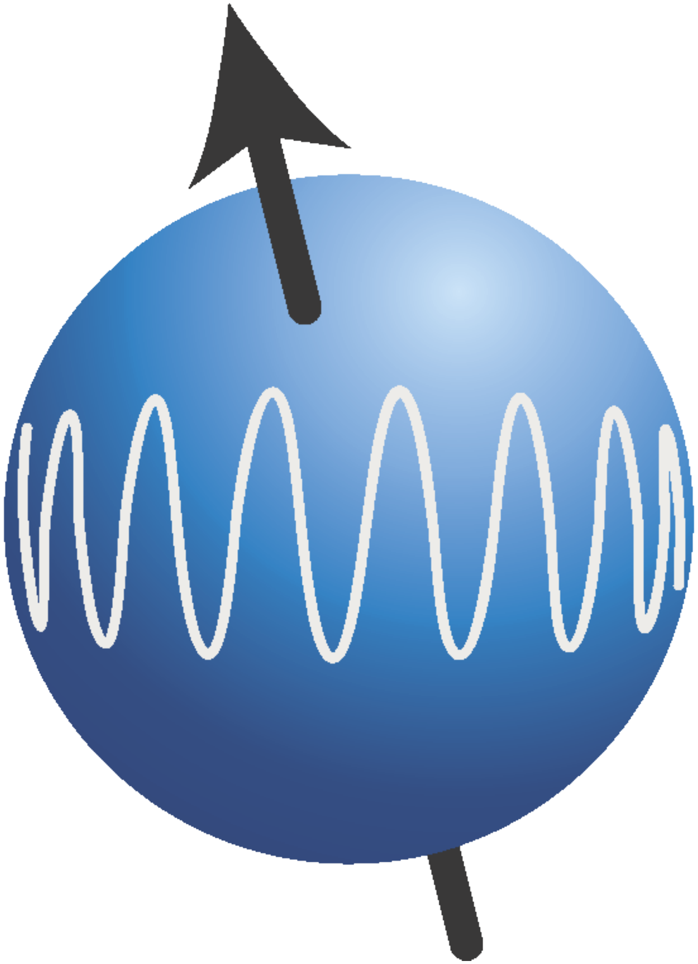


TopSpin

Data Acquisition

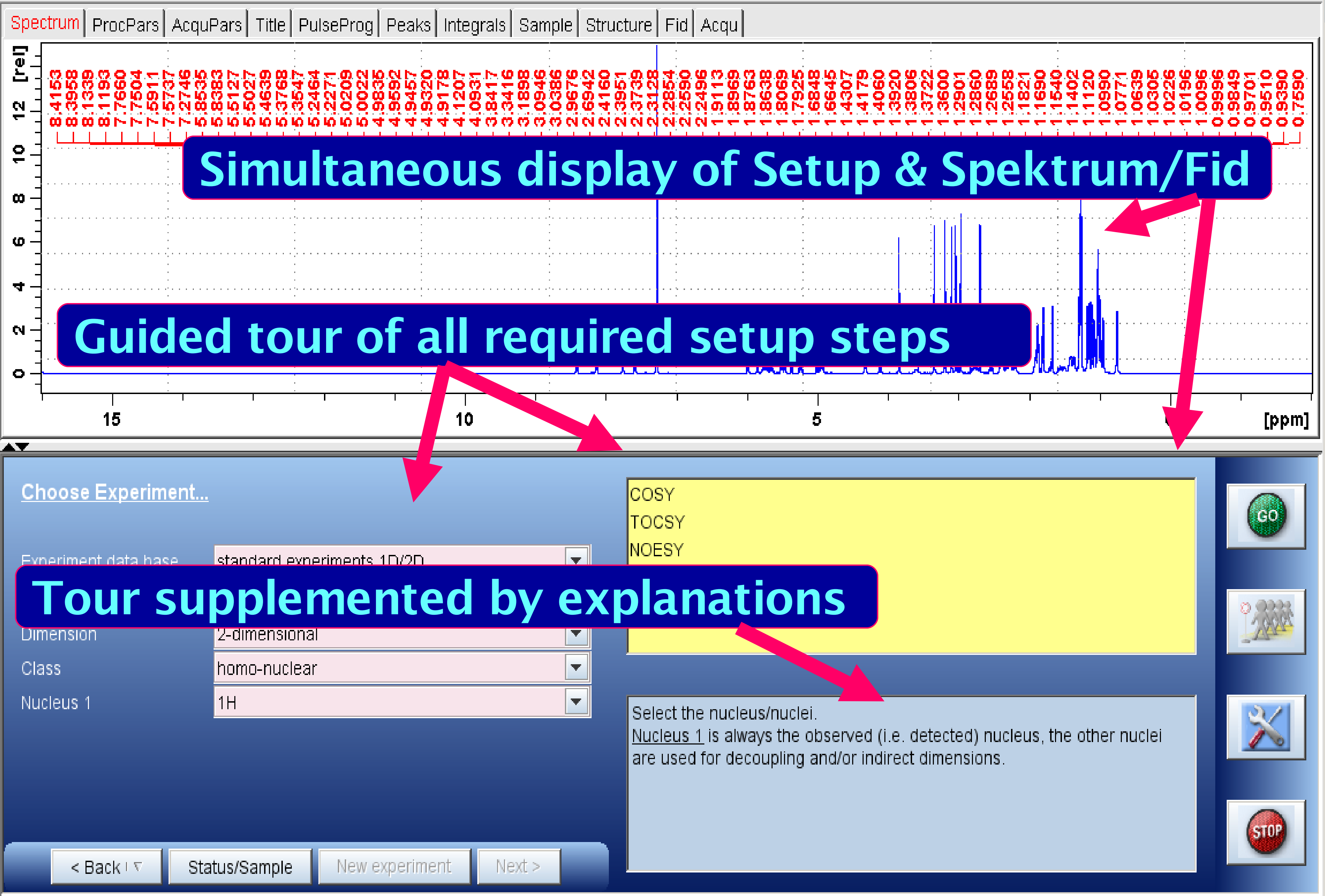
Contents

→ *Please click on a topic to view page*

Data Acquisition: *TopGuide*

- **Guided Acquisition User Interface for:**
  - *First time users*
  - *Occasional users*
  - *Routine users (may skip setup steps)*
- **Supports major 2D experiments**
- **Guarantees successful spectrum acquisition**
- **Includes data processing and plotting!**

Data Acquisition: *TopGuide*



Simultaneous display of Setup & Spektrum/Fid

Guided tour of all required setup steps

Tour supplemented by explanations

Choose Experiment...

Experiment data base: standard experiments 1D/2D

Dimension: 2-dimensional

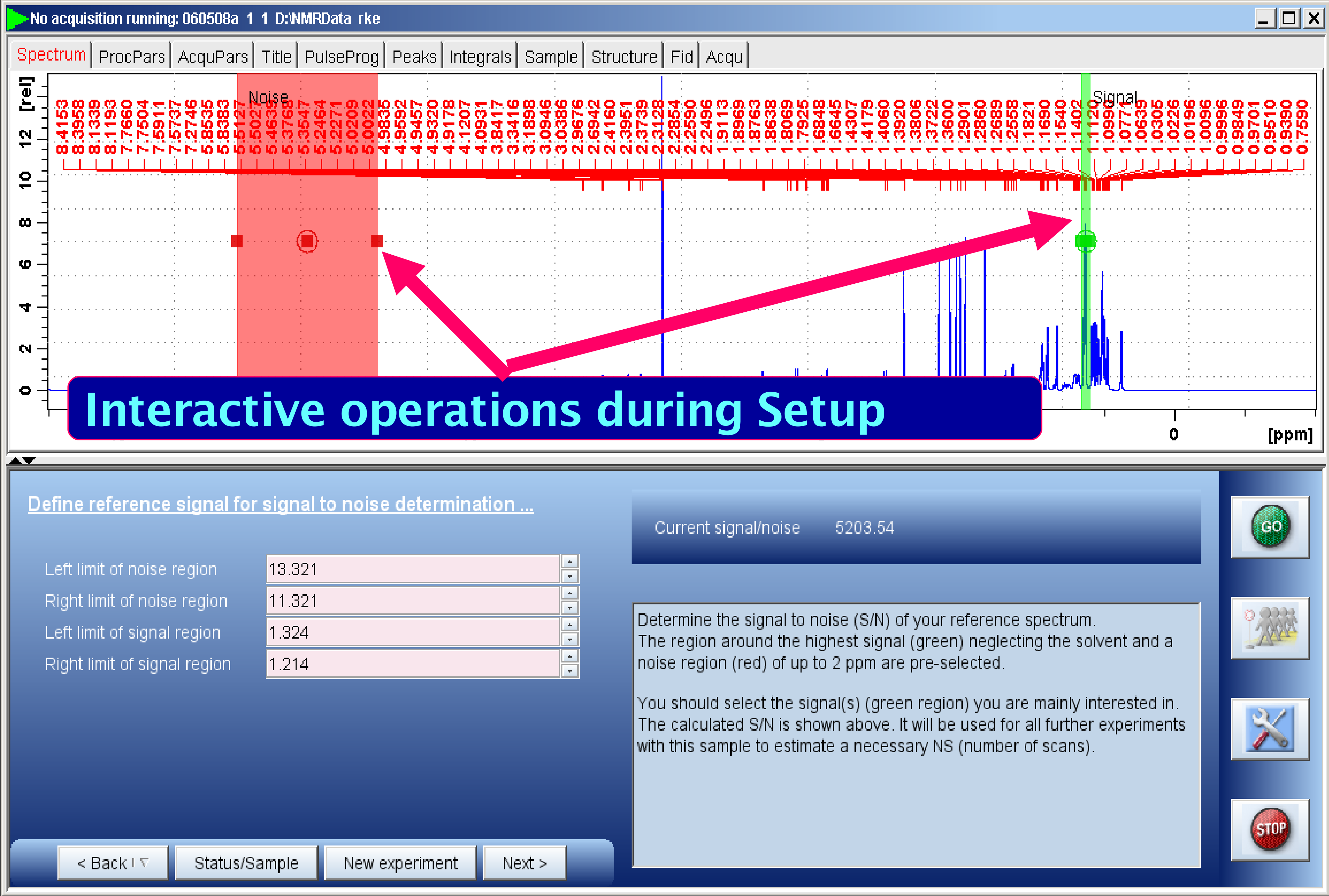
Class: homo-nuclear

Nucleus 1: 1H

COSY
TOCSY
NOESY

Select the nucleus/nuclei.
Nucleus 1 is always the observed (i.e. detected) nucleus, the other nuclei are used for decoupling and/or indirect dimensions.

Data Acquisition: *TopGuide*



No acquisition running: 060508a 1 1 D:\NMRData rke

Interactive operations during Setup

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	1.324
Right limit of signal region	1.214

Current signal/noise 5203.54

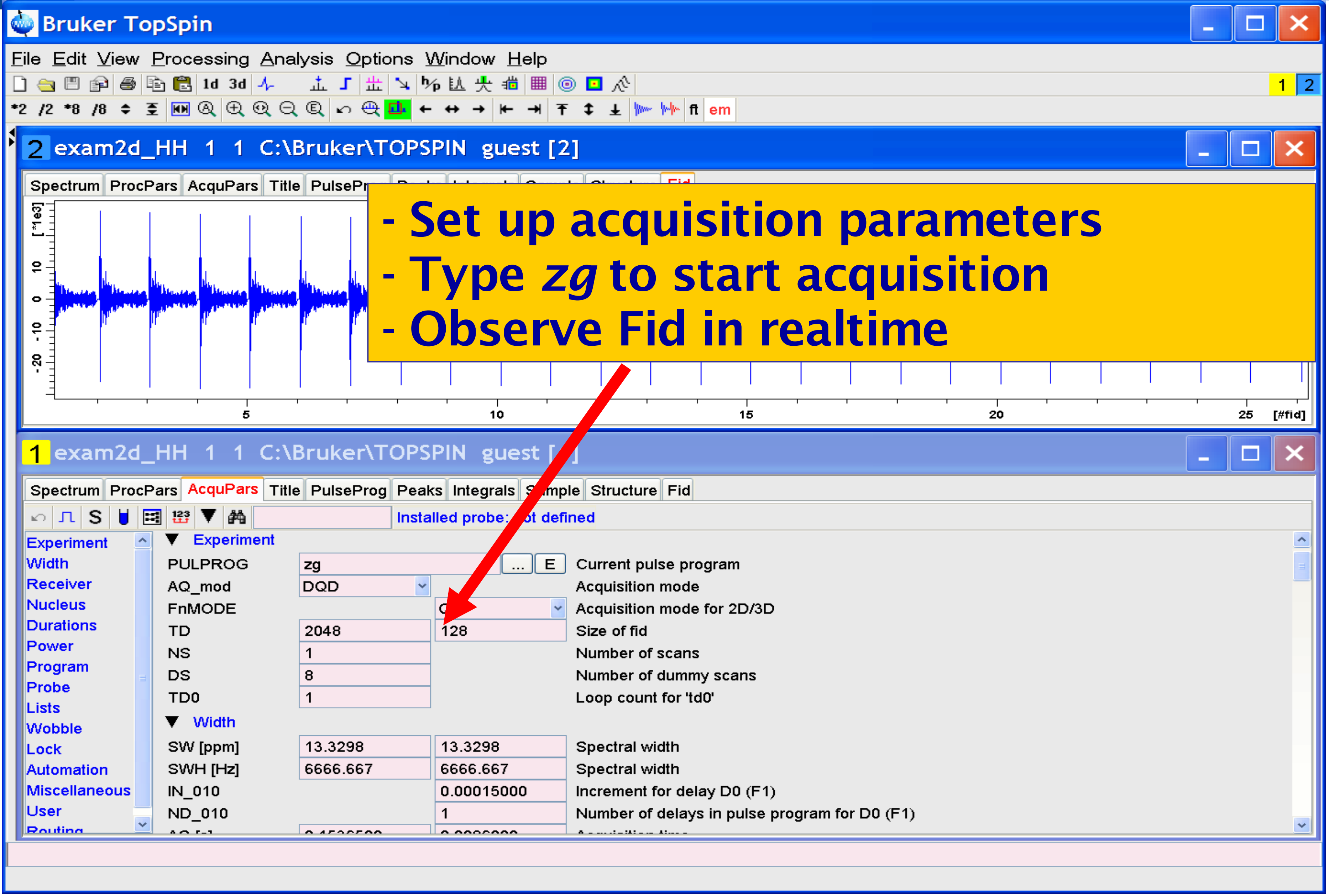
Determine the signal to noise (S/N) of your reference spectrum.
The region around the highest signal (green) neglecting the solvent and a noise region (red) of up to 2 ppm are pre-selected.

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).

Data Acquisition: *Parameter Driven*

- **User Interface for:**
  - *Routine users*
  - *Expert users*
  - *Method development*
- **Provides full flexibility and access to all software modes and hardware accessories**
- **Effective parameter optimization support**

Data Acquisition: *Parameter Driven*



- Set up acquisition parameters
- Type *zg* to start acquisition
- Observe Fid in realtime

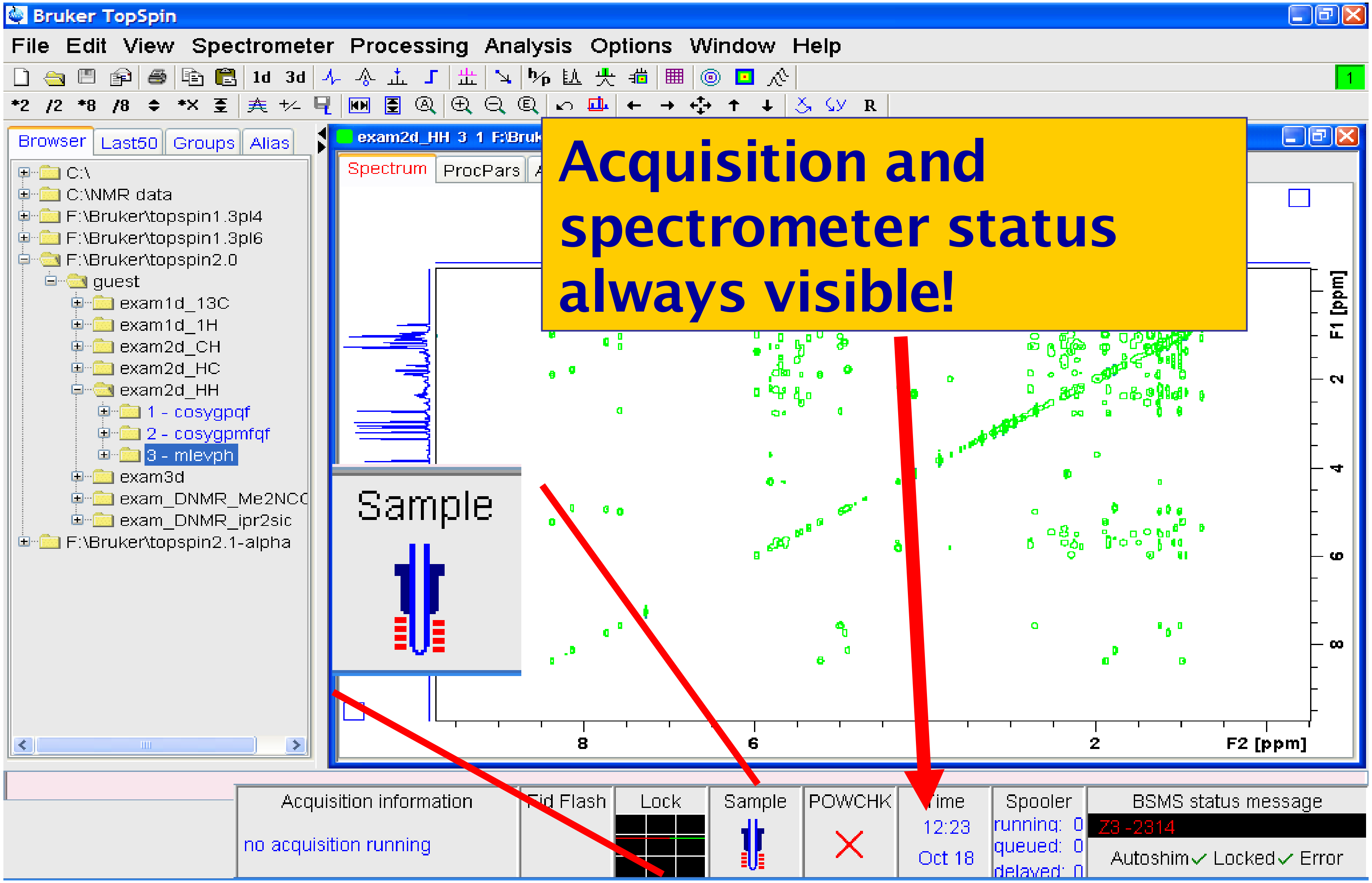
Experiment

PULPROG	zg		Current pulse program
AQ_mod	DQD		Acquisition mode
FnMODE		Q	Acquisition mode for 2D/3D
TD	2048	128	Size of fid
NS	1		Number of scans
DS	8		Number of dummy scans
TD0	1		Loop count for 'td0'

Width

SW [ppm]	13.3298	13.3298	Spectral width
SWH [Hz]	6666.667	6666.667	Spectral width
IN_010		0.00015000	Increment for delay D0 (F1)
ND_010		1	Number of delays in pulse program for D0 (F1)
]

Data Acquisition: *Acquisition Status Panel*



Acquisition and spectrometer status always visible!

Acquisition information: no acquisition running

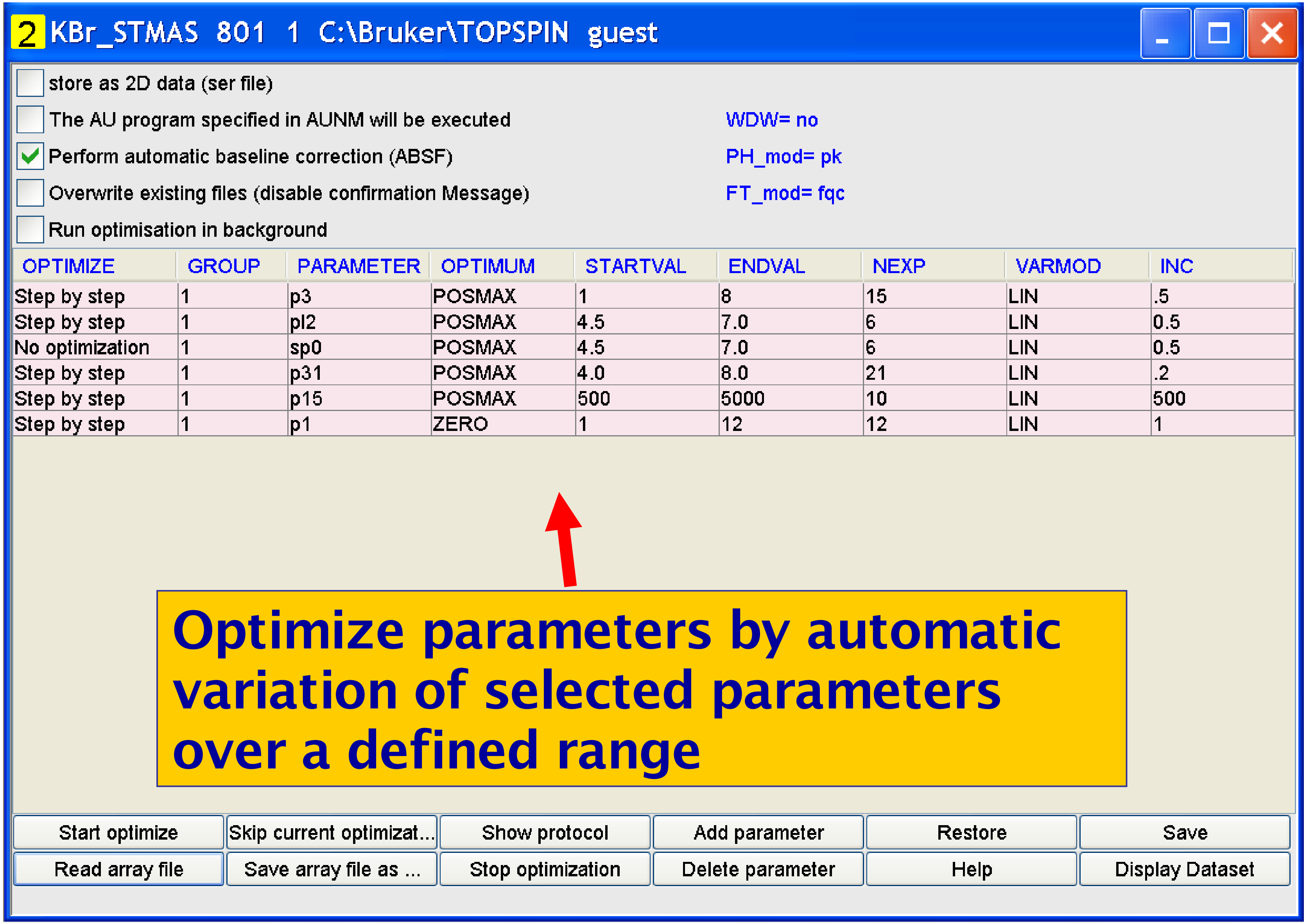
Time: 12:23 Oct 18

Spooler: running: 0 queued: 0 delayed: 0

BSMS status message: Z3 -2314

Autoshim✓ Locked✓ Error

Data Acquisition: *Parameter Optimization*



☐ store as 2D data (ser file)

☐ The AU program specified in AUNM will be executed

☑ Perform automatic baseline correction (ABSF)

☐ Overwrite existing files (disable confirmation Message)

☐ Run optimisation in background

WDW= no

PH_mod= pk

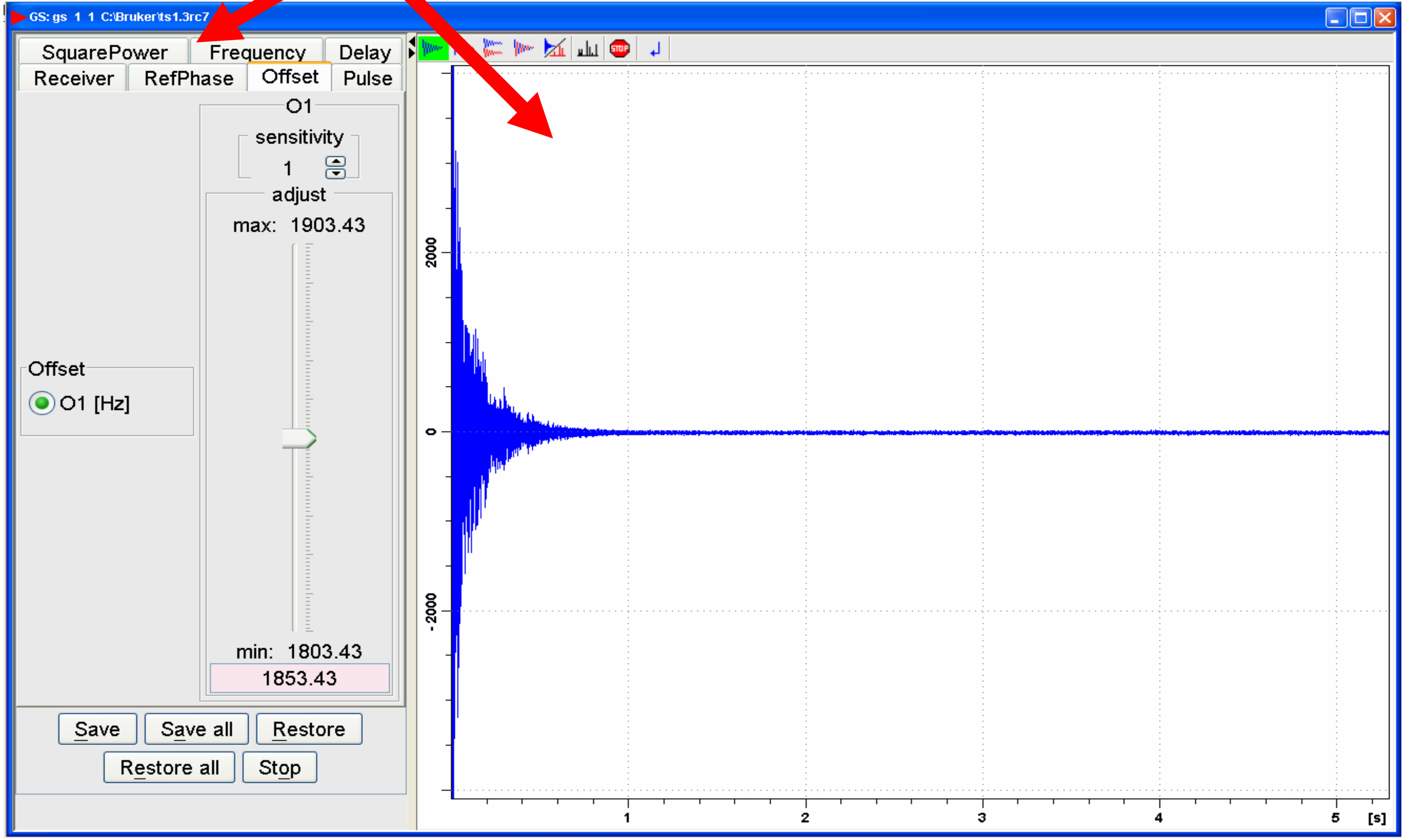
FT_mod= fqc

OPTIMIZE	GROUP	PARAMETER	OPTIMUM	STARTVAL	ENDVAL	NEXP	VARMOD	INC
Step by step	1	p3	POSMAX	1	8	15	LIN	.5
Step by step	1	pl2	POSMAX	4.5	7.0	6	LIN	0.5
No optimization	1	sp0	POSMAX	4.5	7.0	6	LIN	0.5
Step by step	1	p31	POSMAX	4.0	8.0	21	LIN	.2
Step by step	1	p15	POSMAX	500	5000	10	LIN	500
Step by step	1	p1	ZERO	1	12	12	LIN	1

Optimize parameters by automatic variation of selected parameters over a defined range

Data Acquisition: *Parameter Optimization*

Interactive parameter optimization: Adjust parameters and watch the effect on fid or spectrum



GS: gs 1 1 C:\Bruker\ts1.3rc7

Offset

● O1 [Hz]

O1

sensitivity 1

adjust

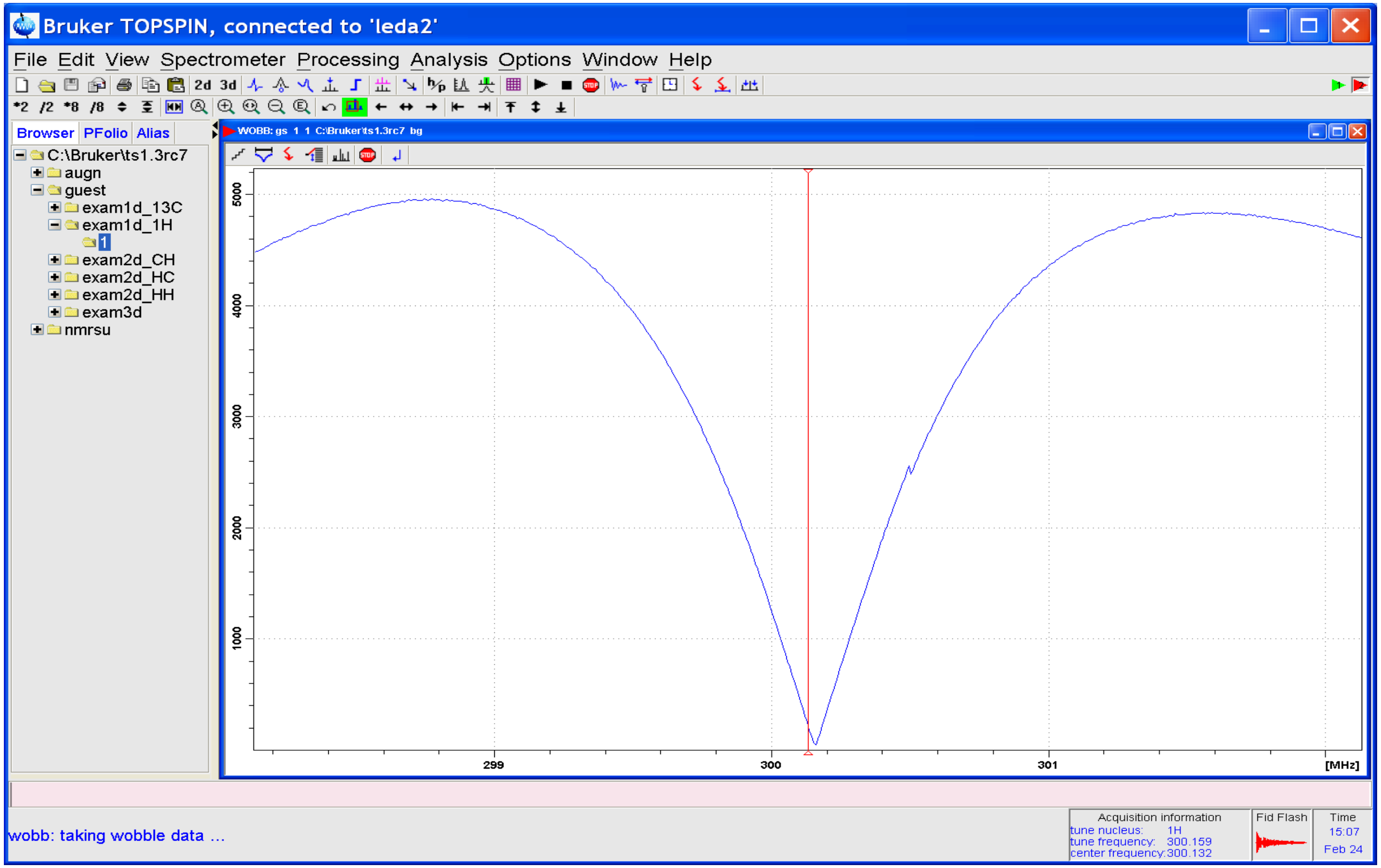
max: 1903.43

min: 1803.43

1853.43

Data Acquisition: *Parameter Optimization*

Optimization of wobble curve during manual tuning and matching



wobb: taking wobble data ...

Acquisition information

tune nucleus: 1H
tune frequency: 300.159
center frequency: 300.132

Time

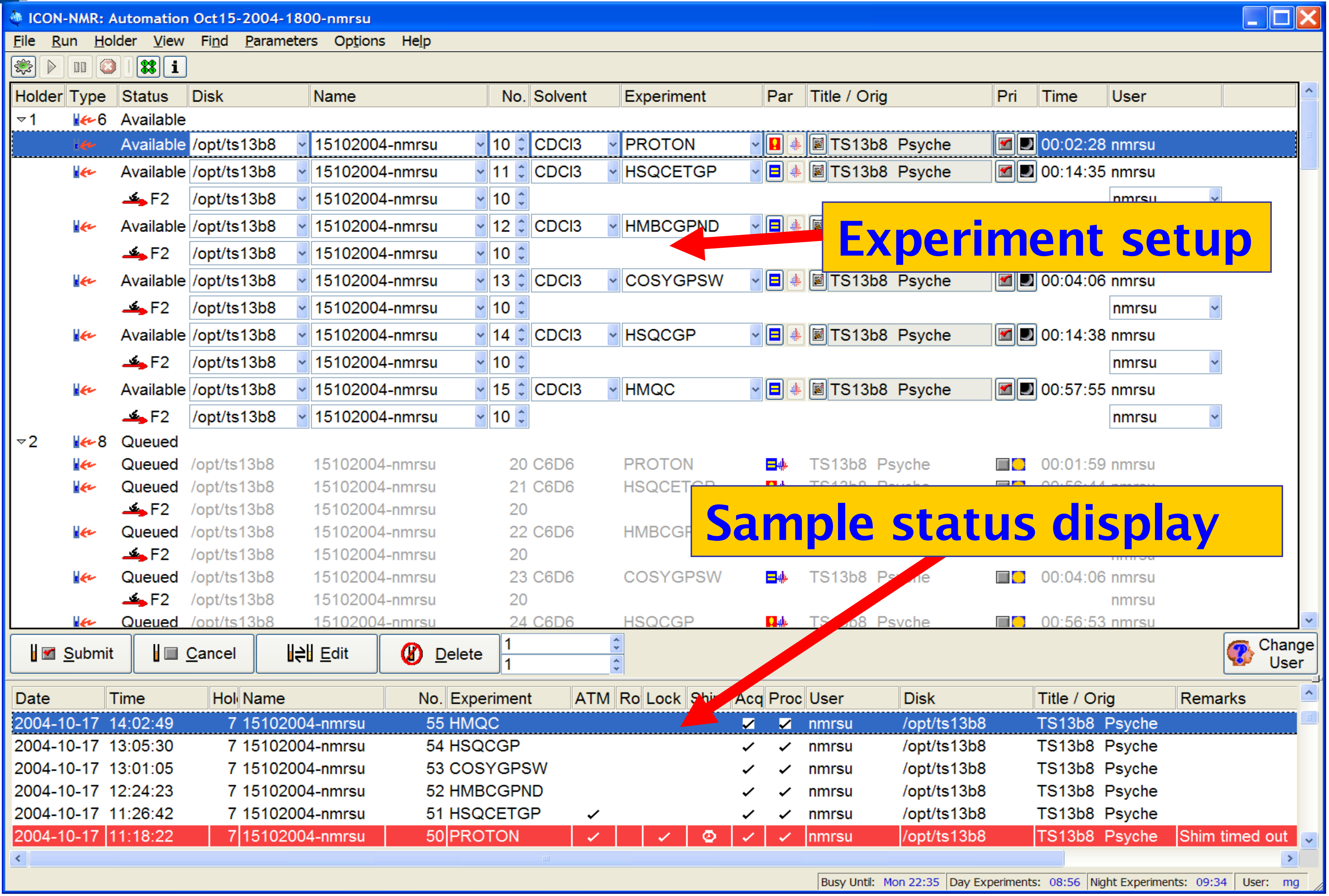
15:07
Feb 24

Automation Interface: *IconNmr*

Graphical user interface for fully automated acquisition and processing

- **Supports sample changers and preparation robots**
- **Configurable 1-click experiment setup**
- **Multi-user support, routine users, walk-up users**
- **Spreadsheet import**
- **Priority sample support**
- **WEB interface for remote setup, incl. small screen Pocket PC support**

Automation Interface : *IconNmr*



Holder	Type	Status	Disk	Name	No.	Solvent	Experiment	Par	Title / Orig	Pri	Time	User
1	6	Available										
		Available	/opt/ts13b8	15102004-nmrsu	10	CDCl3	PROTON		TS13b8 Psyche		00:02:28	nmrsu
		Available	/opt/ts13b8	15102004-nmrsu	11	CDCl3	HSQCETGP		TS13b8 Psyche		00:14:35	nmrsu
	F2		/opt/ts13b8	15102004-nmrsu	10							nmrsu
		Available	/opt/ts13b8	15102004-nmrsu	12	CDCl3	HMBCGPND					
	F2		/opt/ts13b8	15102004-nmrsu	10							
		Available	/opt/ts13b8	15102004-nmrsu	13	CDCl3	COSYGPSW		TS13b8 Psyche		00:04:06	nmrsu
	F2		/opt/ts13b8	15102004-nmrsu	10							nmrsu
		Available	/opt/ts13b8	15102004-nmrsu	14	CDCl3	HSQCGP		TS13b8 Psyche		00:14:38	nmrsu
	F2		/opt/ts13b8	15102004-nmrsu	10							nmrsu
		Available	/opt/ts13b8	15102004-nmrsu	15	CDCl3	HMQC		TS13b8 Psyche		00:57:55	nmrsu
	F2		/opt/ts13b8	15102004-nmrsu	10							nmrsu
2	8	Queued										
		Queued	/opt/ts13b8	15102004-nmrsu	20	C6D6	PROTON		TS13b8 Psyche		00:01:59	nmrsu
		Queued	/opt/ts13b8	15102004-nmrsu	21	C6D6	HSQCETGP		TS13b8 Psyche		00:56:44	nmrsu
	F2		/opt/ts13b8	15102004-nmrsu	20							
		Queued	/opt/ts13b8	15102004-nmrsu	22	C6D6	HMBCGP					
	F2		/opt/ts13b8	15102004-nmrsu	20							nmrsu
		Queued	/opt/ts13b8	15102004-nmrsu	23	C6D6	COSYGPSW		TS13b8 Psyche		00:04:06	nmrsu
	F2		/opt/ts13b8	15102004-nmrsu	20							nmrsu
		Queued	/opt/ts13b8	15102004-nmrsu	24	C6D6	HSQCGP		TS13b8 Psyche		00:56:53	nmrsu

Experiment setup

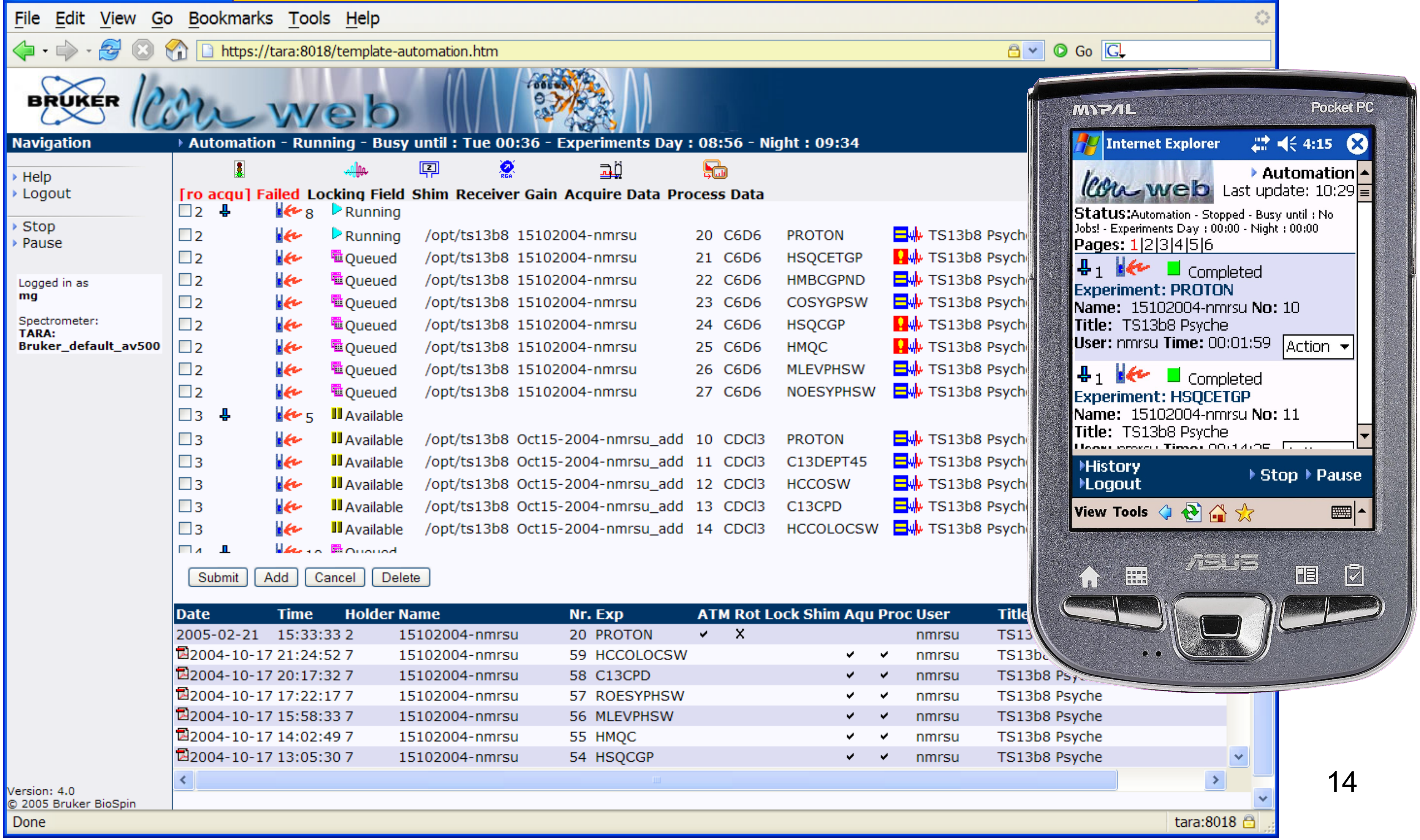
Sample status display

Date	Time	Hol	Name	No.	Experiment	ATM	Ro	Lock	Shi	Acq	Proc	User	Disk	Title / Orig	Remarks
2004-10-17	14:02:49	7	15102004-nmrsu	55	HMQC					✓	✓	nmrsu	/opt/ts13b8	TS13b8 Psyche	
2004-10-17	13:05:30	7	15102004-nmrsu	54	HSQCGP					✓	✓	nmrsu	/opt/ts13b8	TS13b8 Psyche	
2004-10-17	13:01:05	7	15102004-nmrsu	53	COSYGPSW					✓	✓	nmrsu	/opt/ts13b8	TS13b8 Psyche	
2004-10-17	12:24:23	7	15102004-nmrsu	52	HMBCGPND					✓	✓	nmrsu	/opt/ts13b8	TS13b8 Psyche	
2004-10-17	11:26:42	7	15102004-nmrsu	51	HSQCETGP	✓				✓	✓	nmrsu	/opt/ts13b8	TS13b8 Psyche	
2004-10-17	11:18:22	7	15102004-nmrsu	50	PROTON	✓		✓	⊗	✓	✓	nmrsu	/opt/ts13b8	TS13b8 Psyche	Shim timed out

Busy Until: Mon 22:35 | Day Experiments: 08:56 | Night Experiments: 09:34 | User: mg

Automation Interface: *IconNmr*

Experiment setup via WEB browser using PC or Pocket PC



Automation - Running - Busy until : Tue 00:36 - Experiments Day : 08:56 - Night : 09:34

Logged in as **mg**

Spectrometer: **TARA: Bruker_default_av500**

[ro acqu] Failed Locking Field Shim Receiver Gain Acquire Data Process Data

☐2	8	Running						
☐2		Running	/opt/ts13b8	15102004-nmrsu	20	C6D6	PROTON	TS13b8 Psych
☐2		Queued	/opt/ts13b8	15102004-nmrsu	21	C6D6	HSQCETGP	TS13b8 Psych
☐2		Queued	/opt/ts13b8	15102004-nmrsu	22	C6D6	HMBCGPND	TS13b8 Psych
☐2		Queued	/opt/ts13b8	15102004-nmrsu	23	C6D6	COSYGPSW	TS13b8 Psych
☐2		Queued	/opt/ts13b8	15102004-nmrsu	24	C6D6	HSQCGP	TS13b8 Psych
☐2		Queued	/opt/ts13b8	15102004-nmrsu	25	C6D6	HMQC	TS13b8 Psych
☐2		Queued	/opt/ts13b8	15102004-nmrsu	26	C6D6	MLEVPHSW	TS13b8 Psych
☐2		Queued	/opt/ts13b8	15102004-nmrsu	27	C6D6	NOESYPHSW	TS13b8 Psych
☐3	5	Available						
☐3		Available	/opt/ts13b8	Oct15-2004-nmrsu_add	10	CDCl3	PROTON	TS13b8 Psych
☐3		Available	/opt/ts13b8	Oct15-2004-nmrsu_add	11	CDCl3	C13DEPT45	TS13b8 Psych
☐3		Available	/opt/ts13b8	Oct15-2004-nmrsu_add	12	CDCl3	HCCOSW	TS13b8 Psych
☐3		Available	/opt/ts13b8	Oct15-2004-nmrsu_add	13	CDCl3	C13CPD	TS13b8 Psych
☐3		Available	/opt/ts13b8	Oct15-2004-nmrsu_add	14	CDCl3	HCCOLOCSW	TS13b8 Psych
☐4	10	Queued						

Date	Time	Holder	Name	Nr.	Exp	ATM	Rot	Lock	Shim	Aqu	Proc	User	Title
2005-02-21	15:33:33	2	15102004-nmrsu	20	PROTON	✓	X					nmrsu	TS13
2004-10-17	21:24:52	7	15102004-nmrsu	59	HCCOLOCSW					✓	✓	nmrsu	TS13b
2004-10-17	20:17:32	7	15102004-nmrsu	58	C13CPD					✓	✓	nmrsu	TS13b8 Ps
2004-10-17	17:22:17	7	15102004-nmrsu	57	ROESYPHSW					✓	✓	nmrsu	TS13b8 Psyche
2004-10-17	15:58:33	7	15102004-nmrsu	56	MLEVPHSW					✓	✓	nmrsu	TS13b8 Psyche
2004-10-17	14:02:49	7	15102004-nmrsu	55	HMQC					✓	✓	nmrsu	TS13b8 Psyche
2004-10-17	13:05:30	7	15102004-nmrsu	54	HSQCGP					✓	✓	nmrsu	TS13b8 Psyche

Version: 4.0
© 2005 Bruker BioSpin

Last update: 10:29

Status: Automation - Stopped - Busy until : No Jobs! - Experiments Day : 00:00 - Night : 00:00

Pages: 1|2|3|4|5|6

1 Completed

Experiment: PROTON

Name: 15102004-nmrsu **No:** 10

Title: TS13b8 Psyche

User: nmrsu **Time:** 00:01:59

1 Completed

Experiment: HSQCETGP

Name: 15102004-nmrsu **No:** 11

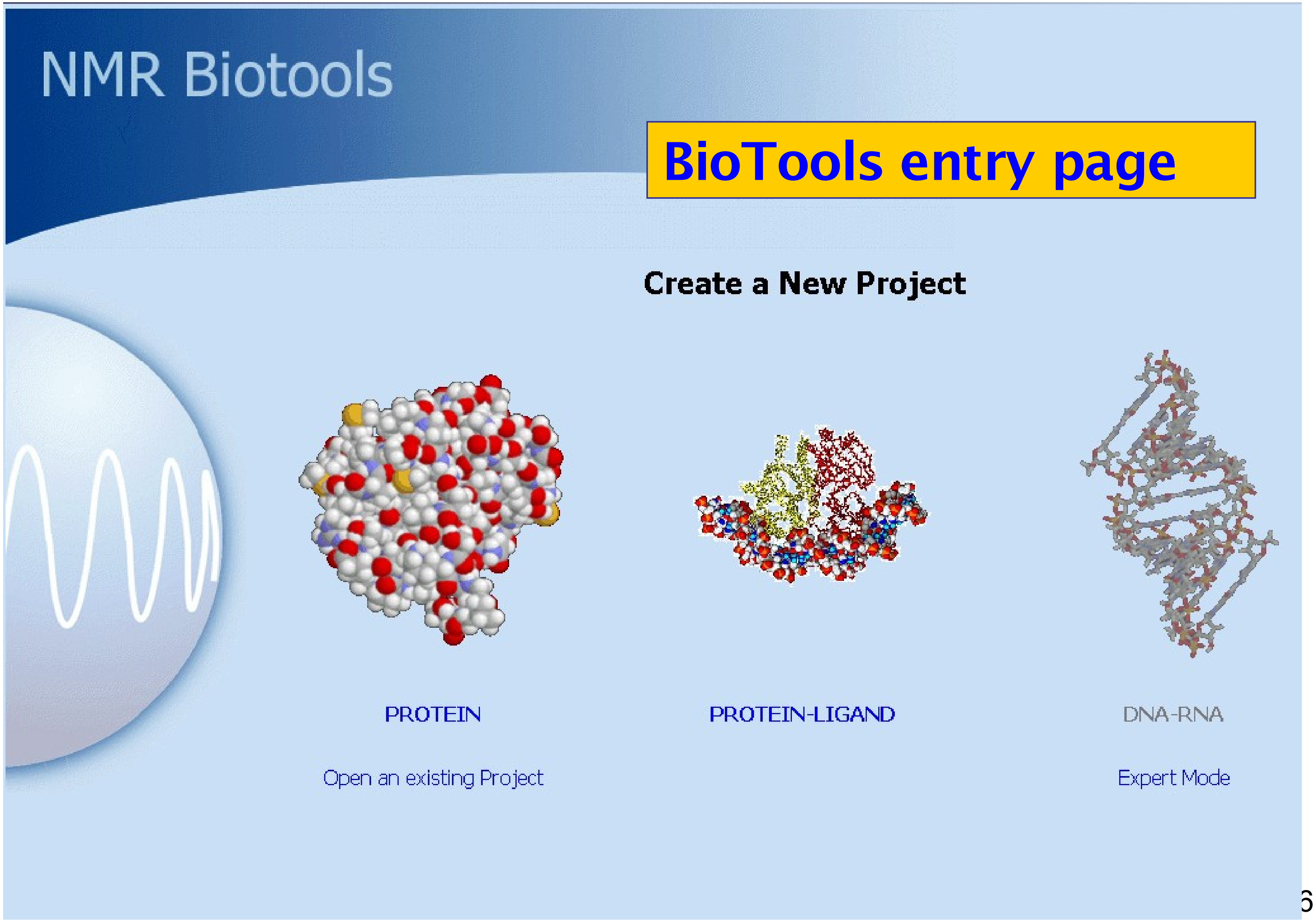
Title: TS13b8 Psyche

Spectra of Biomolecules: *BioTools*

Acquisition user interface tailored for biological applications such as protein structure determination or studying protein-ligand bindings

- **Guided macro-molecule multi-experiment acquisition**
- **Automatic acquisition optimization**
- **1-click multi-acquisition launch**
- **Quick screen / scout spectral overview mode**
- **Experiment tree / operation adaptable via IconNmr.**

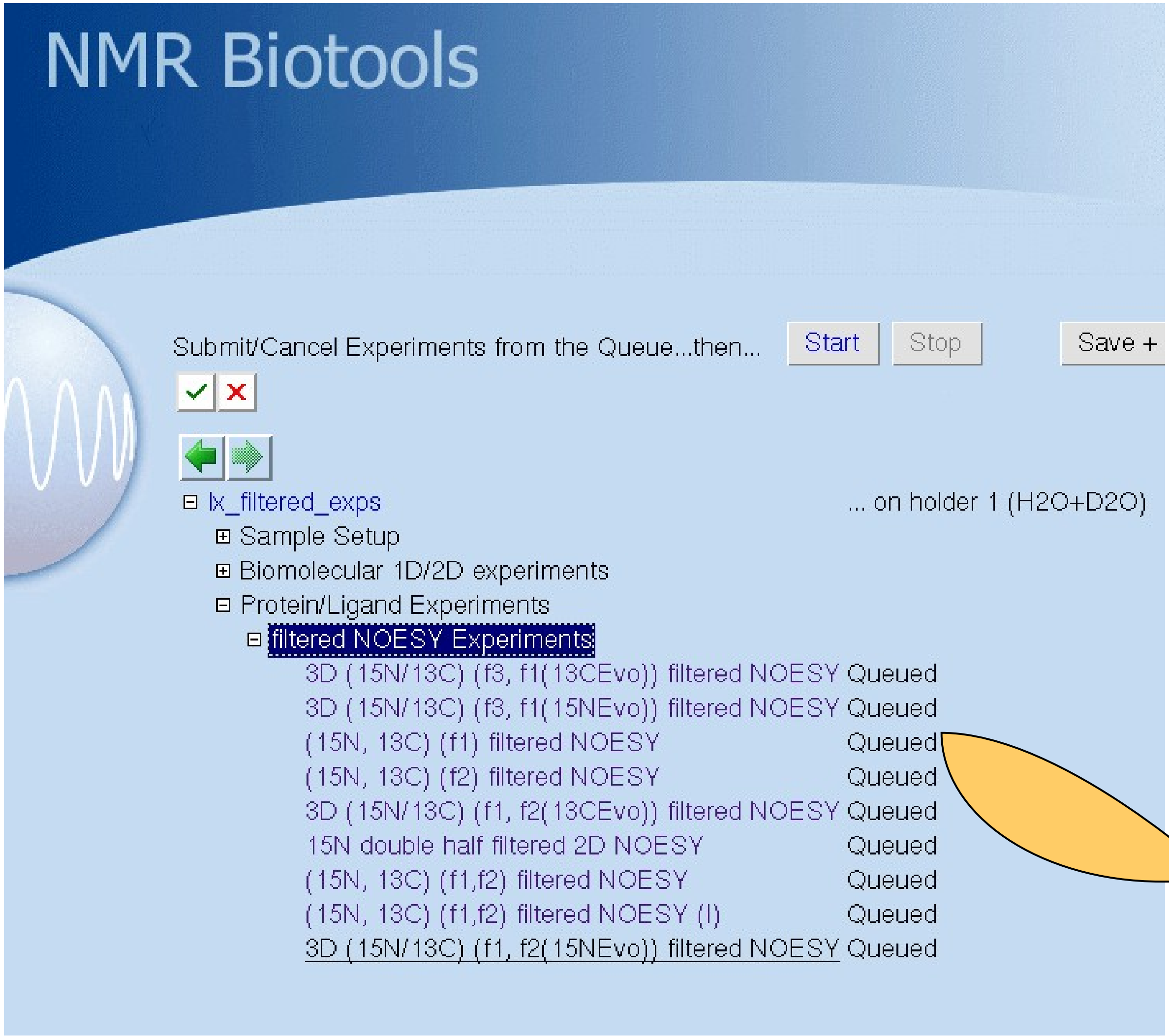
Spectra of Biomolecules: *BioTools*



BioTools entry page

Spectra of Biomolecules: *BioTools*

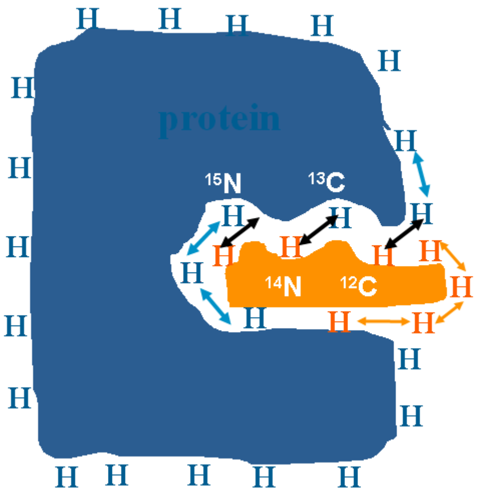
Experiment tree for protein-ligand studies



Submit/Cancel Experiments from the Queue...then...

⊟ lx_filtered_exps ... on holder 1 (H2O+D2O)
- ⊞ Sample Setup
- ⊞ Biomolecular 1D/2D experiments
- ⊟ Protein/Ligand Experiments
  - ⊟ filtered NOESY Experiments

3D (15N/13C) (f3, f1(13CEvo)) filtered NOESY	Queued
3D (15N/13C) (f3, f1(15NEvo)) filtered NOESY	Queued
(15N, 13C) (f1) filtered NOESY	Queued
(15N, 13C) (f2) filtered NOESY	Queued
3D (15N/13C) (f1, f2(13CEvo)) filtered NOESY	Queued
15N double half filtered 2D NOESY	Queued
(15N, 13C) (f1,f2) filtered NOESY	Queued
(15N, 13C) (f1,f2) filtered NOESY (I)	Queued
3D (15N/13C) (f1, f2(15NEvo)) filtered NOESY	Queued



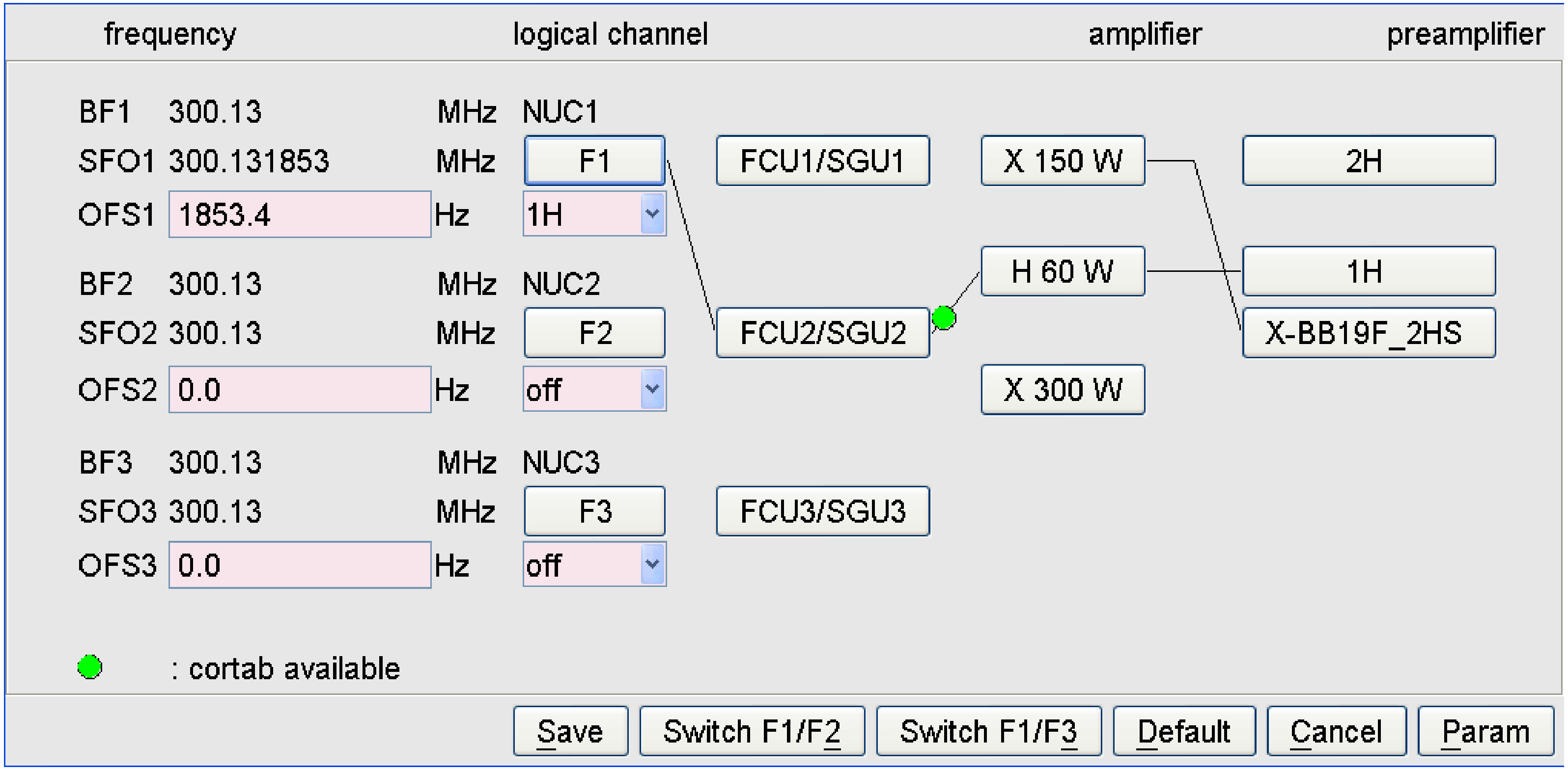
Controlling Spectrometer Sub-Systems

TopSpin provides software panels to access all spectrometer sub-systems

- **Frequency routing**
- **Sample, shim, lock control**
- **Manual and automatic tuning & matching**
- **Interactive parameter optimization**
- **VTU control**
- **Magnet information system**

Controlling Spectrometer Sub-Systems

Visualize and configure the pulse pathway from frequency generation to the probe



BF1 300.13 MHz NUC1
SFO1 300.131853 MHz
OFS1 1853.4 Hz 1H

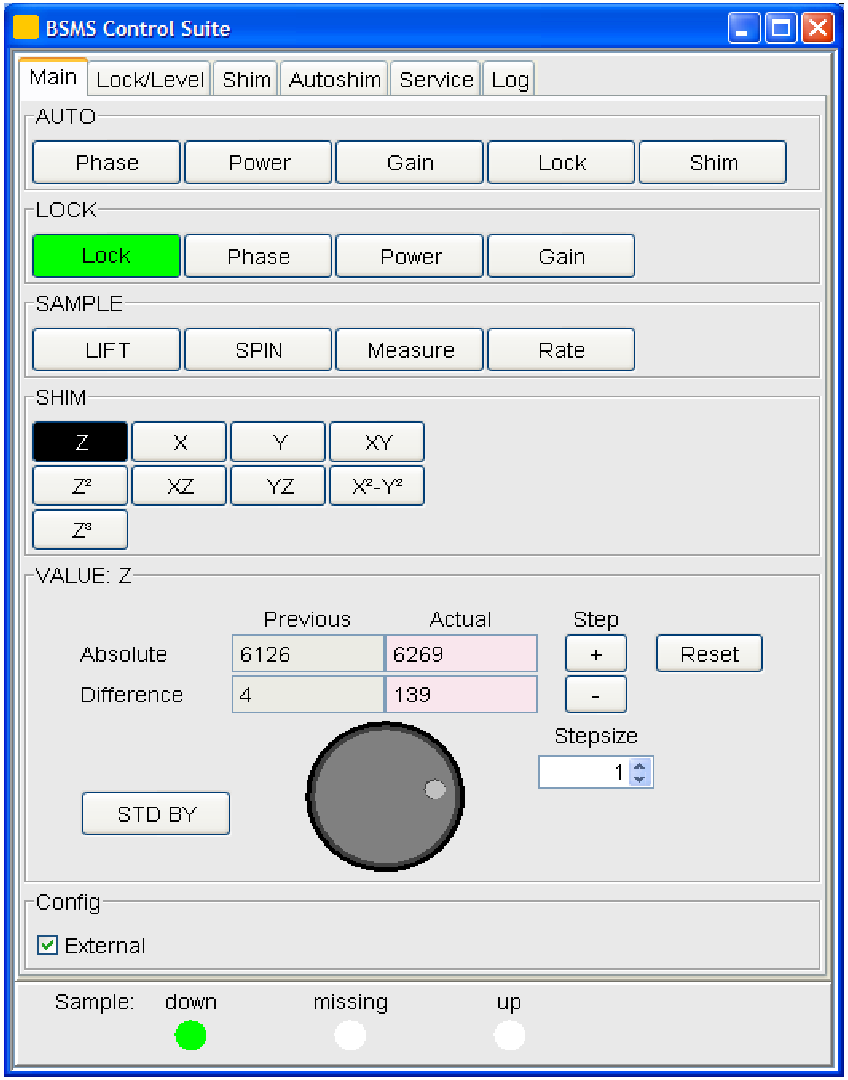
BF2 300.13 MHz NUC2
SFO2 300.13 MHz
OFS2 0.0 Hz off

BF3 300.13 MHz NUC3
SFO3 300.13 MHz
OFS3 0.0 Hz off

● : cortab available

Controlling Spectrometer Sub-Systems

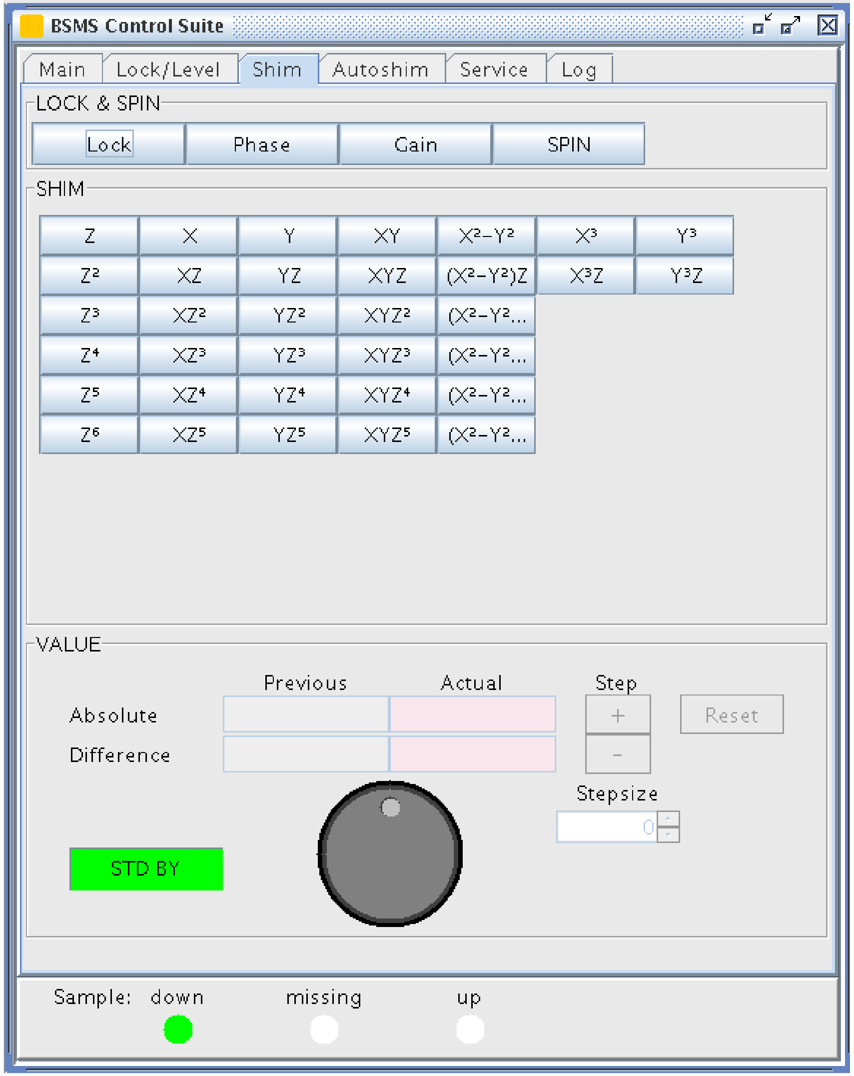
The *BSMS panel* allows you control sample, shims and lock by software



	Previous	Actual
Absolute	6126	6269
Difference	4	139

Stepsize 1

☑ External

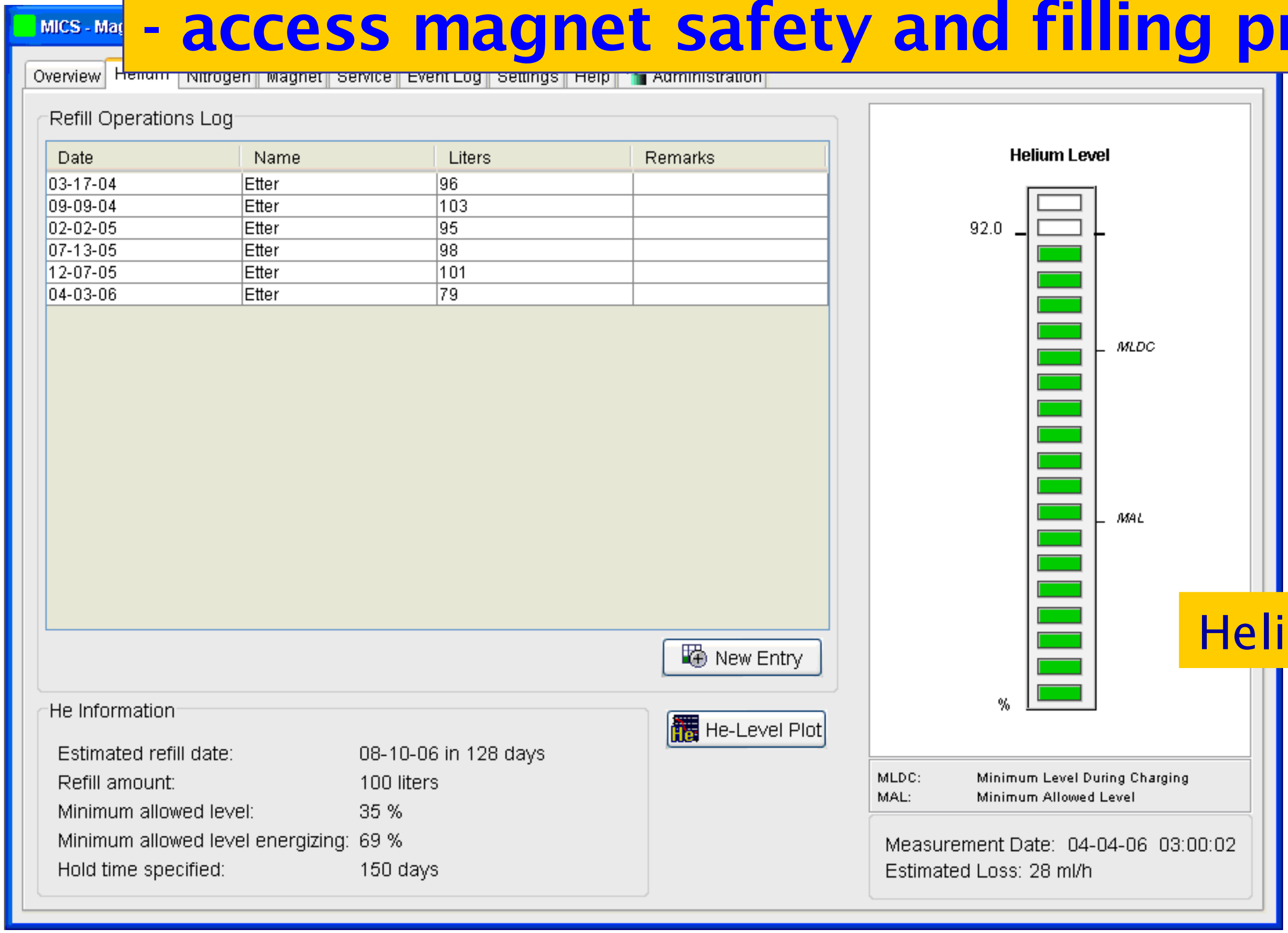


Stepsize 0

Controlling Spectrometer Sub-Systems

Magnet Information & Control System:

- **supervise Helium and Nitrogen levels**
- **receive automatic refill notification**
- **access magnet safety and filling procedures**



Refill Operations Log

Date	Name	Liters	Remarks
03-17-04	Etter	96	
09-09-04	Etter	103	
02-02-05	Etter	95	
07-13-05	Etter	98	
12-07-05	Etter	101	
04-03-06	Etter	79	

He Information

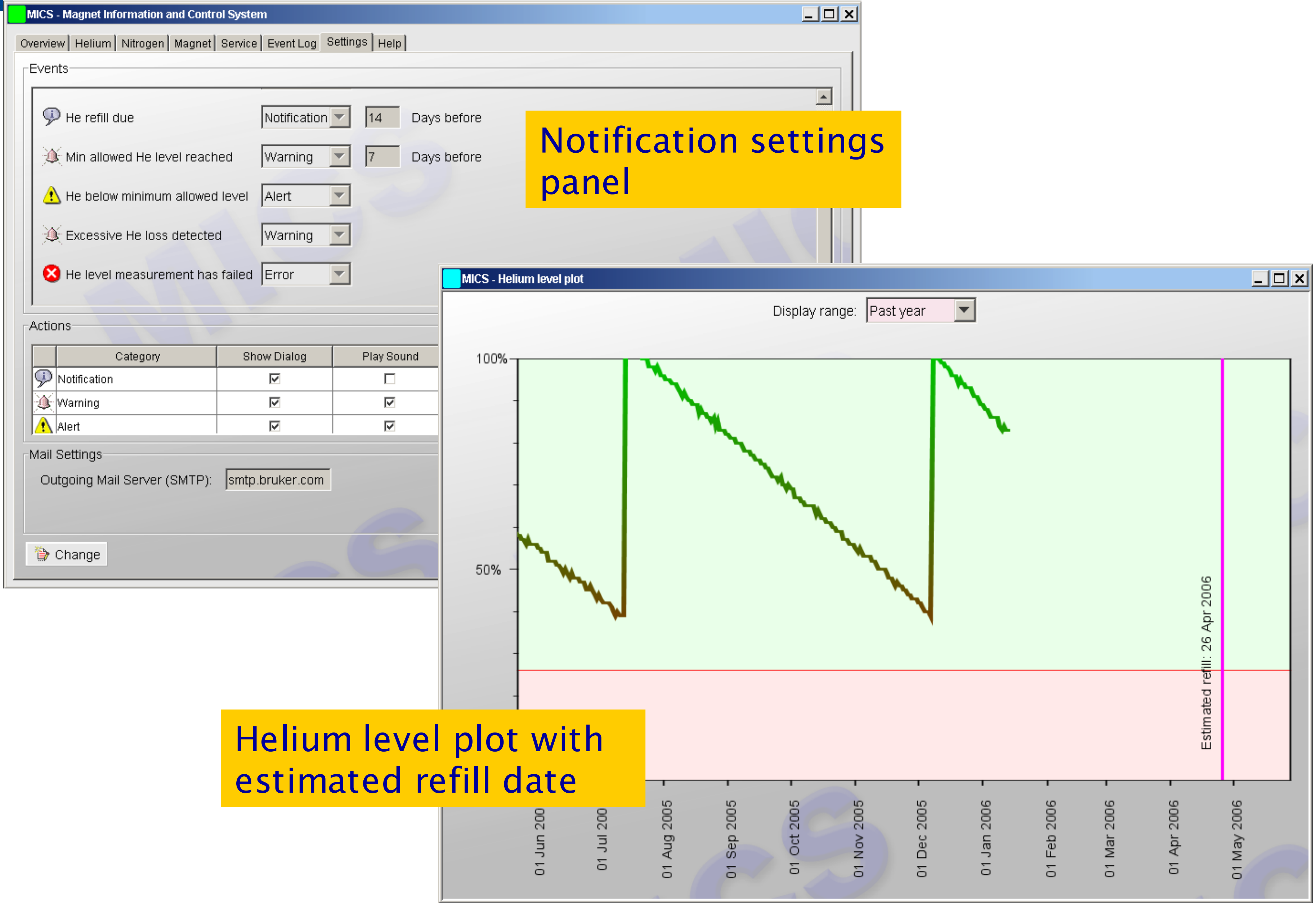
Estimated refill date:	08-10-06 in 128 days
Refill amount:	100 liters
Minimum allowed level:	35 %
Minimum allowed level energizing:	69 %
Hold time specified:	150 days

MLDC:	Minimum Level During Charging
MAL:	Minimum Allowed Level

Measurement Date: 04-04-06 03:00:02
Estimated Loss: 28 ml/h

Helium Watch

Controlling Spectrometer Sub-Systems



MICS - Magnet Information and Control System

Events

He refill due	Notification	14	Days before
Min allowed He level reached	Warning	7	Days before
He below minimum allowed level	Alert		
Excessive He loss detected	Warning		
He level measurement has failed	Error		

Actions

Category	Show Dialog	Play Sound
Notification	☑	☐
Warning	☑	☑
Alert	☑	☑

Mail Settings

Outgoing Mail Server (SMTP): smtp.bruker.com

MICS - Helium level plot

Display range: Past year

Notification settings panel

Helium level plot with estimated refill date

Controlling Spectrometer Sub-Systems

Automatic Shimming

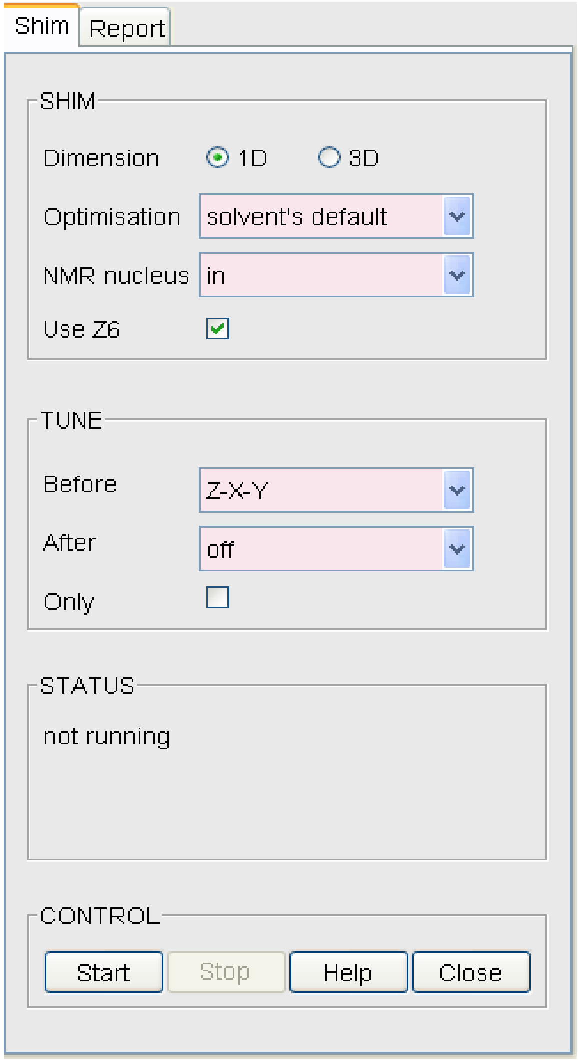
TopShim is ***the*** comprehensive tool for shimming:

→ Obtain excellent resolution and solvent suppression easily and fast.

→ Robust and intelligent implementation of gradient shimming.

→ Optional integrated tune functionality.

→ TopShim can be operated manually as well as during automation



SHIM

Dimension ● 1D ○ 3D

Optimisation: solvent's default

NMR nucleus: in

Use Z6 ☑

TUNE

Before: Z-X-Y

After: off

Only ☐

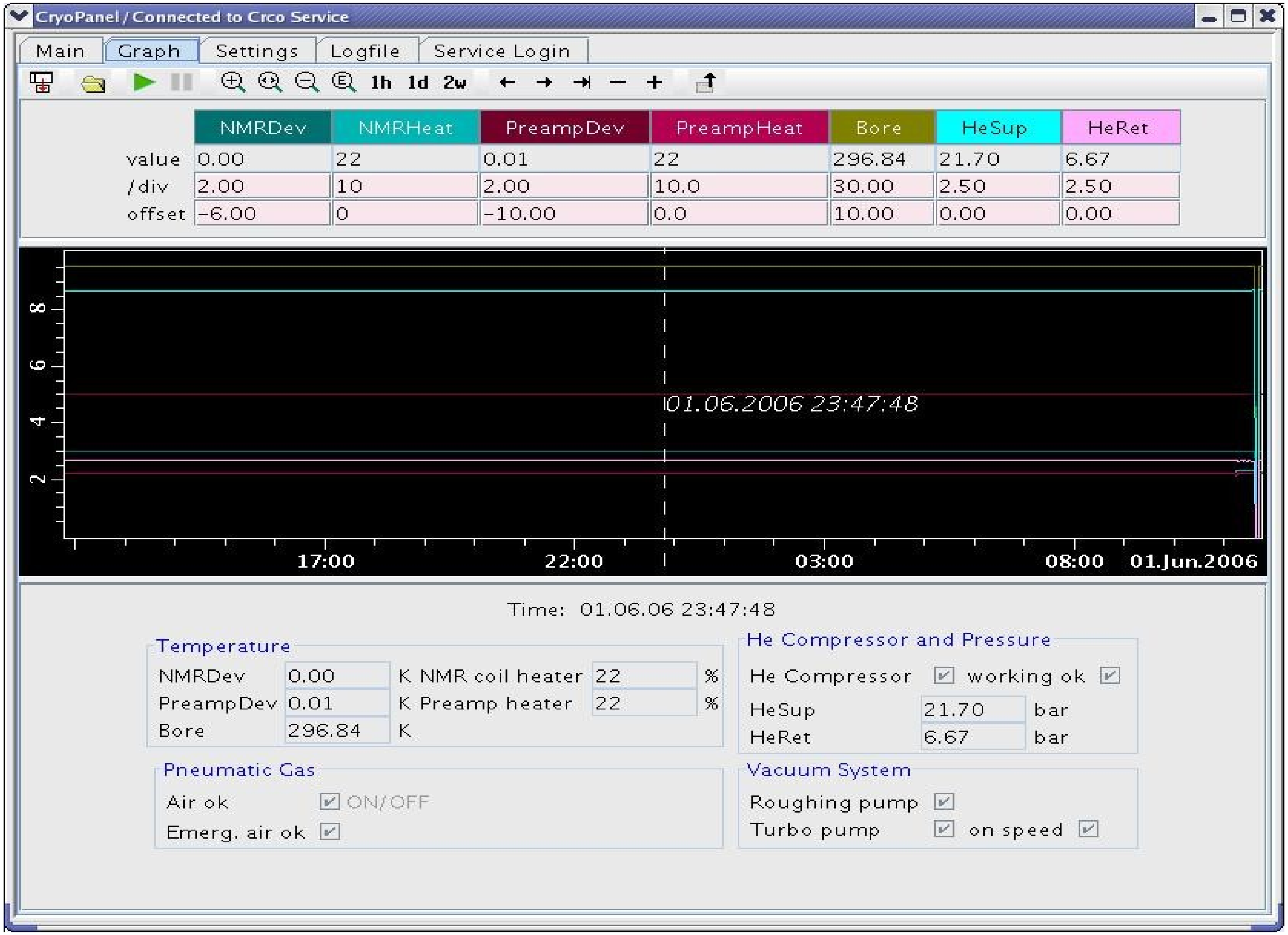
STATUS

not running

CONTROL

Controlling Spectrometer Sub-Systems

Cryoprobe Control Panel



	NMRDev	NMRHeat	PreampDev	PreampHeat	Bore	HeSup	HeRet
value	0.00	22	0.01	22	296.84	21.70	6.67
/div	2.00	10	2.00	10.0	30.00	2.50	2.50
offset	-6.00	0	-10.00	0.0	10.00	0.00	0.00

Time: 01.06.06 23:47:48

Temperature

NMRDev 0.00 K NMR coil heater 22 %
PreampDev 0.01 K Preamp heater 22 %
Bore 296.84 K

He Compressor and Pressure

He Compressor ☑ working ok ☑
HeSup 21.70 bar
HeRet 6.67 bar

Pneumatic Gas

Air ok ☑ ON/OFF
Emerg. air ok ☑

Vacuum System

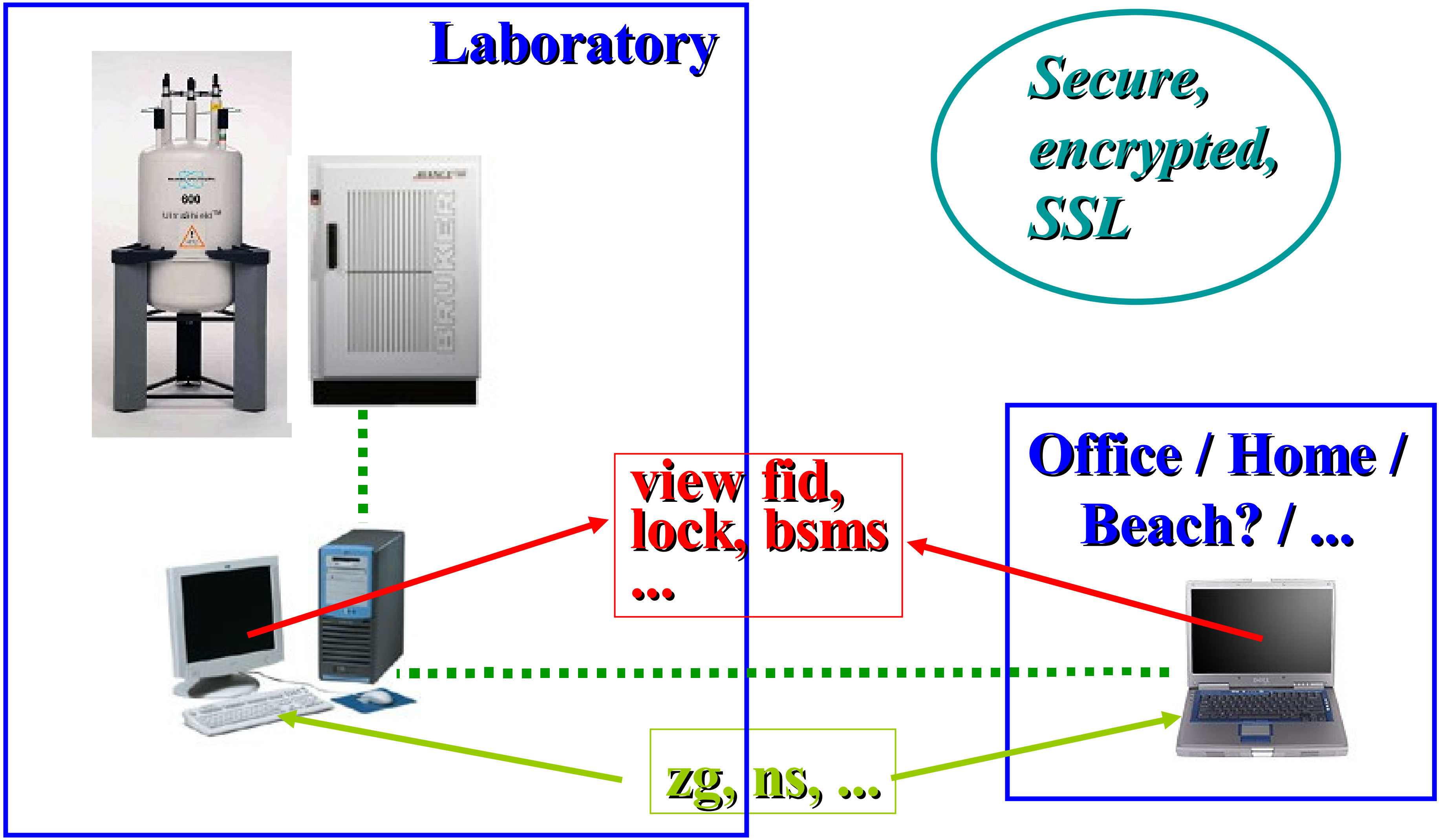
Roughing pump ☑
Turbo pump ☑ on speed ☑

Remote Spectrometer Control

Features:

- Full spectrometer control from remote PC via network
- Several protocol possibilities:
  → telnet / SSH / X11 on Linux systems
  → Windows Terminal Server
  → VNC public domain
  → TopSpin internal protocol (no installation of 3rd party software required, high speed, no extra TopSpin license required)

Remote Spectrometer Access



Laboratory

Secure, encrypted, SSL

view fid, lock, bsms ...

Office / Home / Beach? / ...

zg, ns, ...