

# **Varian NMR Manual (Agilent NMR)**

## **Standard Operation Training Course**



# 1. Software

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<https://github.com/OpenVnmrJ/OpenVnmrJ/blob/master/Install.md>

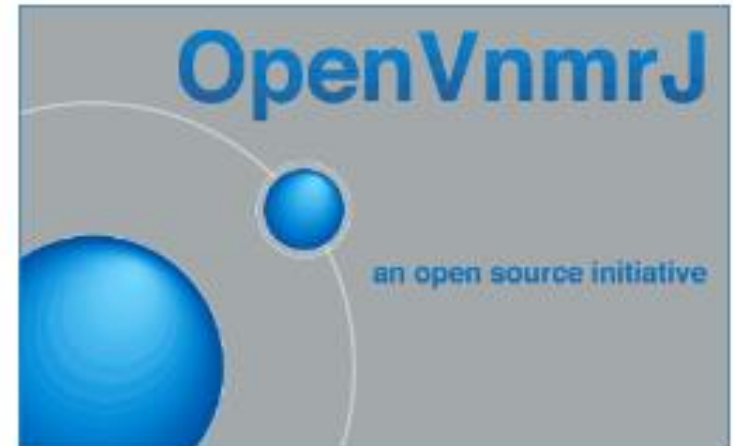
## OpenVnmrJ 3.1A

CentOS: Versions 7.5, 7.6, 7.7, 7.8, 7.9

RHEL: Versions 8.4

AlmaLinux: Version 8.4

Ubuntu: Version 20.



## OpenVnmrJ 2.1A

RHEL/CentOS: Versions 6.8, 6.9, and 6.10

RHEL/CentOS: Versions 7.5, 7.6, 7.7, 8.1, and 8.2



## **2. Turn on /off & Reset Hardware**

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# How to reset Console

1. Open terminal
2. Type *su acqproc* on terminal  
(Disconnect Workstation <-> NMR console communication)
3. Push reset switch on mater board of NMR Console
4. Type *su acqproc* on terminal  
(Connect Workstation <-> NMR console communication)
5. Click Setup hardware (reset software/hardware configuration)
6. Click Reset pneumatics (reset air flow control unit)
7. Click Reset VT (reset Temperature unit)

The screenshot displays the NMR console software interface. The 'Setup hardware' button is highlighted with a red box and the number 5. The 'Spin/Temp' section is also highlighted with a red box. The 'Reset pneumatics' and 'Reset VT' buttons are highlighted with red boxes and the numbers 6 and 7 respectively. A terminal window is overlaid on the right, showing the command 'su acqproc' entered, with the numbers 2 and 4 above it.

Sample Info  
Lock  
Shim  
Spin/Temp

Spinner: liquids  
Regulate speed  
0 Hz Off Spin off

Temperature  
Regulate temp  
60 Regulated FTS 0.0 C  
VT air flow 2 l/min VT air on VT air off

Control spinner from this panel only  
☐ Abort after spinner error  
☐ Warn after spinner error  
☒ Ignore spinner error

Control temperature from this panel only  
☐ Abort after temperature error  
☐ Warn after temperature error  
☒ Ignore temperature error

Reset pneumatics Reset VT Set FTS

Terminal window:  
su acqproc

# How to reset Workstation (PC)

1. Open terminal
2. Type *su acqproc* on terminal  
(Disconnect Workstation <-> NMR console communication)
3. Reset Workstation (PC)
4. Push reset switch on mater board of NMR Console
5. Type *su acqproc* on terminal  
(Connect Workstation <-> NMR console communication)
6. Click Setup hardware (reset software/hardware configuration)
7. Click Reset pneumatics (reset air flow control unit)
8. Click Reset VT (reset Temperature unit)

The screenshot shows the NMR workstation software interface. The 'Sample Info' tab is selected, and the 'Spin/Temp' section is highlighted with a red box and the number 3. The 'Spinner: liquids' section has a 'Regulate speed' button and a 'Spin off' button. The 'Temperature' section has a 'Regulate temp' button and a 'Temp off' button. The 'VT air flow' is set to 2 l/min, and there are 'VT air on' and 'VT air off' buttons. The 'Setup hardware' button is highlighted with a red box and the number 6. The 'Reset pneumatics' and 'Reset VT' buttons are highlighted with red boxes and the numbers 7 and 8 respectively. A terminal window is open in the bottom right corner, showing the command 'su acqproc' entered, with the number 5 next to it.

3 5

su acqproc

6 7 8

Reset pneumatics Reset VT

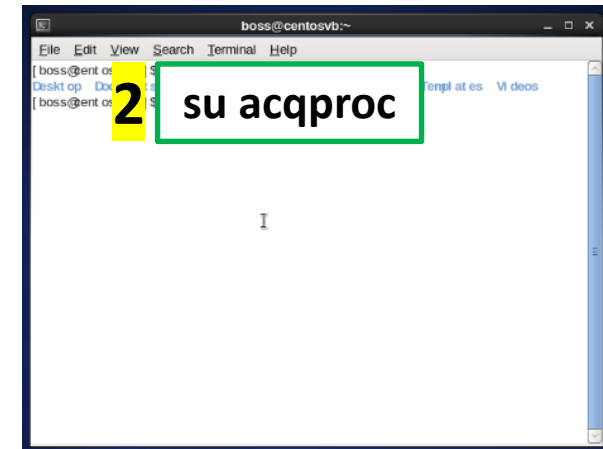
Idle Total acquisition time is 8 min, 31 sec

## <Turn off Console & Workstation>

1. Open terminal
2. Type *su acqproc* on terminal  
(Disconnect Workstation <-> NMR console communication)
3. Turn off Workstation (PC)
4. Turn off NMR Console

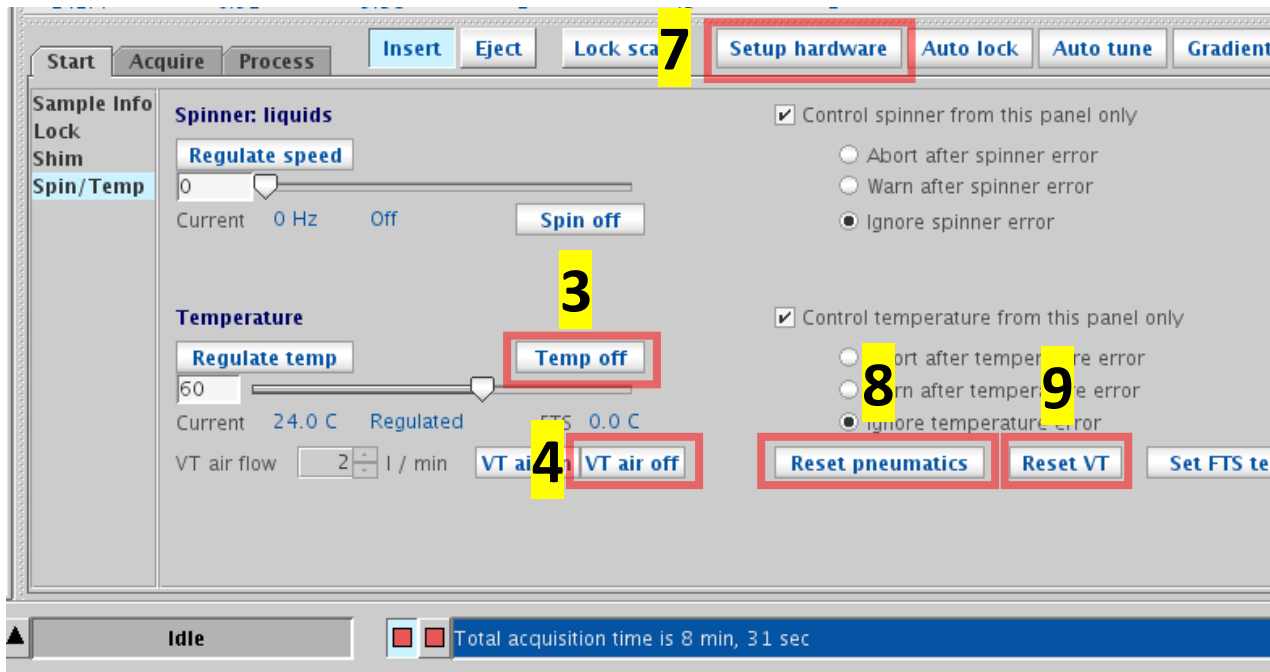
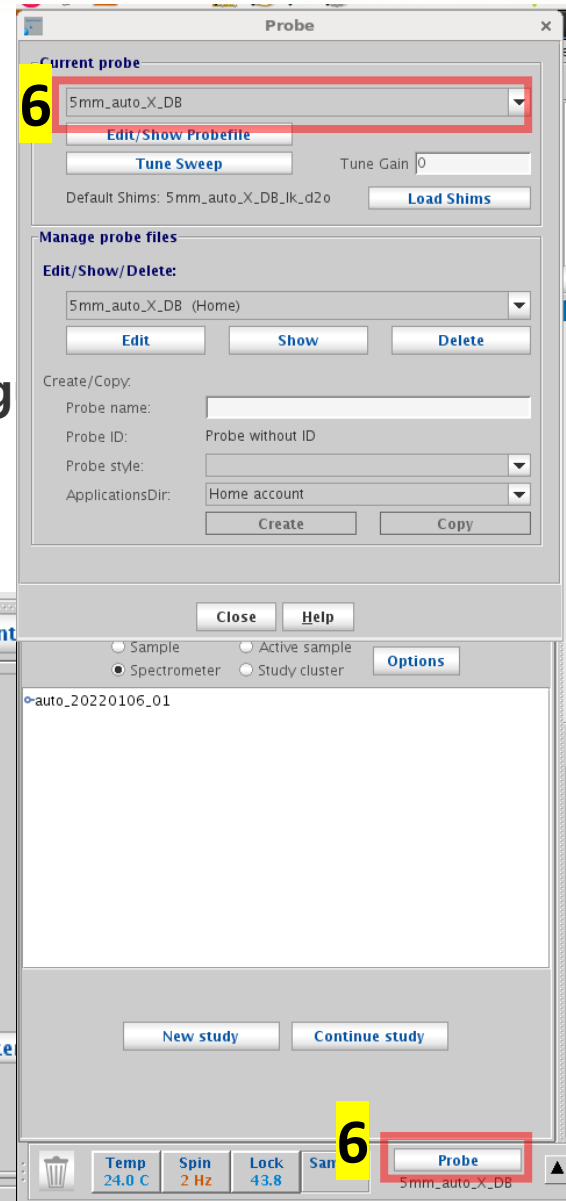
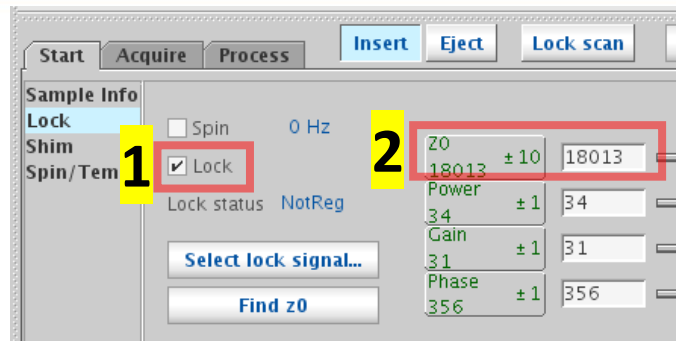
## <Turn on Console & Workstation>

1. Turn on NMR Console
2. Turn on Workstation (PC)
3. Double click 'openvnmrj2.1' (Automatically run 'su acqproc')
4. Click Setup hardware (reset software/hardware configuration)
5. Click Reset pneumatics (reset air flow control unit)
6. Click Reset VT (reset Temperature unit)



# How to change NMR probe

1. Lock off
2. Z0 is 0
3. Regulate Temp off
4. Air flow off
5. **Replace NMR probe**
6. Choice Current probe
7. Click Setup hardware (reset software/hardware config)
8. Click Reset pneumatics (reset air flow control unit)
9. Click Reset VT (reset Temperature unit)
10. If it is not work, follow 'How to reset Console'.





### **3. Quick Guide**

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## 3-1. Automation

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# Automation

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Viewport ProcessPlot ArrayedSpectra

Protocols QuickSubmit Frame

Experiment Selector

Solids Experiments Tests AutoSolids Experiments

Common Liquids Calibration Service

PROTON	CARBON
(H)PRESAT	(H)wet1D
(HH)gCOSY	(HC)HSQCAD
(HC)gHMBCAD	(H)NOESY1D
Studies ▾	

Study Queue

☐ Sample ☐ Active sample ☒ Spectrometer ☐ Study cluster Options

auto\_20220106\_01

**2**

New study Continue study

Temp 24.0 C Spin 0 Hz Lock 43.8 Sample Probe 5mm\_auto\_X\_DB

Viewport ProcessPlot ArrayedSpectra

Protocols QuickSubmit Frame

Experiment Selector

Solids Experiments Tests AutoSolids Experiments

Common Liquids Calibration Service

PROTON	CARBON
(H)PRESAT	(H)wet1D
(HH)gCOSY	(HC)HSQCAD
(HC)gHMBCAD	(H)NOESY1D
Studies ▾	

Study Queue

Submit queue Cancel

New Sample

SampleInfo [0:00]

New study Submit to Background

Clear pending exp from queue

Viewport ProcessPlot ArrayedSpectra

Protocols QuickSubmit Frame

Experiment Selector

Solids Experiments Tests AutoSolids Experiments

Common Liquids Calibration Service

PROTON	CARBON
(H)PRESAT	(H)wet1D
(HH)gCOSY	(HC)HSQCAD
(HC)gHMBCAD	(H)NOESY1D
Studies ▾	

Study Queue

Submit queue Cancel

New Sample

SampleInfo [1:24]  
PROTON\_001 [0:24]

New study Submit to Background

Clear pending exp from queue

Temp 24.0 C Spin 0 Hz Lock 43.8 Sample Probe 5mm\_auto\_X\_DB



# Automation

**11** Automation

**4** Sample\_name (to be submitted)

**7** SampleInfo [1:24]  
PROTON\_001 [0:24]

**5** Sample name: Sample\_name

**6** Solvent: CDCI3

**9** Save

**8** Acquisition options

**10** Submit

Temp 24.0 C Spin 0 Hz Lock 43.8 Sample Probe 5mm\_auto\_X\_DB

Adding PROTON to queue



## 3-2. Manually operation

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# Process

The screenshot displays the OpenVnmrj software interface. The 'Experiments' menu is open, showing various experiment types. The 'Process' tab is selected, showing a list of experiments and a detailed view of the current experiment.

Numbered callouts indicate the following steps:

1. Select 'Proton' in the 'Experiments' menu.
2. Click 'Insert' in the 'Process' tab.
3. Click 'Qect' in the 'Process' tab.
4. Click 'Clear' in the 'Sample information' dialog.
5. Click 'DMSO' in the 'Solvent' dropdown menu.
6. Click 'Auto lock' in the 'Process' tab.
7. Click 'Auto tune' in the 'Process' tab.
8. Click 'Gradient shim' in the 'Process' tab.

# Process

Start Acquire **Process** **Insert** **Eject** Lock scan Setup hardware **Auto lock** **Auto tune** **Gradient shim** Logout

Sample Info Lock Shim Spin/Temp

0 Hz **3** **2** **6** **7** **8**

**Change sample**

Lock status 18013 34 31 356

Select lock signal... Find z0

Gain +1 Phase +1

Autolock

☐ Automatic  
☐ Sample  
☐ z0 only  
☐ Unlocked  
☒ Not used

Run autolock

Start **Acquire** **9** **Process** Show time **Go** Stop MoveSW Est. pw90 Arrays Sequence diagram **14** Reference help

Default H1 **10** Experiment: PROTON Solvent: c6 **12** Observ **13** Decoupler: C13

Acquisition options

Spectral width (select) ppm  
(...or enter) -2.0 to 14.0 ppm

Number of scans 8  
Relaxation delay 1 s  
Pulse angle 45 degrees

**11**

File Edit View Experiments

New Workspace  
Join a New Workspace  
Open... Ctrl-O  
**Save As... Ctrl-S**  
Auto Save  
Printers...  
Print Screen...  
Auto Plot  
Review PDF Plots...  
Switch Operators...  
Exit Vnmrj

DATA  
Labs  
Automation  
Solid\_state\_NMR



## 4. Start tab

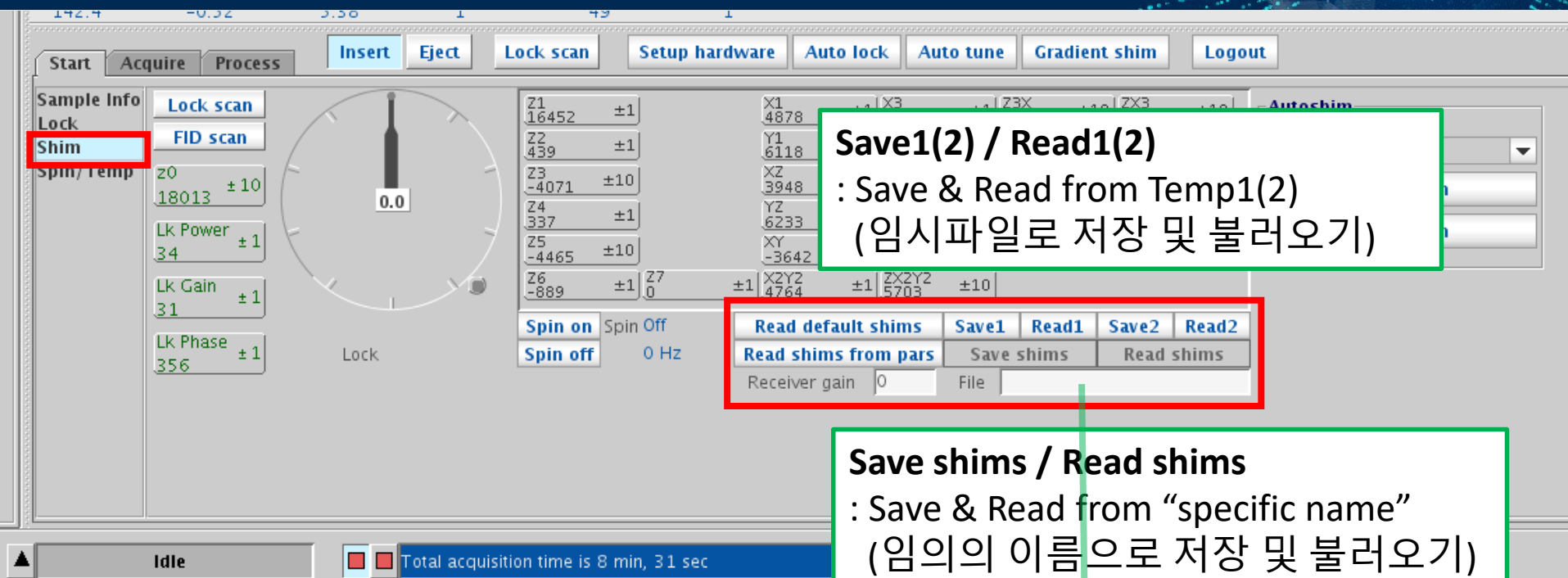
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# Start - Shim



## Read default shims

: Read shim from Gradient shim-map  
(Gradient shim-map을 가져옴)

## Read shims from pars

: Read shim from experiments  
(실험방에서 shim-map을 가져옴)

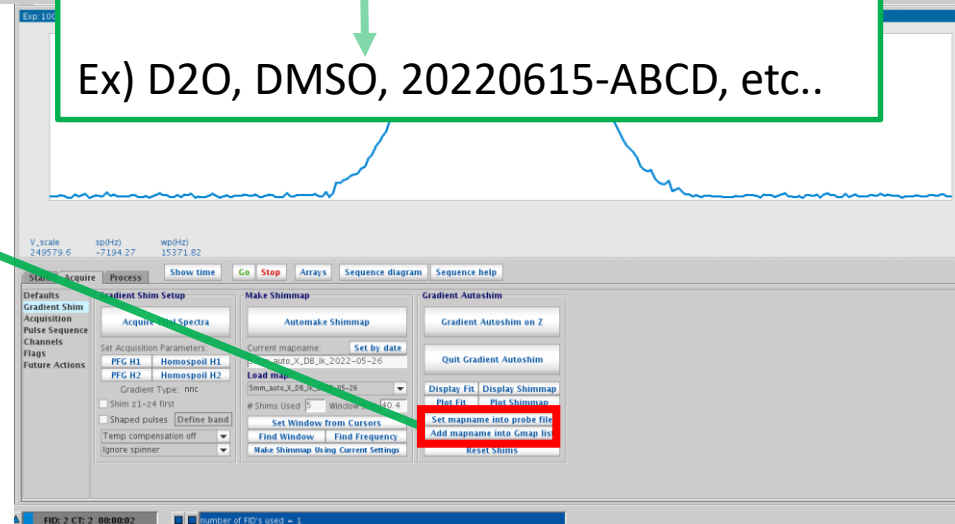
## Save1(2) / Read1(2)

: Save & Read from Temp1(2)  
(임시파일로 저장 및 불러오기)

## Save shims / Read shims

: Save & Read from "specific name"  
(임의의 이름으로 저장 및 불러오기)

Ex) D2O, DMSO, 20220615-ABCD, etc..



# Start – Spin

Start Acquire Process Insert Eject Lock scan Auto tune Gradient shim Logout

Sample Info Lock Shim

**Spinner: liquids**

Regulate speed

0

Current 0 Hz Off Spin off

**Spin**  
Type 20  
Enter  
Click Regulate speed

**Temperature**

Regulate temp

60

Current 24.0 C Regulated FTS 0.0 C

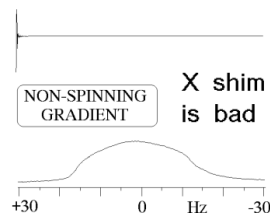
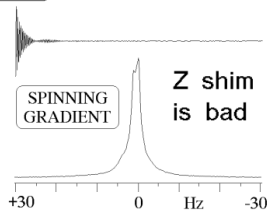
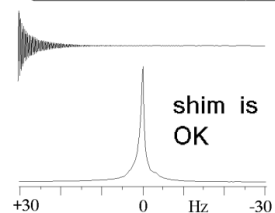
VT air flow 2 l/min VT air on VT air off

Reset pneumatics Reset VT Set FTS temp 25

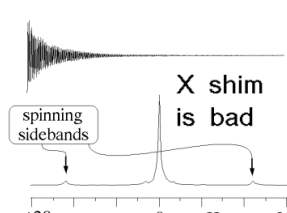
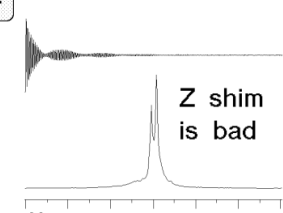
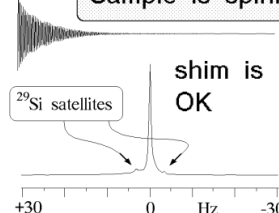
Warn after temperature error  
Ignore temperature error

Idle Total acquisition time is 8 min, 31 sec

Sample is NOT spinning.



Sample is spinning.



[https://medicine.uiowa.edu/nmr/sites/medicine.uiowa.edu.nmr/files/wysiwyg\\_uploads/Shimming%20an%20NMR%20Magnet.pdf](https://medicine.uiowa.edu/nmr/sites/medicine.uiowa.edu.nmr/files/wysiwyg_uploads/Shimming%20an%20NMR%20Magnet.pdf)

# Start – Temp

The screenshot shows the UNIST NMR control software interface. At the top, there are buttons for 'Setup hardware', 'Auto lock', 'Auto tune', 'Gradient shim', and 'Logout'. On the left, a sidebar contains 'Start', 'Acquire', 'Sample Info', 'Lock', 'Chim', and 'Spin/Temp' (which is highlighted with a red box). A green box highlights the 'Temperature' section, containing the text: 'Type 50 (target temp)', 'Enter', and 'Click'. Below this, another green box highlights the 'Temperature' control panel, which includes a 'Regulate temp' button, a 'Temp off' button, a slider set to 60, and a display showing 'Current 24.0 C Regulated FTS 0.0 C'. Below the slider, it shows 'VT air flow 2 l / min' and buttons for 'VT air on' and 'VT air off'. A third green box highlights the text: 'Limit VT air flow -> 6 °C / min', 'Extremely temperature change could break Quartz in Probe.' To the right, a diagram of the NMR probe is shown. A green box points to the top of the probe with the text: 'VT flow cause temp gradient. Stabilization time: 5 – 15 min'. Below the probe, a 'Heater' is shown connected to a 'VT Unit' box.

Start Acquire

Sample Info Lock Chim Spin/Temp

Temperature

Type 50 (target temp)

Enter

Click

Regulate temp Temp off

60

Current 24.0 C Regulated FTS 0.0 C

VT air flow 2 l / min VT air on VT air off

Limit VT air flow -> 6 °C / min

Extremely temperature change could break Quartz in Probe.

VT flow cause temp gradient. Stabilization time: 5 – 15 min

Heater

VT Unit

## **5. Acquire tab**

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# Acquire tab

Start **Acquire** Process Show time Go Stop MoveSW Est. pw90 Arrays Sequence diag

Default H1 **Acquisition** Pulse Sequence Channels Flags Future Actions

**PROTON**

**Data**

Spectral width 9615.4 Hz **Spectrum width (SW)**

Acquisition time 1.704 s **aq (AQ)**

Complex points 16384

**Excitation**

Relaxation delay 1.000 s **D1 (D1)**

First pulse 0.00 μs or 0 degrees

Inter-pulse delay 0.000 s

Observe pulse 5.00 s **pw (P1)**

ation pw90 10.00 μs at power 62 dB

Requested 8 **nt (NS) number of scans**

Completed 0

☐ Steady state 0

☒ Block size 32 **bs (type tr)**

☐ Interleave

Receiver gain 38 **tpwr (plw1)**

Timing (μs) rof2 24.81 **= rga (Bruker)**

alfa 7.2

**AQ = TD \* dwell time**

**ss (DS)**

Start Acquire **Proce** Show time Go Stop MoveSW Est. pw90 **de** ram Sequence help

Default H1 **Channels** Acquisition Pulse Sequence Channels Flags Future Actions Overview

**PROTON**

Channels:

Nucleus / freq. H1 599.826 MHz **Spectrum center (O1)**

Offset 599.80 Hz

Dec on/off ☐ Homo pwr 1

Dec modulation offset 0.00 Hz

90 deg. at pwr 10.00 μs at 62

= dmf

Homodec ---

Waveform ---

at resolution --- degrees

Decouple **set** 2 C13 150.840 MHz

0.00 Hz

nnn

c

28.5 μs at 39

= 35088

W40\_5mm\_auto\_X\_DB

9.00 degrees

Decouple **set** 3 0.000 MHz

0.00 Hz

n

c

31.0 μs at 1

= 32258

1.00 degrees

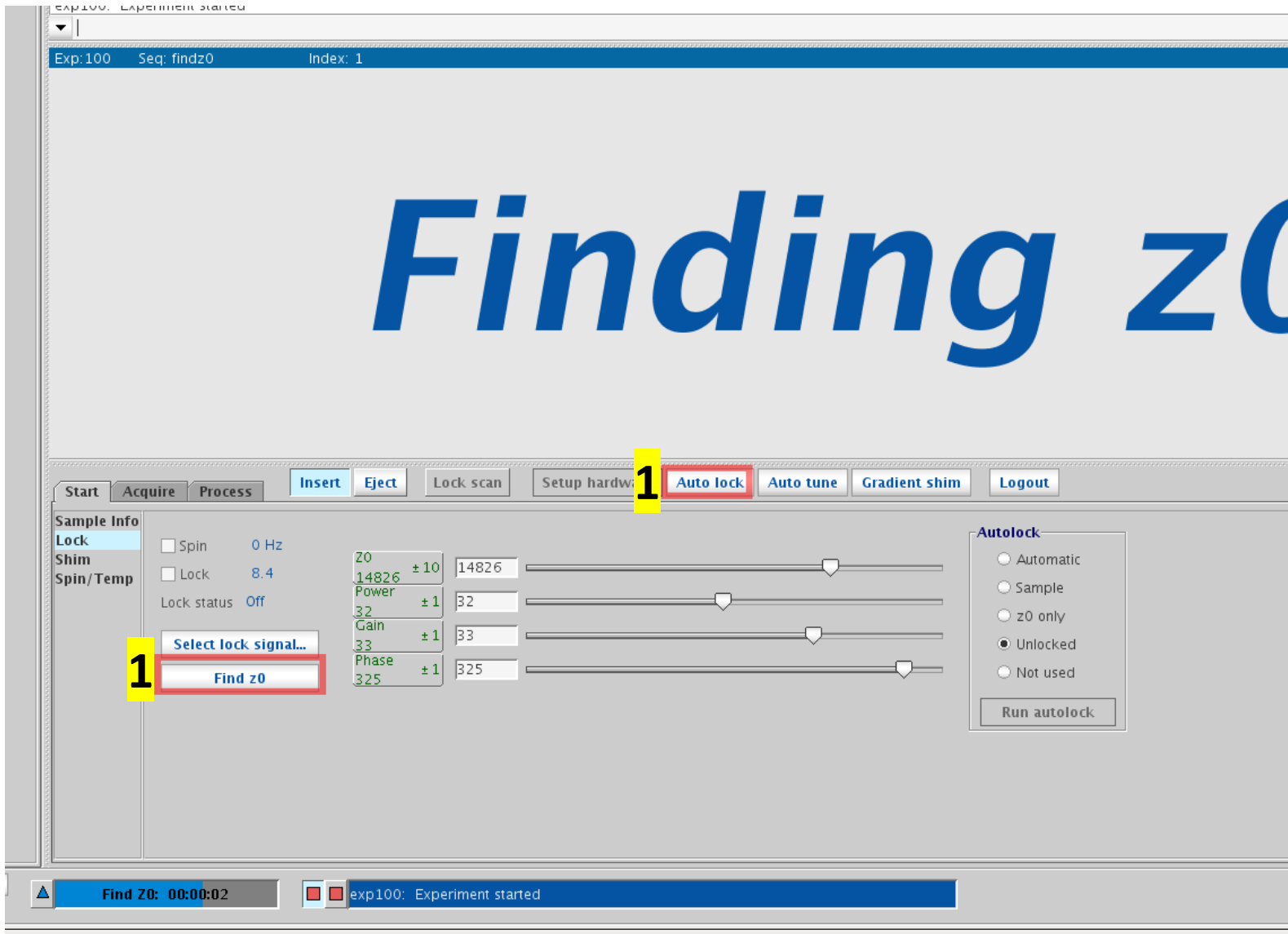
**de (Prescan delay)**

## 6-1. Lock

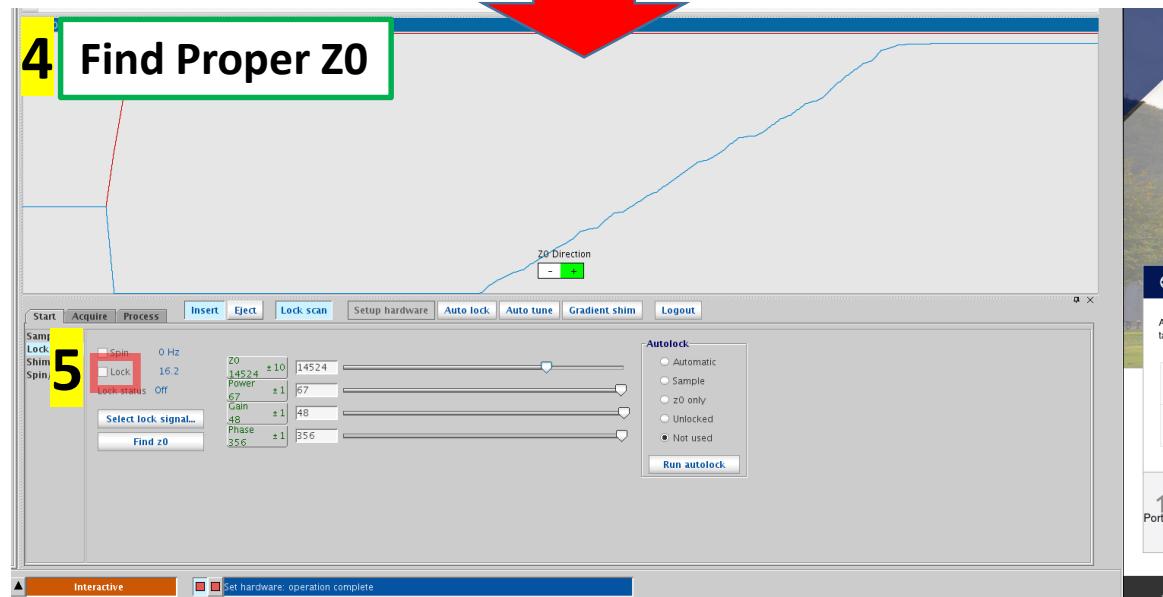
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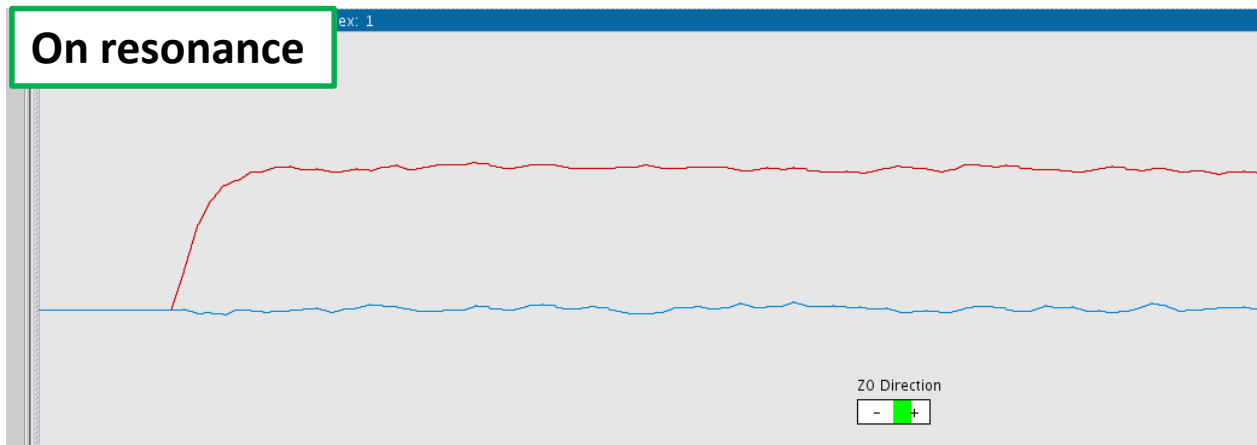


# Lock (Manual)





# Lock (Manual)



## **6-2. Tune & Match**

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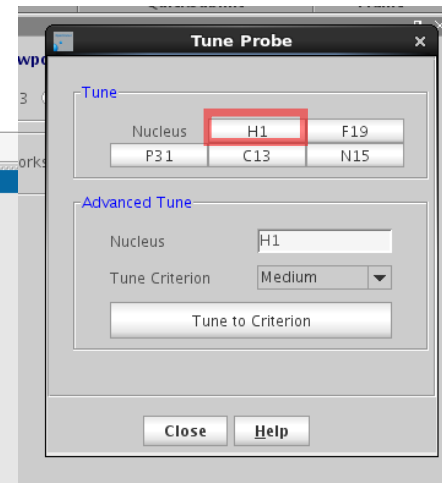
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# Tuning and Matching

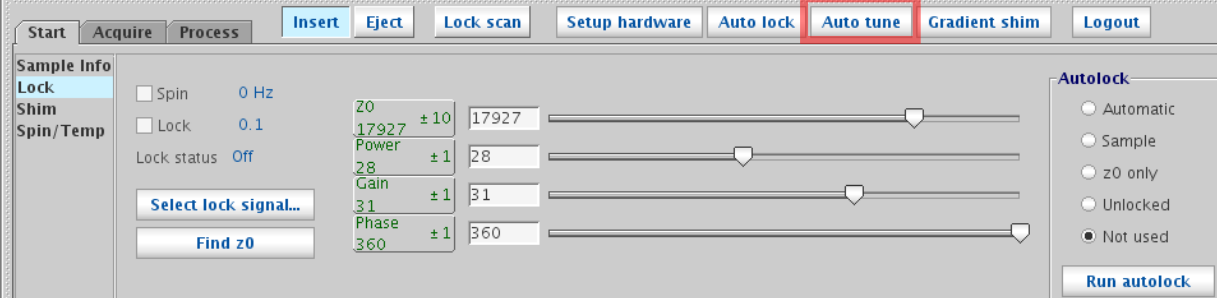
## <Tune method>

1. Click Auto tune
2. Type *protune* on command line
3. Type *protune('calibrate')* on command line
4. Probe -> Tune sweep -> Manual tune

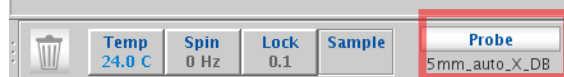
## 2. Type *protune*



## 1. Click Auto tune



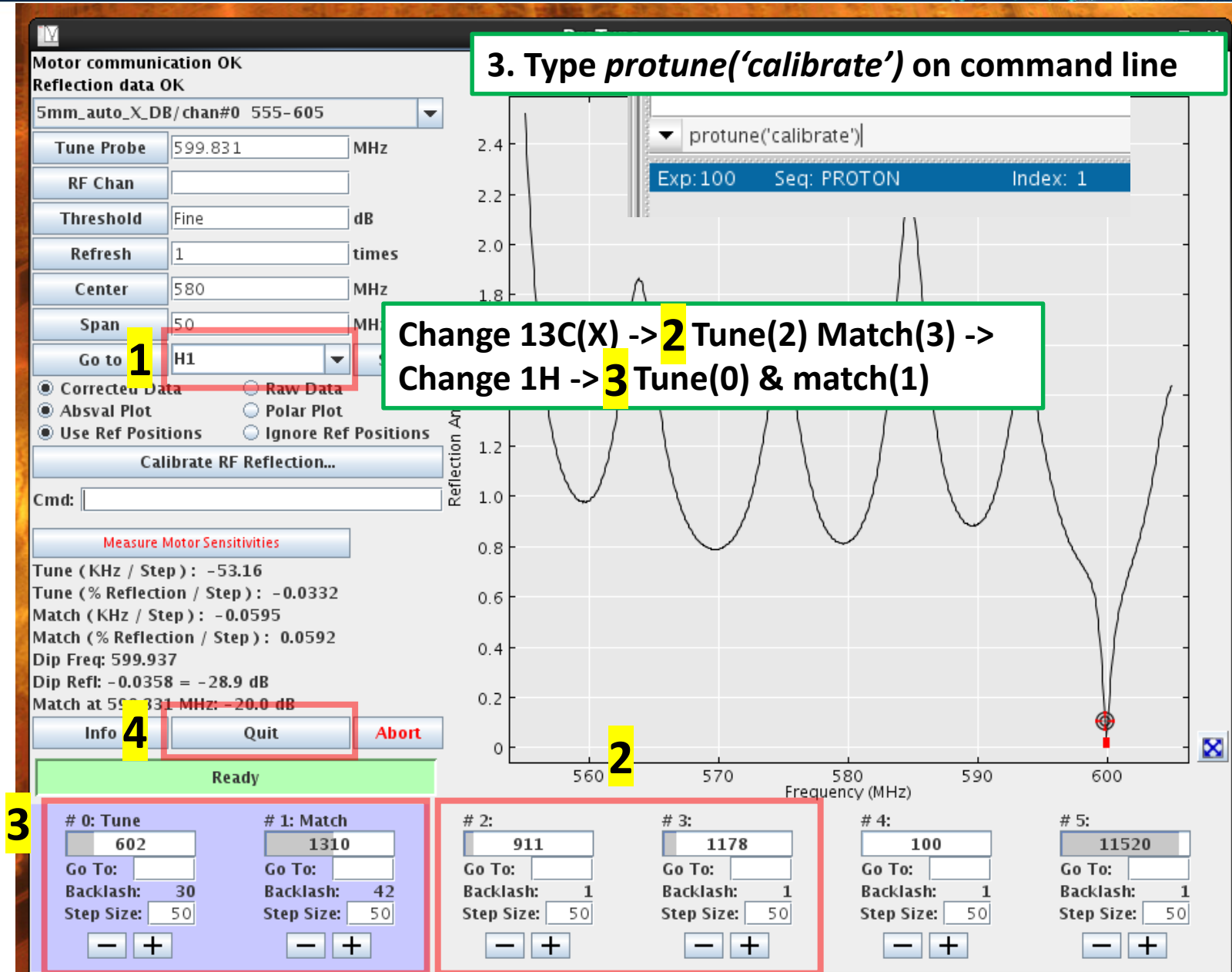
## 4. Probe -> Tune sweep -> Manual tune



# Protune('Calibrate')

## 3. Type *protune('calibrate')* on command line

Change 13C(X) -> **2** Tune(2) Match(3) ->  
Change 1H -> **3** Tune(0) & match(1)





# Manual tune (Original process)

**1** Probe

**2** Edit/Show Probefile  
Tune Sweep

**3** Tune RF channel

**4** Start Probe Tune

**5** Manually control tune stick

Current probe: 5mm\_auto\_X\_DB

Edit/Show Probefile

Tune Sweep

Tune Gain: 0

Default Shims: 5mm\_auto\_X\_DB\_1k\_d2o

Load Shims

Manage probe files

Edit/Show/Delete:

5mm\_auto\_X\_DB (Home)

Edit Show Delete

Create/Copy:

Probe name:

Probe ID: Probe without ID

Probe style:

ApplicationsDir: Home account

Create Copy

Close Help

Options

Sample Active sample Spectrometer Study cluster

auto\_20220106\_01

New study Continue study

Temp 24.0 C Spin 2 Hz Lock 43.8

Probe Tuning

Probe: 5mm\_auto\_X\_DB

Start Acquire Process Insert Eject Lock scan Setup hardware Auto lock Auto tune Gradient shim Logout

Probe: Tune RF channel 1

Center Frequency H1 H1 Freq 599.83 M Span 10.0 M

Choose Marker 1 Choose Marker 2

Center frequency to markers

Power 0 dB Gain 0 dB

Vertical scale \*2 /2 Autoscale # Points 512

Vertical position +20 -20

Start Probe Tune

Stop Probe Tune

Quit

Exp: 100 Seq: mtune Index: 1 mouse: [LEFT] click to set first cursor [RIGHT] click to set second cursor [MIDDLE] click or scroll to scale

H1

5

8000 7000 6000 5000 4000 3000 2000 1000

V\_position 0 V\_scale 1.8 cursor 301.49 delta 4.03

Tuning: ok - tuning to C13 meets Fine criterion  
Tuning: ok - tuning to H1 meets Fine criterion  
Tuning done: ok

Tuning done: ok

## 6-3. Processing

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The screenshot shows the OpenVnmrj software interface. The 'Process' tab is selected, and the 'Transform' button is highlighted with a red box and the number 2. The 'Process' button is also highlighted with a red box and the number 1. A green box highlights the 'Type wft' option in the 'Process' tab. The main window displays a 1D NMR spectrum with a peak at 5.69 ppm. The x-axis is labeled 'ppm' and ranges from 10 to -1. The y-axis is labeled 'V\_position' and ranges from 33.0 to 55141.1. The spectrum shows a complex pattern of peaks, with a prominent peak at 5.69 ppm. The 'Process' tab includes fields for 'Sample information' (Sample: dmsol, Solvent: dmsol, Sample owner: vnmr1) and 'Process options' (FT data size: 64k, LineBroaden: 0.6 Hz). The 'Plot options' section includes 'Parameters: Basic', 'Integrals: Off', and 'Peak Values: Peaks ppm'. The 'Display spectrum' button is also visible.

**Type wft**

1 2

Exp: 100 Seq: PROTON Index: 1

5.69

ppm

V\_position 33.0 55141.1 9.57 delta

Start Acquire **Process** **Transform** Auto process Display spectrum Auto plot preview Clear screen Cancel

**Sample information**

Sample dmsol  
Solvent dmsol  
Sample owner vnmr1

Comments:  
20220520-TM200-2015j6111\_H1

**Process options**

FT data size 64k  
☒ LineBroaden 0.6 Hz

**Plot options**

Parameters Basic  
Integrals Off  
Peak Values Peaks ppm

Process Auto plot Auto preview

Display spectrum Save current process/display parameters

Temp 24.0 C Spin 0 Hz Lock 31.3 Sample Probe 5mm\_auto\_X\_DB

FID: 1 CT: 2 00:01:53 processing: /home/vnmr1/Desktop/DATA/ENF/QC/20220520-TM200-2015j6111\_H1.fid

# Process tab

The screenshot shows the 'Process' tab of an NMR processing software. The interface is divided into several panels: 'Basic', 'Fourier transform', 'Display', 'Reference', 'Peak picking', and 'Integration'. Annotations with green boxes and arrows point to specific features:

- Zero-filling (complex point \* 2~4)**: Points to the 'Transform size' dropdown menu in the 'Fourier transform' panel, which is set to '64k'.
- Referencing**: Points to the 'By solvent' button in the 'Reference' panel.
- Diagonal correction (Type dc)**: Points to the 'DC correct' button in the 'Baseline correct' section of the 'Reference' panel.
- Set integration value**: Points to the 'Set norm to' input field in the 'Integration' panel, which is set to '1000.00'.
- Auto intensity control (Type vsadj)**: Points to the 'Auto LP' button in the 'Fourier transform' panel.
- Auto phase correction (Type aph)**: Points to the 'Autophase' button in the 'Display' panel.
- Baseline correction on Integration area (Type bc)**: Points to the 'BC correct' button in the 'Baseline correct' section of the 'Reference' panel.
- Fine Maximum intensity on peak (Type nl)**: Points to the 'Find nearest line' button in the 'Display' panel.

Other visible buttons and options include: 'Start', 'Acquire', 'Process', 'Transform', 'Auto process', 'Display spectrum', 'Auto plot preview', 'Clear screen', 'Cancel', 'Transform all', 'Transform FID #', 'Acquired points', 'Lin. prediction', 'Autoscale', 'Autophase', 'Full screen', 'Full spectrum', 'Display text', 'By solvent', 'By TMS', '2.50 ppm', 'Baseline correct', 'DC correct', 'Find integrals', 'BC correct', 'Peak threshold', 'Find peaks', 'Autoscale', 'Integral values', 'Normalized values', 'Set norm to', 'Save current process / Display parameters', 'in FID directory', 'Vert scale', 'Axis', 'Disp. mode', and 'Display parameters'.



# Process tab

Start Acquire **Process** Transform Auto process Display spectrum Auto plot preview Clear screen Cancel

Basic  
Default  
**Weighting**  
Display  
More 1D  
Integration  
Cursors/Line Lists  
Plot  
Text Output

**Fourier transform**

Transform all ☒ Transform size 64k  
Transform FID # 1 Acquired points 16,384

**AutoSelect weighting**

exponential	gaussian
sine	cosine
sq-sine	sq-cosine
pseudo	res-enhance
/4 ssqsine	

**Weight parameters**

line broadening	0.6	<input checked="" type="checkbox"/>
sinebell	0	<input type="checkbox"/>
shift	0	<input type="checkbox"/>
gaussian	0.1	<input type="checkbox"/>
shift	0	<input type="checkbox"/>
additive offset	0	<input type="checkbox"/>

Zero-filling  
(Complex point \* 2~4)

Line broadening (LB)  
1H: 0.6 ~ 1  
13C: 3

Linear Prediction (LP)  
: 2 ~ 3 (Case by case)

Start Acquire **Process** Transform Auto process Display spectrum Auto plot preview Clear screen Cancel

Basic  
Default  
Weighting  
Display  
**More 1D**  
Integration  
Cursors/Line Lists  
Plot  
Text Output

**Linear prediction**

☒ LP ON/OFF **Auto**  
☒ Back ☐ Forward

Coefficients 32  
Basis points 64  
starting at 2  
Predicted points 1  
starting at 1  
Acquired points 16,384  
☒ FT size 64k  
Weighting exponential

**Cut off FID signal for Aring (ringing)**  
ex) Short T1 experiments\_17O, 23Na, 79Br, 127I, etc..)

FID phase rotation 0.0 degrees

# Process tab

Start Acquire **Process** Transform Auto process Display spectrum Auto plot preview Clear screen Cancel

Basic Spectral graphics

**Show integration line or not**

Integration  
Cursors/Line Lists  
Plot  
Text Output

Logo  
☐ None ☒ Custom Browse...

☐ Integral lines  
☐ Full ☐ Partial  
☒ Integral values  
☒ Scaled ☐ Normalized  
☐ Horiz ☒ Vert

Peak labels  
ppm  
☒ Axis  
☒ ppm ☐ Hz  
☐ Molecule

Lists

Parameters  
☐ Basic ☒ All ☐ None

Integral values  
☒ Integral list  
☒ Scaled ☐ Normalized

Peak positions  
☒ Peak list  
☒ ppm ☐ Hz

☒ Comments ☒ Miniplots

Send to  
Hz per mm: 28.2  
☐ Print 1 page  
☐ Print 2 pages  
☒ Print double-sided

Preview Print

**Show PDF**

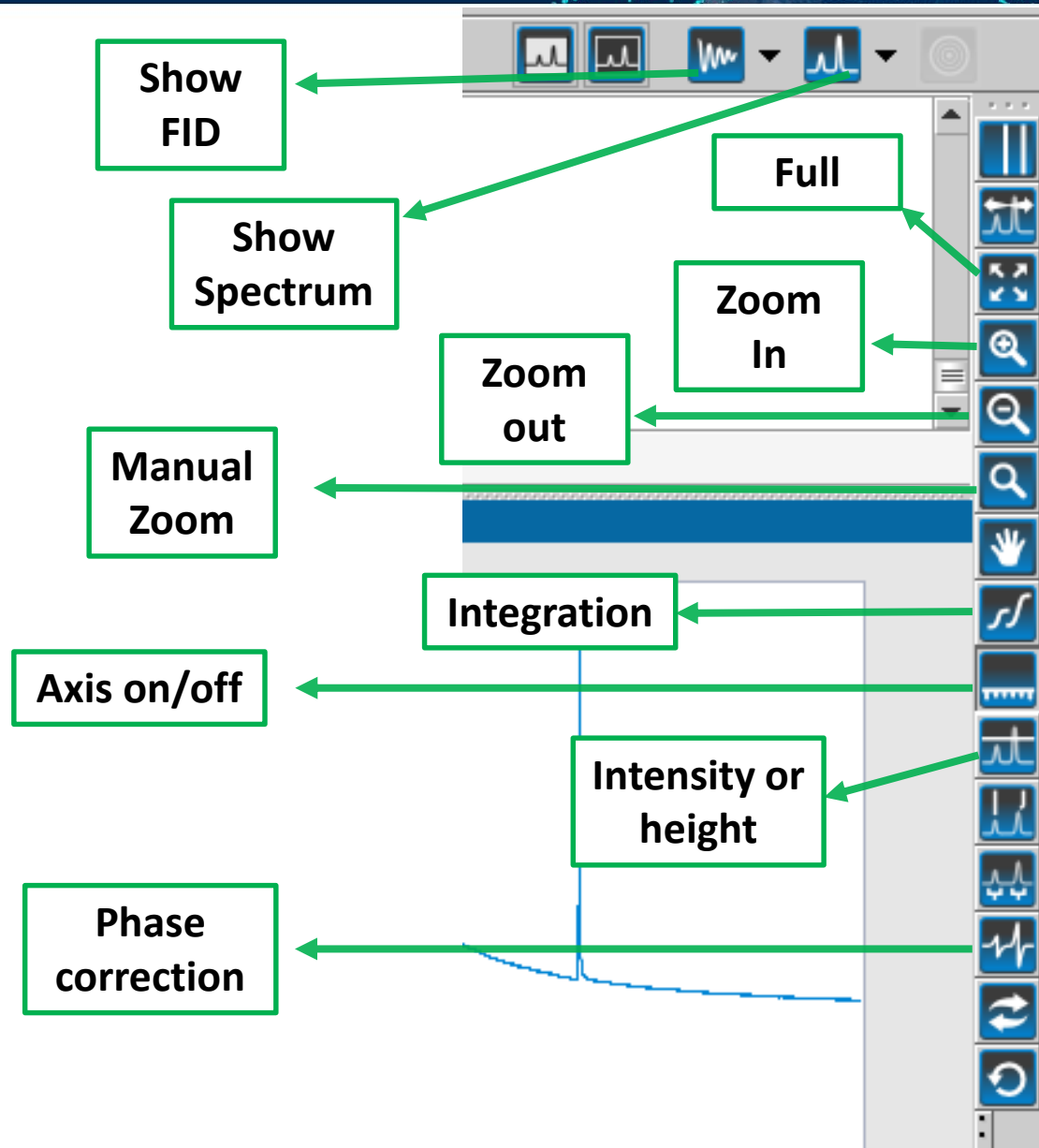
Start Acquire Process **Transform** Auto process Display spectrum Auto plot preview Clear screen Cancel

Basic  
Default  
Weighting  
Display  
More 1D  
Integration  
Cursors/Line Lists  
Plot  
Text Output

ACQUISITION		SAMPLE		PROCESSING		GRADIENT SHIM	
sfrq	92.077	date	Jun 16 2022	fn	not used	gzsize	5
tn	1k	file	/home/vnmr1/v~	sb	not used	gzlvl	2000
at	0.017	nrmrsgs/gshimlib/sh~				gzwin	30.3
np	512	immrps/5mm_auto_X~		wnt wft f vsadj ds~		d2	0.0010
sw	15432.1	DB_1k_2022-06-16-A~		sh		d3	arrayed
ss	1	.fid				vtcomplvl	0
tpwr	45	solvent	D2O			gstab	0.00025
pw	300.0	temp	24.0			shift	0.00300
d1	3.000						
tof	15.1						
		DECOUPLING				FLAGS	
nt	4	dn	H1			n	
ct	4	dof	0			n	
gain	26	dm	n			n	
		dmm	c				
		dmf	200				
		dpwr	30				

**Show sequence manual**

Text  
Basic  
Array  
Channels  
Shims  
Seq manual  
More  
Clear



## 7. Maintenance

---

**UNIST**

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SCIENCE AND TECHNOLOGY



## Affecting factors for Shimming

1. Temperature gradient (Convection effect)
2. Sample tube (Camber, Thickness, Scratch, Material quality, Impurity contents)
3. Sample height
4. Sample (Concentration, Paramagnetic species, Impurity, Ion/salt, Particle)
5. Solvent (Viscosity, Dielectric constant)

Axial shims(on axis): Z1, Z2, Z3, Z4, Z5, Z6, etc..

Radial shims(off axis): X, Y, XY, XZ, YZ, X2Y2, etc..

Ex)  $X = X + Z0$ ,  $XZ = X + Z1$

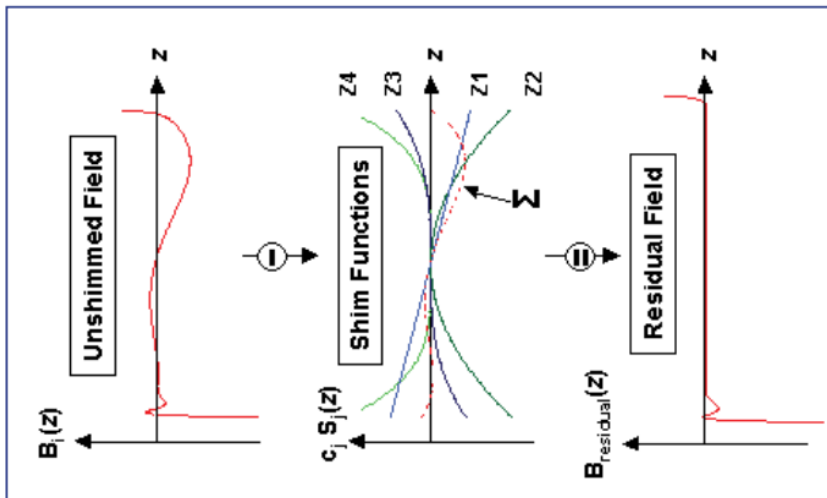
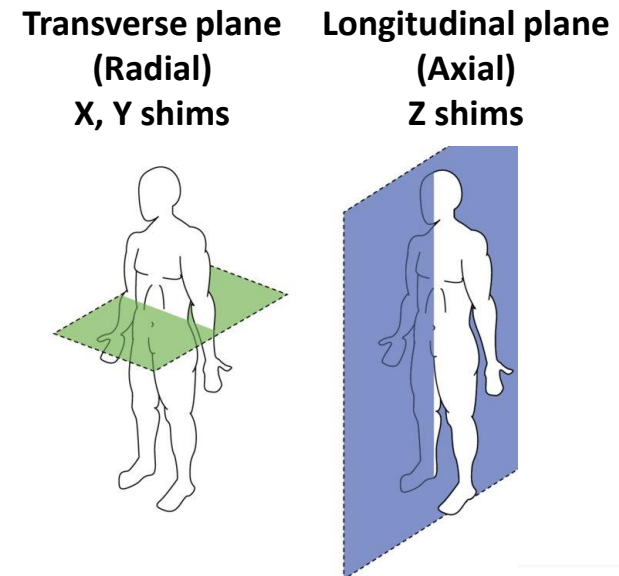


Fig. 7: The 1D gradient shimming algorithm. In a one-time calibration experiment it is necessary to use the method of Fig. 5 to measure the actual

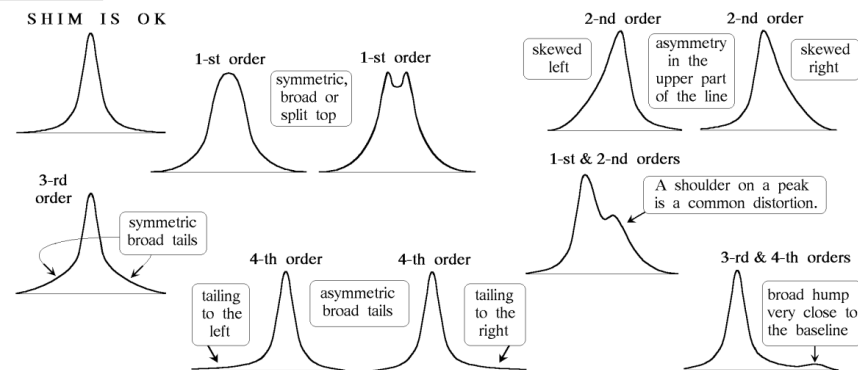


# Class of shim coil

SHIM CONTROLS ON THE SPECTROMETERS					spinning/ non-spin	high/ low	odd/ even	order
FX-90Q	WM-360	MSL-300	AC-300	AMX-600				
Y	Z	Z	Z	Z	spinning	low	odd	1-st
C	Z <sup>2</sup>	Z <sup>2</sup>	Z <sup>2</sup>	Z <sup>2</sup>	spinning	low	even	2-nd
Y <sup>3</sup>	Z <sup>3</sup>	Z <sup>3</sup>	Z <sup>3</sup> Z <sup>5</sup>	Z <sup>3</sup> Z <sup>5</sup>	spinning spinning	high high	odd odd	3-rd 5-th
F	Z <sup>4</sup>	Z <sup>4</sup>	Z <sup>4</sup>	Z <sup>4</sup>	spinning	high	even	4-th
Z X	X Y	X Y	X Y	X Y	non-spin non-spin	low low	odd odd	1-st 1-st
ZX XY YZ X <sup>2</sup> -Y <sup>2</sup>	XY YZ XZ X <sup>2</sup> -Y <sup>2</sup>	XY YZ XZ X <sup>2</sup> -Y <sup>2</sup>	XY YZ XZ X <sup>2</sup> -Y <sup>2</sup>	XY YZ XZ X <sup>2</sup> -Y <sup>2</sup>	non-spin non-spin non-spin non-spin non-spin	low low low low low	even even even even even	2-nd 2-nd 2-nd 2-nd 2-nd
X <sup>3</sup> Z <sup>3</sup>	X <sup>3</sup> Y <sup>3</sup>	X <sup>3</sup> Y <sup>3</sup> XZ <sup>2</sup> YZ <sup>2</sup>	X <sup>3</sup> Y <sup>3</sup> XZ <sup>2</sup> YZ <sup>2</sup>	X <sup>3</sup> Y <sup>3</sup> XZ <sup>2</sup> YZ <sup>2</sup> ZXY Z(X <sup>2</sup> -Y <sup>2</sup> )	non-spin non-spin non-spin non-spin non-spin non-spin non-spin	high high high high high high high	odd odd odd odd odd odd odd	3-rd 3-rd 3-rd 3-rd 3-rd 3-rd 3-rd
				XZ <sup>3</sup> YZ <sup>3</sup>	non-spin non-spin	high high	even even	4-th 4-th
Y	Z				<--- spinning axis for NMR tubes			

**Doped 1% H<sub>2</sub>O in D<sub>2</sub>O  
(0.1 mg/ml GdCl<sub>3</sub> in sample)**

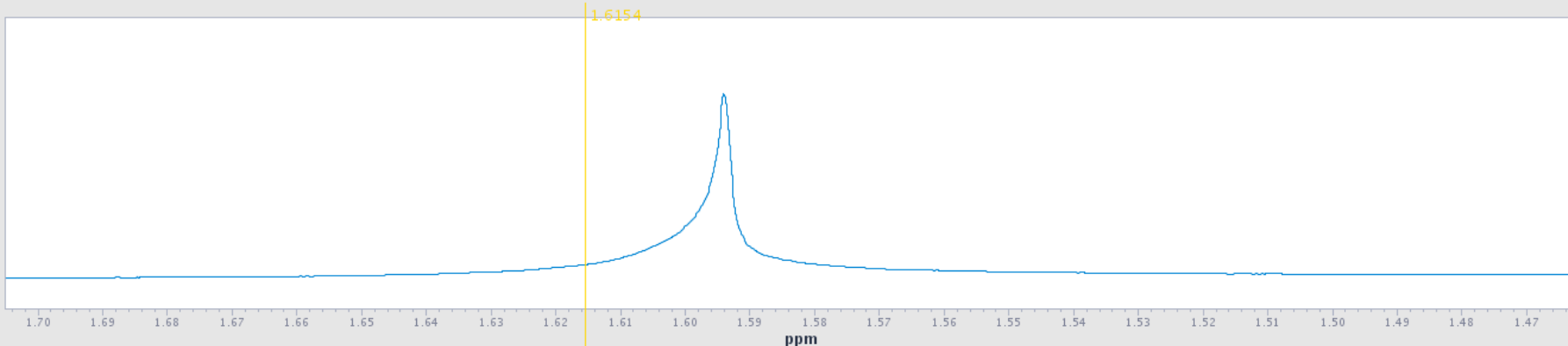
**Bruker 400 MHz linewidth 4 Hz  
Varian 600 MHz linewidth 6 Hz**



SKETCHES OF LINE DISTORTIONS CAUSED BY VARIOUS GRADIENTS

# Manual shim

Exp: 100 Seq: PROTON Index: 1 mouse: [LEFT] click to set first cursor [RIGHT] click to set second cursor [MIDDLE] click or scroll to scale



Shim value +/- 32767

Start 2 Acquire Process Insert Eject Lock scan Setup hardware Auto lock Auto tune Gradient shim Logout

Sample In Lock scan Shim 3 Spectrum FID Disp Linesh 4 DC correct Autophase 6

#1 50.0 % FID area 6.5 Rescale FID area 5

Z1 16452 ±1	X1 4878 ±1	X3 -877 ±1	Z3X -467 ±10	ZX3 -6623 ±10
Z2 439 ±1	Y1 6118 ±1	Y3 125 ±1	Z3Y 4666 ±10	ZY3 -6320 ±10
Z3 -4071 ±10	XZ 3948 ±1	XZ2 6225 ±1	Z2XZ2 -3089 ±10	Z4X 4174 ±10
Z4 337 ±1	YZ 6233 ±1	YZ2 11877 ±10	Z2XY -2404 ±10	Z4Y -4745 ±10
Z5 -4465 ±10	XY -3642 ±10	ZXY 267 ±10		
Z6 -889 ±1	Z7 0 ±1	X2Y2 4764 ±1	ZX2Y2 5703 ±10	

Spin on Spin Off Read default shims Save1 Read1 Save2 Read2  
Spin off 0 Hz Read shims from pars Save shims Read shims  
Receiver gain 0 File

Autoshim  
Start shim  
Stop shim

1. Z1 (+/- 10)
2. Z2

At least 30 min (1 cycle)  
Poor shim -> Long time (3-4 cycle)

## <Line shape sample>

**1H: CHCl<sub>3</sub> in Acetone-D<sub>6</sub>**

**13C: Dioxane in Benzene-D<sub>6</sub>**

## <Routine shim>

**1) Spin off**

**2) Adjust Lock level 80**

**3) Z1 -> Z2 -> Z1**

**4) Z3 -> Z1 -> Z2 -> Z3 -> Z1 -> Z2**

**5) Z4 -> Z1 -> Z2 -> Z4 -> Z1 -> Z2**

**6) Turn off spin -> Repeat step 3), 4), 5)**

**7) Turn on spin -> 3)**

## <Remove spinning sideband>

**1) Spin off**

**2) Adjust Lock level 80**

**3) X-Y-X-Y**

**4) X-ZX-X**

**5) Y-ZY-Y**

**6) X**

**7) XY-ZXY**

**8) X-Y-X-Y**

**9) Spin on**

**10) Z4 (asymmetry peak)**

**11) Z3-Z1-Z2**

Typical interactions for axial shims:

- Z1 and all other axial shims, to some extent
- Z2 and Z1
- Z3 and Z1
- Z4 and Z2 (with large delta Z4s: Z4 and Z3)
- Z5 and both Z3 and Z1 (Z5 not available on 13-channel shim systems)

**Table 42.** Lineshape Effects and Their Associated Shims

<i>Lineshape Effect</i>	<i>Shims</i>
Split peak	Z4 and Z1
Asymmetry greater than half-way up	Z2
Asymmetric foot	Z4
Symmetric feet and or low broad base	Z5
Symmetrically broad base	Z3
Spinning sidebands	Low-order radials X1, Y1
Symmetric broad base	High-order radials X3, Y3, etc.



## Tools > Standard Calibration Experiments > Shim Editor

**Current method**

1 pfg\_xyz\_extended

2 Start shim in background

Stop shim

Show shim log

Set as default on profile

**Manage shim method files**

Edit/Show/Delete

Edit Show Delete

**Method**

	Tol	Range	Steps	Delay	Spin
pfg & lock1d	x1 y1 xz x1 yz y1				0
lock1d	xz2 xz x1 yz2 yz y1 xy x2y2 x1 y1				
pfg & lock1d	x1 y1 z1				

**FID-shim parameters**

Set for current sample...

tpwr 53

pw 5.05

Acqtime 2.93601

d1 2.5

gain 42

offset 699.7

sw 11160.7

OR use default parameters for lineshape sample:

Default lineshape

Close Help

- lock—optimizes the lock shim variables as a group.
- lock1d—optimizes the lock shim variables independently in listed order.
- fid—optimizes the FID shim variables as a group.
- fid1d—optimizes the FID shim variables independently in listed order.
- Pfg – optimizes the shims using a z-gradient shim method.
- Gxyz – optimizes the shims using a 3D gradient shim method.

**Lineshape sample**

1H: CHCl<sub>3</sub> in Acetone-D<sub>6</sub>

13C: Dioxane in Benzene-D<sub>6</sub>

# Create Gradient shim-map (Simple)

1H shimming: 10% H<sub>2</sub>O in 90% D<sub>2</sub>O  
2H shimming: Doped 1% H<sub>2</sub>O in 99% D<sub>2</sub>O

The screenshot displays the Bruker QNP software interface with several key components highlighted for creating a gradient shim-map:

- Tools Menu (6):** The 'Tools' menu is open, and 'Set Up Gradient Shimming' is selected.
- Gradient Shim Setup (5):** The 'Acquire Trial Spectra' button is highlighted.
- Make Shimmap (4):** The 'Automake Shimmap' button is highlighted.
- Gradient Autoshim (2):** The 'Gradient Autoshim on Z' button is highlighted.
- Sequence Diagram (2):** The 'Sequence diagram' button is highlighted.
- Shimmap Plot (3):** A plot showing the shimmap results is highlighted.

The main window displays a 1D NMR spectrum with a peak at 2172.57 Hz. The status bar at the bottom indicates 'Idle' and 'exp100: Acquisition complete'.

# Create Gradient shim-map (Manually)

Exp: 100 Seq: gmapz Index: 1

1372.57

5 Type ds(1)  
Set Window size (check height and Hz)

V\_scale 249579.6 sp(Hz) -7194.27 wp(Hz) 15371.82 first 1 last 2 step 1

1

4

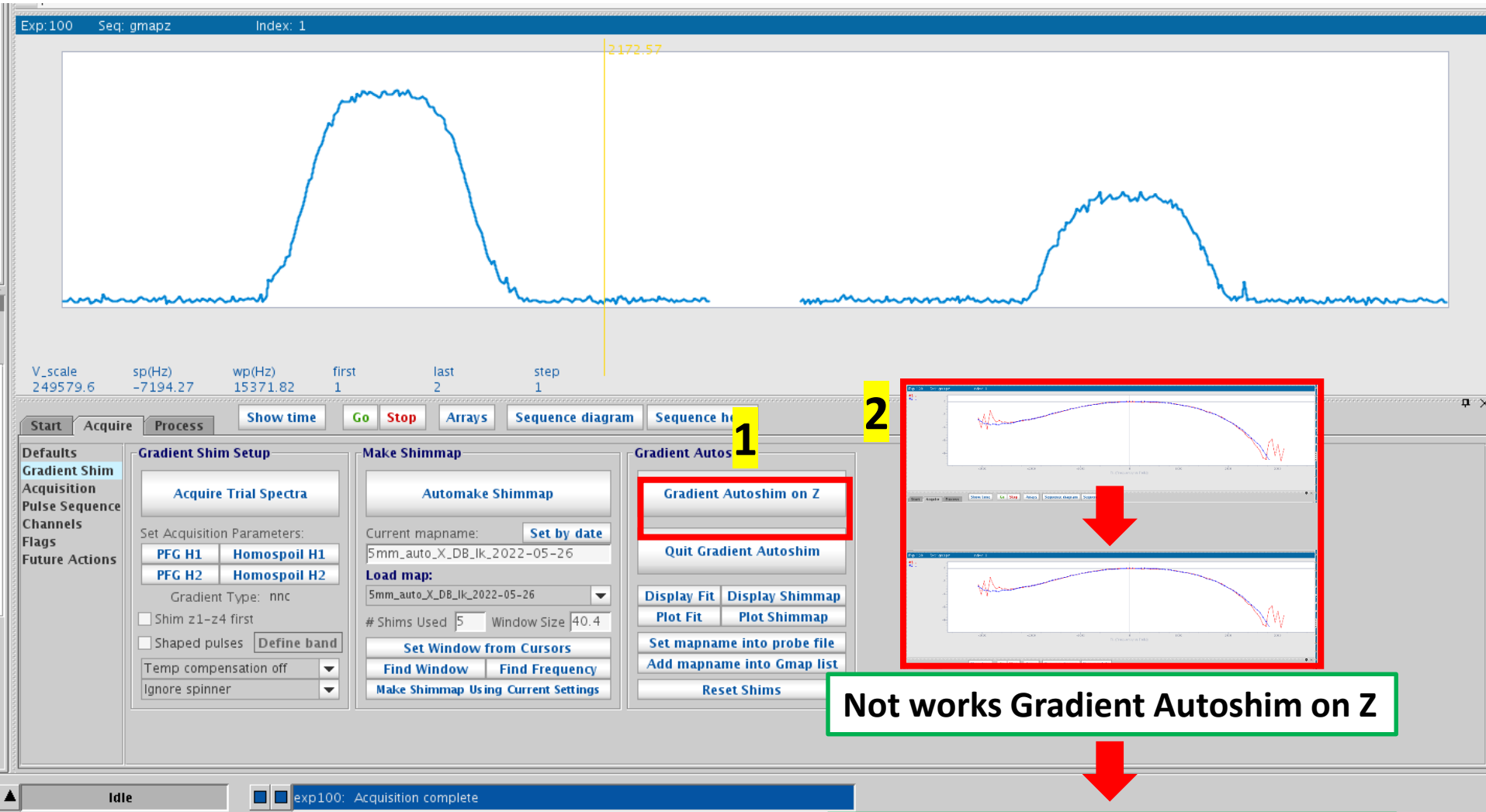
3

6

7

2

# Create Gradient shim-map (Trouble shooting)

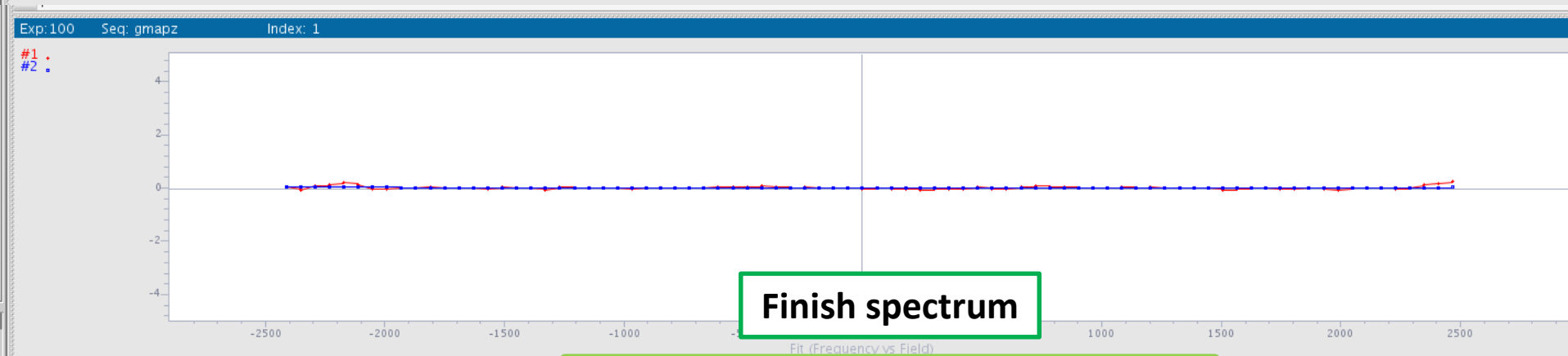
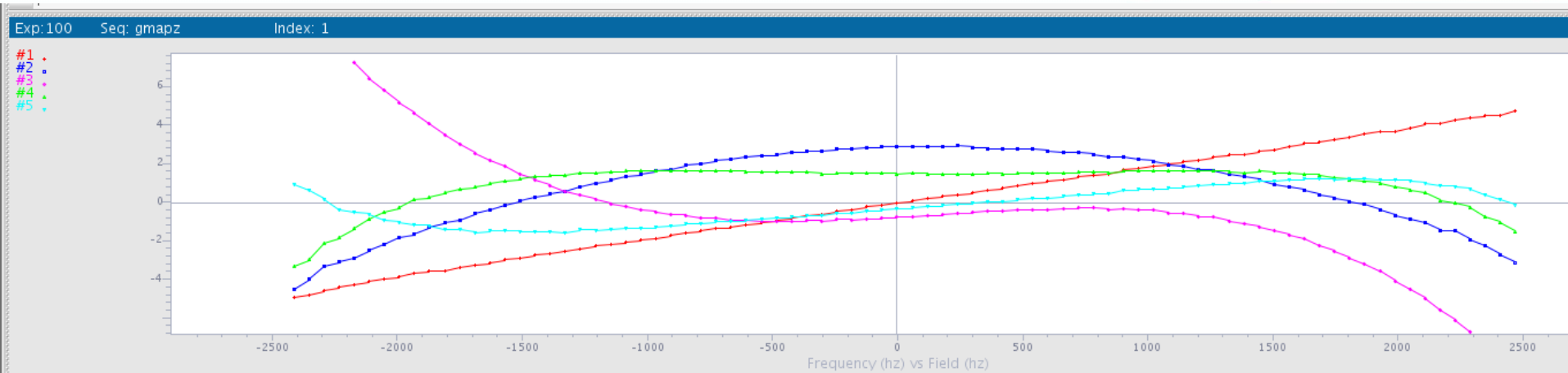


Not works Gradient Autoshim on Z

Try to use 3D shim or Shim editor



# Finish shim-map



Finish spectrum

Start Acquire Process Show time Go Stop Arrays Seq

Defaults Gradient Shim Acquisition Pulse Sequence Channels Flags Future Actions

Gradient Shim Setup

Acquire Trial Spectra

Set Acquisition Parameters:

PFG H1 Homospoil H1

PFG H2 Homospoil H2

Gradient Type: nnc

Shim z1-z4 first

Make Shimmap

Automake Shimmap

Current mapname: 5mm\_auto\_X\_DB\_Ik\_2022-06-09

Load map: 5mm\_auto\_X\_DB\_Ik\_2022-06-09

# Shims Used 5 Window Size 31.6

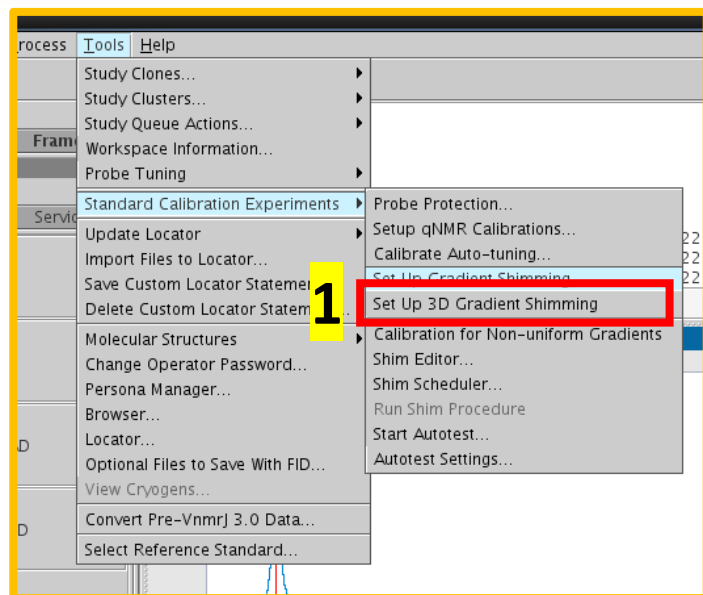
Display Fit Display Shimmap Plot Fit Plot Shimmap

Exp: 100 Seq: PROTON Index: 1

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50% Inwidth: 2.09  
95% Inwidth: 28.36  
11% Inwidth: 63.80

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# 3D shim



At least 30 min for 1 cycle

Poor shim -> Try to use manual shim or shim editors

