

Introduction to TopSpin



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Introduction to TopSpin



- Overview of Topspin interface
- Basic procedure for setting up an acquisition
 - setting up your dataset
 - controlling the spectrometer
- Basic 1D processing
- A little about acquiring and processing 2D's
- A few other useful features

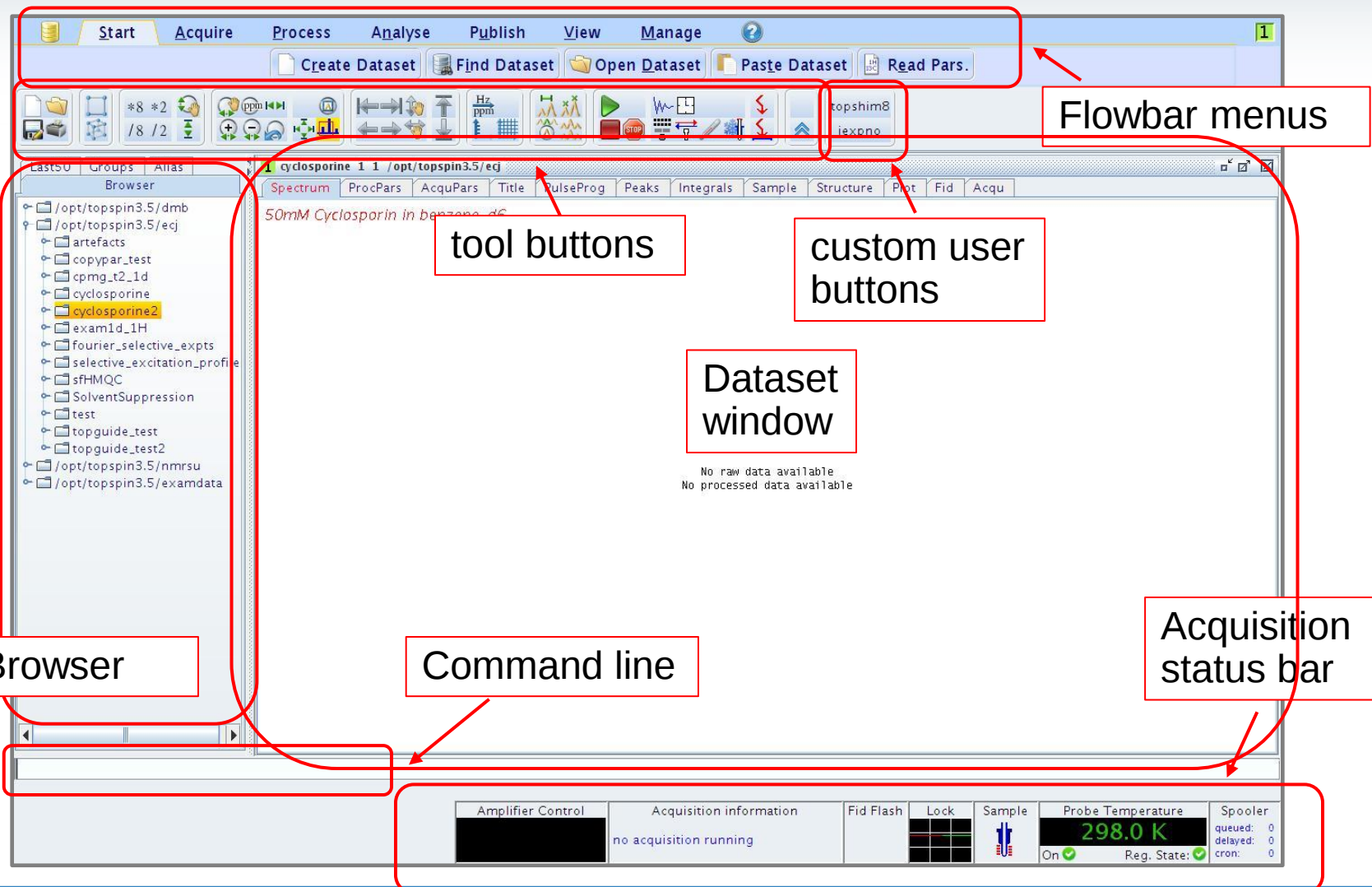
Starting Topspin



TopSpin 3.5

- If Topspin isn't already running, click the desktop ICON to start
- It's yet to be decided whether each user will have an individual Linux login, or if there will be shared group logins...

Topspin layout



The screenshot displays the Bruker Topspin software interface. The top menu bar includes 'Start', 'Acquire', 'Process', 'Analyse', 'Publish', 'View', and 'Manage'. Below the menu bar is a toolbar with icons for file operations and data processing. The main window is divided into several panes: a 'Data Browser' on the left showing a file tree, a 'Dataset window' in the center displaying '50mM Cyclosporin in benzene-d6', and an 'Acquisition status bar' at the bottom right showing '298.0 K' and 'no acquisition running'. Red boxes and arrows highlight specific areas: 'Flowbar menus' (top right), 'tool buttons' (middle left), 'custom user buttons' (middle right), 'Data Browser' (left), 'Command line' (bottom left), and 'Acquisition status bar' (bottom right).

Flowbar menus

tool buttons

custom user buttons

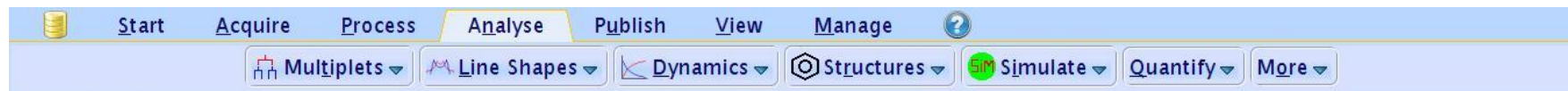
Dataset window

Data Browser

Command line

Acquisition status bar

Flowbars – guiding your workflow



Experiment Setup



Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

NAME: cyclosporine

EXPNO: 1

PROCNO: 1

☐ Use current parameters

☒ Experiment: PROTON Select

Options

☐ Set solvent: C6D6

☒ Execute 'getprosol'

☐ Keep parameters: P 1, O1, PLW 1 Change

DIR: /opt/topspin3.5/ecj

☐ Show new dataset in new window

Receivers (1,2, ...16): 1

TITLE: 50mM Cyclosporin in benzene-d6

Buttons: OK, Cancel, More Info..., Help

Amplifier Control: no acquisition running

Reg. State: On, cron: 0

Experiment Setup



Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

NAME	cyclosporine		
EXPNO	1		
PROCNO	1		
☐ Use current parameters			
☒ Experiment	PROTON	Select	
Options			
☐ Set solvent	C6D6	v	
☒ Execute 'getprosol'			
☐ Keep parameters	P 1, O1, PLW 1	Change	
DIR	/opt/topspin3.5/ecj		
☐ Show new dataset in new window			
Receivers (1,2, ...16)	1		
TITLE	50mM Cyclosporin in benzene-d6		
OK Cancel More Info... Help			

1. Where do you want to store your data
2. What experiment do you want to run?

Experiment Setup – data storage location



Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

NAME

EXPNO

PROCNO

☐ Use current parameters

☒ Experiment

☒ Options

☐ Set solvent

☒ Execute 'getprosolv'

☐ Keep parameters

☐ Show new dataset in new window

Receivers (1,2, ...16)

TITLE

New experiment dataset will be created in the directory specified by

DIR/NAME/EXPNO/

/opt/topspin3.5/ecj/cyclosporine/1/

NAME is a directory which can contain several experiments

EXPNO is any positive integer

Experiment Setup – data storage location



Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

NAME

EXPNO

PROCNO

☐ Use current parameters

☒ Experiment

☒ Options

☐ Set solvent

☒ Execute 'getprosol'

☐ Keep parameters

DIR

☐ Show new dataset in new window

Receivers (1,2, ...16)

TITLE

Some recommendations:

- Remember, *DIR* and *NAME* are directories.
- Limit directory names to letters and numbers
- dashes "-" and underscores "_" are OK
- spaces or special characters such as %, #, (, etc. can sometimes cause problems
- Always store data on a locally mounted hard drive
- The software will allow you to specify a network drive, but it's not recommended!

Experiment Setup – parameter sets



Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

NAME

EXPNO

PROCNO

☐ Use current parameters

☒ Experiment

Options

☐ Set solvent

☒ Execute 'getprosol'

☐ Keep parameters

DIR

☐ Show new dataset in new window

Receivers (1,2, ...16)

TITLE

What is a parameter set?

- All of the information necessary to run your experiment:
 - pulse program name
 - nuclei
 - excitation frequencies and sweep widths
 - durations of pulses* and delays
 - pulse power levels*
 - gradient strengths
 - number of scans
 - relevant spectrometer configuration
 - etc...

* pulse durations and power levels will usually be set in a later step

Experiment Setup – parameter sets



File Options Help

Source = /opt/topspin3.5/exp/stan/nmr/par

Find file names: enter any string, *, ? Exclude: Clear

Class = Any Dim = Any ☐ Show Recommended

Type = Any SubType = Any SubTypeB = Any Reset Filters

AL27ND	APSY_HNCA_32	APSY_HNCACB_32	APSY_HNCO_32	APSY_HNCOCA_42
APSY_HNCOACB_32	APSY_HNCOCANH_62	ASSURE_13C	ASSURE_19F	ASSURE_1H
ASSURE_31P	B_HNCACBGP3D	B_HNCACBIGP3D	B_HNCACOGP3D	B_HNCACOGP4D
B_HNCAGP3D	B_HNCAIGP3D	B_HNCOACBGP3D	B_HNCOACBGP4D	B_HNCOACGP3D
B_HNCOACGP4D	B_HNCOGP3D	B_HNCOIGP3D	B_HSQCET3GPSI	B_TRHNCAACBGP3D
B_TRHNCAACBIGP3D	B_TRHNCAACOGP3D	B_TRHNCAIGP3D	B_TRHNCAIGP3D	B_TRHNCOACBGP3D
B_TRHNCOACGP3D	B_TRHNCOGP3D	B_TRHNCOIGP3D	B_TROSY	
B11ZG	BESTPROFILE	C_CACO	C_CACO	
C_CAN_IASQ	C_CAN_MQ	C_CAN_MQ.2	C_CANCO	
C_CANCOI_3D	C_CBCACO_3D	C_CBCACO_S33D	C_CBCAC	
C_CCCO_3D	C_CCCO_S33D	C_CCCON_3D	C_CCFLO	
C_CCFLOPSY16_CTIA	C_CCFLOPSY16_IA	C_CCNOESY	C_CCNOE	
C_COCA	C_COCA_IA	C_COCA_MQ	C_COCA	
C_CON_MQ	C_CON_MQIA	C_CON_SQ	C_COSY	
C_COSY2_CT	C_HCACO_3D	C_HCACO_3D	C_HCACO_S33D	C_HCAN_3D
C_HCANCO_3D	C_HCANCOI_3D	C_HCBCA_3D	C_HCBCACO_3D	C_HCBCACO_S33D
C_HCBCAN_3D	C_HCCFLOPSY16_3D	C_HNCA_3D	C_HNCACO_3D	C_HNCACO_S33D
C_HNCO_3D	C_HNCOCA_3D	C_HNCOCA2_3D	C13APT	C13CPD
C13CPD32	C13CPDSN	C13DE45SN	C13DEPT135	C13DEPT135p
C13DEPT45	C13DEPT90	C13GD	C13HUMP	C13IG
C13MULT	C13MULT135	C13MULT90	C13MULTCOMP	C13OFF
C13PPTI	C13RESOL	C13SENS	CBCACONHGP3D	CBCACONHGPWG3D
CBCACONHGPWG3D.2	CBCACONHGPWG4D	CBCANHGP3D	CBCANHGPWG3D	CCACONHGP2H3D
CCACONHGP3D	CCACONHGP3D.2	CCANHGP2H3D	CCANHGP3D	CCANHGP3D.2
CCCONHGP2H3D	CCCONHGP3D	CD111ZG	CD113ZG	CL35ZG
CL37ZG	CMC_13C	CMC_HSQC	CMC_PROTON	CMC_SINGLE
CMC_WET	CMCQ_WET	CMCse_13C	CMCse_15NHMBcf2	CMCse_15NHSQCf2
CMCse_1H	CMCse_ADEQ	CMCse_COSY	CMCse_H2BC	CMCse_HMBC
CMCse_HSQC	CMCse_INAD	COSY45SW	COSY90SW	COSYCWGPPSQF
COSYCWPHPS	COSYDCPHWT	COSYDFGPPH19	COSYDQFPHSW	COSYGPDPHPSW
COSYGPFIXSW	COSYGPMSFW	COSYGPSW	COSYPHPR	DECP90
DECP90F3	diff1H5mm	diffGradRec	diffPreemp	diffWaterDiff
DIPS12ESFBGPPH	DIPS12ESGPPH	DIPS12ETGPSI19	DIPS12GPPH19	DIPS1HSQCf3GPSI3D
DIPS1TRETf3GP3D	DOSY	F19	F19CPD	FHSQCCXf3GPPH
FHSQCf3GPPH	GA71ZG	gradshim1d1h	gradshim1d1h_f	gradshim1d2h
gradshim1d2h_f	gradshimdata	gradshimrcb3d	H2OSUPMLEV	H2OSUPNOESY

Set selected item in editor Close

Standard parameter sets exist for (almost) any experiment you want to run

Experiment Setup – parameter sets



File Options Help Source = /opt/topspin3.5/exp/stan/nmr/par

Find file names: Exclude: Clear

Class = Any Dim = Any ☐ Show Recommended

Type = Any Sub Type = Any Sub TypeB = Any Reset Filters

COSY45SW	COSY90SW	COSYCWGPPSQF	COSYCWPHP	COSYDCPHWT
COSYDFGPPH19	COSYDQFPHSW	COSYGPDPHPSW	COSYGPFIWSW	COSYGPMFSW
COSYGPSW	COSYPHPR			

You can search through parameter set names

Read... Close

Experiment Setup – parameter sets



File Options Help Source = /opt/topspin3.5/exp/stan/nmr/par

Find file names: Enter any string(s) Exclude: Clear

Class = Any Dim = Any ☒ Show Recommended

Type = Any SubType = Any SubTypeR = Any Reset Filters

C13CPD	C13DEPT135	COSYGPDPHWS	COSYGPSW	HMBCEGTL3ND
HMBGCP	HMBGCP_15N	HSQC_TOCSY	HSQC_TOCSY_ADIA	HSQCEDETPSISP
HSQCEDETPSISP_ADIA	HSQCETGP_15N	HSQCETGPSISP	HSQCETGPSISP_ADIA	MLEVPHPR
MLEVPHSW	NOESYPHPR	NOESYPHWS	PROTON	ROESYPHPR
ROESYPHWS	WATERSUP			

Set selected item in editor Close

“Show Recommended” button gives list of most common small molecule experiments

I'll discuss these a little more towards the end of this presentation...

Experiment Setup – parameter sets



File Options Help

Find file names: Exclude: Clear

Class = Dim = ☐ Show Recommended

Type = SubType = SubTypeB = Reset Filters

15N_rcCPMG_ALEE	C13_solvent	C13-1scan	C13HSQC	C13HSQC_edited
CE_zgpr30	DOSY	DOSY_Setup	H1-1scan	KBK_SELDPFGPE
LC2DWTUS	P31CPD_DSM	PROTEIN_SETUP	SELDIHMBC.ecj	SELMHBC
SELMLEVHSQCETGPSI.ecj	SEMLGPPHF2.ecj	SELNOGP	SHSQCETGPSISP2.2.old	STEP-NOESY.ecj
STEP-NOESY-old				

Source =

Set selected item in editor Close

User modified parameter sets are stored in a separate directory

The command “wpar” is used to *write parameters*

Experiment Setup – parameter sets



File Options Help Source = /opt/topspin3.5/exp/stan/nmr/par

Find file names: Exclude: Clear

Class = Any Dim = Any ☒ Show Recommended

Type = Any SubType = Any SubTypeB = Any Reset Filters

C13CPD	C13DEPT135	COSYGPDPHWSW	COSYGPSW	HMBCETGPL3ND
HMBCGP	HMBCGP_15N	HSQC_TOCSY	HSQC_TOCSY_ADIA	HSQCEDETPSISP
HSQCEDETPSISP_ADIA	HSQCETGP_15N	HSQCETGPSISP	HSQCETGPSISP_ADIA	MLEVPHPR
MLEVPHSW	NOESYPHPR	NOESYPHWS	PROTON	ROESYPHPR
ROESYPHWS	WATERSUP			

Select parameter set of interest, then click "Set selected item in editor"

Set selected item in editor Close

Experiment Setup – creating new dataset



Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

NAME

EXPNO

PROCNO

☐ Use current parameters

☒ Experiment

☒ Options

☐ Set solvent

☒ Execute 'getprosol'

☐ Keep parameters

DIR

☐ Show new dataset in new window

Receivers (1,2, ...16)

TITLE

After defining data storage location and parameter set name, click "Ok"

Controlling the spectrometer – the Acquire tab



The screenshot shows the Bruker Topspin software interface. The top menu bar includes 'Start', 'Acquire', 'Process', 'Analyse', 'Publish', 'View', and 'Manage'. Below the menu is a toolbar with various icons for sample, lock, tune, spin, shim, prosol, gain, go, and more. The left sidebar shows a file browser with a tree structure of folders and files. The main window displays the 'Acquire' tab, showing a spectrum plot. A red box highlights the text 'But first... ... a few more details on the Topspin flowbar'. The status bar at the bottom shows various parameters and controls.

But first...

... a few more details on the
Topspin flowbar

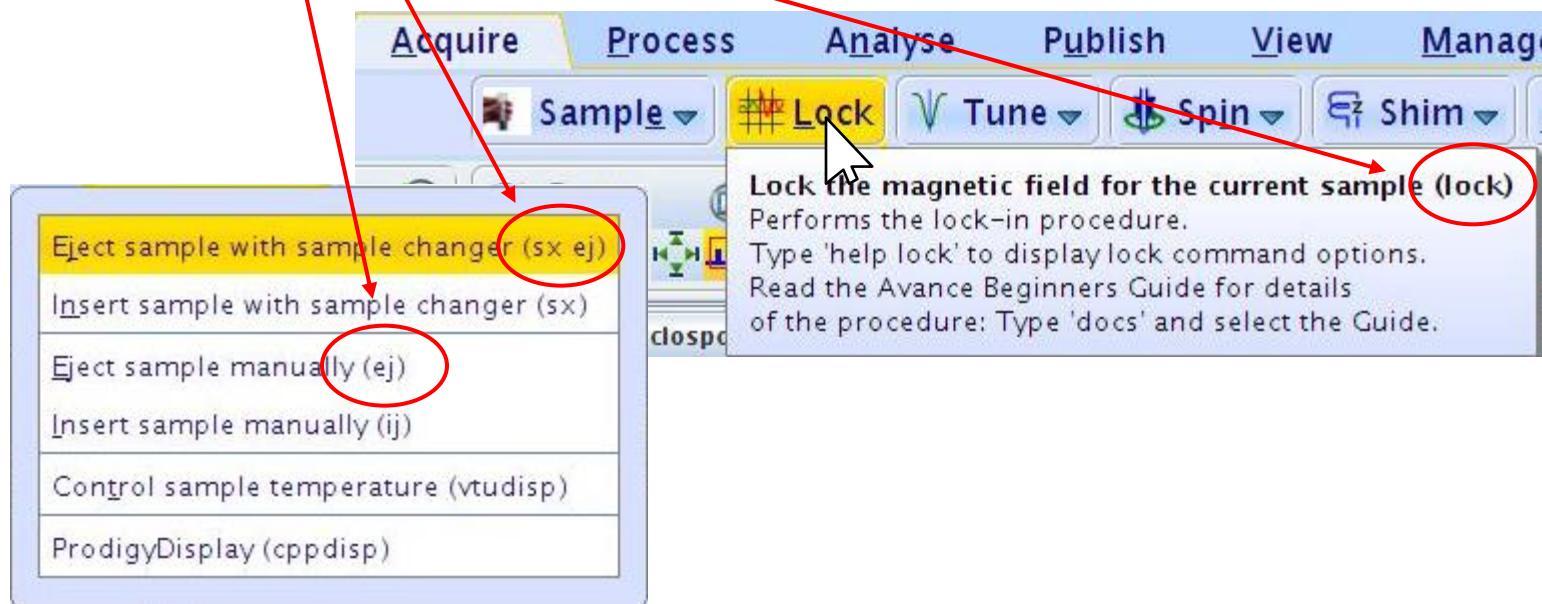
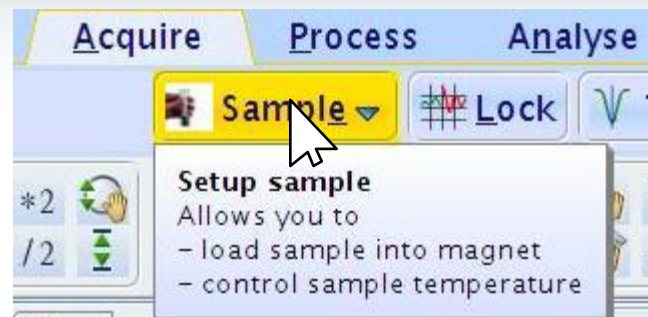
No raw data available
No processed data available

Amplifier Control	Acquisition information	Fid Flash	Lock	Sample	Probe Temperature	Spooler
	no acquisition running				298.0 K	queued: 0 delayed: 0 cron: 0
					On	Reg. State: ✓

some Flowbar details



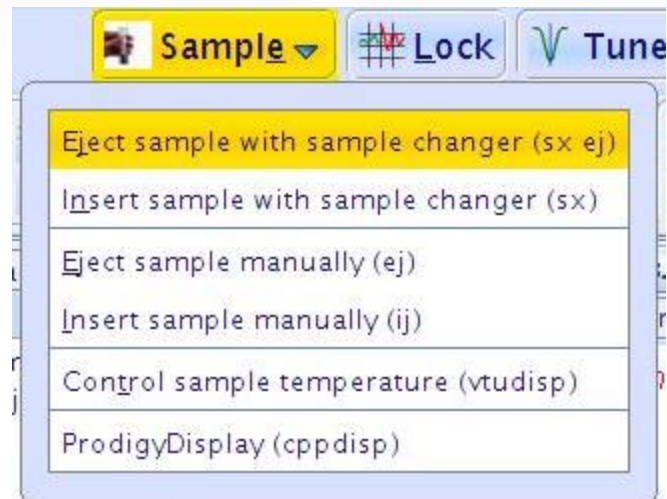
- Hovering the mouse over a button will open a tool tip
- command line commands are usually shown in parentheses



3 types of Flowbar buttons



- 1) Some buttons (like "Sample") open a pull-down menu of options



3 types of Flowbar buttons



- 2) Some buttons (like “Lock”) execute a single command



3 types of Flowbar buttons



3) Some buttons (like "Tune") have two parts

- clicking on the left part executes a default command
- clicking on the right opens a list of related options



Back to data acquisition...

- click Flowbar buttons from left to right



The screenshot displays the Bruker TopSpin software interface. The 'Acquire' tab is selected in the top menu bar. The 'Sample' button in the flowbar is highlighted, and its context menu is open, showing options: 'Eject sample with sample changer (sx ej)', 'Insert sample with sample changer (sx)', 'Eject sample manually (ej)', 'Insert sample manually (ij)', 'Control sample temperature (vtudisp)', and 'ProdigyDisplay (cppdisp)'. The left sidebar shows a file tree with 'cyclosporine2' selected. The bottom status bar includes sections for 'Amplifier Control', 'Acquisition information' (showing 'no acquisition running'), 'Fid Flash', 'Lock', 'Sample', 'Probe Temperature' (displaying '298.0 K'), and 'Spooler'.

“Sample” button

- Control the sample changer
- Turn on or off the sample change lift air
- Open the sample temperature control panel

More info on loading samples...



- Use Bruker spinners!
 - Varian/Agilent spinners are slightly different and won't work
- Use depth gauge to determine how far to insert NMR tube into spinner
 - Don't adjust position of gauge – it should be at 2cm



^2H Lock



The screenshot shows the Bruker software interface with the 'Lock' button highlighted. A tooltip for the 'Lock' button reads: 'Lock the magnetic field for the current sample (lock). Performs the lock-in procedure. Type 'help lock' to display lock command options. Read the Advance Beginners Guide for details of the procedure: Type 'docs' and select the Guide.'

A solvent selection dialog box is open, displaying a list of solvents and their descriptions. The solvent 'C6D6' (benzene-d6) is highlighted in red.

Solvent	Description
Acetic	acetic acid-d4
Acetone	acetone-d6
C6D6	benzene-d6
CD2Cl2	dichloromethane-d2
CD3CN	acetonitrile-d3
CDCl3	chloroform-d
D2O	deuteriumoxide
D2O_salt	deuteriumoxide with salt
Dioxane	dioxane-d8
DMF	N,N-dimethylformamide-d7
DMSO	dimethylsulfoxide-d6
EtOD	ethanol-d6
H2O+D2O	90%H2O and 10%D2O
HDMSO	90%DMSO and 10%DMSO-d6
MeOD	methanol-d4
Pyr	pyridine-d6
TFE	trifluoroethanol-d3
THF	tetrahydrofuran-d8
Tol	toluene-d8

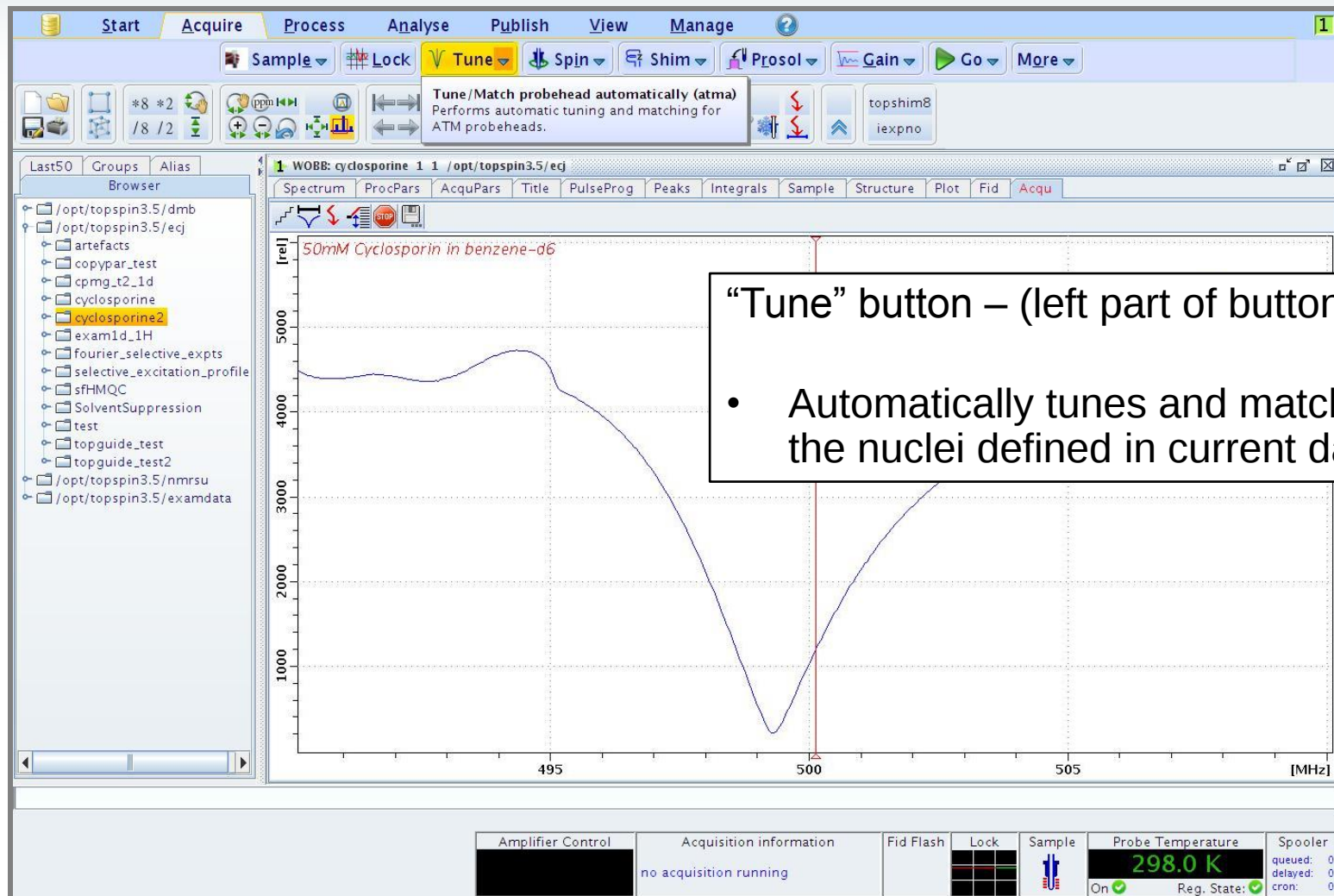
The bottom status bar shows the following information:

- Amplifier Control: [Status]
- Acquisition information: no acquisition running
- Fid Flash: [Status]
- Lock: [Status]
- Sample: [Status]
- Probe Temperature: 298.0 K
- Spooler: queued: 0, delayed: 0, cron: 0

“Lock” button

- Select the solvent from list
- All relevant lock parameters are set and the lock is automatically optimized
- “D2O” vs. “H2O+D2O” – this will determine whether automatic shimming will use ^2H or ^1H observe

Automatic tune and match



Sample Spinning - optional



The screenshot shows the Bruker TopSpin software interface. The 'Spin' menu is open, displaying options for controlling sample rotation and MAS spinning. The 'cyclosporine' experiment is selected in the left-hand browser. The main window displays the 'Spectrum' tab, showing a 2D raw data plot. A text box in the center of the interface provides advice on when to use spinning.

Spin Menu Options:

- Turn sample rotation on (ro on)
- Turn sample rotation off (ro off)
- Change sample rotation rate (ro)
- MAS Pneumatic Unit (masdisp)
- Start MAS Spinning (masg)
- Stop MAS Spinning (mash)
- Get MAS Spinning Rate (masrget)
- Set MAS Spinning Rate (masrset)

Text Box:

If spinning lineshape is significantly better than non-spinning, then X/Y shims should be touched up

Status Bar:

Amplifier Control	Acquisition information	Fid Flash	Lock	Sample	Probe Temperature	Spooler
	no acquisition running				298.0 K	queued: 0 delayed: 0 cron: 0

Shimming – topshim



The screenshot shows the Bruker TopSpin software interface. The top menu bar includes Start, Acquire, Process, Analyse, Publish, View, and Manage. Below the menu bar is a toolbar with icons for Sample, Lock, Tune, Spin, Shim, Prosol, Gain, Go, and More. A tooltip for the Shim icon reads: "Autoshim sample using TopShim (topshim). The core method of TopShim is gradient shimming. A quality criterion for the final lineshape ensures best results for all situations." The left sidebar shows a file browser with a tree structure. The main window displays the "Spectrum" tab for a file named "1 cyclosporine 1 1 /opt/topspin3.5/ecj". The sample name "50mM Cyclosporin in benzene-d6" is visible. The bottom status bar shows various system parameters: Amplifier Control, Acquisition information (no acquisition running), Fid Flash, Lock, Sample, Probe Temperature (298.0 K), and Spooler status.

1 cyclosporine 1 1 /opt/topspin3.5/ecj

50mM Cyclosporin in benzene-d6

- Default gradient shimming (topshim) usually works quite well from sample to sample
- fully automated
- usually takes less than a minute
- uses info from lock solvent to specify shimming method

Amplifier Control	Acquisition information	Fid Flash	Lock	Sample	Probe Temperature	Spooler
	no acquisition running				298.0 K	queued: 0
					On	delayed: 0
					Reg. State: ✓	cron: 0

Shimming – topshim



The screenshot displays the Bruker Topspin software interface. The 'Shim' menu is open, showing various shimming options. A red arrow points from the text box below to the 'Open topshim graphical user interface (topshim gui)' option in the menu.

Shim Menu Options:

- Display topshim report (topshim report)
- Additional topshim options
- Shim manually using BSMS panel (bsmsdisp)
- Traditional gradient shimming (gradshim)
- Set Shim Values (setshim)
- Read shim values (rsh)
- Write shim values (wsh)
- View Shim Values (vish)
- Delete Shim File (delsh)
- Autoshim using tune file (tune)
- Autoshim using tune file for current probe (tune.sx)
- Edit autoshim definition (tune) file (edtune)
- Open topshim graphical user interface (topshim gui)
- Stop topshim optimization (topshim stop)
- 3D topshim (H2O sample) (topshim 3d)
- Tune shim after topshim (topshim tunea)
- Run topshim unlocked (topshim lockoff)

Text Box:

topshim's GUI offers more automatic shimming options

Bottom Status Bar:

Amplifier Control	Acquisition information	Fid Flash	Lock	Sample	Probe Temperature	Spooler
	no acquisition running				298.0 K	queued: 0 delayed: 0 cron: 0

Shimming – topshim



The screenshot displays the Bruker TopSpin software interface. The top menu bar includes 'Start', 'Acquire', 'Process', 'Analyse', 'Publish', 'View', and 'Manage'. Below the menu bar is a toolbar with various icons for sample, lock, tune, spin, shim, and processing. A 'Manuals (docs)' dropdown menu is open, showing a list of manuals. The 'TopShim' manual is highlighted with a red circle and a red arrow pointing to it. A text box on the right says 'A lot more details in the Topshim manual...'. The status bar at the bottom shows 'no acquisition running' and 'Probe Temperature: 298.0 K'.

Manuals (docs)

- Commands
- Parameters
- General
 - User Manual
 - Control & Function Keys
 - Release Letter
 - Beginner Guide
- Acquisition – User Guides
 - 1D and 2D Step-by-Step – Basic
 - 1D and 2D Step-by-Step – Advanced
 - Basic 1D and 2D Experiments
 - 3D/Triple-Resonance experiments
- Acquisition – Application Manuals
 - Eretic2
 - Multi-Receive Acquisition
 - Solids Introduction
 - Solids
 - TopSolids
 - Cross Polarization Dynamics
 - SB/MAS
 - BEST-NMR
 - LC-NMR
 - Dosy
 - Diffusion
 - Shapetool
 - Gradient Shimming
 - TopShim
 - CMCO
- APSY
- Acquisition & Processing References
 - Acqu. Commands & Parameters
 - Proc. Commands & Parameters
 - Edprosol Manual
 - Edlock Guide
 - Pulse Program Catalogue, 1D/2D
 - Pulse Program Catalogue, BIO
 - NUS Parameters
- Automation and Plotting
 - ICON-NMR Automation Interface
 - Plotting
- Analysis and Simulation
 - Structure Analysis Tools
 - NMR-SIM Experiment Simulator
 - Daisy

Close this dialog when a manual is opened

Multi-Doc Search Books Close

no acquisition running

Probe Temperature: 298.0 K

Reg. State: On

Spooler: queued: 0, delayed: 0, cron: 0

Getprosol



The screenshot shows the Bruker TopSpin software interface. The 'Acquire' tab is selected. The 'Sample' dropdown is set to 'cyclosporine 1 1 /opt/topspin3.5/ecj'. The 'Prosol' button is highlighted, and a tooltip explains its function: 'Update 'prosol' parameters (getprosol) Reads the probehead and solvent dependent parameters as defined by "edprosol" and copies them to the corresponding acquisition parameters.' The 'Spectrum' tab is active, showing a plot of '50mM Cyclosporin in benzene-d6'. The 'Browser' on the left shows the file structure, with 'cyclosporine2' selected. The status bar at the bottom indicates 'no acquisition running' and 'Probe Temperature: 298.0 K'.

- Prosol = **probe** and **solvent** dependent parameters
- reads calibrated pulses for installed into current dataset
- RF pulse power levels are all set to zero in standard parameter sets

Automatic receiver gain



The screenshot displays the Bruker TopSpin software interface. The top menu bar includes 'Start', 'Acquire', 'Process', 'Analyse', 'Publish', 'View', and 'Manage'. Below the menu is a toolbar with various icons for sample, lock, tune, spin, shim, and prosol. A 'Gain' button is highlighted in yellow. A tooltip for the 'Gain' button reads: 'Auto-adjust receiver gain (rga) Optimizes the receiver gain. Performs acquisitions with varying receiver gain RG and finally sets this just below the value where no digitizer overflow occurs.'

The left sidebar shows a file browser with a tree structure. The selected file is 'cyclosporine2' under the path '/opt/topspin3.5/ecj'. The main window displays the 'Spectrum' tab with the title '50mM Cyclosporin in benzene-d6'. The bottom status bar shows various acquisition parameters:

Amplifier Control	Acquisition information	Fid Flash	Lock	Sample	Probe Temperature	Spooler
	no acquisition running				298.0 K	queued: 0
					On	delayed: 0
					Reg. State: ✓	cron: 0

- Sets the receiver gain to optimal value
- Acquired data will use full dynamic range of the analogue to digital converter in the receiver

Start acquiring data



The screenshot shows the Bruker TopSpin software interface. The 'Acquire' tab is selected in the top menu. The left sidebar shows a file tree with the following structure:

- /opt/topspin3.5/dmb
- /opt/topspin3.5/ecj
 - artefacts
 - copypar_test
 - cpmg_t2_1d
 - cyclosporine
 - cyclosporine2**
 - exam1d_1H
 - fourier_selective_expts
 - selective_excitation_profile
 - sfHMQC
 - SolventSuppression
 - test
 - topguide_test
 - topguide_test2
- /opt/topspin3.5/nmrslu
- /opt/topspin3.5/examdata

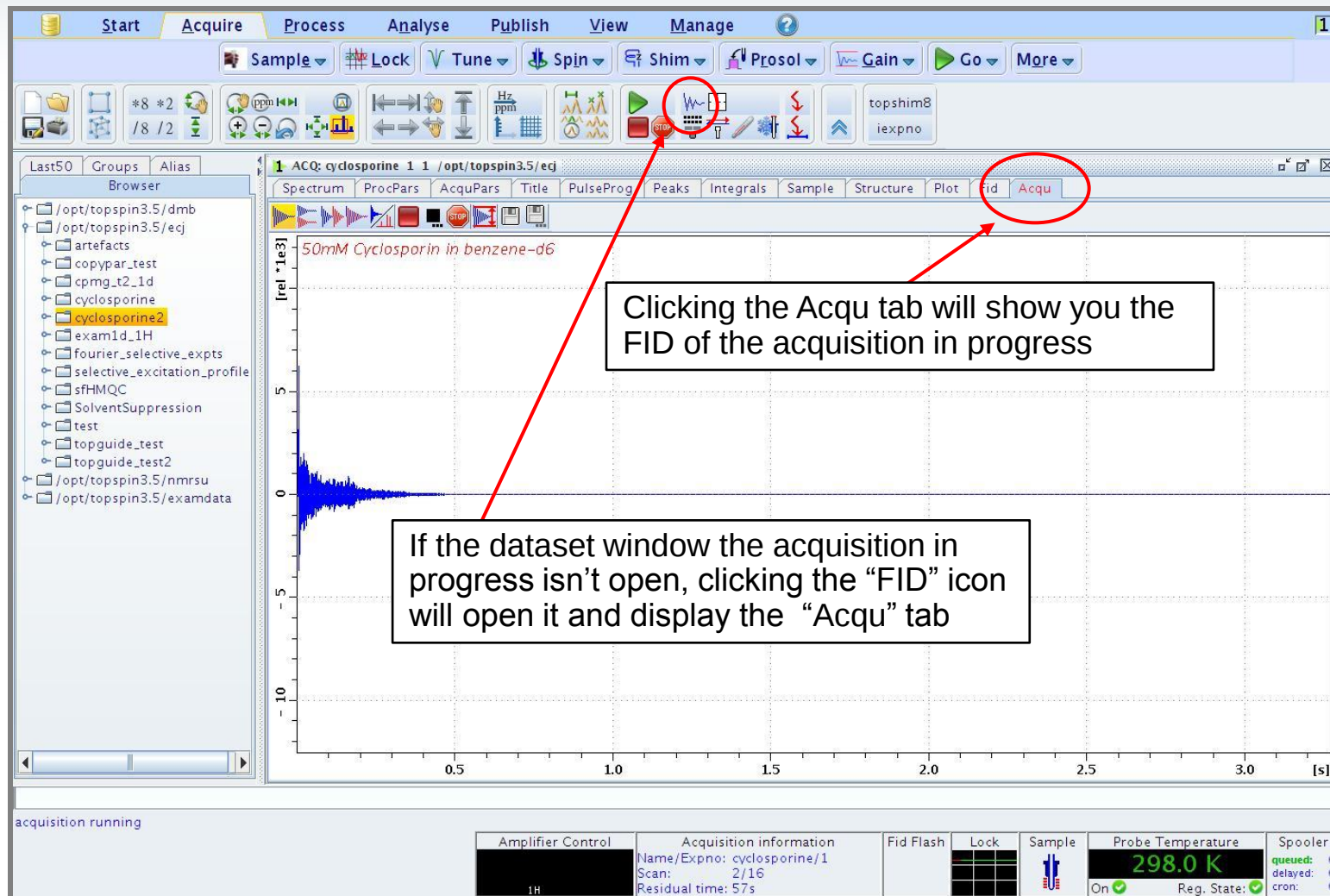
The main window displays the 'Spectrum' tab for the dataset '1 cyclosporine 1 1 /opt/topspin3.5/ecj'. The title bar indicates '50mM Cyclosporin in benzene-d6'. A warning dialog box titled 'Start acquisition (zg)' is open, displaying the following text:

Start acquisition (zg)
Uses the acquisition parameters of the currently active dataset. If a dataset exists, zg will ask to override it, unless this feature was disabled (command "set", ZG safety off). You may also enable "auto-archiving" so as to avoid inadvertent data data loss. (command "set", Configure accounting and data archiving).

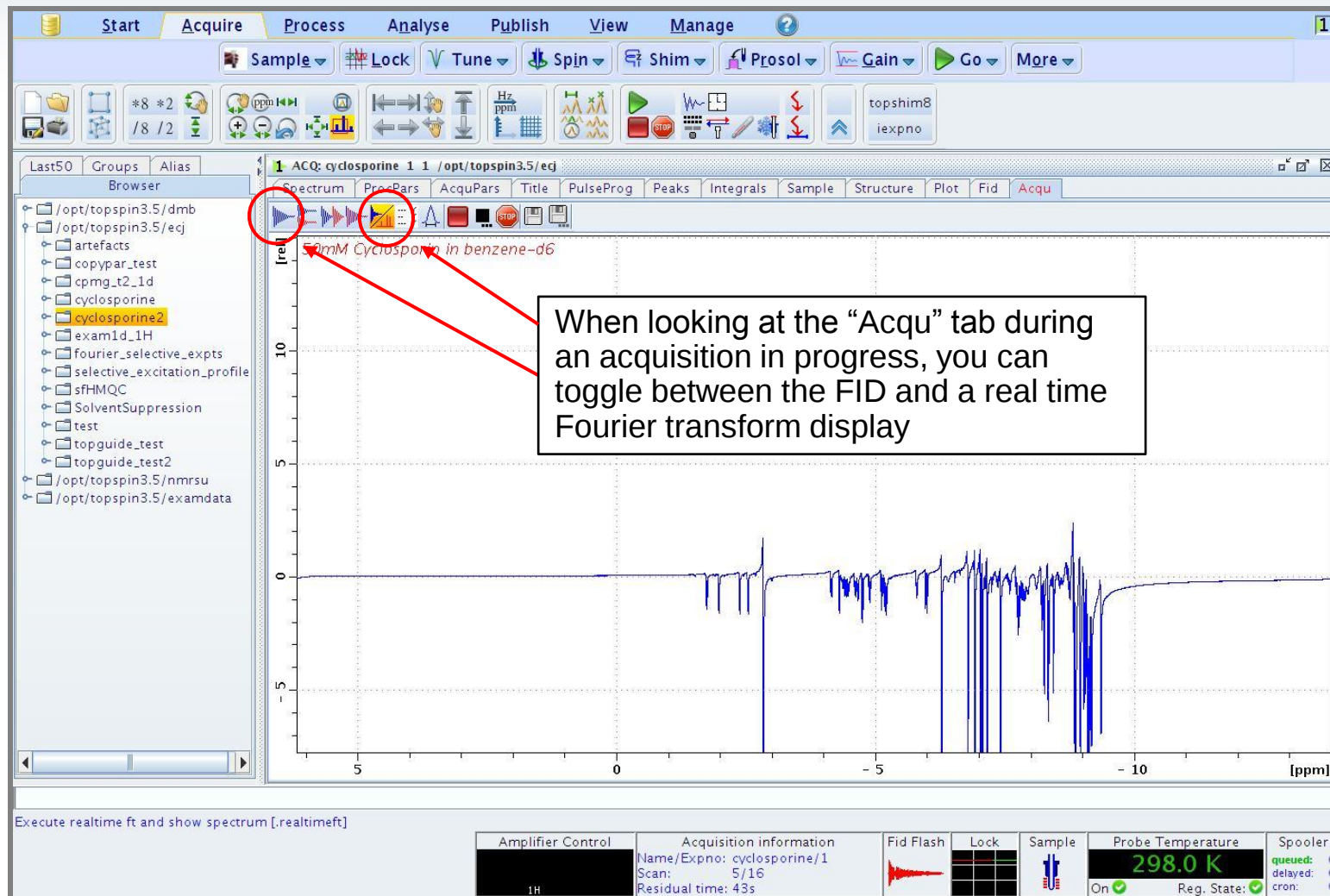
At the bottom of the interface, the 'Amplifier Control' section shows 'no acquisition running'. The status bar displays '298.0 K' and 'On' with a green checkmark, and a 'Reg. State' section with 'queued: 0', 'delayed: 0', and 'cron: 0'.

- The Go button starts the acquisition using all of the parameters in the current dataset.
- *Warning: you can potentially overwrite data if you click "Go" in a dataset which already contains spectral data.*
- *User configurable preferences will determine whether you get a warning before overwriting data.*

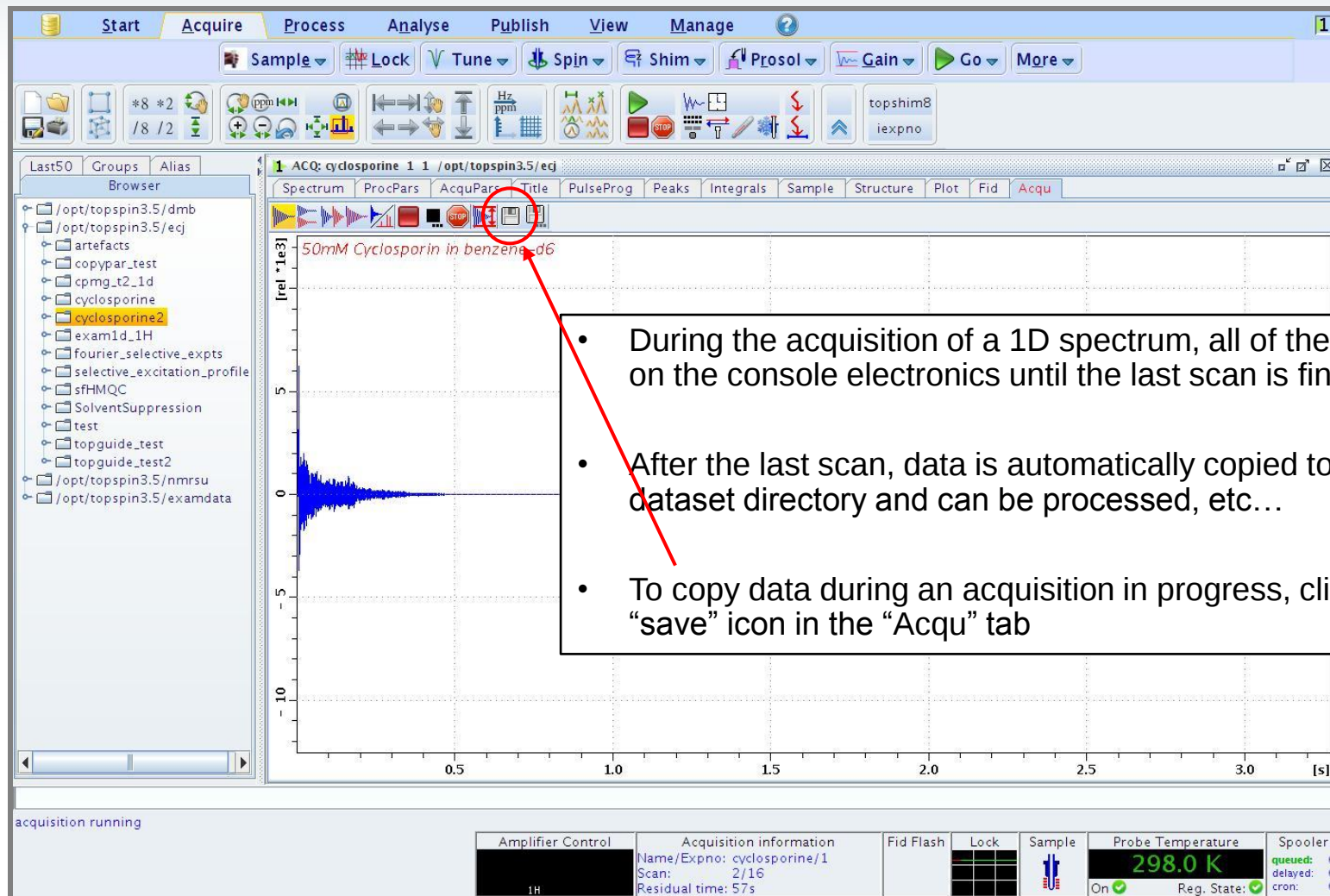
Some info on data acquisition



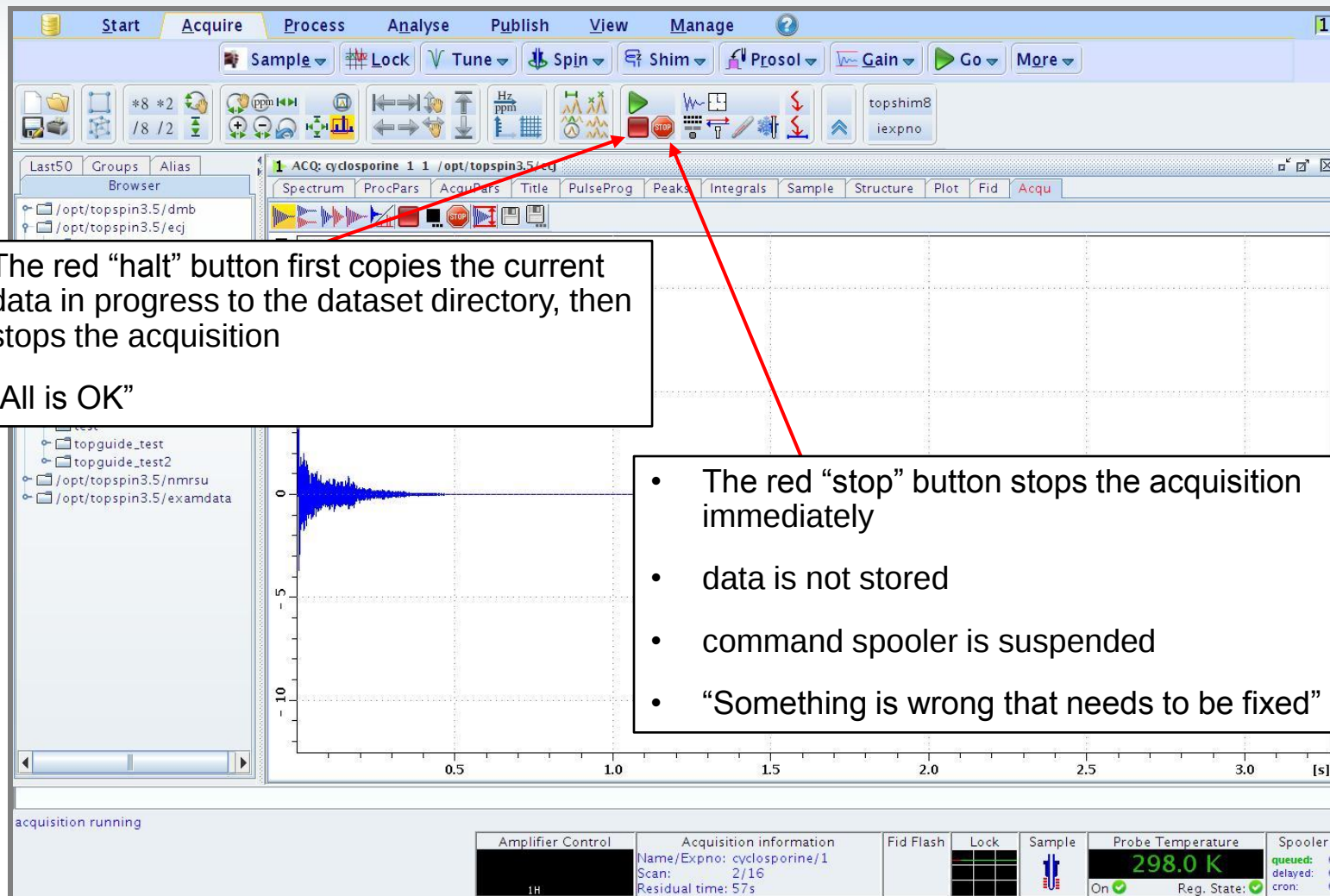
Some info on data acquisition



Some info on data acquisition



Stopping an acquisition in progress



Command Spooler – queuing multiple acquisitions



The screenshot displays the Bruker TopSpin software interface. The main window shows a file browser on the left with a tree view of directories. The central panel displays the acquisition parameters for a specific experiment, including the sample name '50mM Cyclosporin in benzene-d6'. A text box in the center lists the following points:

- all acquisition commands can automatically be sent to a spooler
- once one process finishes, the next will start
- you can queue up multiple experiments as well as shimming, tuning, etc.
- This must be tuned on in the user settings

A callout box labeled 'Spooler' shows the following status:

```
Spooler
queued: 3
delayed: 0
cron: 0
```

The bottom status bar provides additional information, including the acquisition name 'cyclosporine/2', the scan number '1/128', the residual time '5m21s', and the probe temperature '298.0 K'.

Command Spooler – queuing multiple acquisitions



Spooler Queue Job Tools

Queued jobs (3) | Scheduled jobs (0) | Cron jobs (0)

Command	Status	Data object	Owner	Estimated t...	Estimated start
zg yes	Running	/opt/topspin3.5/ecj/cyclosporine/2/pdata/1	nmrsu	0:05:30	July 8, 2015 2:29 PM
atma	Waiting	/opt/topspin3.5/ecj/cyclosporine/3/pdata/1	nmrsu	n/a	n/a
rga	Waiting	/opt/topspin3.5/ecj/cyclosporine/3/pdata/1	nmrsu	n/a	n/a
zg yes	Waiting	/opt/topspin3.5/ecj/cyclosporine/3/pdata/1	nmrsu	0:09:59	July 8, 2015 2:35 PM

finished

Amplifier Control | Acquisition information | Fid Flash | Lock | Sample | Probe Temperature: 298.0 K | Pooler: queued: 3, delayed: 0, cron: 0

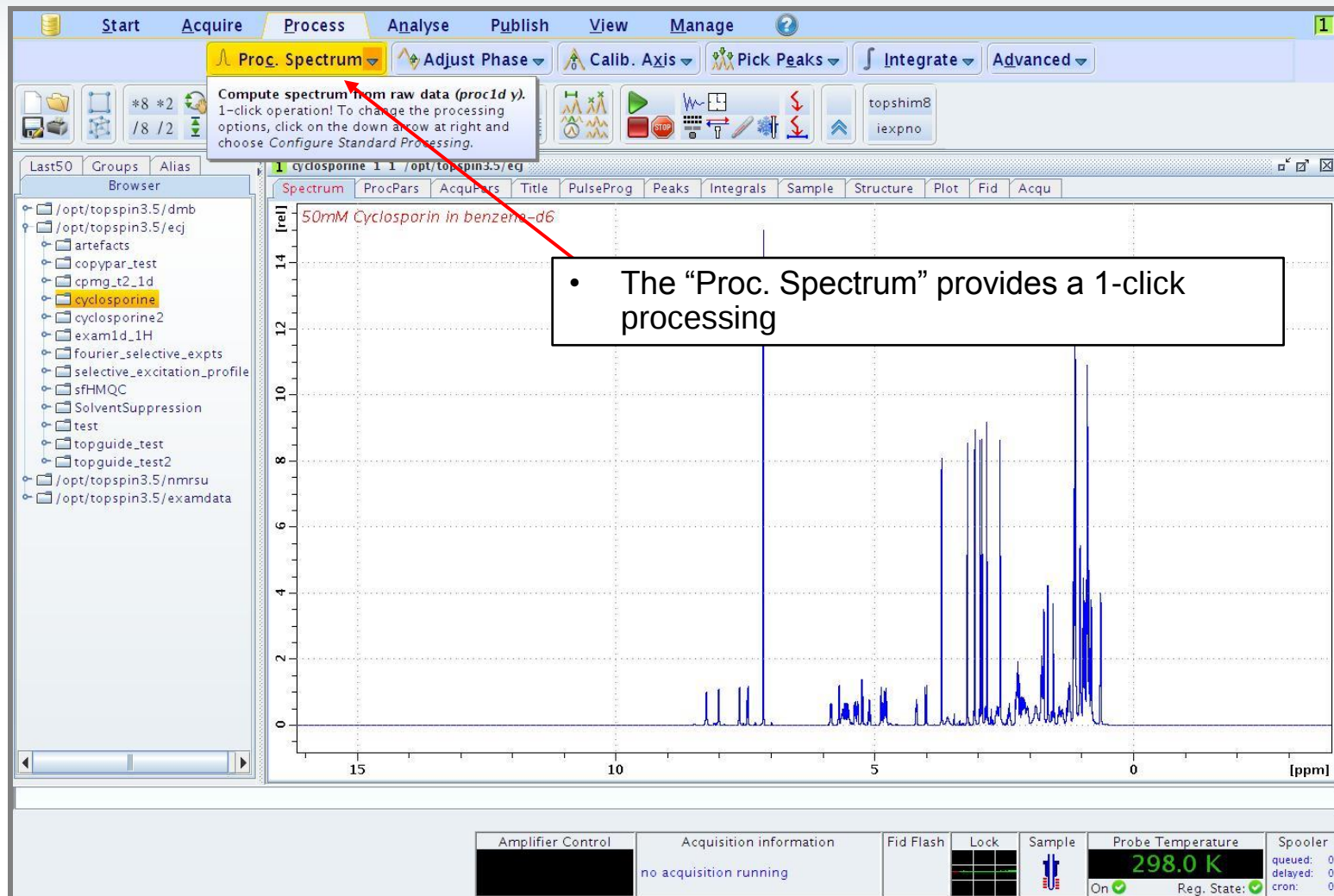
List of spooled commands

Datasets used for each spooled command will

- Clicking on “queued” will show a list of the spooled jobs

- Right-clicking on a spooled job will give options for changing or deleting it

Basic data processing...



Basic data processing...



The screenshot displays the Bruker TopSpin software interface. The 'Proc. Spectrum' menu is open, showing options like 'Configure Standard Processing (proc1d)', 'Window Multiplication (wm)', 'Fourier Transform (ft)', 'Fourier Transform Options ... (ftf)', and 'Start Automation AU Program (xaup)'. A red arrow points from the 'Configure Standard Processing (proc1d)' option to a text box. The text box contains the following text:

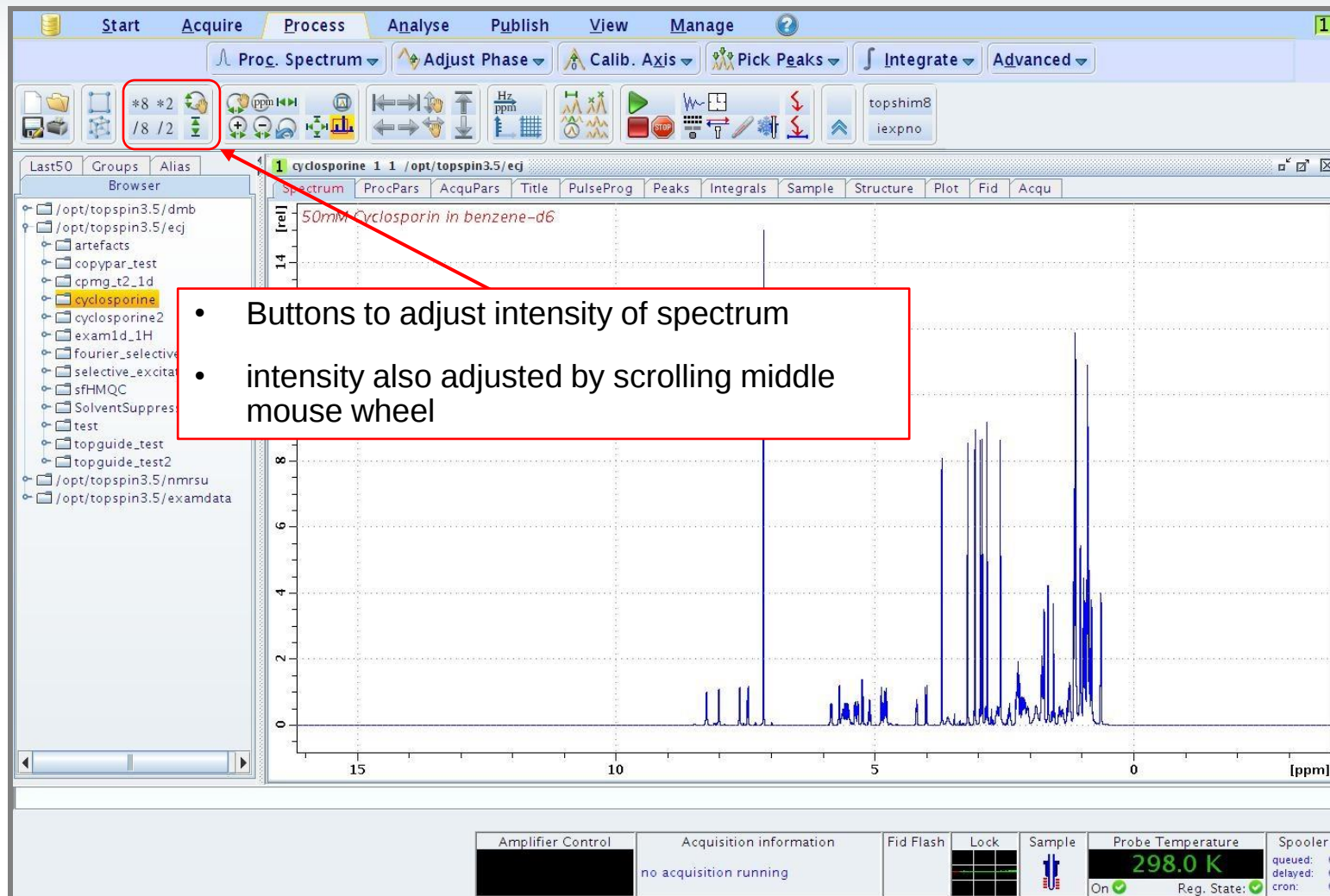
- The details of exactly what Proc Spectrum does can be configured

The 'Configure Standard Processing' dialog box is also visible, showing various processing options and their settings:

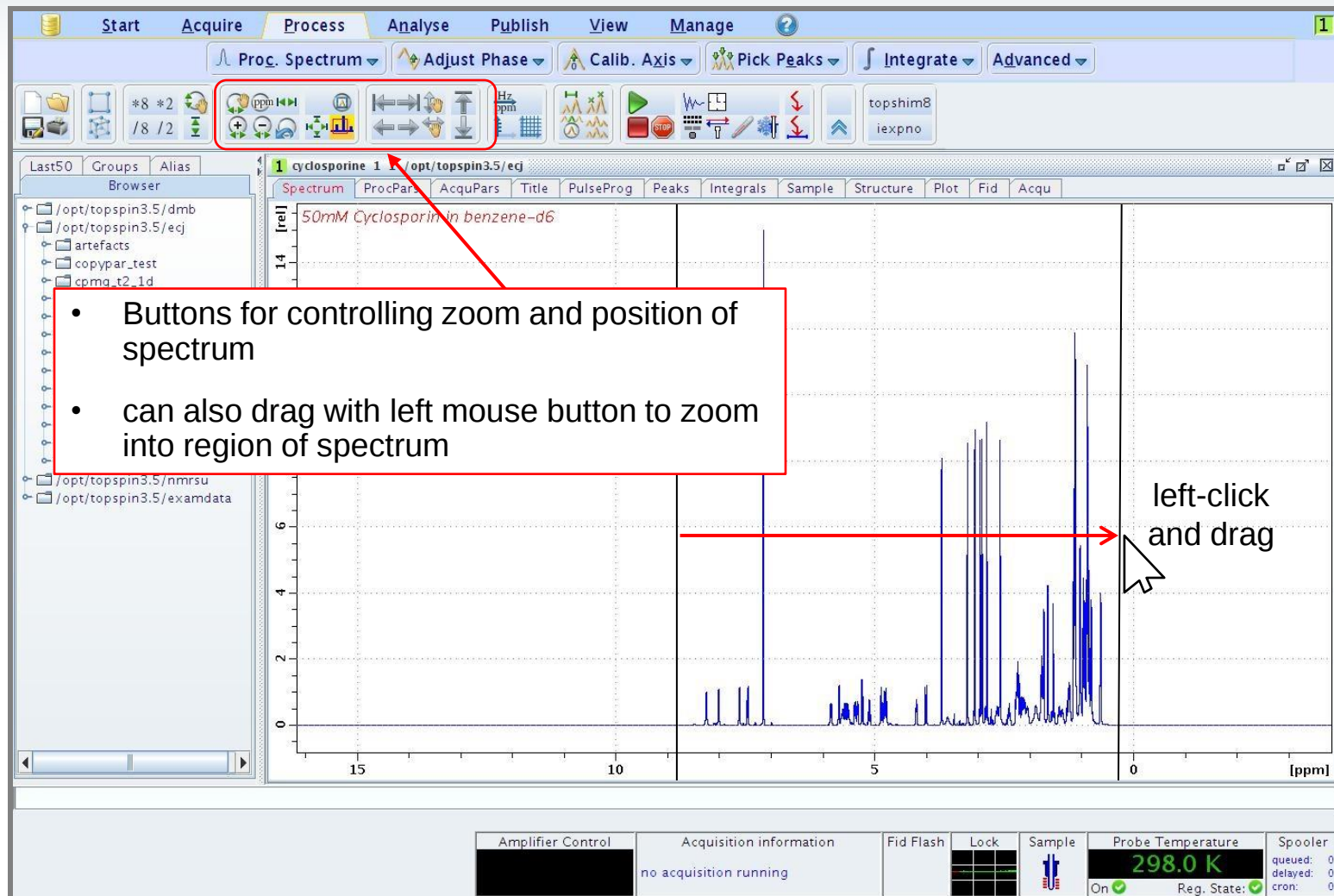
- Exponential Multiply (em) ☒ LB [Hz] = 0.3
- Fourier Transform (ft) ☒
- Auto - Phasing (apk) ☒
- Set Spectrum Reference (sref) ☐
- Auto - Baseline Correction (absn) ☒ Include integration = no
- Plot (autoplot) ☐ LAYOUT = +/1D_H.xwp
- Warn if processed data exist ☒

The dialog box has 'Save', 'Execute', and 'Cancel' buttons. The background shows a spectrum plot with chemical shift in ppm on the x-axis (ranging from 15 to 0) and intensity on the y-axis. The status bar at the bottom indicates 'no acquisition running' and 'Probe Temperature: 298.0 K'.

Manipulating spectrum display



Manipulating spectrum display



Basic data processing – manual phasing



The screenshot displays the Bruker TopSpin software interface. The 'Process' tab is active, and the 'Adjust Phase' button is highlighted with a red circle. A text box labeled 'Start manual phasing mode' points to the 'Adjust Phase' button. The main window shows a 1D NMR spectrum of cyclosporine in benzene-d6. The x-axis is labeled 'ppm' and ranges from 15 to 0. The y-axis is labeled 'I [a.u.]' and ranges from 0 to 15. The spectrum shows several peaks, with the most prominent ones between 0 and 5 ppm. A red circle highlights the '0' and '1' buttons in the top left corner of the spectrum window. A text box labeled 'When done, click "save and return" icon' points to the 'save and return' icon (a floppy disk with a checkmark) in the top right corner of the spectrum window. Two text boxes provide instructions for adjusting the phase:

To adjust zero-order phase:

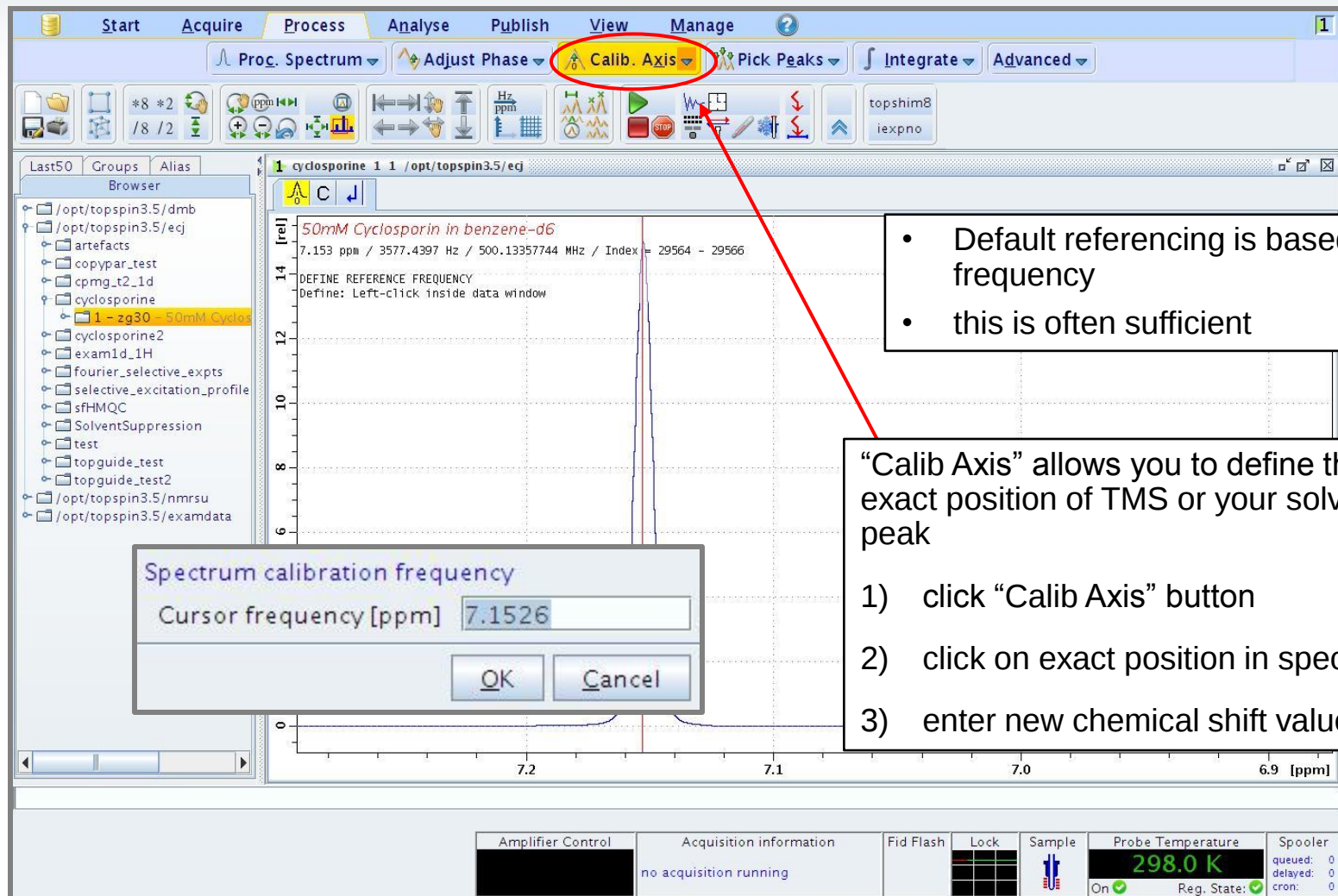
- left-click on "0"
- move mouse up and down while continuing to hold down left mouse button

To adjust first-order phase:

- left-click on "1"
- move mouse up and down while continuing to hold down left mouse button

The bottom status bar shows '0 order correction' and 'no acquisition running'. The 'Probe Temperature' is 298.0 K, and the 'Reg. State' is 'On'.

Basic data processing – chemical shift referencing

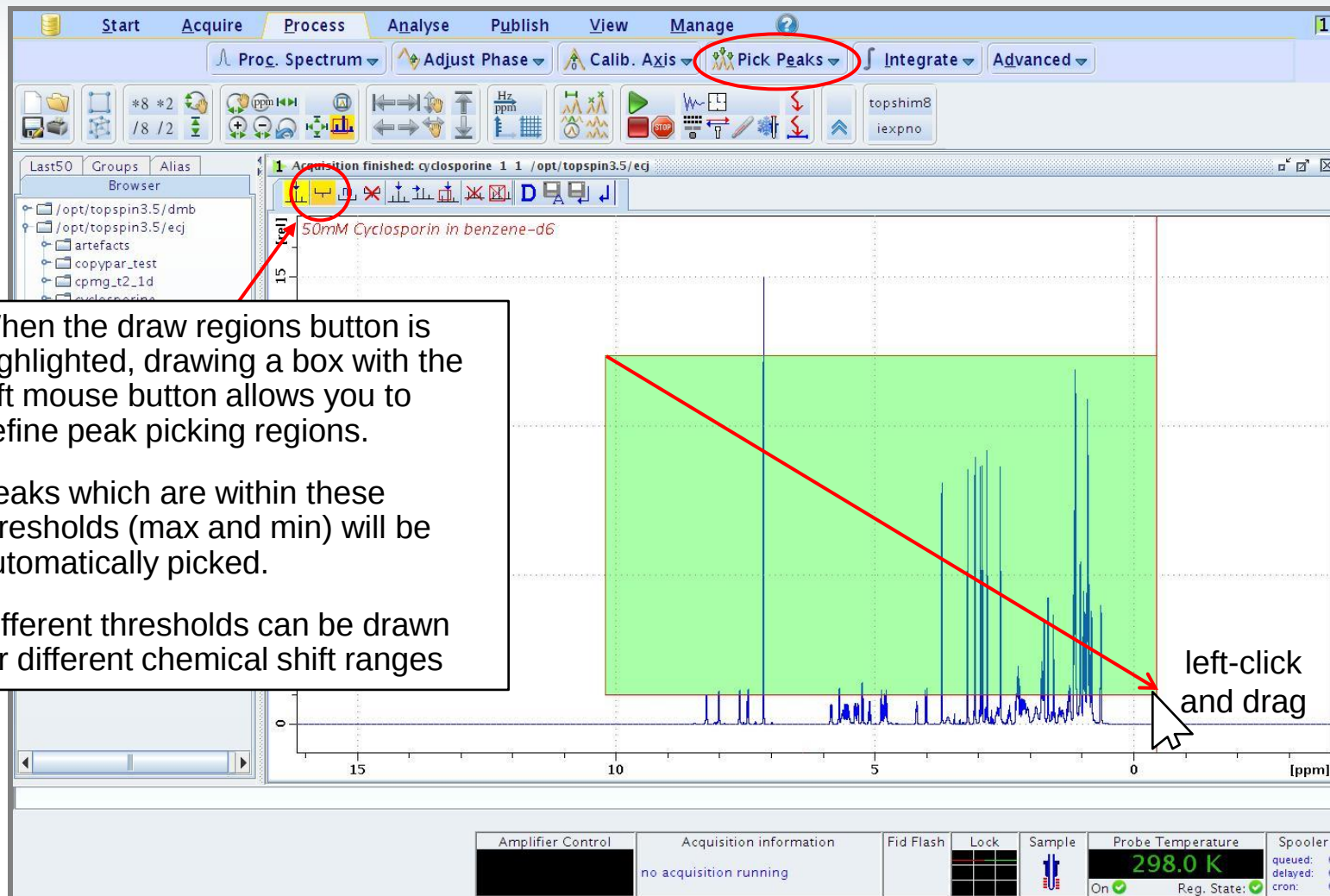


- Default referencing is based on lock frequency
- this is often sufficient

“Calib Axis” allows you to define the exact position of TMS or your solvent peak

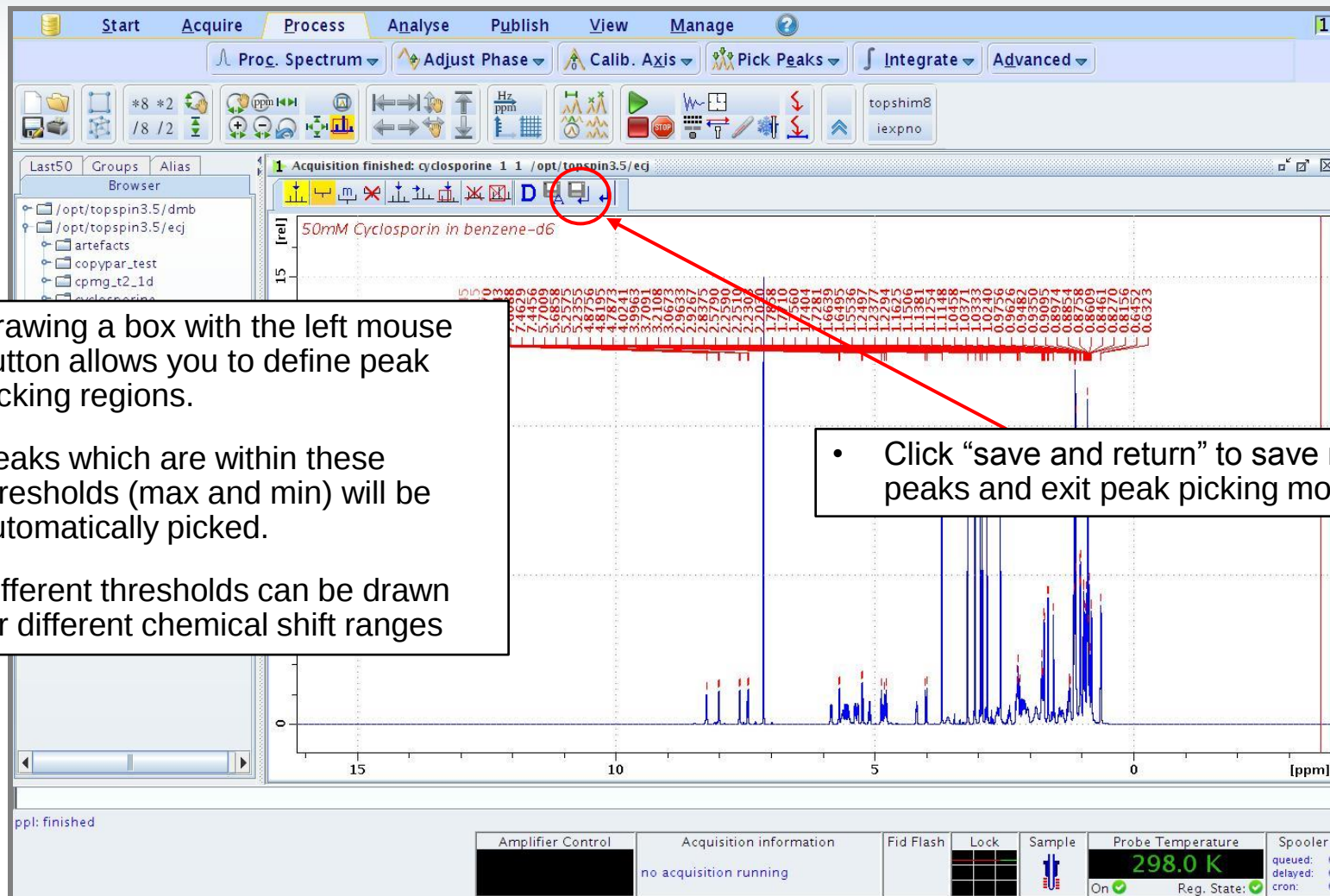
- 1) click “Calib Axis” button
- 2) click on exact position in spectrum
- 3) enter new chemical shift value

Basic data processing – manual peak picking



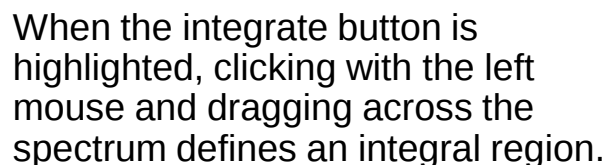
- When the draw regions button is highlighted, drawing a box with the left mouse button allows you to define peak picking regions.
- Peaks which are within these thresholds (max and min) will be automatically picked.
- Different thresholds can be drawn for different chemical shift ranges

Basic data processing – manual peak picking

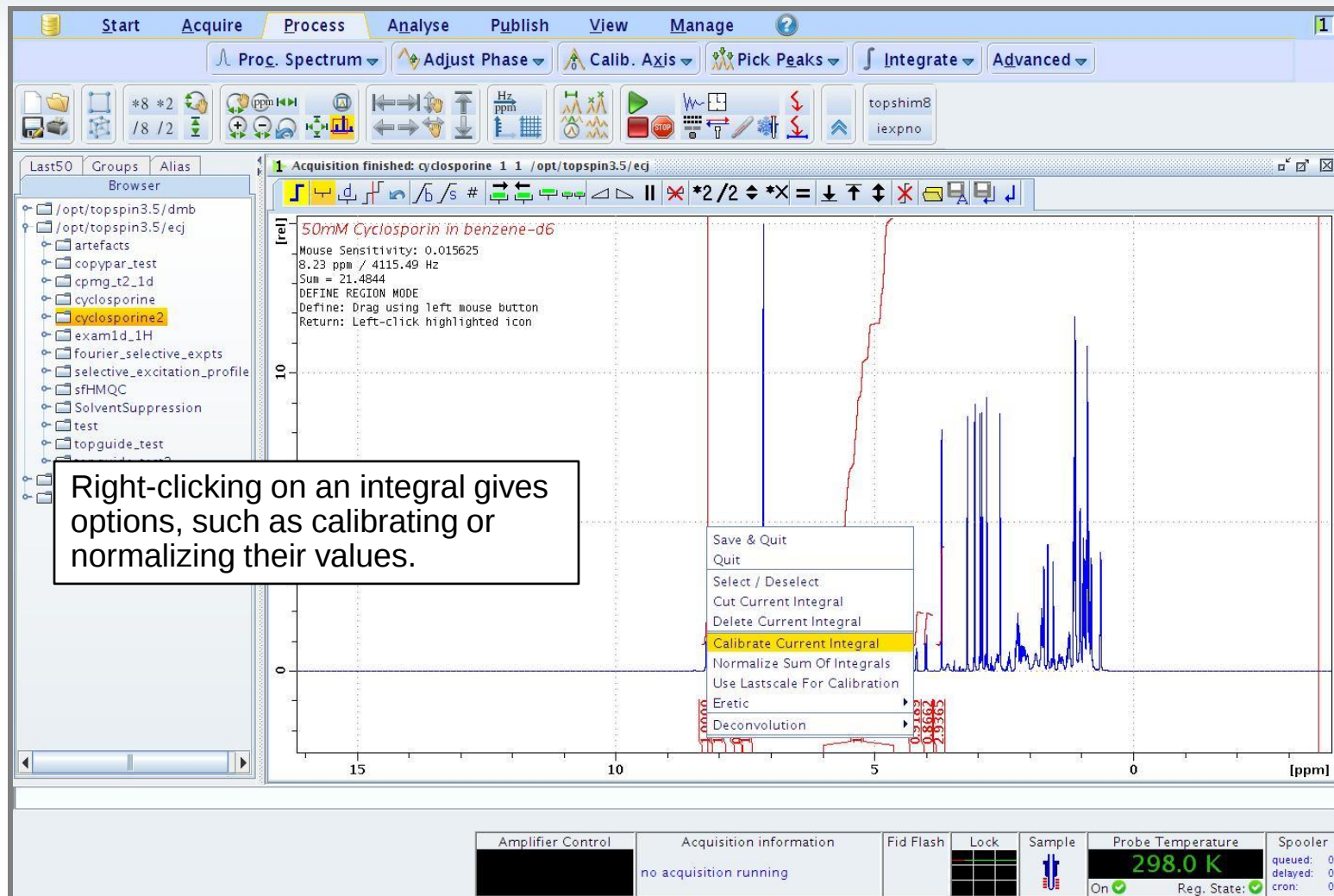


- Drawing a box with the left mouse button allows you to define peak picking regions.
- Peaks which are within these thresholds (max and min) will be automatically picked.
- Different thresholds can be drawn for different chemical shift ranges

- Click “save and return” to save new peaks and exit peak picking mode

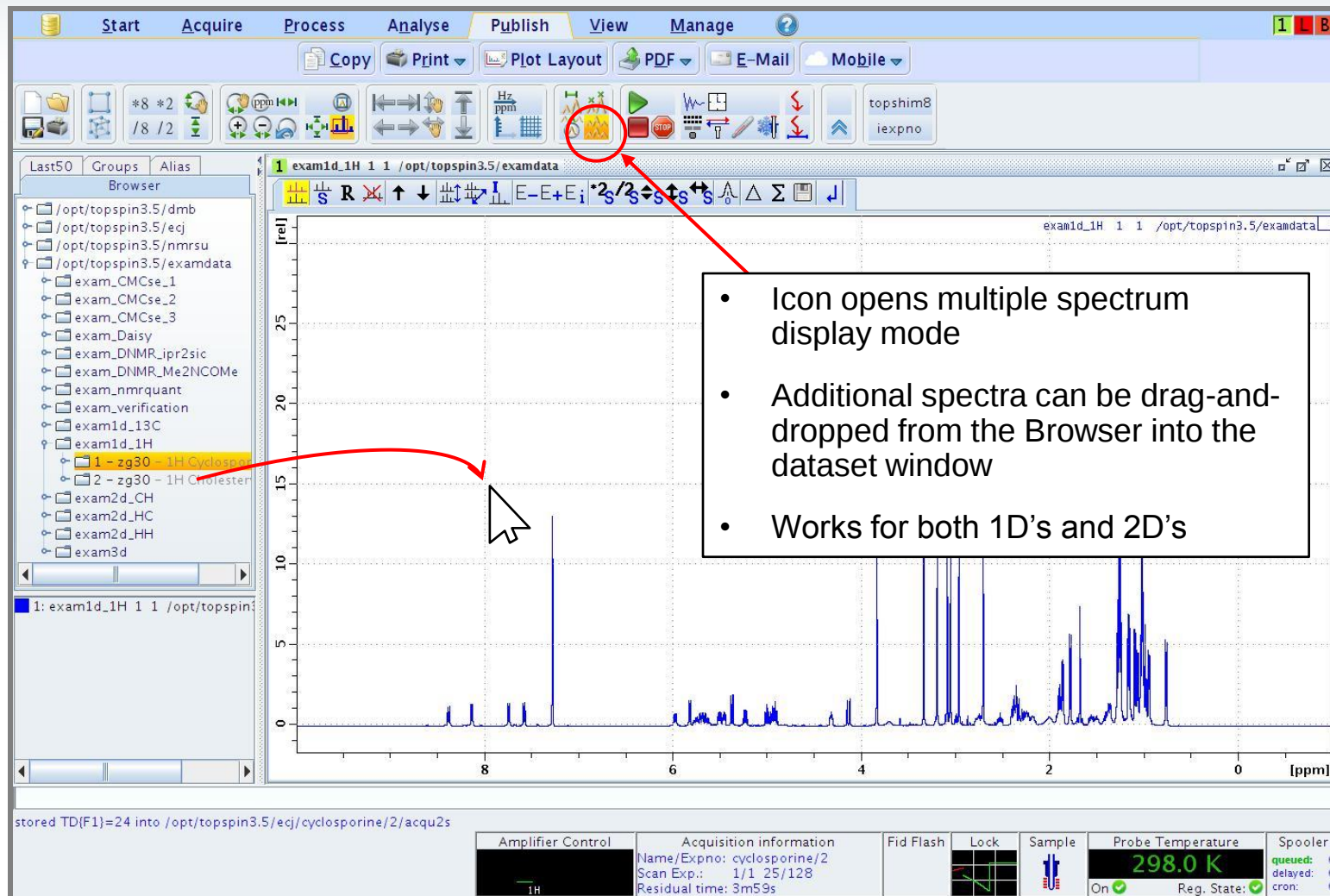


Basic data processing – manual integration



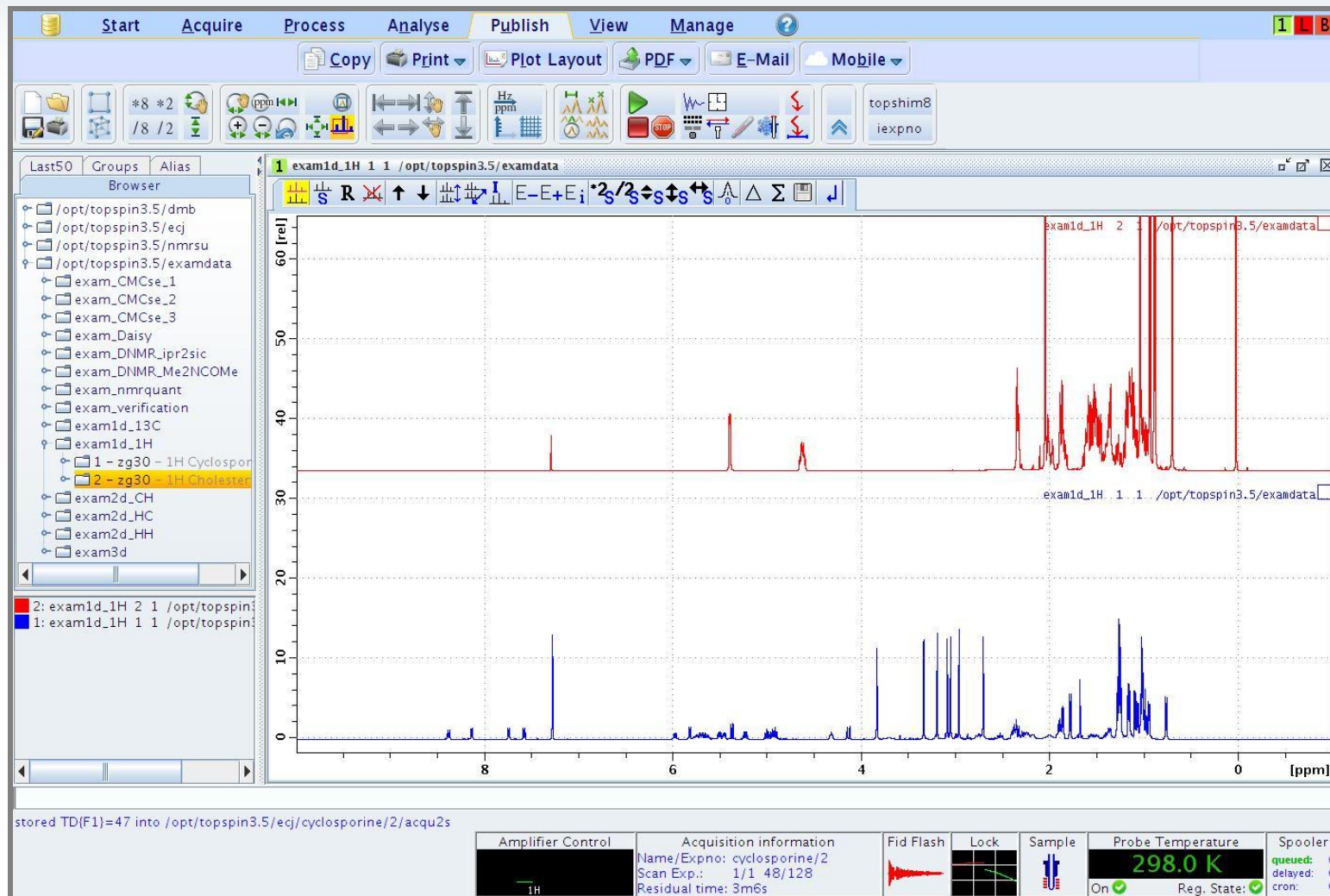
Additional 1D display options

- overlaying spectra



Additional 1D display options

- overlaying spectra



2D experiments...pretty much the same as 1D's



Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

NAME: cyclosporine

EXPNO: 2

PROCNO: 1

☐ Use current parameters

☒ Experiment: COSYGPSW

Options:

- ☐ Set solvent: C6D6
- ☒ Execute 'getprosol'
- ☐ Keep parameters: P 1, O1, PLW 1
- DIR: /opt/topspin3.5/ecj
- ☐ Show new dataset in new window
- Receivers (1,2, ...16): 1

TITLE: 50mM Cyclosporin in benzene-d6

- Define location for new experiment (new EXPNO used here)
- Define parameter set for new experiment

Additional setup option for 2D's - Setlimits



The screenshot displays the Bruker TopSpin software interface. The 'SetLimits' menu option is highlighted with a red circle and a red arrow pointing to it. A tooltip for 'SetLimits' is visible, explaining its function: 'Setup limits for 2D in F2 and F1 (setlimits). Set the limits for Homo and Hetero 2D experiments as obtained from 1D spectra. Sets the sweep width and excitation frequency for a 2D dataset. It will prompt you to open a reference 1D dataset from the Topspin browser, and zoom into the region of interest. The SW and center of the region of the 1D spectrum will be copied to the 2D spectrum. This can be used for either homonuclear or heteronuclear experiments. The nucleus of the 1D dataset used determines the dimension(s) of the 2D to which the SW and O1 is copied.'

A red arrow points from the 'SetLimits' menu option to a text box containing the following information:

- Setlimits provides a graphics tool for setting the spectral regions for 2D experiments (direct and indirect dimensions)

The interface also shows a file browser on the left with a tree view of files, including '1 - zg30 - 50mM Cyclosporin'. The main window displays a spectrum plot with the title '50mM Cyclosporin in benzene-d6'. The status bar at the bottom indicates 'no acquisition running' and shows various system parameters like 'Probe Temperature: 298.0 K'.

Additional setup option for 2D's - Setlimits



The screenshot shows the Bruker TopSpin software interface. The 'Acquire' tab is selected in the top menu. The 'SetLimits' button is highlighted in the top toolbar. A file browser on the left shows a directory structure with '1 - 50mM Cyclosporine' selected. A 'setlimits' dialog box is open in the center, displaying instructions for setting frequencies. The status bar at the bottom shows 'no acquisition running' and a probe temperature of 298.0 K.

- New window pops up giving instructions for “setlimits”
- keep this window open for now!

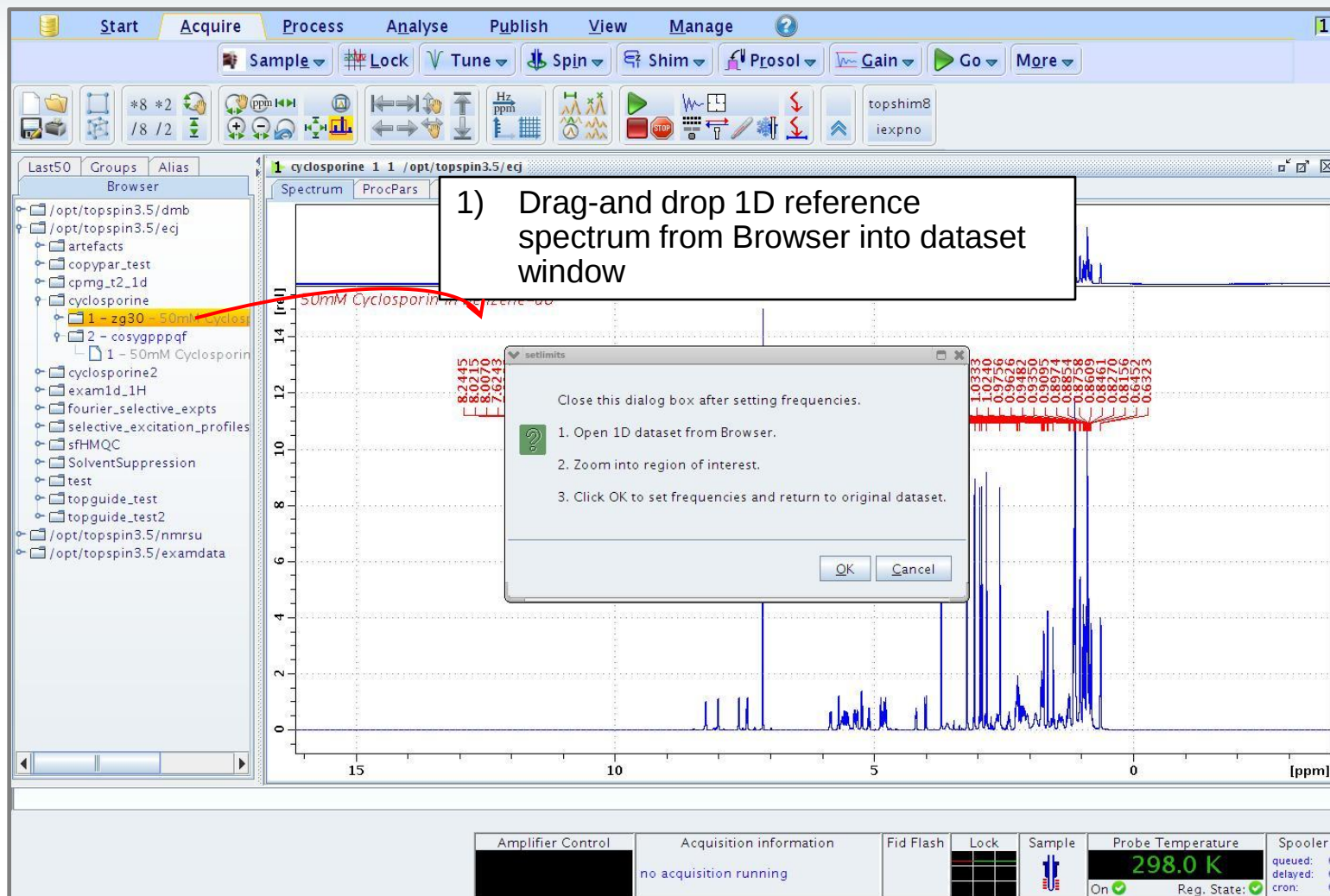
Close this dialog box after setting frequencies.

1. Open 1D dataset from Browser.
2. Zoom into region of interest.
3. Click OK to set frequencies and return to original dataset.

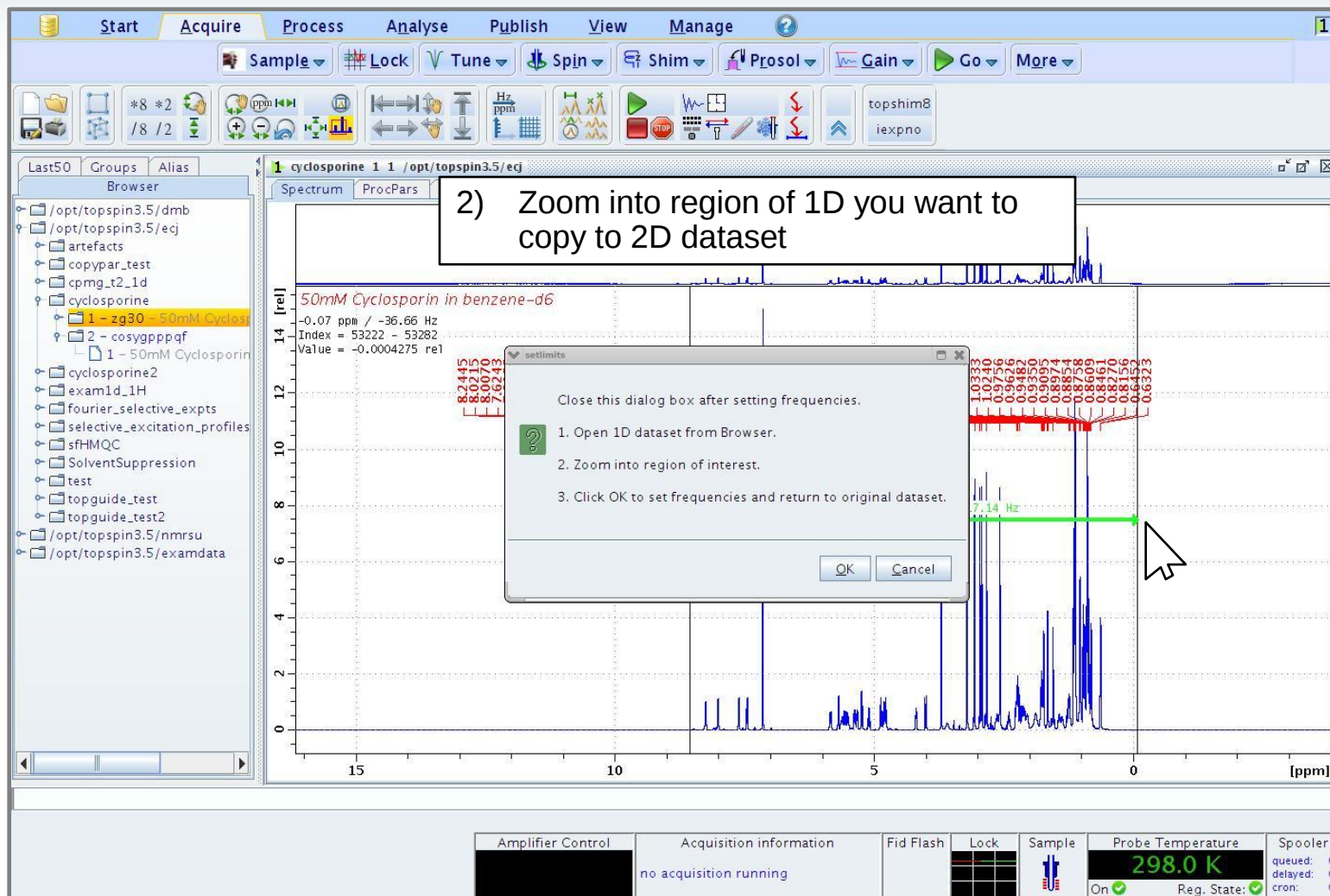
OK Cancel

Amplifier Control Acquisition information FID Flash Lock Sample Probe Temperature Spooler
no acquisition running 298.0 K
On Reg. State: cron: 0

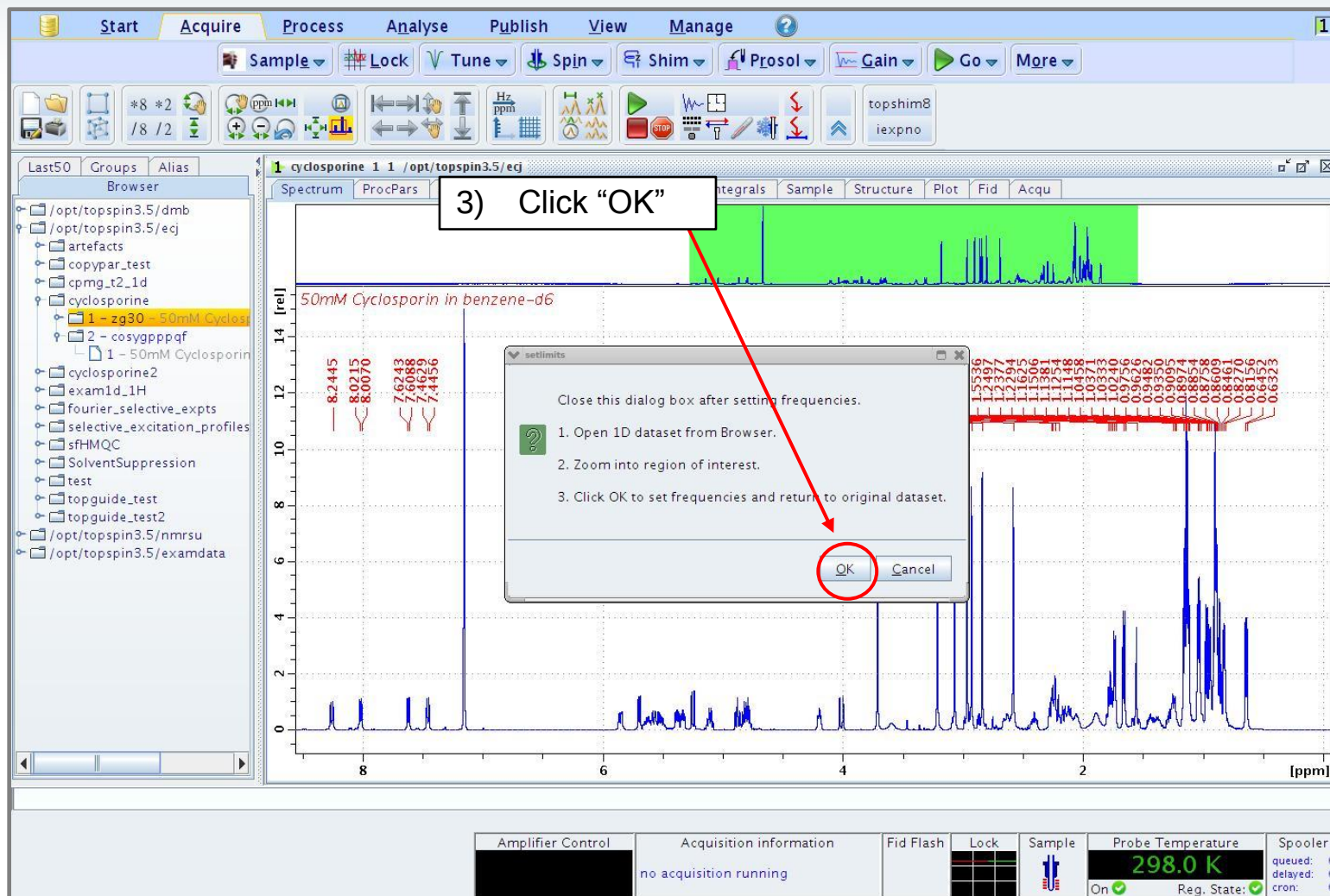
Additional setup option for 2D's - Setlimits



Additional setup option for 2D's - Setlimits



Additional setup option for 2D's - Setlimits



Additional setup option for 2D's - Setlimits



The screenshot shows the Bruker TopSpin software interface. The 'Acquire' tab is selected. The 'SetLimits' button is highlighted in the top toolbar. The left sidebar shows a file tree with the following structure:

- /opt/topspin3.5/dmb
- /opt/topspin3.5/ecj
 - artefacts
 - copypar_test
 - cpmg_t2_1d
 - cyclosporine
 - 1 - zg30 - 50mM Cyclosporin
 - 2 - cosygpppqf
 - 1 - 50mM Cyclosporin
 - cyclosporine2
 - exam1d_1H
 - fourier_selective_expts
 - selective_excitation_profiles
 - sfHMQC
 - SolventSuppression
 - test
 - topguide_test
 - topguide_test2
- /opt/topspin3.5/nmrstu
- /opt/topspin3.5/examdata

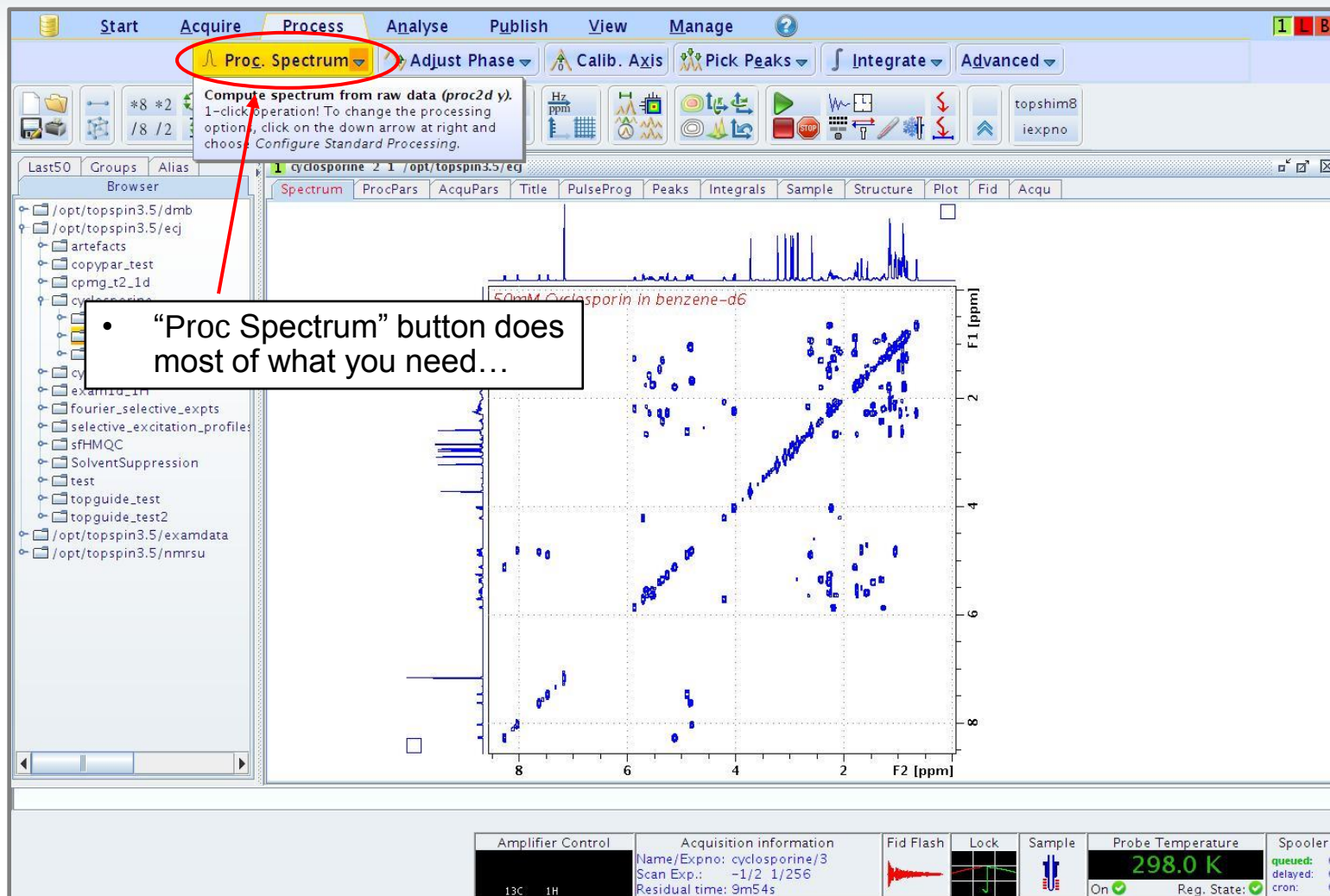
The main window displays the 'Spectrum' tab for the file '1 cyclosporine 2 1 /opt/topspin3.5/ecj'. The title bar indicates '50mM Cyclosporin in benzene-d6'. A dialog box titled '1H spectral limits copied for F1 and F2 dimensions.' is open, showing the following information:

- SW: 8.6383 ppm
- O1P: 4.243 ppm

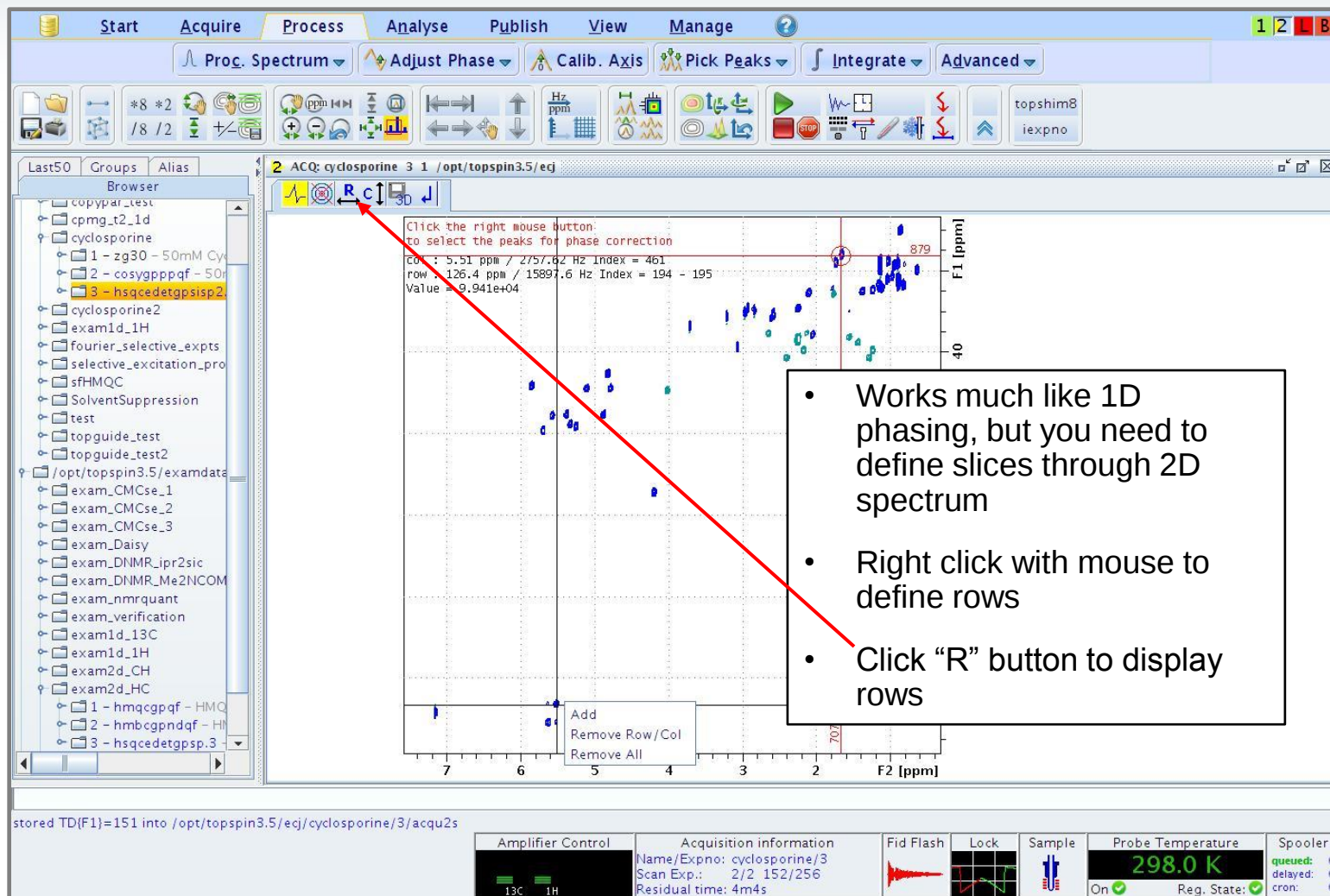
The status bar at the bottom shows 'setlimits: finished' and various system controls including Amplifier Control, Acquisition information (no acquisition running), Fid Flash, Lock, Sample, Probe Temperature (298.0 K), and Spooler status.

- Relevant sweep widths and excitation frequencies are automatically copied to 2D dataset
- Rest of setup is the same:
 - “Prosol”
 - “Gain”
 - “Go”

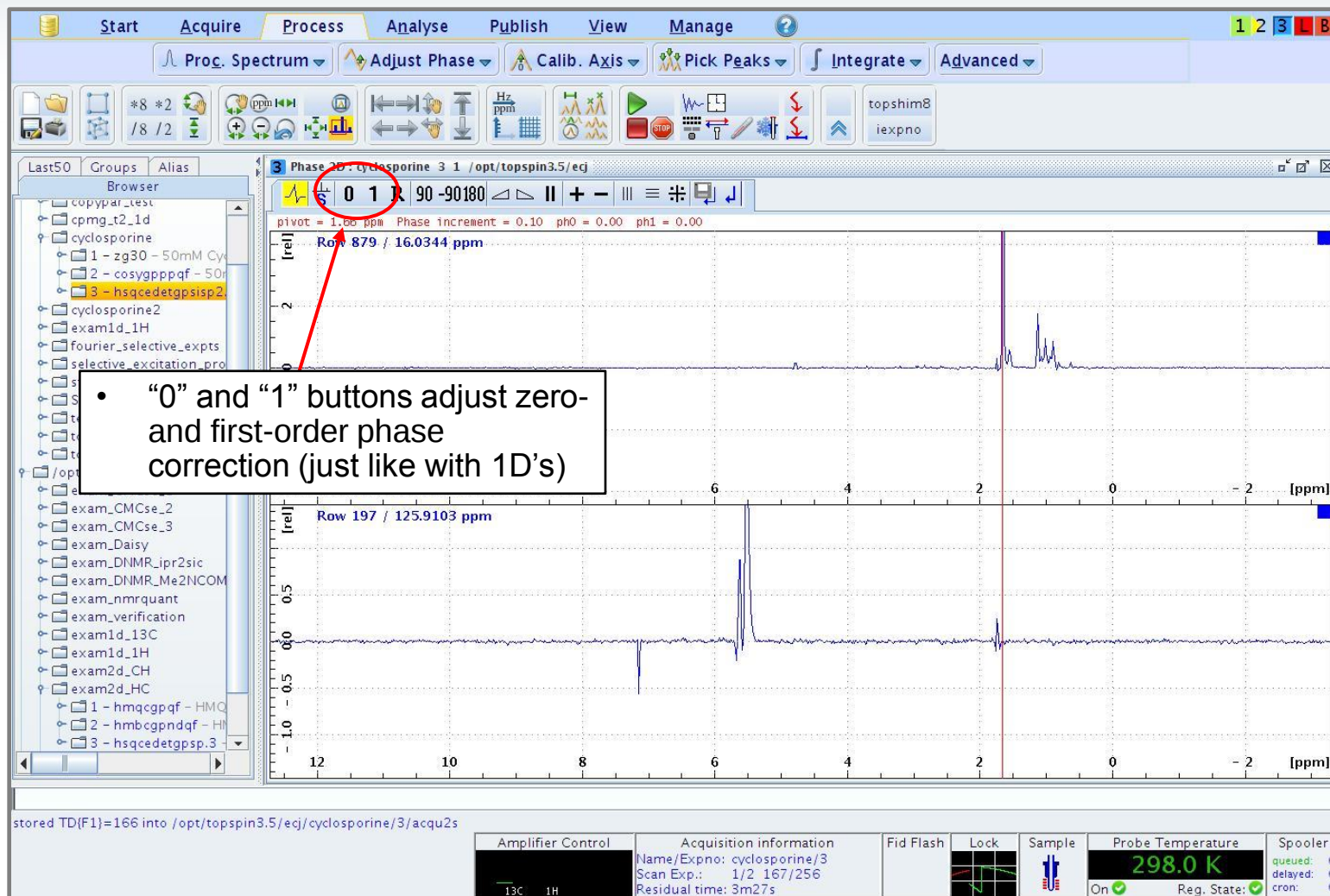
Processing 2D's



Processing 2D's – manual phasing



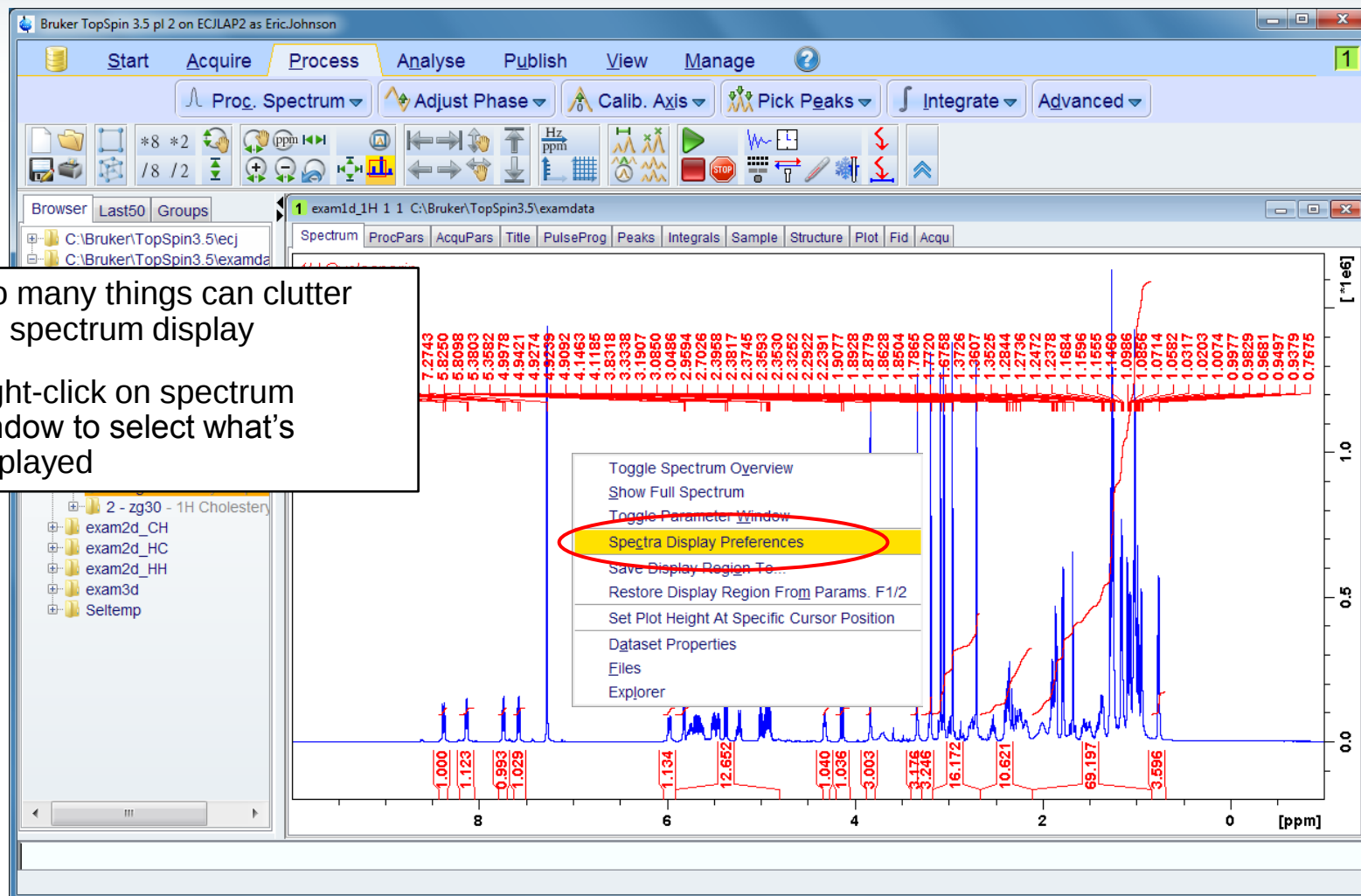
Processing 2D's – manual phasing



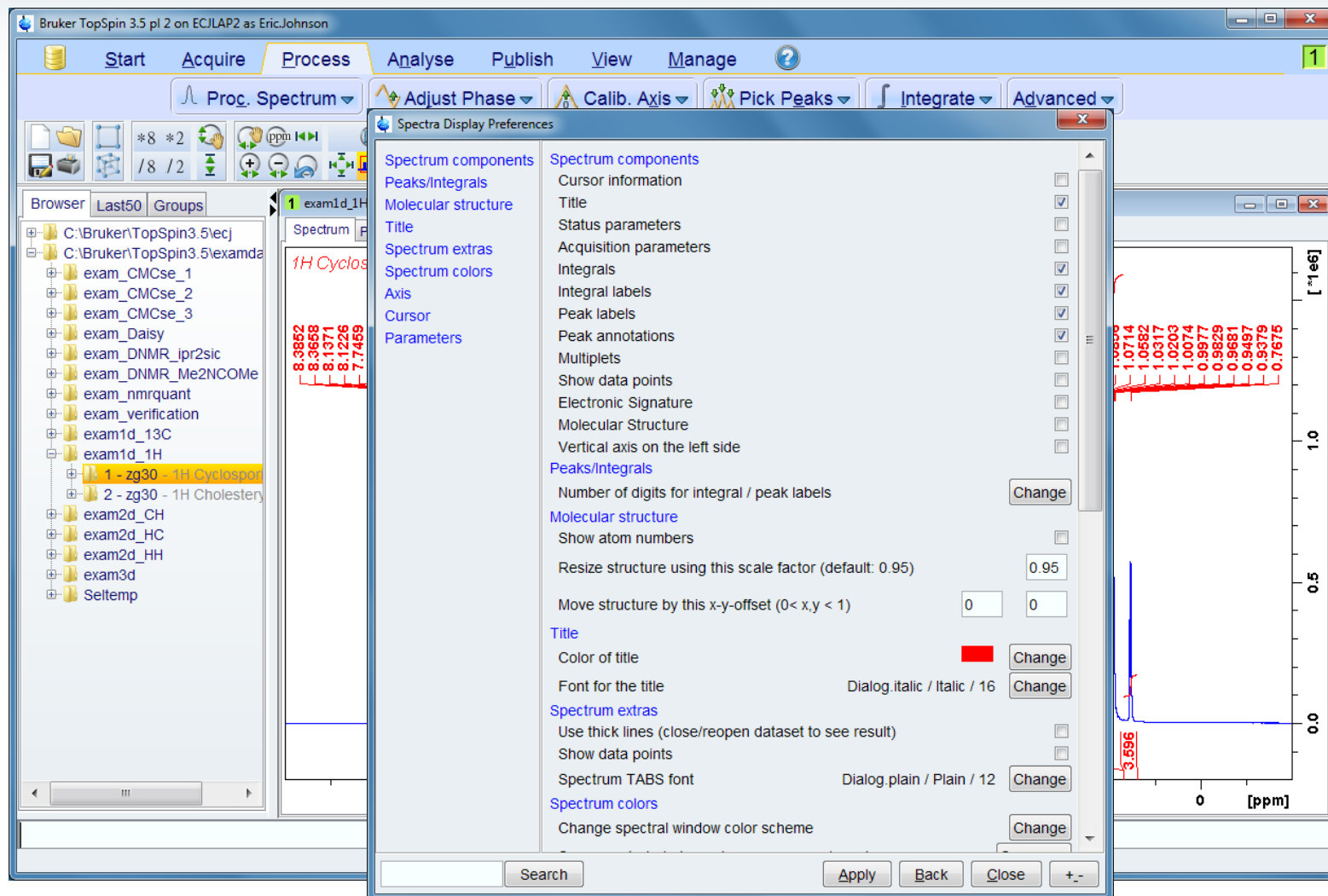
More about the Topspin spectrum display



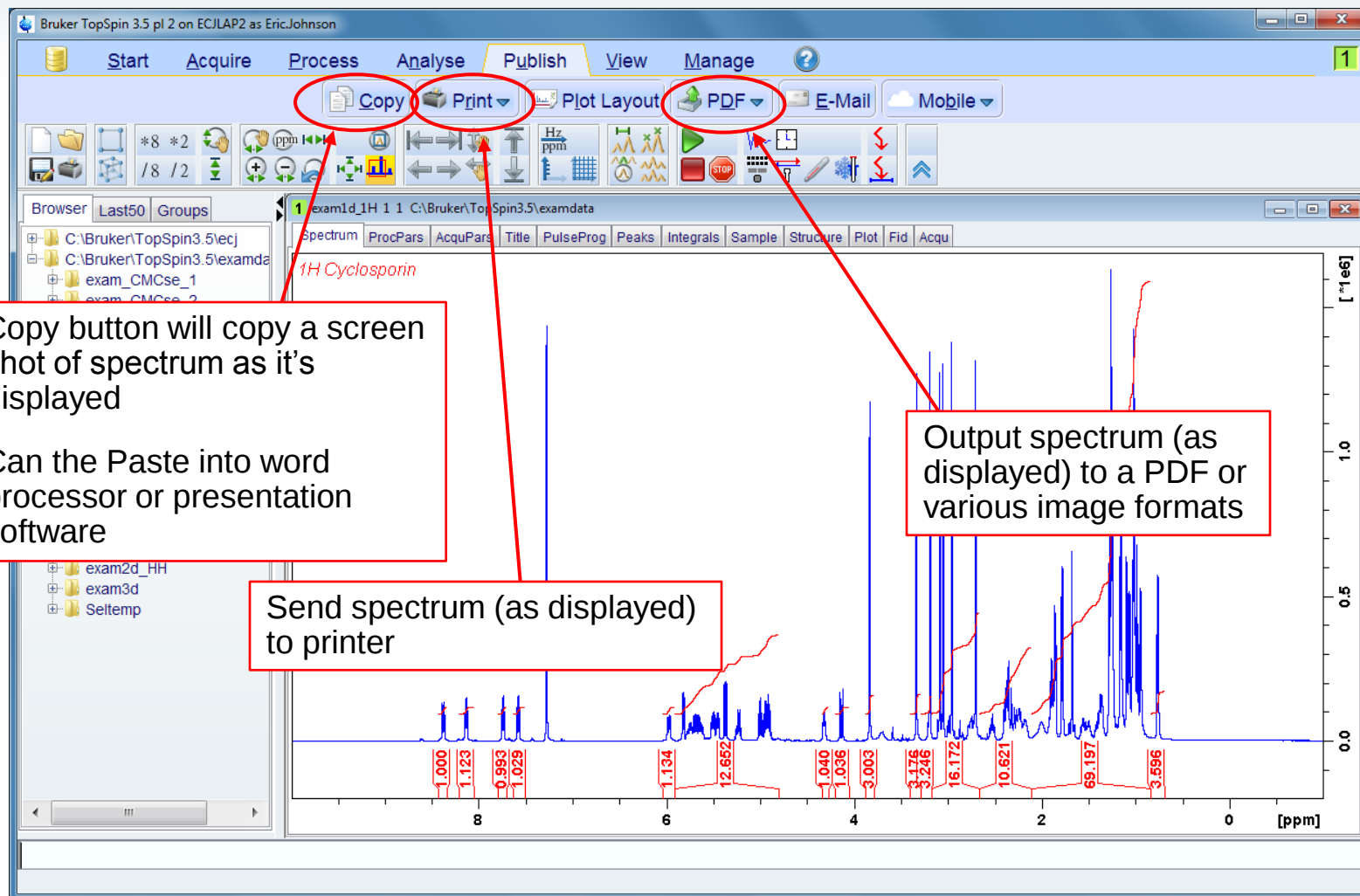
- Too many things can clutter the spectrum display
- Right-click on spectrum window to select what's displayed



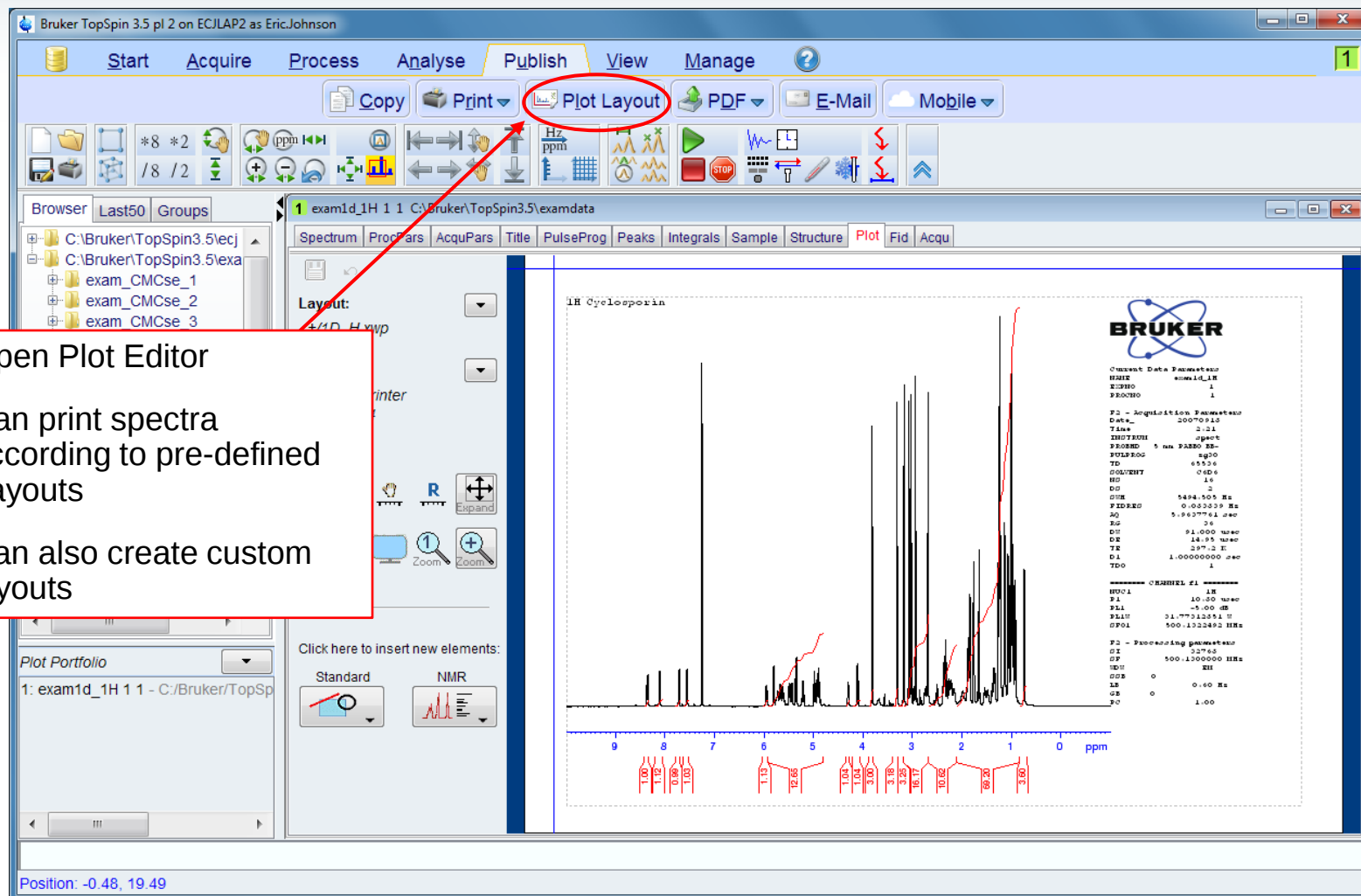
More about the Topspin spectrum display



Plotting – copying/pasting spectra



Plotting – copying/pasting spectra



- Open Plot Editor
- Can print spectra according to pre-defined Layouts
- Can also create custom layouts

Back to recommended parameter sets...



Parameter Sets: rpar

File Options Help

Source = C:\Bruker\TopSpin3.5\exp\stan\nmr\par

Find file names: [] Exclude: [] Clear

Class = Any Dim = Any ☒ Show Recommended

Type = Any SubType = Any SubTypeB = Any Reset Filters

Class	Type	SubType	SubTypeB	Description
C13CPD				13C with 1H decoupling, 1024 scans, 235 ppm
C13DEPT135				DEPT 135 experiment, CH3/CH positive, CH2 negative, 256 scans, 160 ppm
COSYGPDFPSW				Gradient selected double quantum filtered phase sensitive COSY
COSYGPSW				Gradient selected COSY
HMBCETGPL3ND				1H-13C HMBC with gradient selection using 3-fold low pass filter for better 1J suppression
HMBCGP				1H-13C HMBC with gradient selection
ADIA				1H-15N HMBC with gradient selection
SISP				1H-13C HSQC-TOCSY with gradient selection 600 MHz >= BF1
SISP_ADIA				1H-13C HSQC-TOCSY with gradient selection BF1 >= 700 MHz
N				1H-13C multiplicity edited HSQC with gradient selection 600 MHz >= BF1
HSQCETGPSISP				1H-13C multiplicity edited HSQC with gradient selection BF1 >= 700 MHz
HSQCETGPSISP_ADIA				1H-15N HSQC with gradient selection
MLEVPHPR				1H-13C HSQC with gradient selection 600 MHz >= BF1
MLEVPHSW				1H-13C HSQC with gradient selection BF1 >= 700 MHz
NOESYPHPR				Phase sensitive TOCSY with solvent suppression
NOESYPHSW				Phase sensitive TOCSY
PROTON				Phase sensitive NOESY with solvent suppression
ROESYPHPR				Phase sensitive NOESY
ROESYPHSW				1H experiment
WATERSUP				Phase sensitive ROESY with solvent suppression
				Phase sensitive ROESY
				1H with water suppression

Read... Close

- Options -> Show Comment will display brief description of parameter sets

Brief description of parameter sets names...



The screenshot shows a window titled "Parameter Sets: rpar" with a menu bar (File, Options, Help) and a toolbar. The "Source" dropdown is set to "C:\Bruker\TopSpin3.5\exp\stan\nmr\par". The window displays a list of parameter sets with columns for Name, Class, Type, and a list of codes. The codes are organized into groups, with some highlighted in blue.

Name	Class	Type	Codes
C13C	Refresh From File System		COSYGPDPHSW, COSYGPSW, HMBCEGPL3ND
HMBC	Manage Source Directories		HSQC_TOCSY, HSQC_TOCSY_ADIA, HSQCEDETGPSISP
HSQCCEDETGPSISP_ADIA			HSQCETGPSISP, HSQCETGPSISP_ADIA, MLEVPHPR
MLEVPHSW			NOESYPHPR, NOESYPHSW, PROTON, ROESYPHPR
ROESYPHSW			WATERSUP

Buttons at the bottom right: Read..., Close

- Parameter set (and pulse program) names often have several 2-letter codes
- HSQCEDETGPSISP:
 - ED = with multiplicity editing
 - ET = echo-Antiecho
 - GP = with gradients
 - SI = sensitivity improved
 - SP = with shaped pulses
- for full list of 2-letter codes, look at the file "Pulprog.info" in the pulse program directory
- "edpul" will display list of pulse programs

Acquisition parameters



The screenshot displays the Bruker TopSpin software interface. The 'Acquire' tab is selected, and the 'AcqPar' sub-tab is active. The left sidebar shows a file browser with the 'cyclosporine2' folder highlighted. The main panel displays acquisition parameters for the experiment 'cyclosporine 1'.

Parameter	Value	Description
PULPROG	zg30	Current pulse program
AQ_mod	DQD	Acquisition mode
TD	65536	Size of fid
DS	2	Number of channels
NS	16	Number of scans
TD0	1	Loop count for 'td0'
SW [ppm]	19.9947	Spectral width
SWH [Hz]	10000.000	Spectral width
AQ [sec]	3.2767999	Acquisition time
FIDRES [Hz]	0.305176	Fid resolution
FW [Hz]	4032000.000	Filter width
RG	32	Receiver gain
DW [μsec]	50.000	Dwell time
DWOV [μsec]	0.025	Oversampling dwell time
DECIM	2000	Decimation rate of digital filter
DSPFIRM	sharp(standard)	DSP firmware filter
DICTYP	DDU	Digitization

At the bottom, the status bar shows 'no acquisition running' and a probe temperature of 298.0 K.

Clicking the “pulse” or “A” icon will toggle between pulse program specific pulses and delays, and all acquisition parameters

The “AcqPar” tab show full list of acquisition parameters

Acquisition parameters



1 Acquisition finished: cyclosporine 1 /opt/topspin3.5/eq

Probe: CPP BBO 500S2 BB-H&F-D-05 Z

General

Parameter	Value	Description
PULPROG	zg30	Pulse program for acquisition
TD	65536	Time domain size
SWH [Hz, ppm]	10000.00	Sweep width
AQ [sec]	3.2767999	Acquisition time
RG	32	Receiver gain
DW [μsec]	50.000	Dwell time
DE [μsec]	10.00	Pre-scan-delay
D1 [sec]	1.000000000	Relaxation delay; 1-5 * T1
DS	2	Number of dummy scans
NS	16	1 * n, total number of scans: NS * TD0
TD0	1	Number of averages in 1D

Channel f1

Parameter	Value	Description
SFO1 [MHz]	500.1330883	Frequency of ch. 1
O1 [Hz, ppm]	3088.30	Frequency of ch. 1
NUC1	1H	Nucleus for channel 1
P1 [μsec]	12.400	F1 channel - 90 degree high power pulse
PLW1 [W, dB]	15	F1 channel - power level for pulse (default)

finished

Amplifier Control | Acquisition information | F1d Flash | Lock | Sample | Probe Temperature: 298.0 K | Spooler

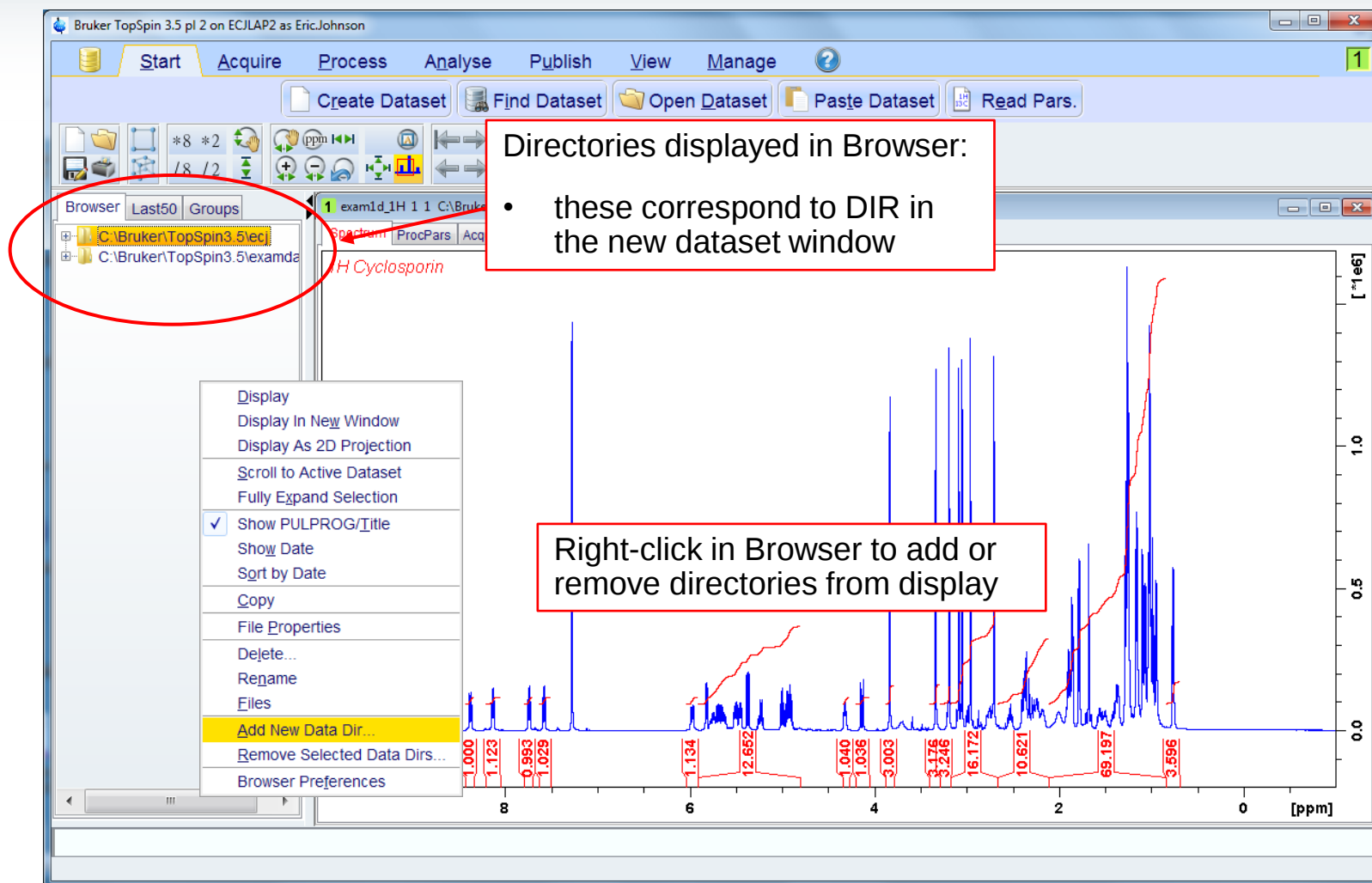
no acquisition running

On | Reg. State: |

Clicking the “pulse” or “A” icon will toggle between pulse program specific pulses and delays, and all acquisition parameters

The “AcquPars” tab show full list of acquisition parameters

Some User preferences (for different Linux or Windows login users)



Some User preferences



A screenshot of the Bruker TopSpin software interface. The main window shows a file browser on the left with a tree view of directories like /opt/topspin3.5/dmb and /opt/topspin3.5/ecj. The central panel displays a spectrum plot titled "50mM Cyclosporin in benzene-d6". The top menu bar includes "Start", "Acquire", "Process", "Analyse", "Publish", "View", and "Manage". The "Analyse" menu is open, and the "Preferences" option is highlighted with a red circle. A "User preferences" dialog box is open on the right, showing various settings. The "Administration items" section is highlighted with a red box, and the "Automatic command spooling" option is checked. A red arrow points from a text box labeled "Automatic command spooling" to the checked checkbox. Other options in the "Administration items" section include "Auto-open last used dataset when restarting TopSpin" (checked), "Show TopSpin data examples directory in data browser" (checked), "Setup users for TopSpin-internal login/logoff and esign" (Change), "Automatic termination of TopSpin when idle time exceeded" (Change), and "Automatic locking of TopSpin when idle time exceeded" (Change). The "Processing preferences" section includes "Enable automatic data processing" (unchecked). The "Text editors" section includes "Preferred text editor" (Internal) and "Text editor for edpul, edmac, edpy, ... always in foreground" (unchecked). The "Miscellaneous" section includes "Collapse parameter editors" (unchecked), "Display EXPNO/PROCNO list when opening data" (checked), "Record commands in protocol file" (checked), and "Language (change requires program restart!)" (English). The dialog box has "Search", "Apply", "Close", and "Reset..." buttons at the bottom.

Automatic command spooling

Some User preferences

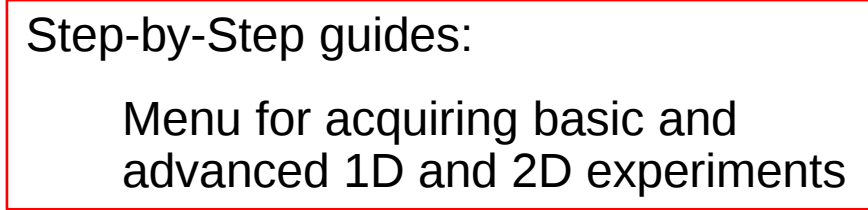


Whether to warn before overwriting data when starting acquisition

Select tools displayed in Status Bar

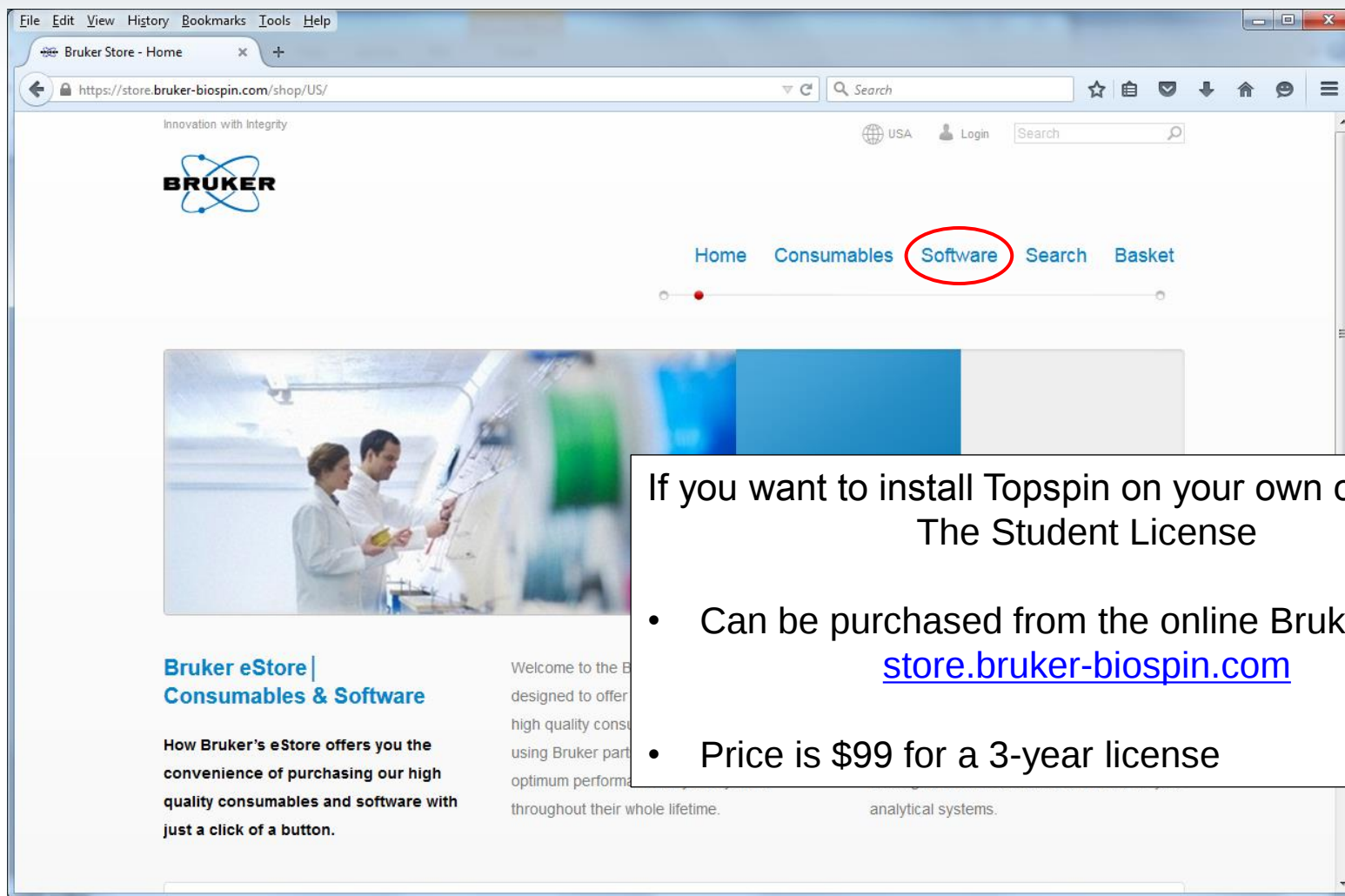
User preferences

- Administration items
- Window settings
- Processing preferences
- Text editors
- Miscellaneous
- Remote connection
- Directories
- Acquisition
 - Show "ased" parameter selection with "oda"
 - Overwrite existing FID without inquiry (ZG safety off)
 - Display digital resolution in FID display window
 - Auto open acquisition window after 'zg'
 - Configure accounting & data archiving after 'zg'
 - Automatically perform getprosol during rpar/edc/new
- More preferences
 - Spectra Display Preferences
 - Spectra Printing Preferences
 - Browser Preferences
 - Status Bar Preferences
 - Lock Display Preferences
 - BSMS Display Preferences



- Basic introduction to NMR
- Basic description of spectrometer components
- Some explanation of the various steps of setting up an acquisition

Topspin student licenses

A screenshot of a web browser displaying the Bruker eStore homepage. The browser's address bar shows the URL "https://store.bruker-biospin.com/shop/US/". The website header includes the Bruker logo, the tagline "Innovation with Integrity", and navigation links for "Home", "Consumables", "Software", "Search", and "Basket". The "Software" link is circled in red. Below the navigation bar, there is a large banner image showing two scientists in a laboratory setting. To the left of the banner, the text reads "Bruker eStore | Consumables & Software" and "How Bruker's eStore offers you the convenience of purchasing our high quality consumables and software with just a click of a button." To the right of the banner, there is a text block that begins with "Welcome to the B" and continues with "designed to offer high quality consu using Bruker part optimum performa throughout their whole lifetime. analytical systems."

If you want to install Topspin on your own computer...
The Student License

- Can be purchased from the online Bruker store:
store.bruker-biospin.com
- Price is \$99 for a 3-year license