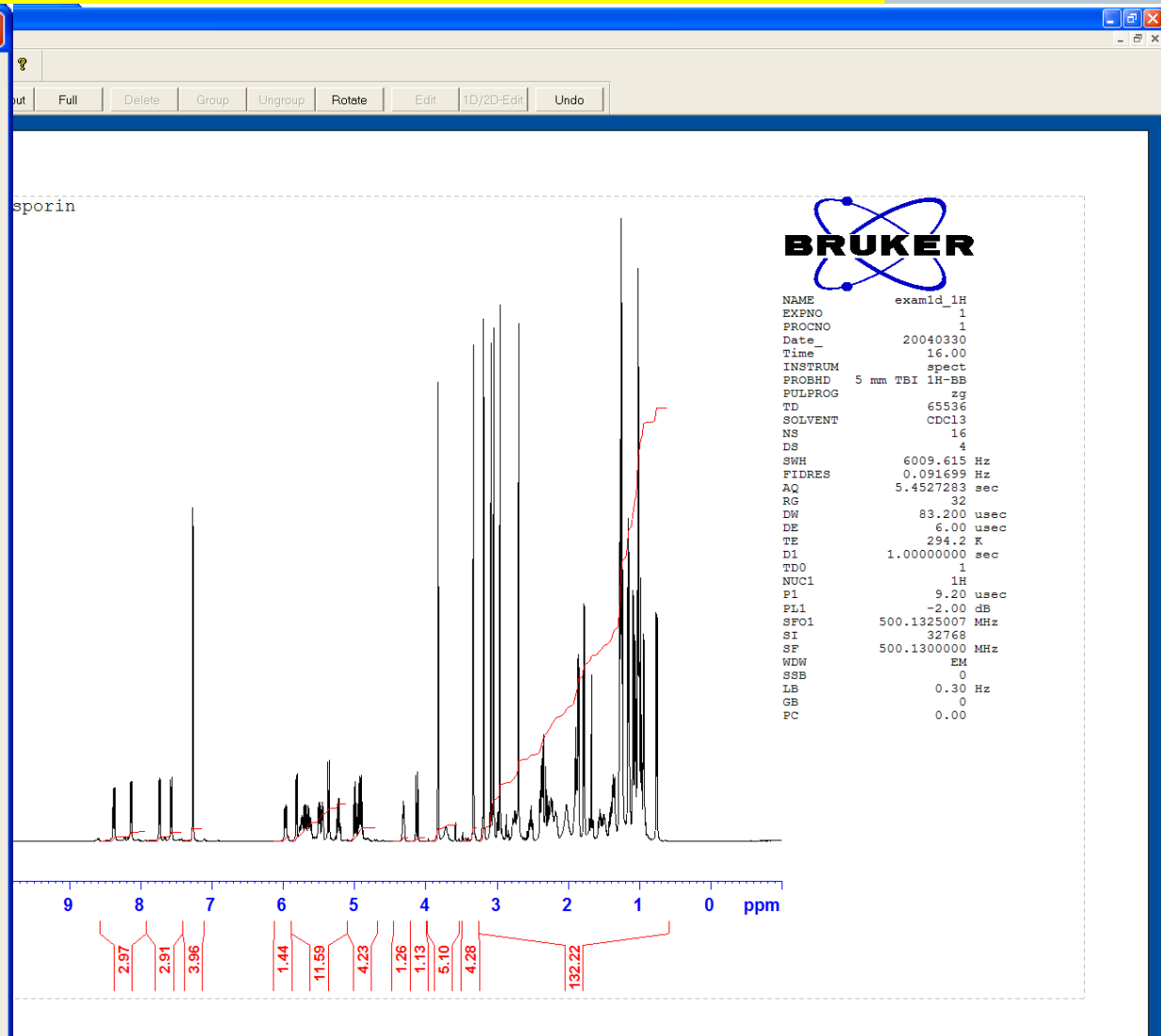
After reset, size of biggest integral is  cm

Base lines

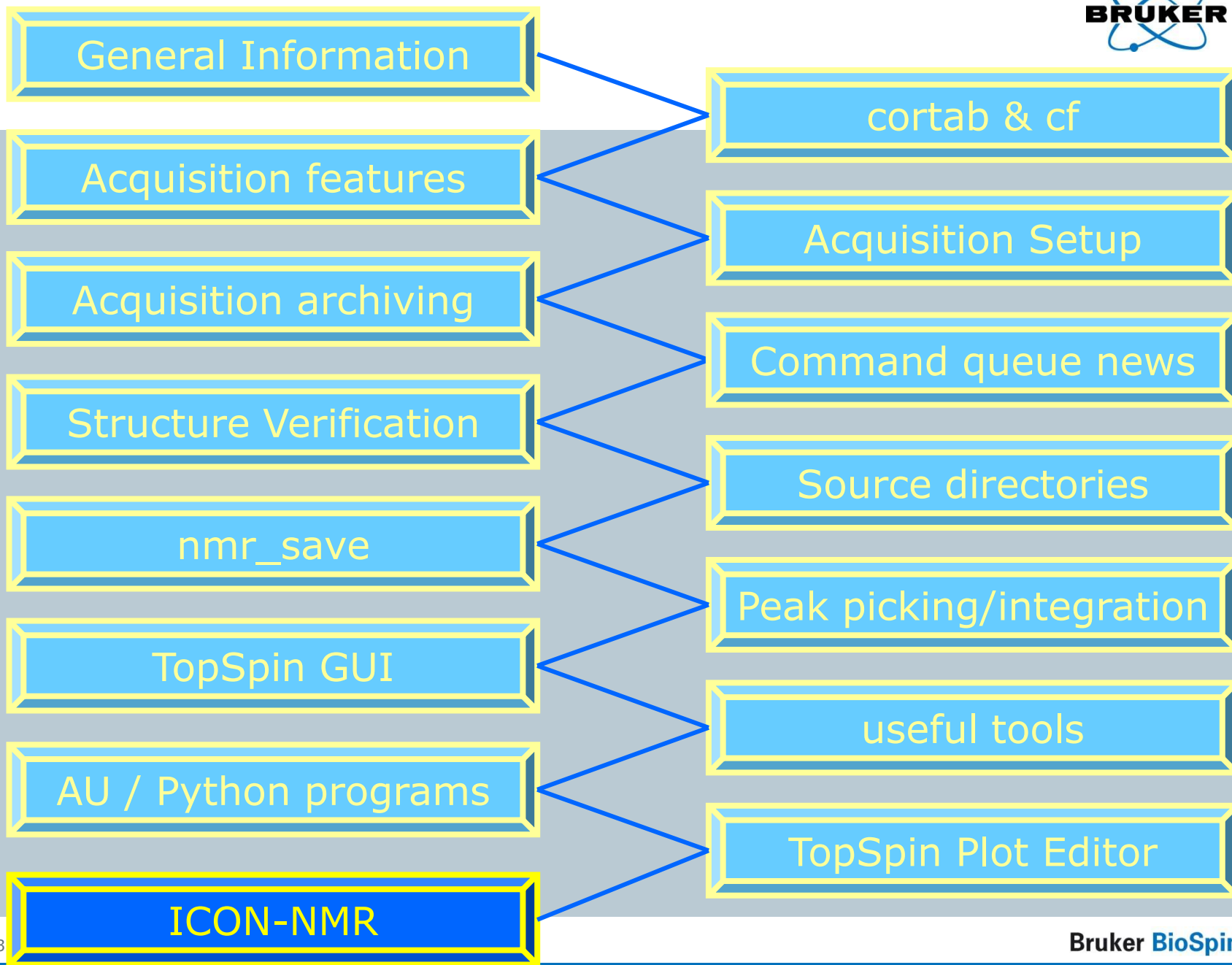
Keep zero line fixed on  % of box

Keep integrals fixed on  % of box

OK Cancel Apply Help



# Content





Icon 4.2 includes support for the new Bruker SampleJet Sample Changer.

A dedicated Sample Holder overview window along with a configuration option to control the measurement sequence order of experiments is provided. The Automation driver routines have also been optimized to take full advantage of the improved performance.

Icon also fully supports the interfacing of this new unit to the SampleTrack Laboratory Management software.



# ICON-NMR 4.2 – SampleJet support



ICON-NMR: 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
- ToolBox Setup
- Accounting

**Run Control**

Default Automation Mode: **Sample Jet**

Rack Sample Sequence:

Eject last sample in queue

Never Rotate the Sample

Start run at user login

**Processing Control**

Generate a Spectrum Printout

Process Data Sets after Acquisition: **Ask on Startup**

Generate Spectrum Print-Out file in data set for possible dispatch to E-mail recipient: **Off**

Perform Structure Consistency Check (HSQC Experiments only)

**DataSet Management**

Ignore the TopSpin Prosol Parameters

Delete temporary datasets after experiment end

Allow Overwrite of existing Acquisition Data

**BEST Mode Settings**

Enable BEST-NMR

BEST-NMR Automation Mode: **Standard (No Barcodes)**

Force Solvent Change after (Number of Hours - Day Time only): **0**

BEST Administration Tool:

next page

# ICON-NMR 4.2 – SampleJet support



The screenshot displays the ICON-NMR software interface with three overlapping windows. The top window shows a menu bar (File, Run, Holder, View, Find, Parameters, Options, Tools, Help) and a toolbar with icons for settings, play, and stop. The middle window shows a list of holders on the left and a table of experiment details in the main area. The bottom window shows a toolbar with buttons for Submit, Cancel, Edit, Delete, Add, Copy, and Change User, along with a 'Preceding Experiments' table.

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri
▷ 41		Available								
▷ 42		Available								
▷ 43		Available								
▷ 44		Available								
▷ 45		Available								
▷ 46		Available								
▷ 47		Available								
▷ 1 A1 - 101		Available								
▷ 1 B1 - 102		Available								
▷ 1 C1 - 103		Available								
▷ 1 D1 - 104		Available								

#	Date	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq
---	------	--------	------	-----	------------	------	-----	----------	------	------	-----

Search Preceding   include previous runs

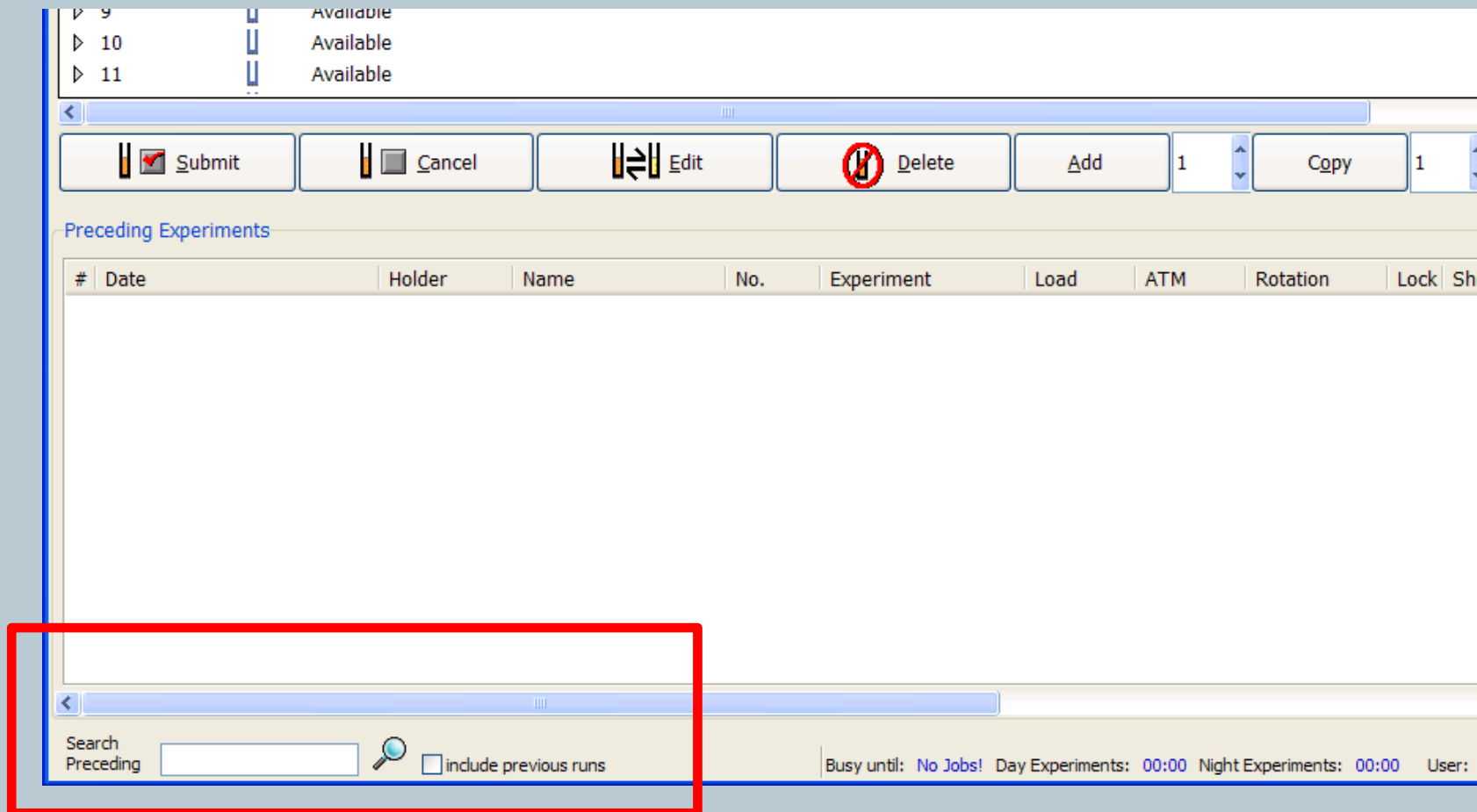
Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: BRUKER\svcu



## Search history files

A convenient search tool has been added to search all entries from preceding experiments performed within Icon-Nmr. Search for multiple items in an experiment's title text, dataset name or a particular remarks message. A list of items is generated in the same manner as the Preceding Experiments (history) list which may be then used to navigate under TopSpin or Amix Viewer to the respective dataset.

## Search history files



The screenshot displays the Bruker ICON-NMR software interface. At the top, there is a list of available experiments with columns for experiment number and status. Below this is a toolbar with buttons for Submit, Cancel, Edit, Delete, Add, and Copy. The main area is titled "Preceding Experiments" and contains a table with columns: #, Date, Holder, Name, No., Experiment, Load, ATM, Rotation, Lock, and Shi. The table is currently empty. At the bottom, there is a search bar with a magnifying glass icon and a checkbox labeled "include previous runs". A red box highlights the search bar and the checkbox. To the right of the search bar, there is a status bar showing "Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User:".



## **Web-Icon Improvements**

Experiments may now be remotely edited via the Web interface.

A timeout feature has also been added to logout idle web users, improving security and throughput.



**Remarks field** now shows process messages

Should any procedure generate an error or warning during sample measurement, a copy of the text of the warning or error will appear in the “Remarks” column of the Preceding Experiments (history) list.



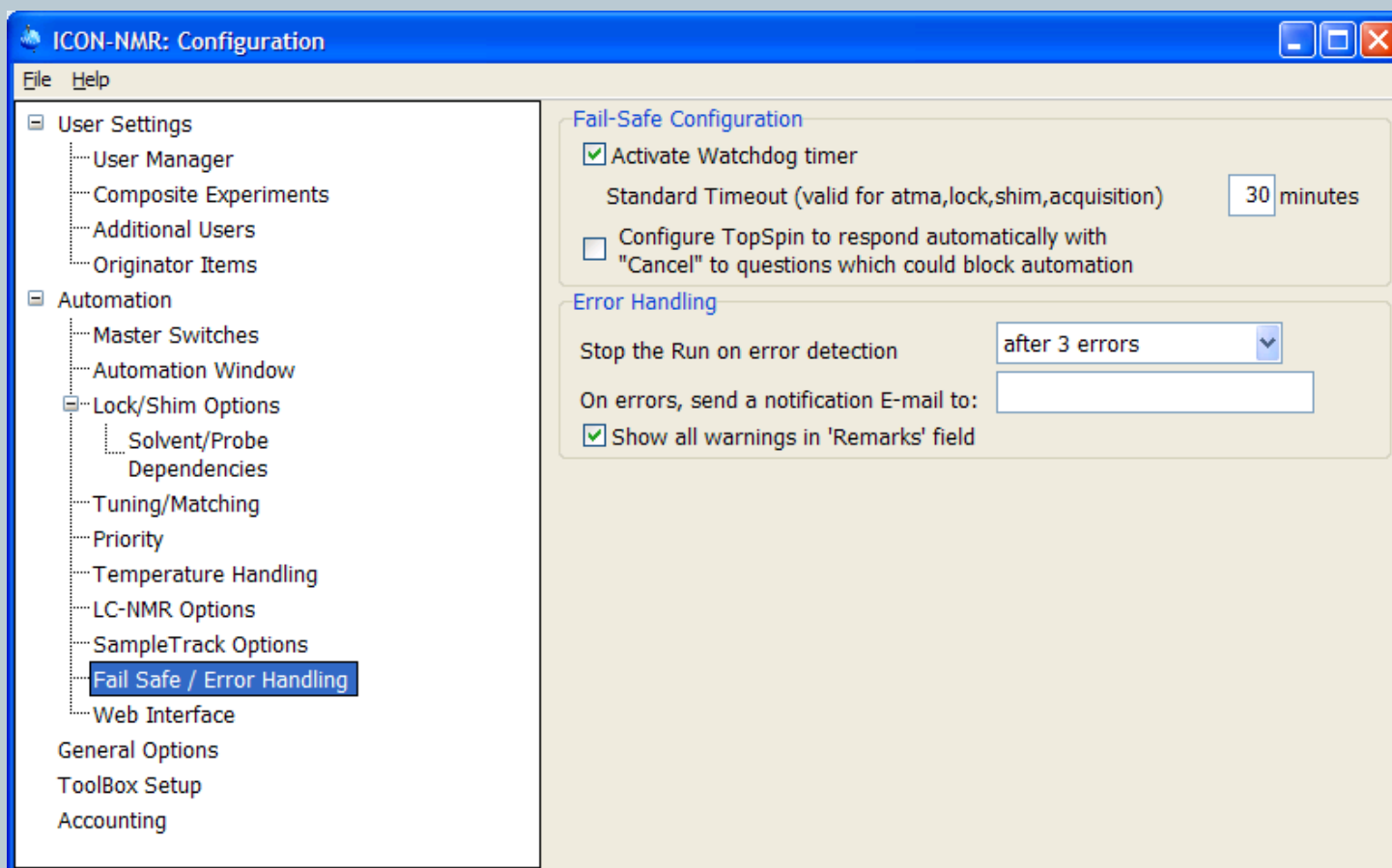
## **Failsafe watchdog timer**

If any action takes longer than expected during the automation process, the run will be restarted. The action which failed to complete will be also restarted, but if it fails again, it will be skipped.

The Automation run will no longer be blocked by any processes which fail to respond.

The time allotted for waiting may be configured and where necessary this system may be circumvented.

## Failsafe watchdog timer



The screenshot shows the 'ICON-NMR: Configuration' dialog box. The left sidebar contains a tree view with the following items: 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, ToolBox Setup, and Accounting. The 'Fail Safe / Error Handling' item is highlighted. The main area is divided into two sections: 'Fail-Safe Configuration' and 'Error Handling'. In 'Fail-Safe Configuration', the 'Activate Watchdog timer' checkbox is checked, and the 'Standard Timeout' is set to 30 minutes. The 'Configure TopSpin to respond automatically with "Cancel" to questions which could block automation' checkbox is unchecked. In 'Error Handling', the 'Stop the Run on error detection' dropdown is set to 'after 3 errors'. The 'On errors, send a notification E-mail to:' field is empty. The 'Show all warnings in "Remarks" field' checkbox is checked.





## **Zip copy, Zip data mail** (User Manager) permission

Icon can now generate Zip files of the generated datasets as part of the run. These can be emailed in the same manner as JDX files have been up to now.

Zip Files may also be copied to a particular directory if required, in the same manner as the JDX-Copy mode.

ICON-NMR: 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**
- ToolBox Setup
- Accounting

**Title**

- Include Originator Information in Title
- Include Experiment/Sample Information in Title

**Data Set**

- Modify DataSet permissions after processing

Experiment Number Automatic Increment

**Passwords**

Check Passwords

**Display**

Language

Font Size Adjuster

**TopSpin**

- Display all TopSpin Warnings

**Mail**

SMTP Mail Server  "From:" Address

**JDX Copy Mode (linked to JDX Copy flag in User Manager)**

Include these data types

JDX Compression Mode: (Also affects DataMail)

File naming format

Create JDX file in this directory

**ZIP Copy Mode (linked to ZIP Copy flag in User Manager)**

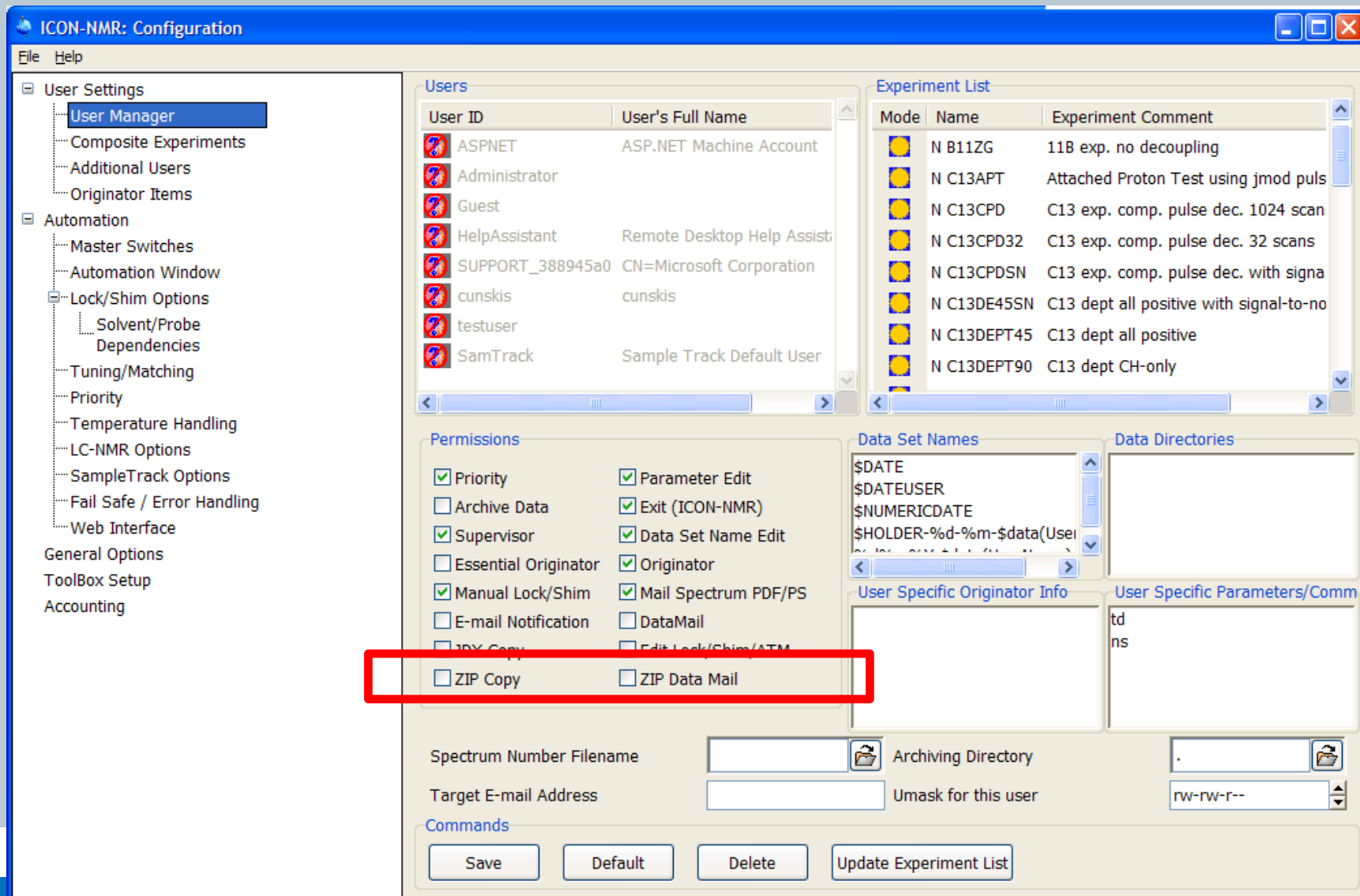
Include these data types

ZIP Compression Mode: (Also affects Zip DataMail)

File naming format

Create ZIP file in this directory

## Zip copy, Zip data mail (User Manager) permission



The screenshot shows the 'ICON-NMR: Configuration' window. The 'User Manager' option is selected in the left-hand navigation pane. The main window is divided into several sections:

- Users:** A list of users with columns for User ID and User's Full Name. Users include ASPNET, Administrator, Guest, HelpAssistant, SUPPORT\_388945a0, cunskis, testuser, and SamTrack.
- Experiment List:** A table with columns for Mode, Name, and Experiment Comment. It lists various experiments like N B11ZG, N C13APT, N C13CPD, etc.
- Permissions:** A section with two columns of checkboxes. The 'ZIP Copy' and 'ZIP Data Mail' options are highlighted with a red box. Other checked options include Priority, Supervisor, Manual Lock/Shim, and Mail Spectrum PDF/PS.
- Data Set Names:** A list of names including \$DATE, \$DATEUSER, \$NUMERICDATE, and \$HOLDER-%d-%m-\$data(User).
- Data Directories:** A field for specifying data directories.
- User Specific Originator Info:** A field for user-specific originator information.
- User Specific Parameters/Comm:** A field for user-specific parameters and commands.
- General Options:** Fields for Spectrum Number Filename, Target E-mail Address, Archiving Directory, and Umask for this user.
- Commands:** Buttons for Save, Default, Delete, and Update Experiment List.



## **Originator ,Regular expression` check**

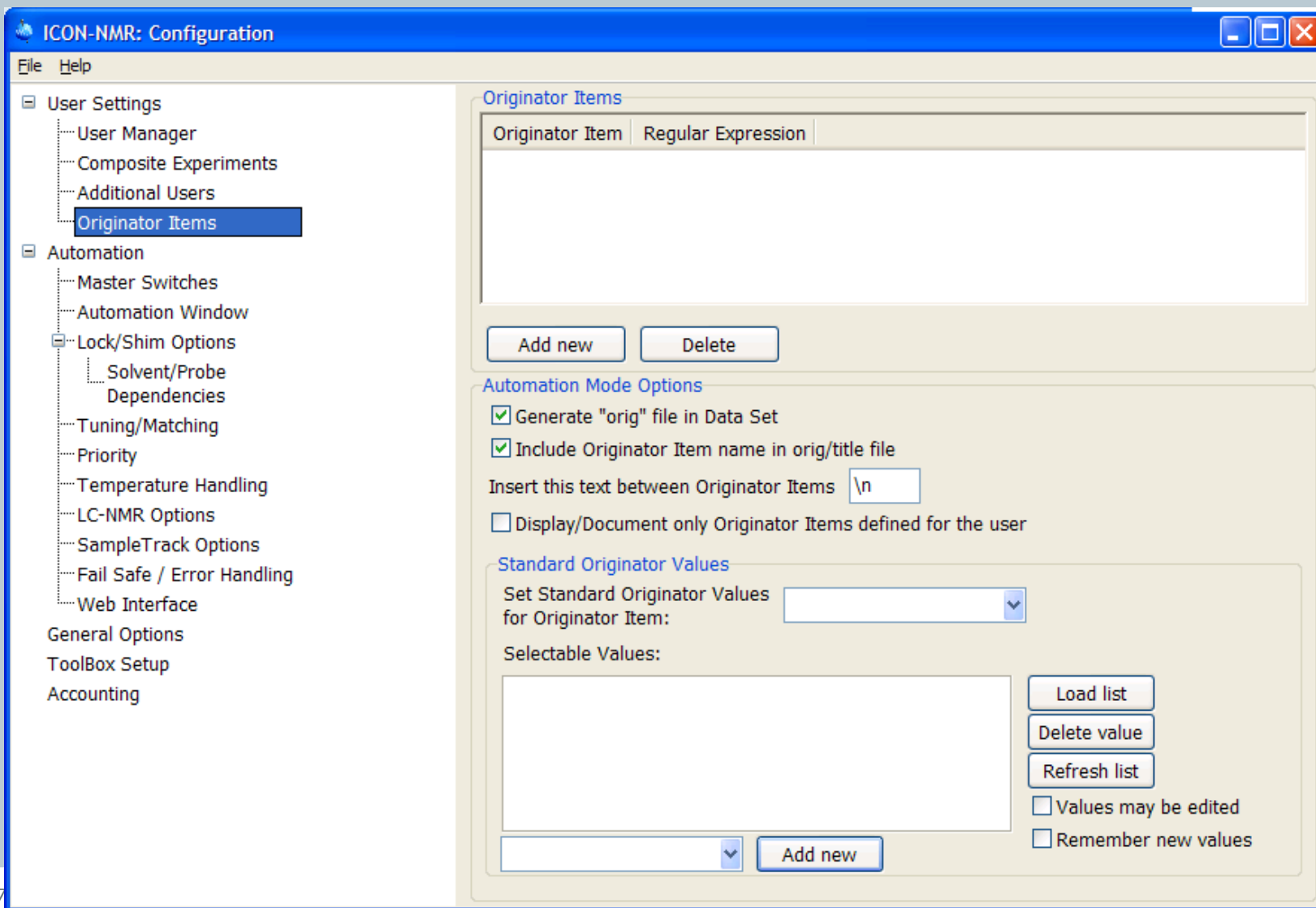
Originator item information may be screened according to syntax rules.

This will further reduce the likelihood of incorrect sample information being entered when samples are being submitted.

More information on how to use/set up `regular expressions` can be found e.g. here:

<http://www.regular-expressions.info>

## Originator Regular expression check



The screenshot shows the 'ICON-NMR: Configuration' window. The left sidebar contains a tree view with the following items: User Settings (expanded), User Manager, Composite Experiments, Additional Users, Originator Items (highlighted), Automation (expanded), Master Switches, Automation Window, Lock/Shim Options (expanded), Solvent/Probe Dependencies, Tuning/Matching, Priority, Temperature Handling, LC-NMR Options, SampleTrack Options, Fail Safe / Error Handling, Web Interface, General Options, ToolBox Setup, and Accounting.

The main area is divided into two sections:

- Originator Items:** A table with two columns: 'Originator Item' and 'Regular Expression'. Below the table are 'Add new' and 'Delete' buttons.
- Automation Mode Options:** Contains several checkboxes:
  - Generate "orig" file in Data Set
  - Include Originator Item name in orig/title file
  - Insert this text between Originator Items:
  - Display/Document only Originator Items defined for the user

Below these options is the **Standard Originator Values** section:

- Set Standard Originator Values for Originator Item:
- Selectable Values:
- Buttons: Load list, Delete value, Refresh list
- Options:  Values may be edited,  Remember new values
- Bottom:  Add new

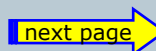


## Experimental Form Style entry mode

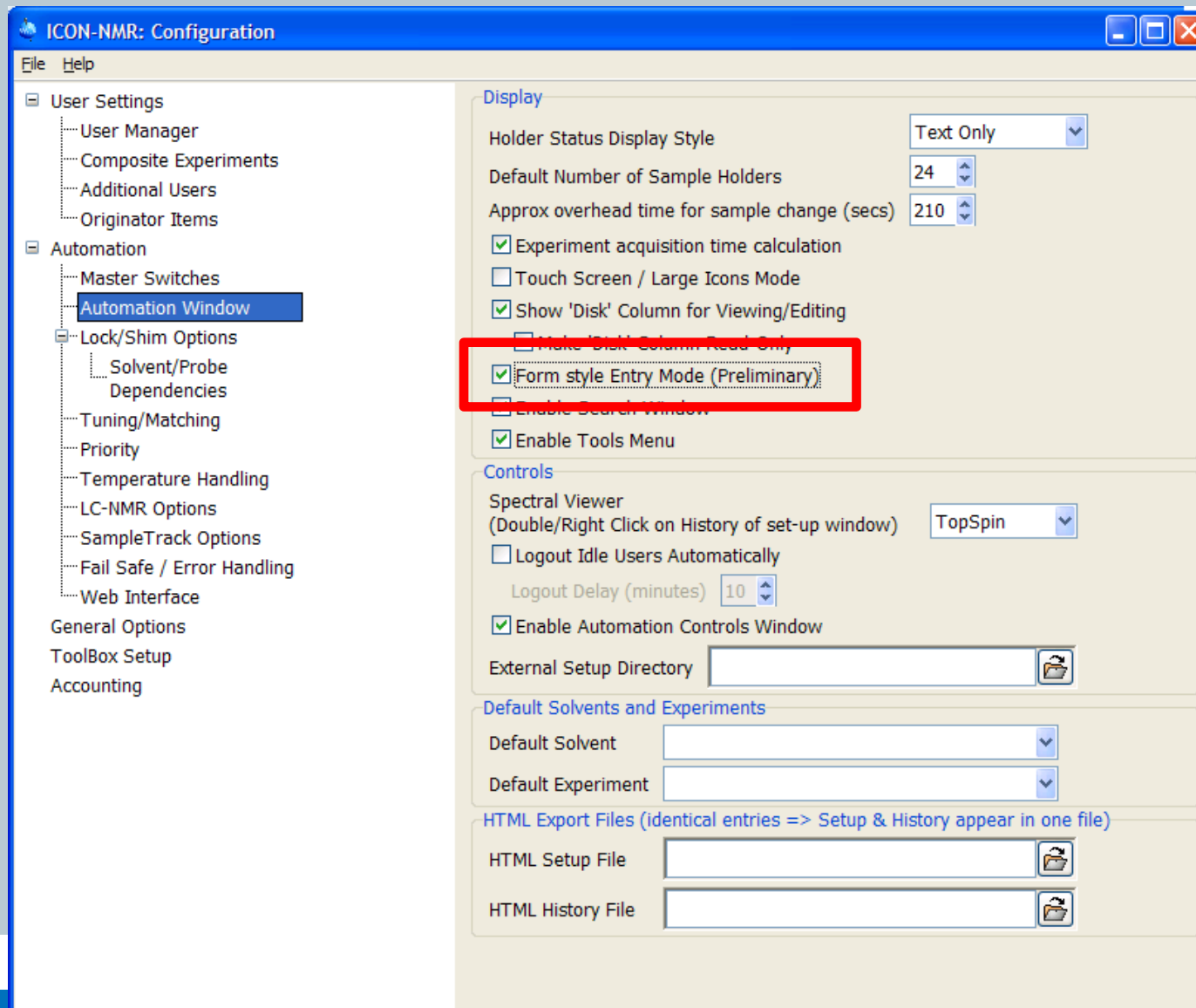
This method of submission may be useful when the instrument is working in environments where access to the instrument needs to be streamlined.

Here the sample position, dataset name and experiment number is set automatically (using either the Spectrum Number Filename or User Manager Dataset Name entry). All that remains is for the user to set Solvent and Experiment and Title/Originator Info.

Comments on this new system please to [nmr-software-support@bruker.de](mailto:nmr-software-support@bruker.de)

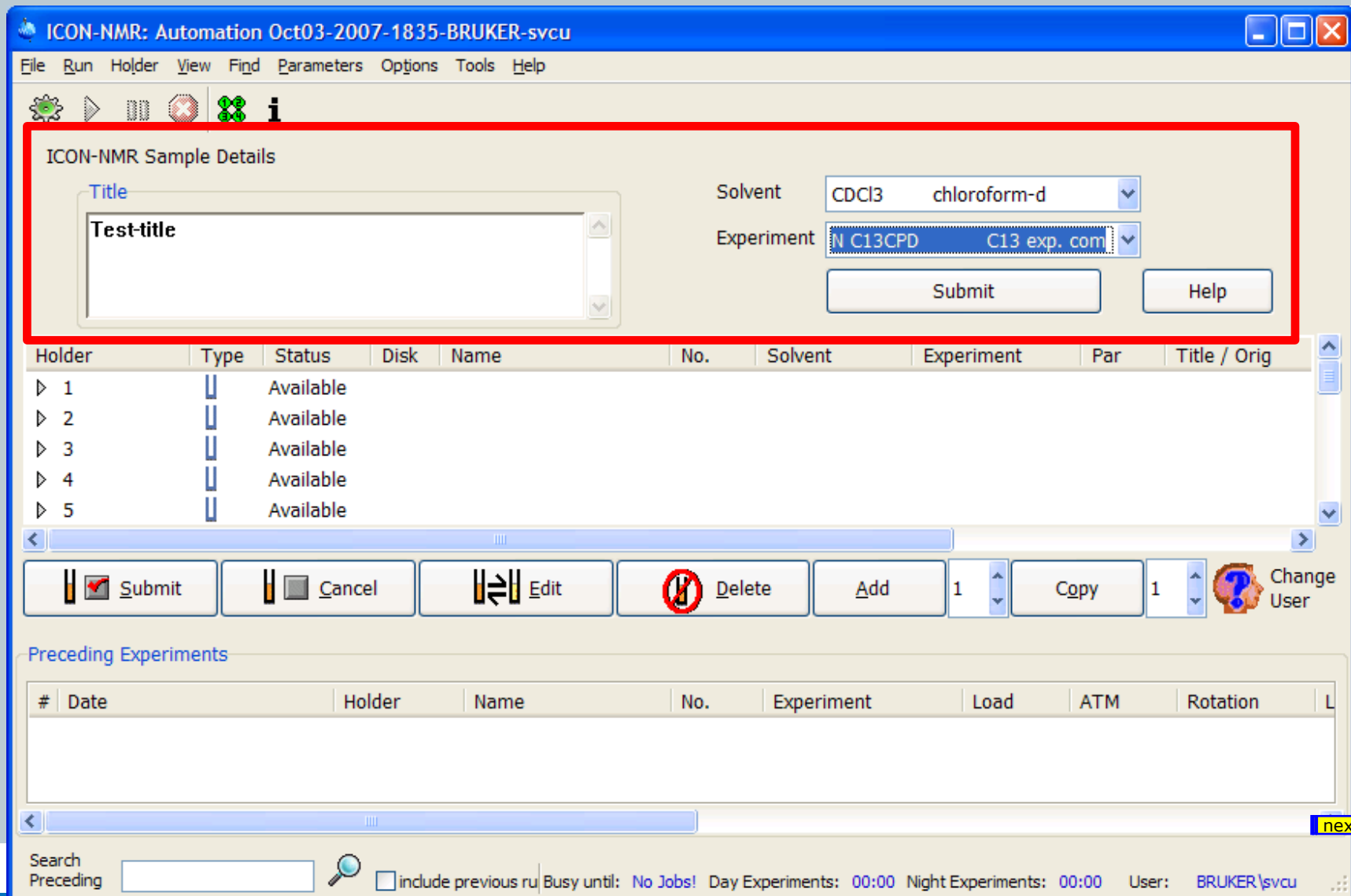


## Experimental Form Style entry mode



The screenshot shows the 'ICON-NMR: Configuration' window. The left sidebar contains a tree view with categories: User Settings, Automation, Lock/Shim Options, Tuning/Matching, Priority, Temperature Handling, LC-NMR Options, SampleTrack Options, Fail Safe / Error Handling, Web Interface, General Options, ToolBox Setup, and Accounting. The 'Automation Window' is selected and highlighted in blue. The main panel is divided into sections: Display, Controls, Default Solvents and Experiments, and HTML Export Files. In the 'Display' section, the 'Form style Entry Mode (Preliminary)' checkbox is checked and highlighted with a red rectangular box. Other settings include 'Holder Status Display Style' set to 'Text Only', 'Default Number of Sample Holders' at 24, and 'Approx overhead time for sample change (secs)' at 210. The 'Controls' section has 'Spectral Viewer' set to 'TopSpin' and 'Enable Automation Controls Window' checked. The 'Default Solvents and Experiments' section has empty dropdowns for 'Default Solvent' and 'Default Experiment'. The 'HTML Export Files' section has empty text boxes for 'HTML Setup File' and 'HTML History File'.

## Experimental Form Style entry mode



ICON-NMR: Automation Oct03-2007-1835-BRUKER-svcu

File Run Holder View Find Parameters Options Tools Help

ICON-NMR Sample Details

Title: Test-title

Solvent: CDCl3 chloroform-d

Experiment: C13CPD C13 exp. com

Submit Help

Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig
▶ 1	U	Available							
▶ 2	U	Available							
▶ 3	U	Available							
▶ 4	U	Available							
▶ 5	U	Available							

Submit Cancel Edit Delete Add Copy Change User

Preceding Experiments

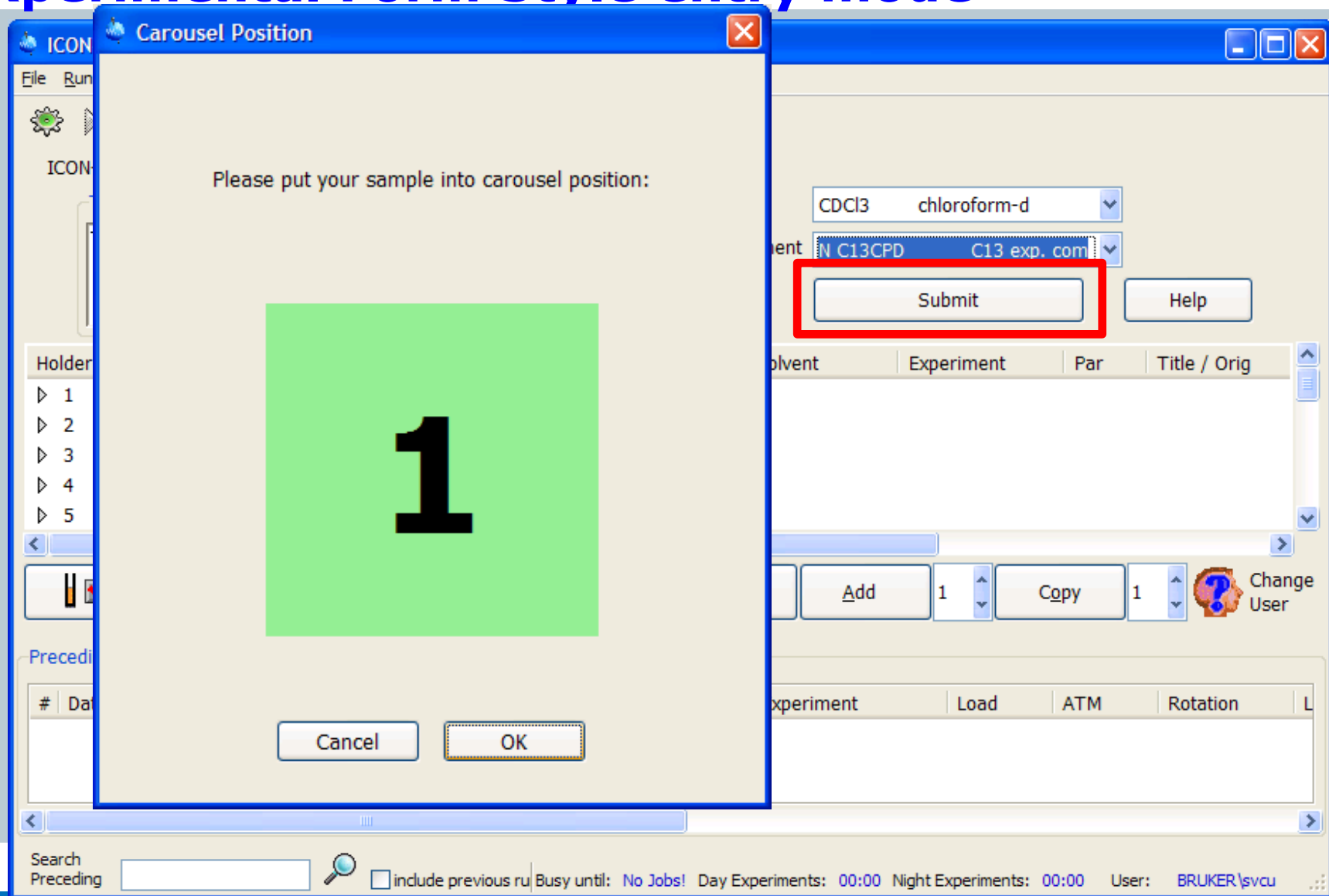
#	Date	Holder	Name	No.	Experiment	Load	ATM	Rotation	L
---	------	--------	------	-----	------------	------	-----	----------	---

Search Preceding [ ] include previous ru Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: BRUKER\svcu

next page

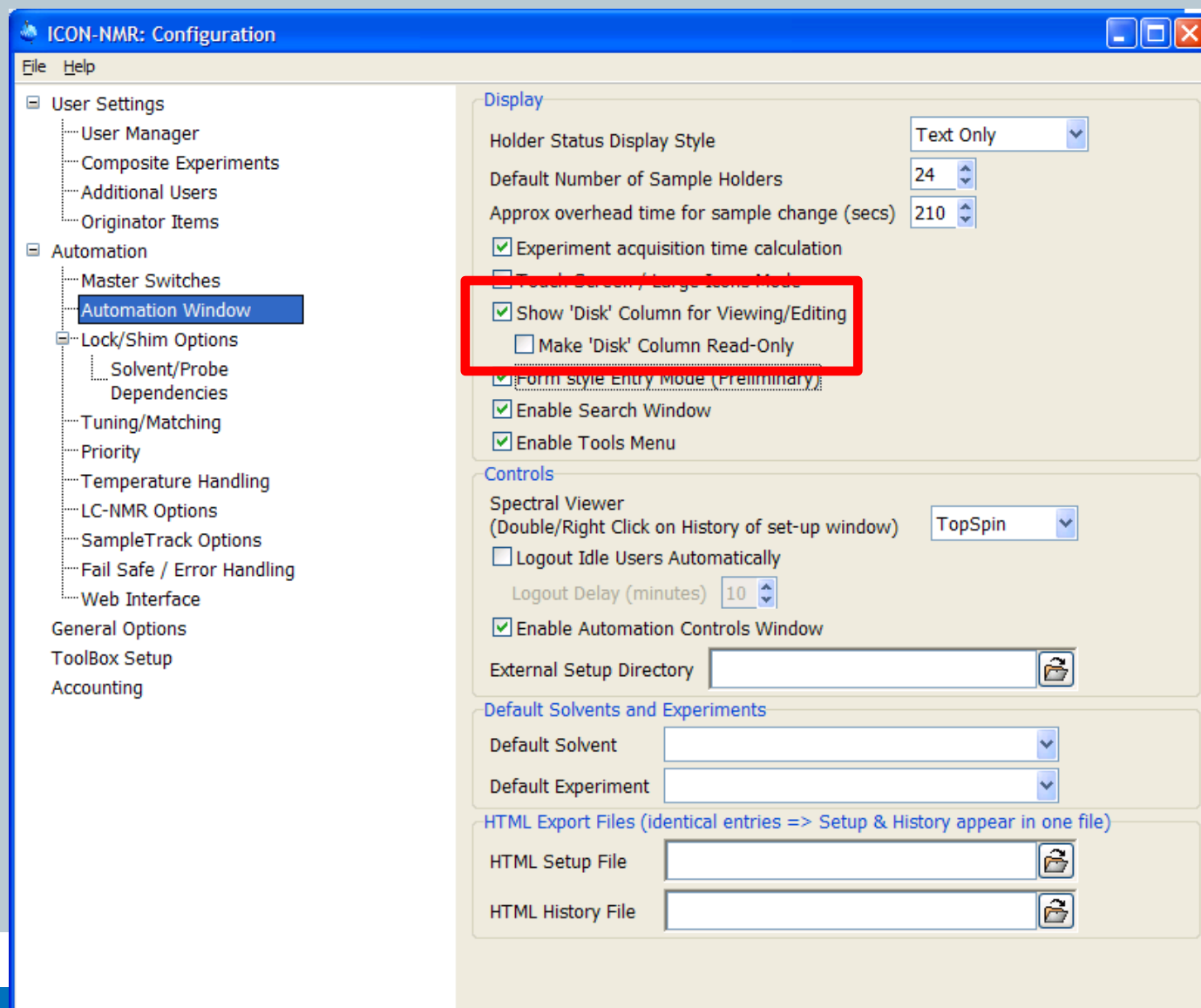


## Experimental Form Style entry mode



The screenshot displays the ICON-NMR 4.2 software interface. A dialog box titled "Carousel Position" is open, prompting the user to "Please put your sample into carousel position:". The dialog features a large green square with a black number "1" in the center, indicating the required position. Below the square are "Cancel" and "OK" buttons. The background shows the "Experimental Form Style" entry mode, which includes a dropdown menu for solvent (set to "CDCl3 chloroform-d") and another dropdown for experiment (set to "C13CPD C13 exp. com"). A red box highlights the "Submit" button. Below these dropdowns are "Add" and "Copy" buttons, each with a "1" in a small box, and a "Change User" button with a question mark icon. The interface also shows a table with columns for "Solvent", "Experiment", "Par", and "Title / Orig". At the bottom, there is a search bar and a status bar with information such as "Busy until: No Jobs!", "Day Experiments: 00:00", "Night Experiments: 00:00", and "User: BRUKER\svcu".

## Disk column ... ... can be hidden optionally.



The screenshot shows the 'ICON-NMR: Configuration' window. The left sidebar contains a tree view with the following categories:

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

The main configuration area is divided into several sections:

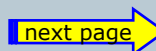
- Display**
  - Holder Status Display Style: Text Only (dropdown)
  - Default Number of Sample Holders: 24 (spinner)
  - Approx overhead time for sample change (secs): 210 (spinner)
  - Experiment acquisition time calculation
  - Touch Screen / Large Icons Mode
  - Show 'Disk' Column for Viewing/Editing (highlighted with a red box)
    - Make 'Disk' Column Read-Only
  - Form style Entry Mode (Preliminary)
  - Enable Search Window
  - Enable Tools Menu
- Controls**
  - Spectral Viewer (Double/Right Click on History of set-up window): TopSpin (dropdown)
  - Logout Idle Users Automatically
    - Logout Delay (minutes): 10 (spinner)
  - Enable Automation Controls Window
  - External Setup Directory: [text field]
- Default Solvents and Experiments**
  - Default Solvent: [dropdown]
  - Default Experiment: [dropdown]
- HTML Export Files** (identical entries => Setup & History appear in one file)
  - HTML Setup File: [text field]
  - HTML History File: [text field]



## Structure consistency check

An additional entry field may optionally be added to the Automation window where a Mol/SD file may be set which will be used on HSQC experiments to perform an automated structure consistency check.

This feature requires the Perch Software Tools.



# ICON-NMR 4.2 – structure verification aid



ICON-NMR: 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
- ToolBox Setup
- Accounting

**Run Control**

Default Automation Mode: Manual Inject/Eject

- Eject last sample in queue
- Never Rotate the Sample
- Start run at user login

**Processing Control**

- Generate a Spectrum Printout
- Process Data Sets after Acquisition: Ask on Startup
- Generate Spectrum Print-Out file in data set for possible dispatch to e-mail recipient: Off
- Perform Structure Consistency Check

**DataSet Management**

- Ignore the TopSpin Prosol Parameters
- Delete temporary datasets after experiment end
- Allow Overwrite of existing Acquisition Data

**BEST Mode Settings**

- Enable BEST-NMR
- BEST-NMR Automation Mode: Standard (No Barcodes)
- Force Solvent Change after (Number of Hours - Day Time only): 0
- BEST Administration Tool: 'bestadm'

next page

# ICON-NMR 4.2 – structure verification aid



ICON-NMR: Automation May03-2007-1433-BRUKER-svcu

File Run Holder View Find Parameters Options Help

Available 2 Available

Hol...	Type	Status	Disk	Name	No.	Solvent	Experiment	Structure/Processing	Par	Title / Orig	Pri	Time	User
1		Available	F:\	03052007-BRUKERsvc	10	CDCI3	PROTON						BRUKER\svc
		Available	F:\	03052007-BRUKERsvc	11	CDCI3	HSQCEDETGP	+	bru10059.mol				BRUKER\svc
		F2	F:\	03052007-BRUKERsvc	10								BRUKER\svc
2		Available											
3		Available											
4		Available											
5		Available											
6		Available											
7		Available											
8		Available											

Submit Cancel Edit Delete Add 1 Copy 1 Change User

Preceding Experiments

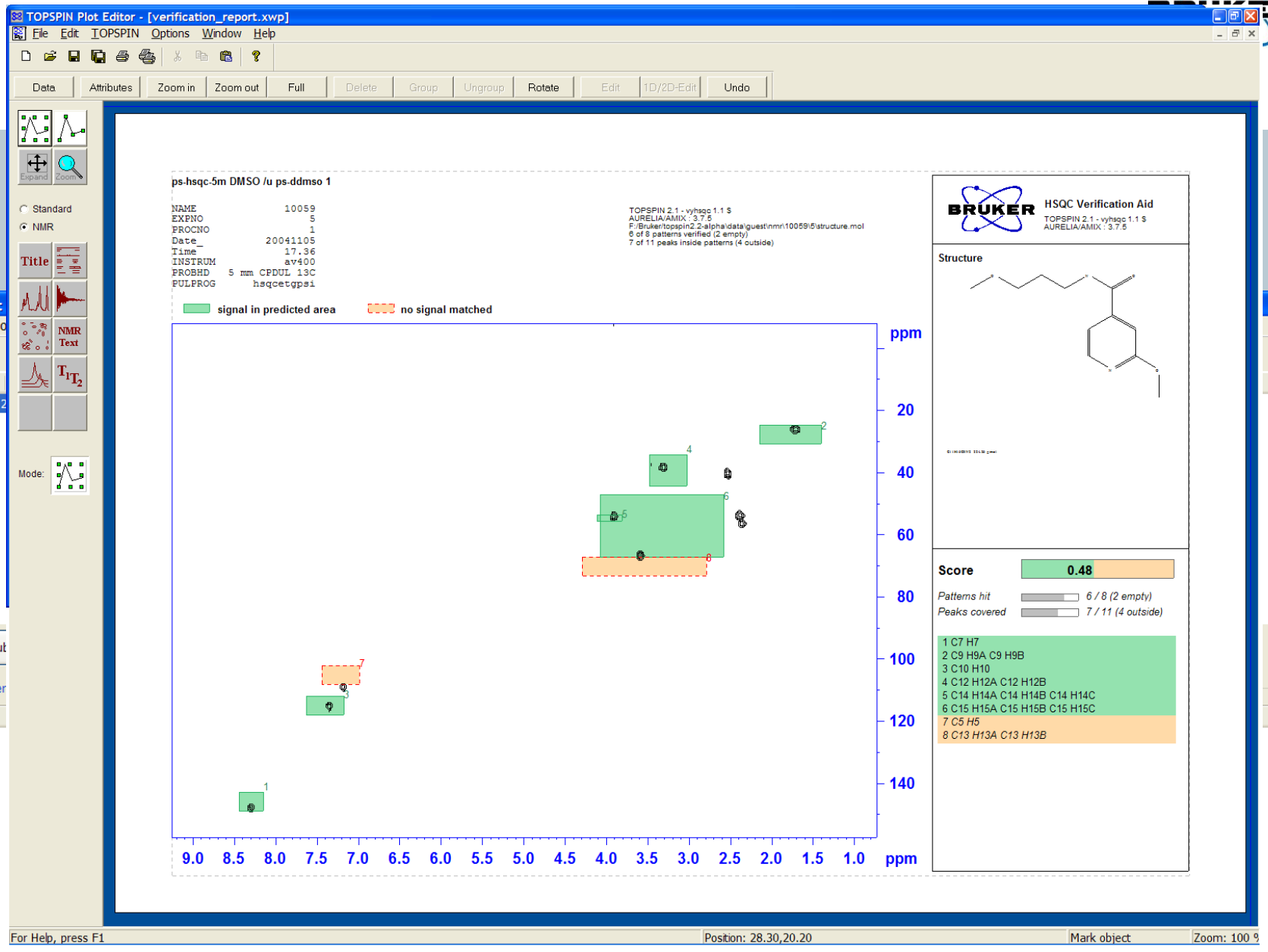
#	Date	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title / Orig	Remarks
---	------	--------	------	-----	------------	------	-----	----------	------	------	-----	------	------	------	--------------	---------

Search   search previous runs

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

next page

# ICON-NMR 4.2 – structure verification aid



ICON-NMR:

File Run Ho

Hol... Type

1 2

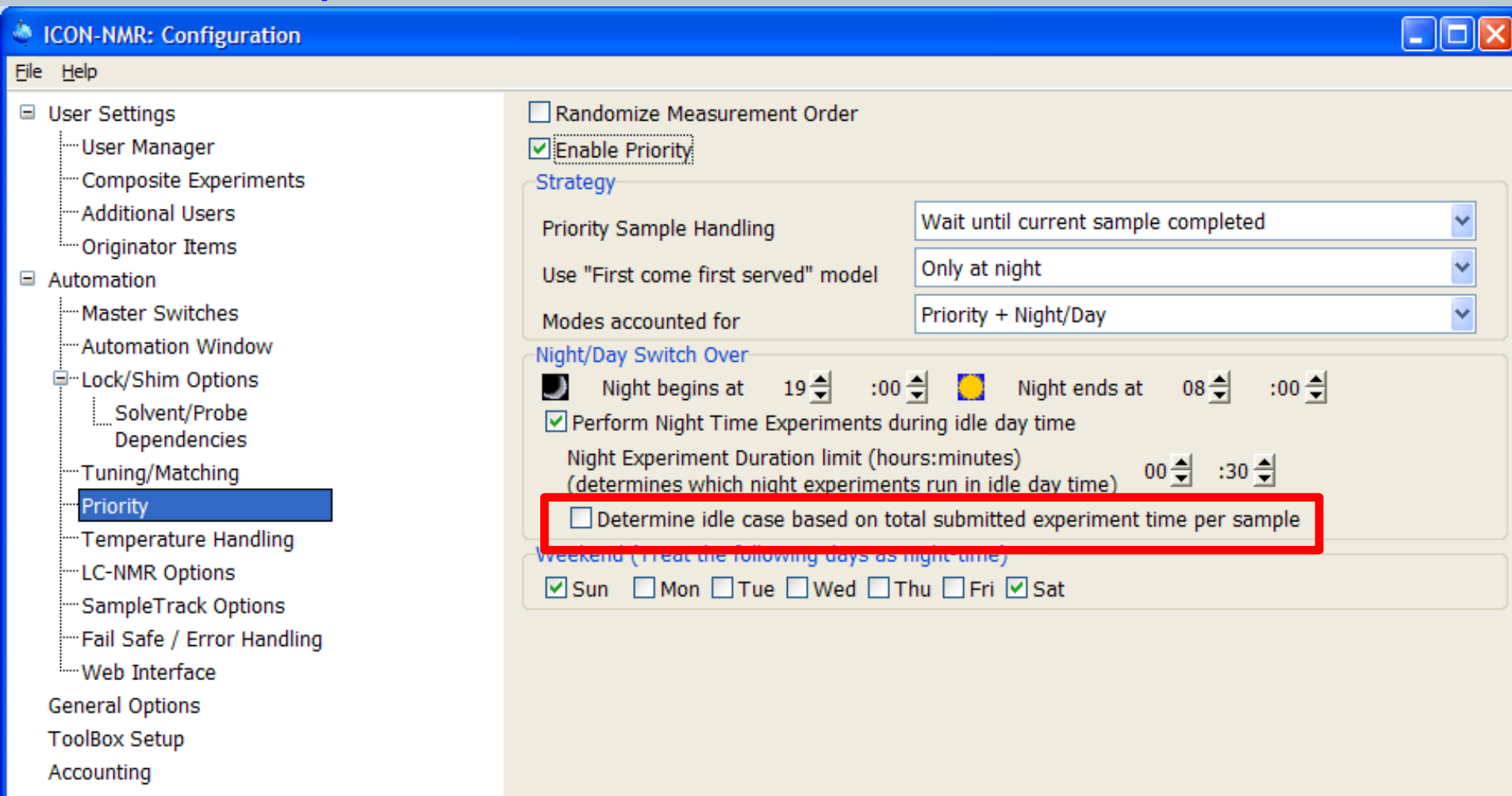
2 3 4 5 6 7 8

Sut

Change User

## Night time experiments ...

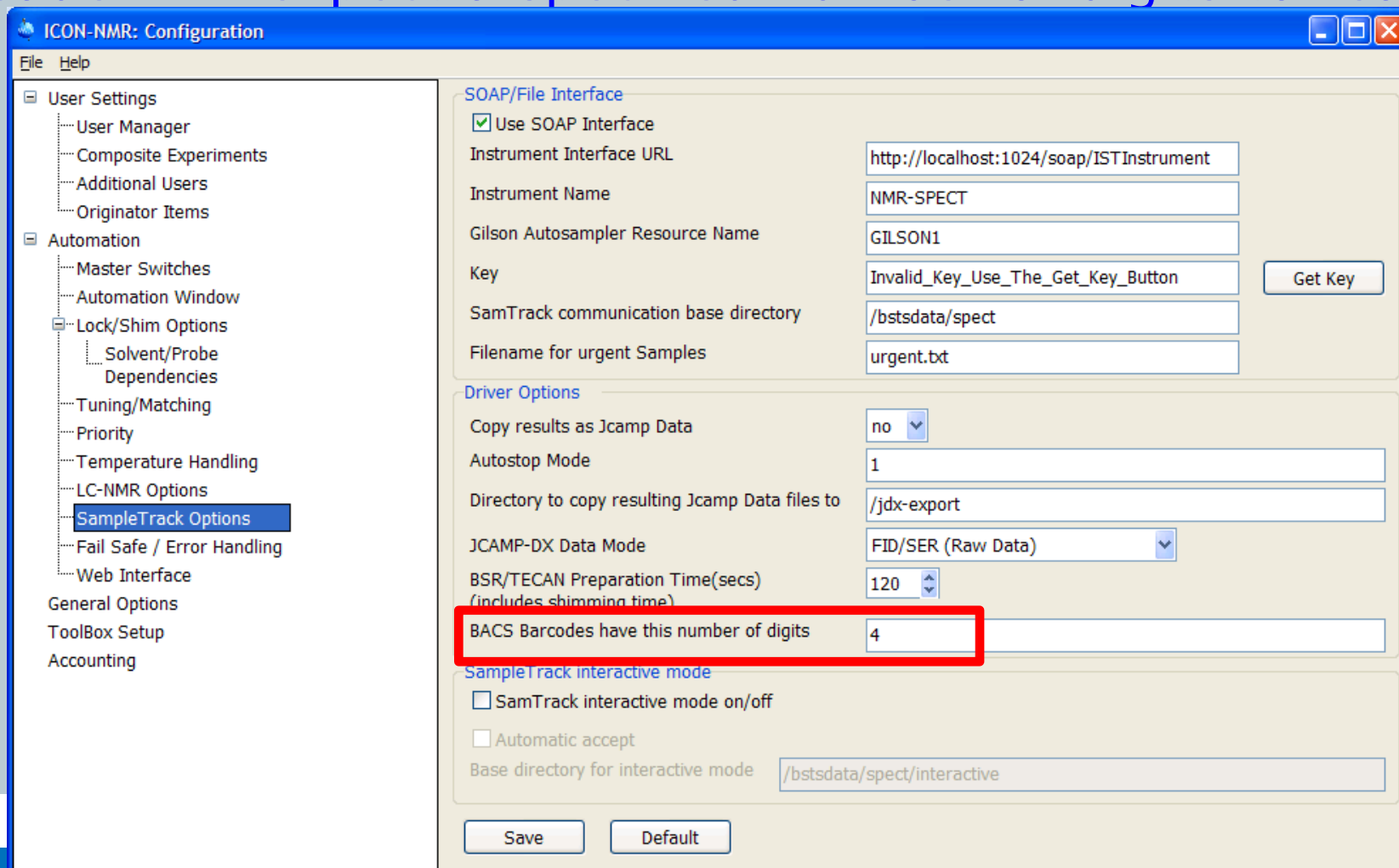
...may now be treated as single entities when determining whether they should be run in idle instrument time.



The screenshot shows the 'ICON-NMR: Configuration' window. The left sidebar contains a tree view with categories: User Settings, Automation, Lock/Shim Options, Tuning/Matching, Priority (highlighted), Temperature Handling, LC-NMR Options, SampleTrack Options, Fail Safe / Error Handling, Web Interface, General Options, ToolBox Setup, and Accounting. The main panel shows the 'Priority' settings. Under 'Strategy', 'Enable Priority' is checked. 'Priority Sample Handling' is set to 'Wait until current sample completed', 'Use "First come first served" model' is 'Only at night', and 'Modes accounted for' is 'Priority + Night/Day'. Under 'Night/Day Switch Over', 'Night begins at' is 19:00 and 'Night ends at' is 08:00. 'Perform Night Time Experiments during idle day time' is checked. 'Night Experiment Duration limit (hours:minutes) (determines which night experiments run in idle day time)' is set to 00:30. A red box highlights the checkbox 'Determine idle case based on total submitted experiment time per sample', which is currently unchecked. At the bottom, 'Weekend (Treat the following days as night time)' is checked for Sun and Sat.

## BACS bar code reader

ICON-NMR can be configured that the BACS bar code reader will expect a specified number of digits to read.



The screenshot shows the 'ICON-NMR: Configuration' window. The left sidebar contains a tree view with 'SampleTrack Options' selected. The main area is divided into sections: 'SOAP/File Interface', 'Driver Options', and 'SampleTrack interactive mode'. In the 'Driver Options' section, the 'BACS Barcodes have this number of digits' field is highlighted with a red box and contains the value '4'. Other fields include 'Instrument Interface URL', 'Instrument Name', 'GILSON1', 'Key', 'SamTrack communication base directory', 'Filename for urgent Samples', 'Copy results as Jcamp Data', 'Autostop Mode', 'Directory to copy resulting Jcamp Data files to', 'JCAMP-DX Data Mode', 'BSR/TECAN Preparation Time(secs)', and 'Base directory for interactive mode'. Buttons for 'Save' and 'Default' are at the bottom.

Section	Field	Value
SOAP/File Interface	Use SOAP Interface	<input checked="" type="checkbox"/>
	Instrument Interface URL	http://localhost:1024/soap/ISTInstrument
	Instrument Name	NMR-SPECT
	Gilson Autosampler Resource Name	GILSON1
	Key	Invalid_Key_Use_The_Get_Key_Button
	SamTrack communication base directory	/bstdata/spect
Driver Options	Filename for urgent Samples	urgent.txt
	Copy results as Jcamp Data	no
	Autostop Mode	1
	Directory to copy resulting Jcamp Data files to	/jdx-export
	JCAMP-DX Data Mode	FID/SER (Raw Data)
	BSR/TECAN Preparation Time(secs)	120
SampleTrack interactive mode	BACS Barcodes have this number of digits	4
	SamTrack interactive mode on/off	<input type="checkbox"/>
	Automatic accept	<input type="checkbox"/>
Base directory for interactive mode		/bstdata/spect/interactive





## **Toolbox/BioTools ...**

... contains a new updated default Bio Experiment definition file, with lots more experiments.



## Spreadsheet Import ...

... allows to specify that the sample position will be taken from a particular column of the sheet.



## External Setup Files ...

... may contain new keywords:

- NIGHT for night experiments and
- MOLFILE to perform the Structure Consistency Check with a particular Molfile.



## **History** of previous experiments ...

... offers new "Load" column, depicts whether a sample was inserted into the magnet correctly or not.



## Questions ...

... issuing from TopSpin may be automatically answered with an automatically generated "Cancel" click, thus preventing any Automation Lockup when no operator is present.

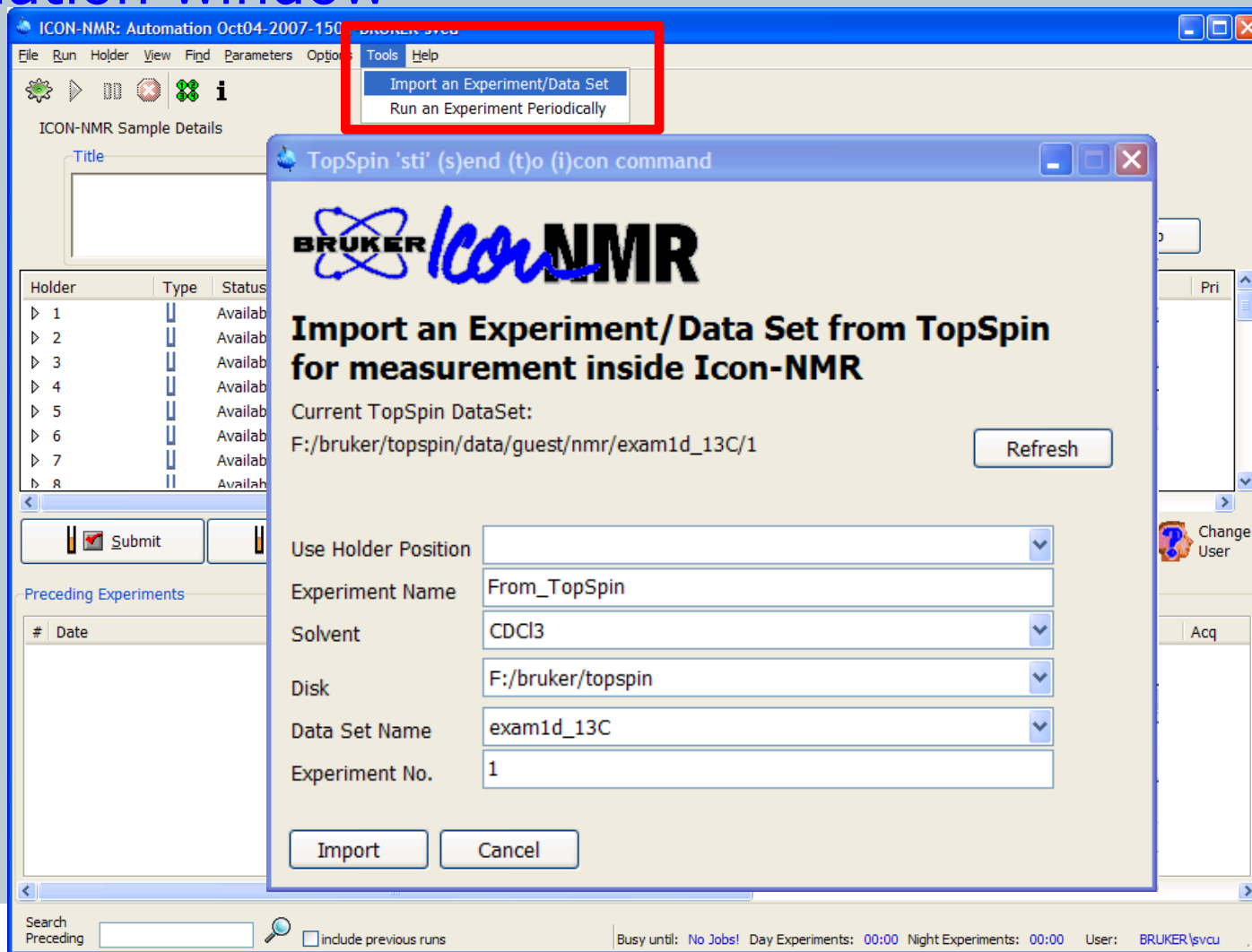


**Import any experiment/dataset** directly into the Automation window

Set up a dataset as you like it in TopSpin and have this dataset sent to Icon-Nmr for measurement inside ICON's Automation interface on any sample.

The dataset may be sent to icon directly from TopSpin using the **sti** (send to icon) command.

## Import any experiment/dataset directly into the Automation window



The screenshot displays the ICON-NMR software interface. The 'Tools' menu is highlighted with a red box, and the 'Import an Experiment/Data Set' option is selected. A dialog box titled 'TopSpin 'sti' (s)end (t)o (i)con command' is open, showing the Bruker logo and the text 'Import an Experiment/Data Set from TopSpin for measurement inside Icon-NMR'. The dialog includes a 'Refresh' button and a text field for the 'Current TopSpin DataSet' containing the path 'F:/bruker/topspin/data/guest/nmr/exam1d\_13C/1'. Below this, there are several input fields: 'Use Holder Position' (a dropdown menu), 'Experiment Name' (text field with 'From\_TopSpin'), 'Solvent' (dropdown menu with 'CDCl3'), 'Disk' (dropdown menu with 'F:/bruker/topspin'), 'Data Set Name' (dropdown menu with 'exam1d\_13C'), and 'Experiment No.' (text field with '1'). At the bottom of the dialog are 'Import' and 'Cancel' buttons. The background interface shows a table of holders with columns for Holder, Type, and Status, and a 'Submit' button.

Holder	Type	Status
1		Availab
2		Availab
3		Availab
4		Availab
5		Availab
6		Availab
7		Availab
8		Availab



## Run an experiment periodically

Up to 10 different experiments (including composites) may be queued for automatic periodic submission on any sample. Queue an experiment to run any number of times. The experiments will be submitted automatically at regular intervals and run with the priority flag set.





## Run an experiment periodically

The screenshot displays the ICON-NMR software interface. The main window, titled "ICON-NMR: Automation Oct04-2007-1453-BRUKER-svcu", has a menu bar with "Tools" and "Help". The "Tools" menu is open, showing "Import an Experiment/Data Set" and "Run an Experiment Periodically".

The "Run an Experiment Periodically" dialog box is open, showing the following settings:

- Use Holder Position: 2
- Experiment: N PROTON 1H experiment 16 s
- Number of experiments: 10
- Delay between experiment submissions: 5 Min
- Disk: F:\Bruker\topspin2.1
- Data Set Name: test-cron
- Start Expno: 10
- Solvent: CDCl3 chloroform-d
- Title: Testrun periodic experiments

The dialog box has "Start" and "Stop" buttons at the bottom.

The main application window shows a table with columns: No., Solvent, Experiment, Par, Title / Orig, Pri. Below the table is a toolbar with buttons: Edit, Delete, Add, Copy, and Change User. At the bottom of the main window, there is a status bar with the text: "Busy until: No Jobs! Day Experiments: 00:00 Night Experiments: 00:00 User: BRUKER\svcu".



## **Color/Theme support** under Linux

Change the colors used and look and feel of ICON-NMR directly from the Linux Desktop Control Panel.

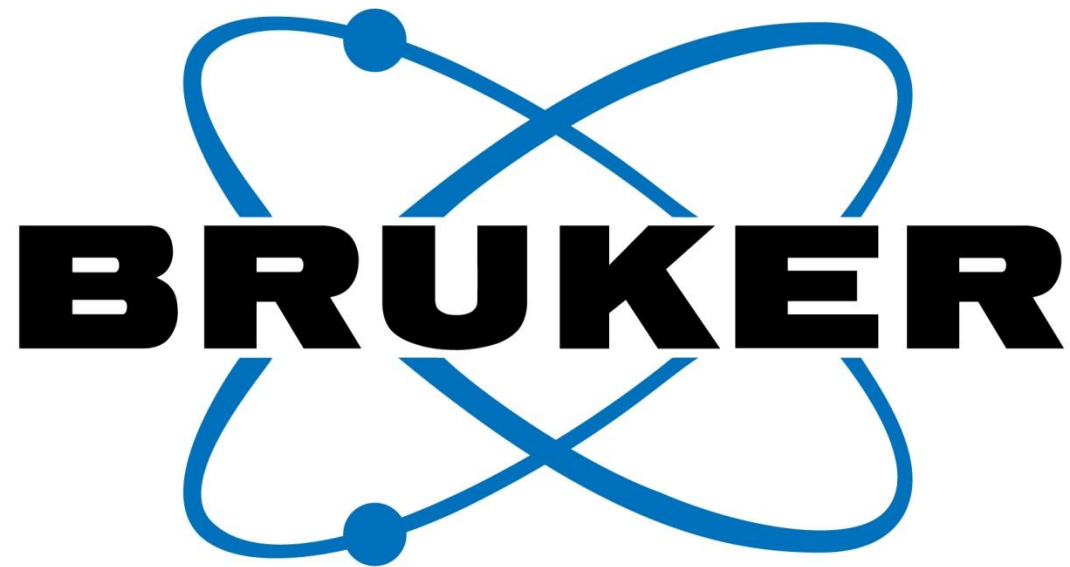
Icon will adopt the standard look and feel of other programs running under Linux.

Windows Users will also notice more conformity with the desktop settings.



## Mouse behaviour

On Microsoft Windows, the Mouse will jump to default buttons automatically when this mouse option has been activated in the "Control Panel".



[www.bruker-biospin.com](http://www.bruker-biospin.com)

# ??Picture digital resolution



**User preferences**

Administration items | Text editor for edpul, edmac, edpy, ... always in foreground

Spectrum | Setup remote systems | pdv-400 | Change

Contour plot | Configure remote access | Change

Spectrum title | Language (change requires program restart!) | English | Change

Spectrum cursor | Define right-click action on a menu item | Change

**Acquisition**

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'  Change

include spectra

Include time

Include sample temperature

Include acquisition status

Include acquisition indicator

Include lock signal

Include MAS spinning rate

Include peak power check (POWCHK) indicator

Include sample state

Include BSMS status

Include amplifier control

**Acquisition**

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'  Change

BSMS display

Auto open BSMS display

