

**Not So Short Introduction To
TopSpin**

Spring 2016

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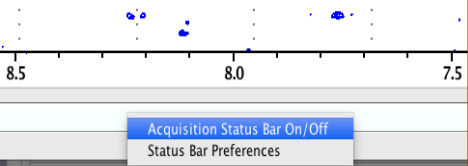
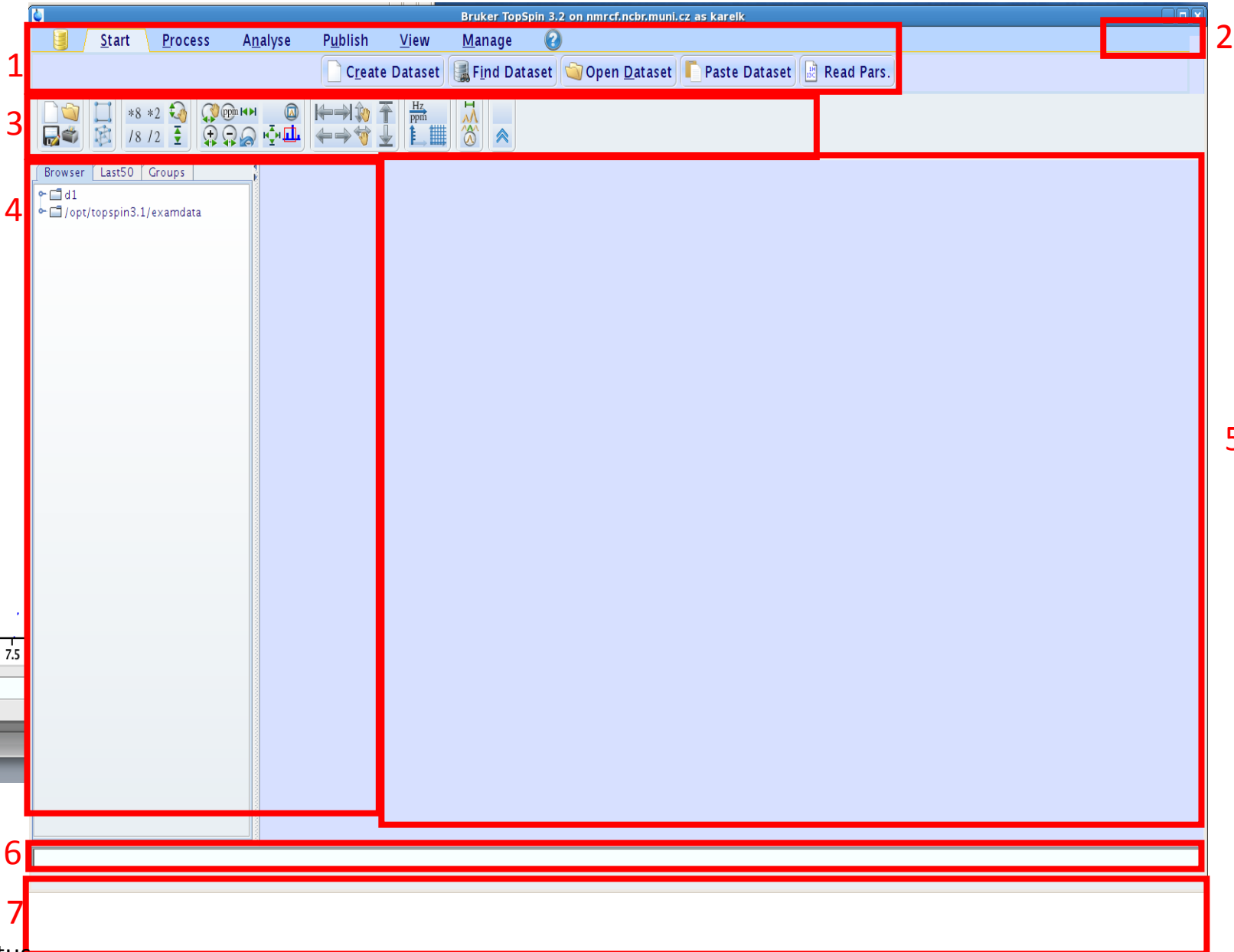
Data Processing

using

TopSpin 3.X

Topspin 3.X – layout description

- 1 – Menu/submenu bar
- 2 – Windows navigator
- 3 – Toolbar
- 4 – Browser
- 5 – Data/window area
- 6 – Command line
- 7 – Status panel



Right mouse click in the status bar area toggles it on/off

Topspin 3.X – layout description

- 1 – Menu bar
- 2 – Windows navigator
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- 7 – Status panel

The screenshot shows the Bruker TopSpin 3.2 software interface. The title bar reads "Bruker TopSpin 3.2 on nmr950.ncbr.muni.cz as karek". The interface is annotated with red boxes and numbers 1 through 7:

- 1**: Menu bar (Start, Acquire, Process, Analyse, Publish, View, Manage)
- 2**: Windows navigator (1 2 LIB T)
- 3**: Toolbar (Proc. Spectrum, Adjust Phase, Calib. Axis, Pick Peaks, Integrate, Advanced)
- 4**: Browser (Last50, Groups, file tree)
- 5**: Data/window area (BSMS Control Suite)
- 6**: Command line
- 7**: Status panel

BSMS Control Suite window details:

- Lock: Phase, Power, Gain, Shim
- LOCK: On-Off, Phase, Power, Gain
- SAMPLE: **LIB T**, SPIN, Measure, Rate, Lock Lost
- SHIM: Spin (Z, Z², Z³, Z⁴), NonSpin (X, XZ, Y, YZ, XY, X²-Y²)
- STD BY: Absolute, Difference, Previous, Actual, Step (+, -), Stepsize, Reset, **STD BY** button
- Config: External
- Sample: down, missing, up, Shim coil temperature: **301 K**

Status Panel details:

- Amplifier Control: [Black]
- Acquisition information: no acquisition running
- Fid Flash: [Grid]
- Lock: [Grid]
- Sample: [Blue icon]
- POWCHK: [Green checkmark]
- Sample Temperature: **Corr. 310.2 K**, Reg. State: [Green checkmark]
- Spooler: queued: 0, delayed: 0, cron: 0
- BSMS status message: **Δ Z 1**, Autoshim: [Green checkmark], Locked: [Red X], Error: [Red X]
- Time: 09:24:27 Dec 23



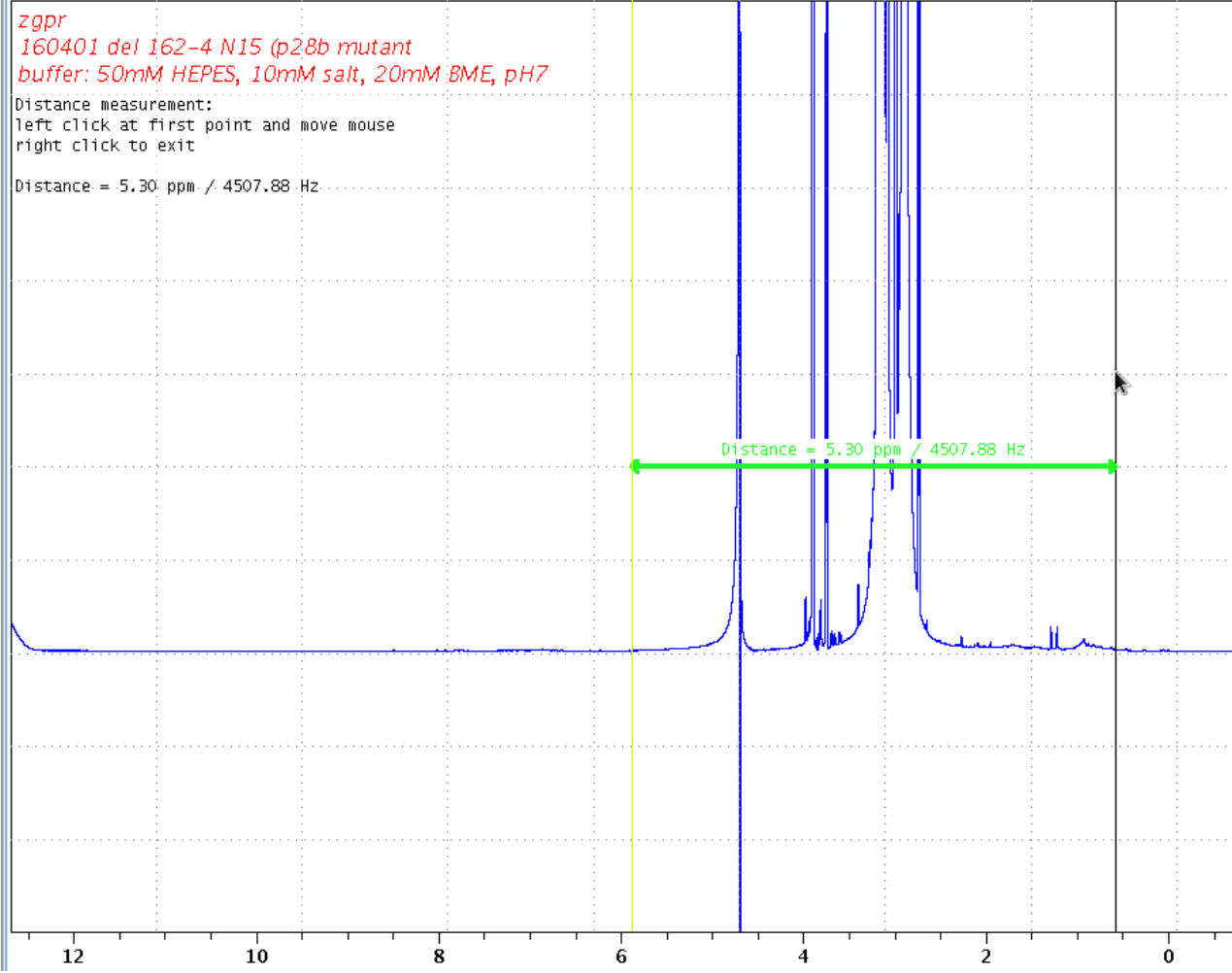
1 160401_850_del162az4 1 1 /d1/data/karek/nmr

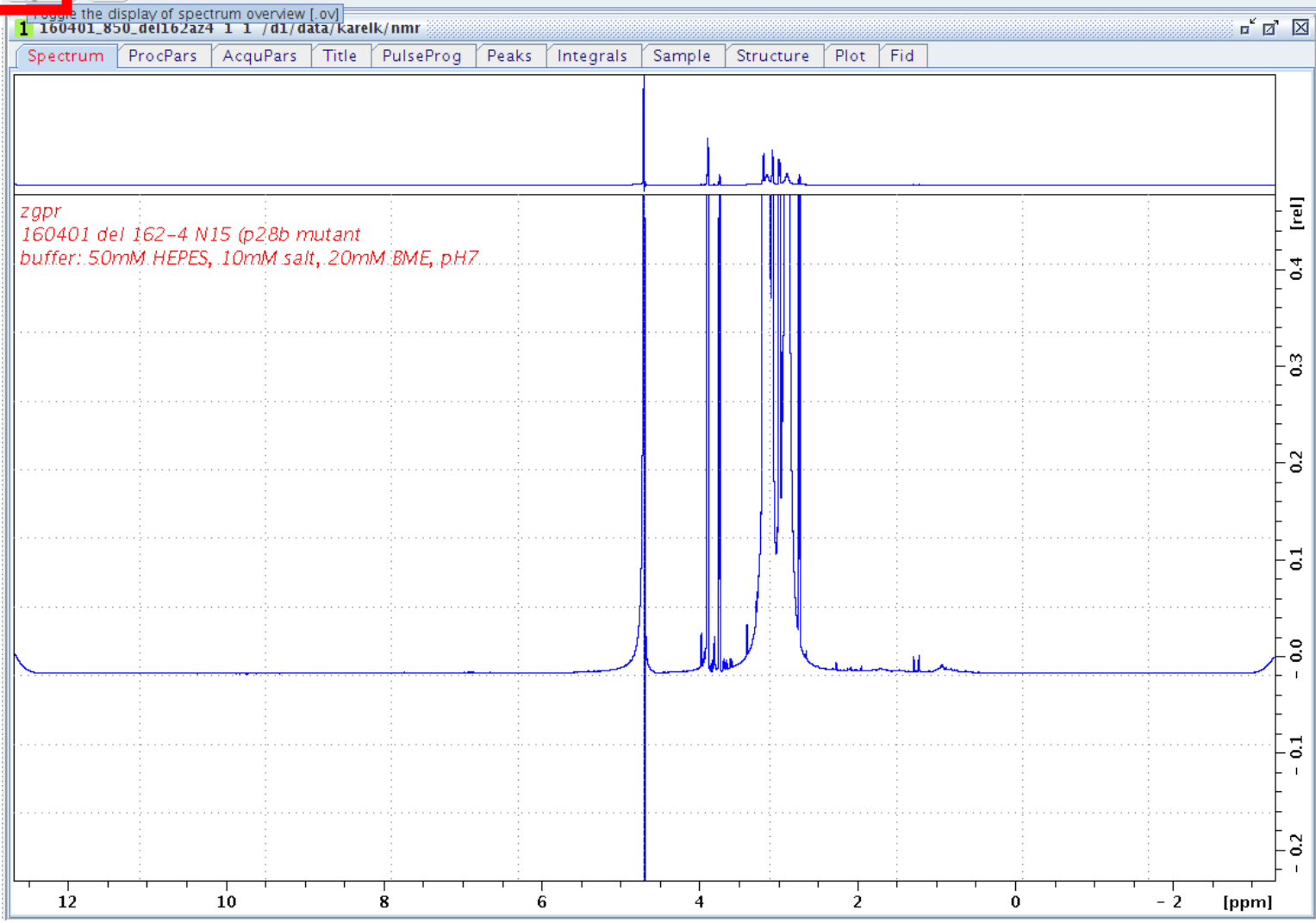
Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Plot Fid

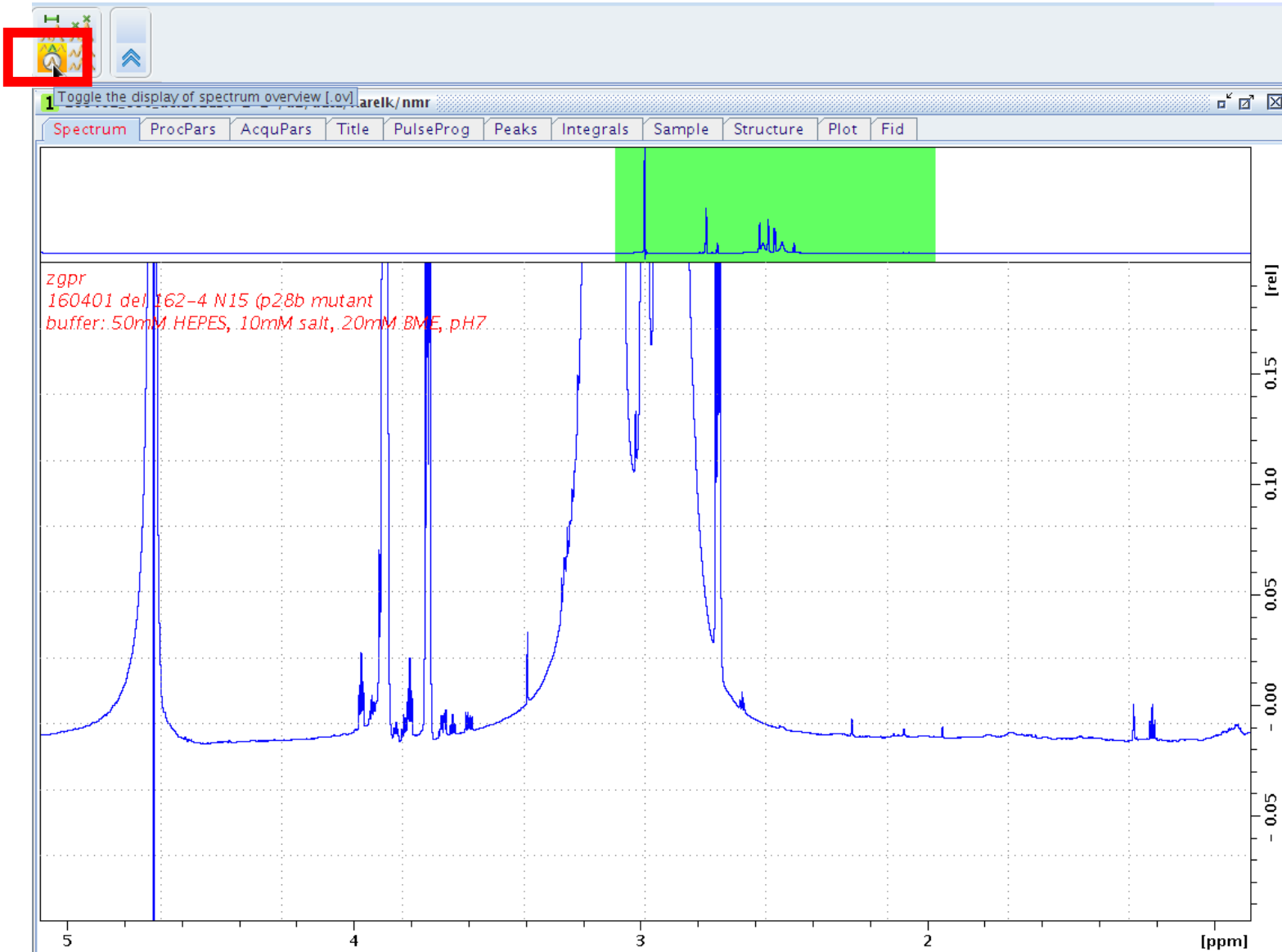
zgpr
I60401 del 162-4 N15 (p28b mutant)
buffer: 50mM HEPES, 10mM salt, 20mM BME, pH7

Distance measurement:
left click at first point and move mouse
right click to exit

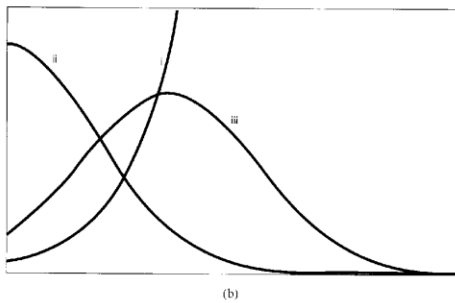
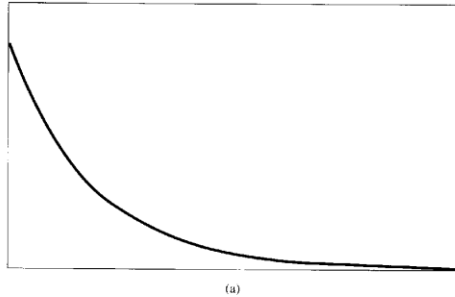
Distance = 5.30 ppm / 4507.88 Hz







NMR data processing

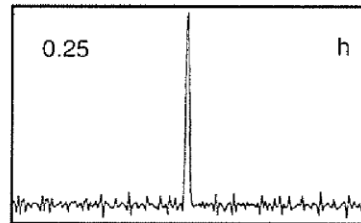
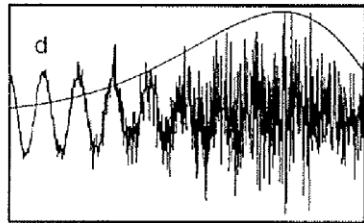
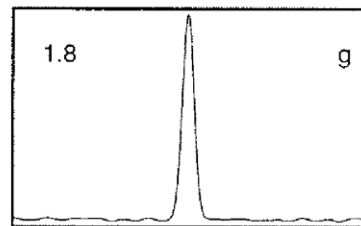
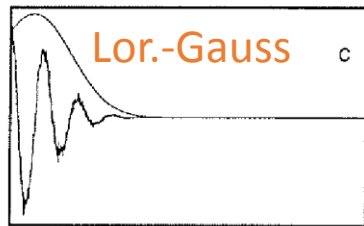
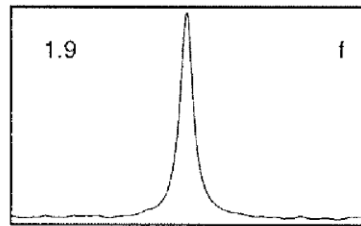
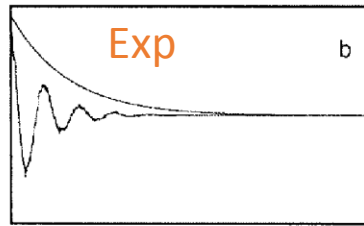
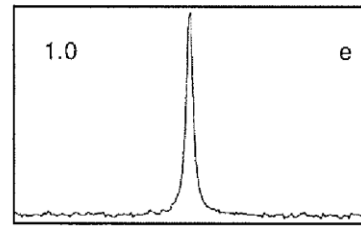
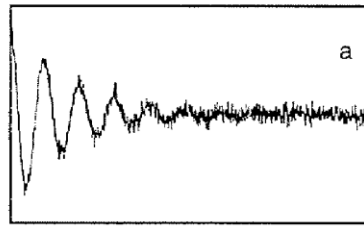


Window functions:

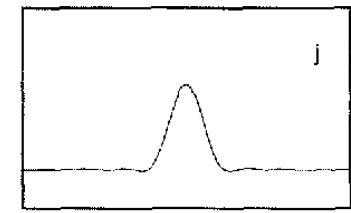
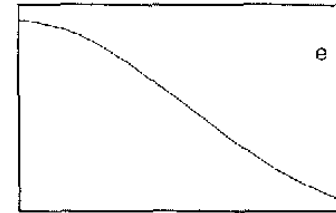
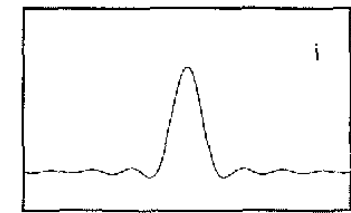
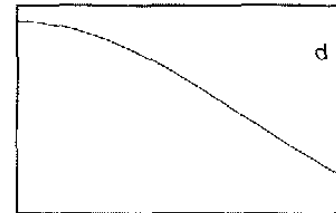
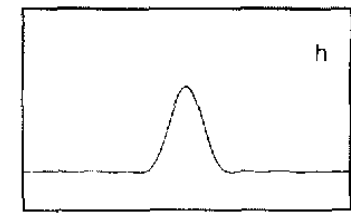
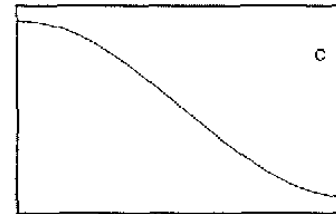
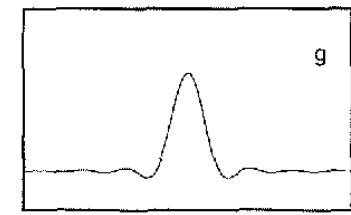
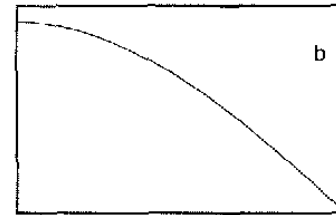
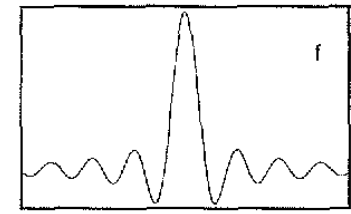
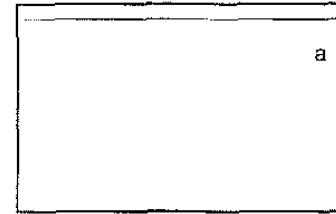
1) improvement of S/N ratio

2) improvement of resolution

NMR data processing – window functions - apodization

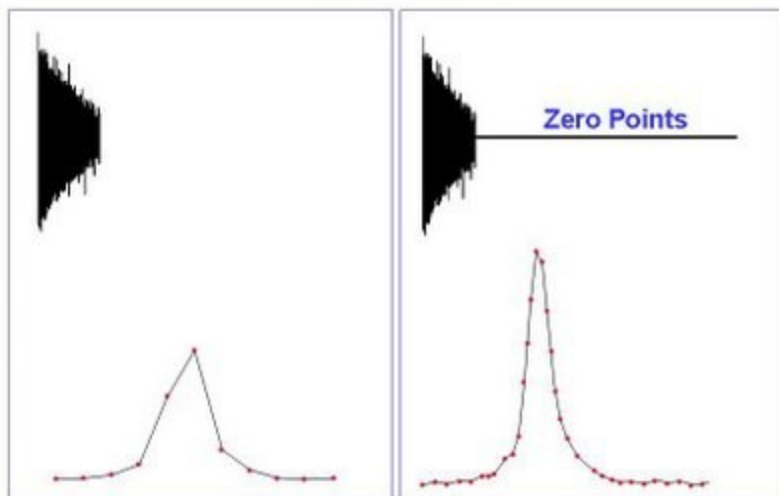


Kaiser w. f'tion

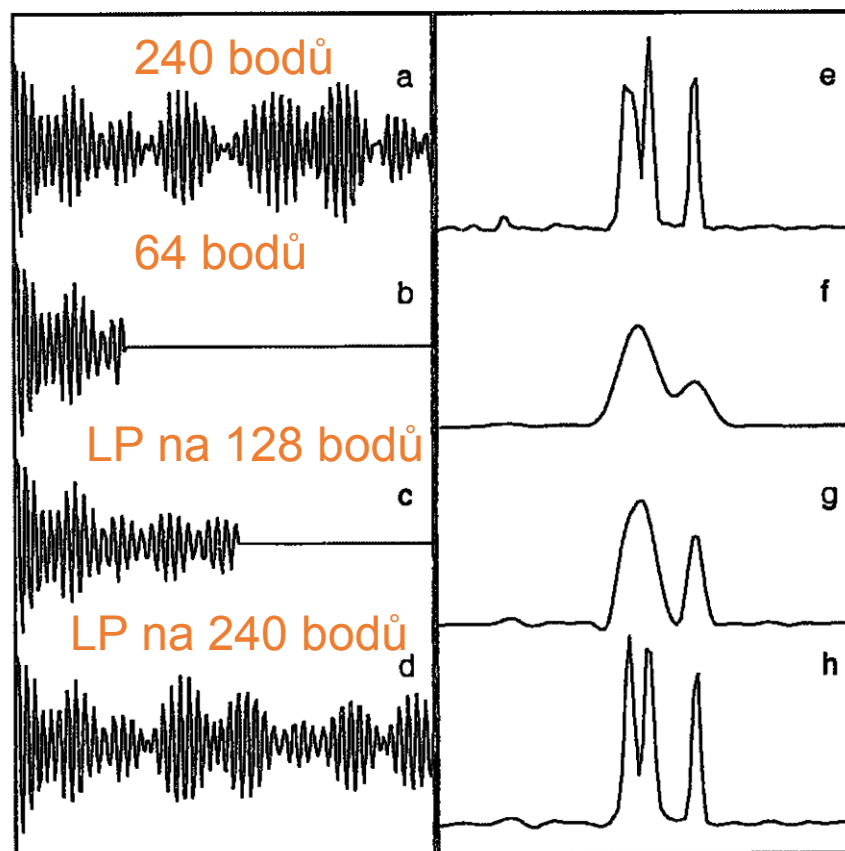


Zpracování NMR dat – Zero Filling, Lineární predikce

Zero filling



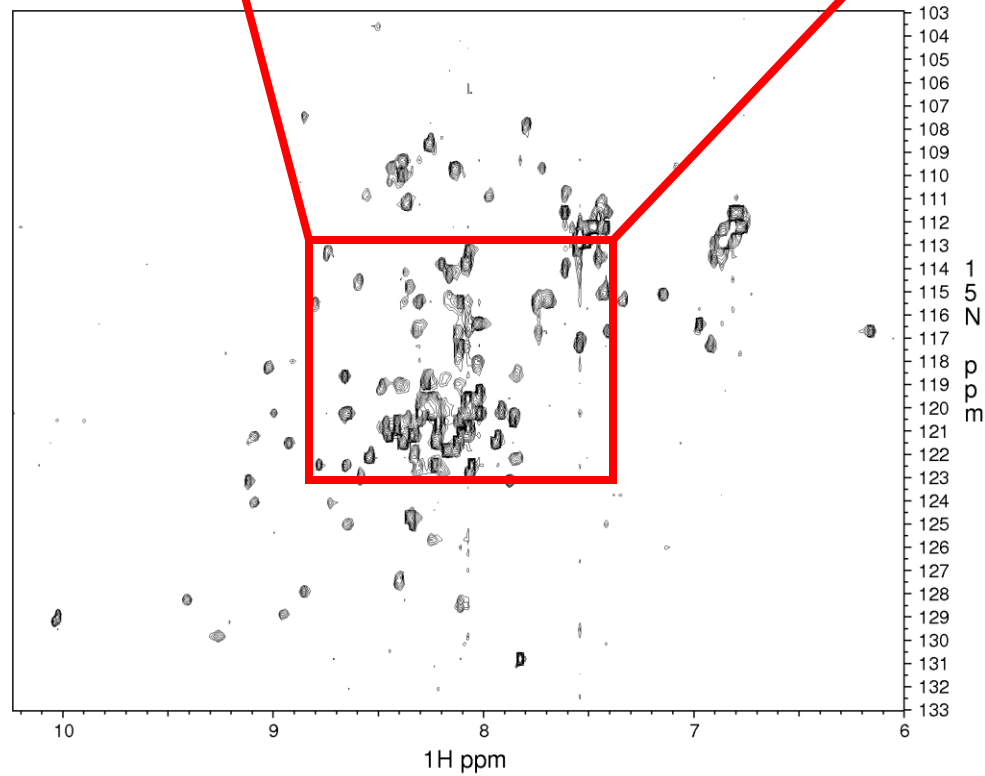
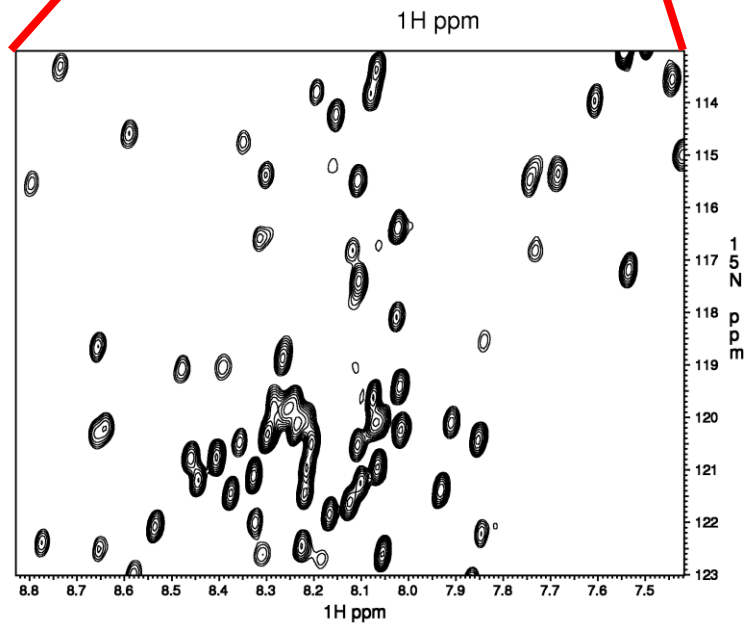
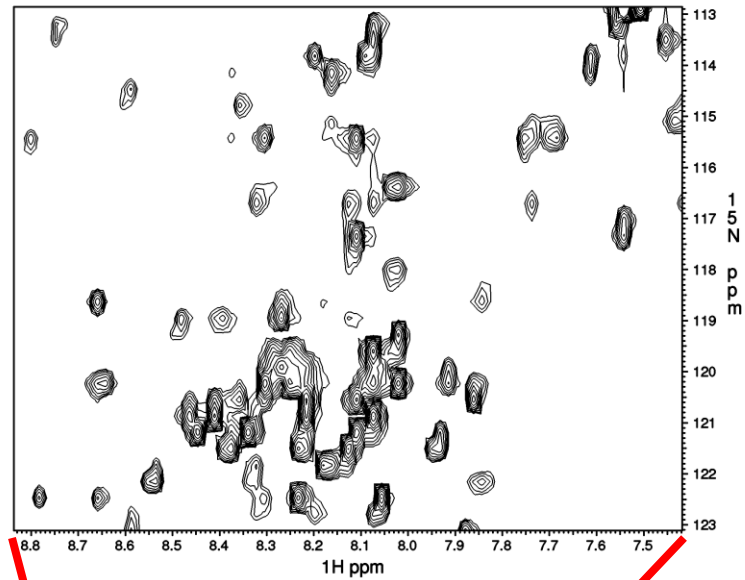
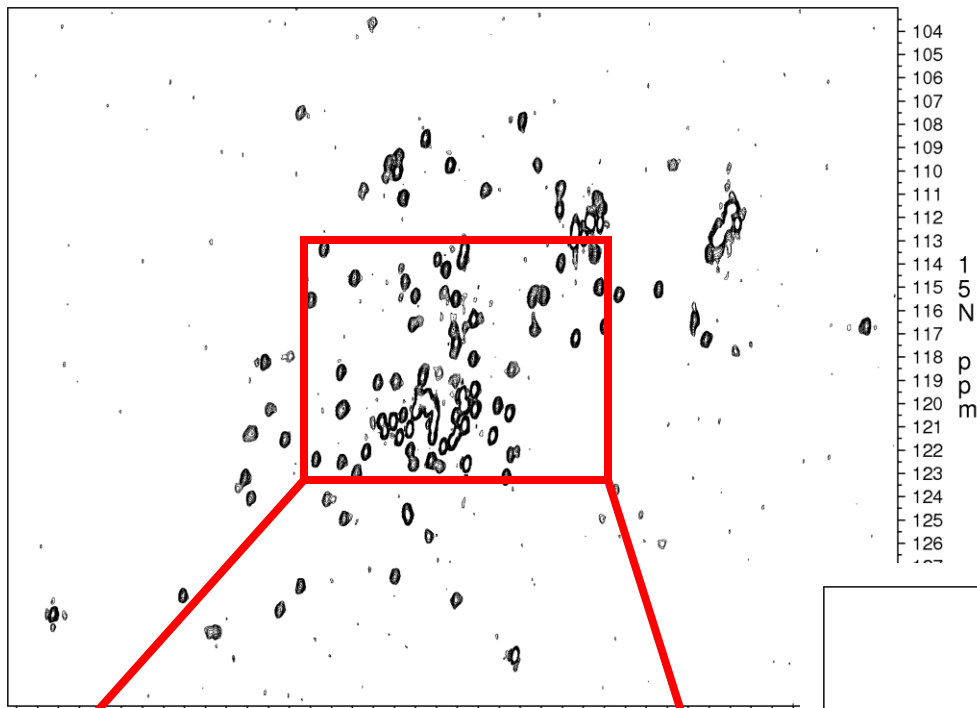
Lineární predikce



NMR data processing – summary

- I) Solvent suppression
- II) Window functions
- III) Zero-filling
- IV) FT
- V) Transposition

```
|nmrPipe -fn POLY -time \  
|nmrPipe -fn SP -off 0.33 -end 0.98 -pow 2 -c 1.0 \  
|nmrPipe -fn ZF -size 2048 \  
|nmrPipe -fn FT -auto \  
|nmrPipe -fn PS -p0 -76.0 -p1 0.0 -di \  
|nmrPipe -fn EXT -x1 11.0ppm -xn 6.0ppm -sw \  
|nmrPipe -fn POLY -ord 3 -auto \  
|nmrPipe -fn TP \  
F2
```



1 160401 / d1/data/karelk/nmr

Spectrums ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Plot Fid

S 12... ME

Reference
Window
Phase
Baseline
Fourier
Integration
Peak
Deconvolution
Automation
Miscellaneous
User

Reference

SI	32768	Size of real spectrum
SF [MHz]	850.2800000	Spectrometer frequency
OFFSET [ppm]	12.68500	Low field limit of spectrum
SR [Hz]	0	Spectrum reference frequency
HZPPT [Hz]	0.414641	Spectral resolution
SPECTYP	UNDEFINED	Type of spectrum e.g. COSY, HMQC, ...

Window function

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

Phase correction

PHC0 [degrees]	-79.041	0th order correction for pk
PHC1 [degrees]	-106.400	1st order correction for pk
PH_mod	pk	Phasing modes for trf, xfb, ...

Baseline correction

ABSG	5	Degree of polynomial for abs (0..5)
ABSF1 [ppm]	10.00000	Left limit for absf
ABSF2 [ppm]	0	Right limit for absf, abs1, abs2

1 160401 / d1/data/karelk/nmr

Spectr ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Plot Fid

S 12. ME

Reference PHC0 [degrees] -79.041 0th order correction for pk
Window PHC1 [degrees] -106.400 1st order correction for pk
Phase PH_mod pk Phasing modes for trf, xfb, ...
Baseline PH_mod pk
Fourier Baseline correction
Integration ^ Baseline correction
Peak ABSF1 [ppm] 10.00000 Degree of polynomial for abs (0..5)
Deconvolution ABSF2 [ppm] 0 Left limit for absf
Automation BCFW [ppm] 1.00000 Right limit for absf, abs1, abs2
Miscellaneous COROFFS [Hz] 0 Filter width for bc (sfil/qfil)
User BC_mod quad Correction offset for BC_MOD=spol etc.
Fid baseline modes for em, ft, xfb, ...
Fourier transform
TDef 0 Number of fid data points used by ft
STSR 0 First output point of strip transform
STSI 0 Total number of output points of strip transform
ME_mod no Linear prediction for ft, xfb, ...
NCOEF 0 Number of LP coefficients
LPBIN 0 Number of output points for LP
TDo 0 Number of back-predicted points
REVERSE FALSE Reverse spectrum during transform
FCOR 0.5 Weighting factor for first fid point
PKNL TRUE Group delay compensation
FT_mod fsc Fourier transform mode for trf, xtrf*
Mdd_mod mdd MDD mode

Process Analyse Publish View Manage

Proc. Spectrum Adjust Phase Calib. Axis Pick Peaks Integrate Advanced

8 *2 8 /2

Groups

- .700b_Nab3_aRRM_Assignm
- .850_Spt6_withoutHisTag_CTD
- .600_Nab3_aRRM_hncaco
- .600_C9320A_Ubq
- .500_C9320B_Ubq
- .700m_C9320C_Ubq
- .500_C9320C_Ubq

el162az4 1 1 /d1/data/karelk/nmr

ProcPars	AcquPars	Title	PulseProg	Peaks	Integrals	Sample	Structure	Plo
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62-4 N15 (p28b mutant)
buffer: 50mM HEPES, 10mM salt, 20mM BME, pH7

Process Analyse Publish View Manage

Proc. Spectrum Adjust Phase Calib. Axis Pick Peaks Integrate Advanced

Groups

160401_850_del162az4 1 1 /d1/data/karelk/nmr

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Plot

zgpr
 160401 del 162-4 N15 (p28b mutant
 buffer: 50mM HEPES, 10mM salt, 20mM BME, pH7

Options
 Manual window adjustment

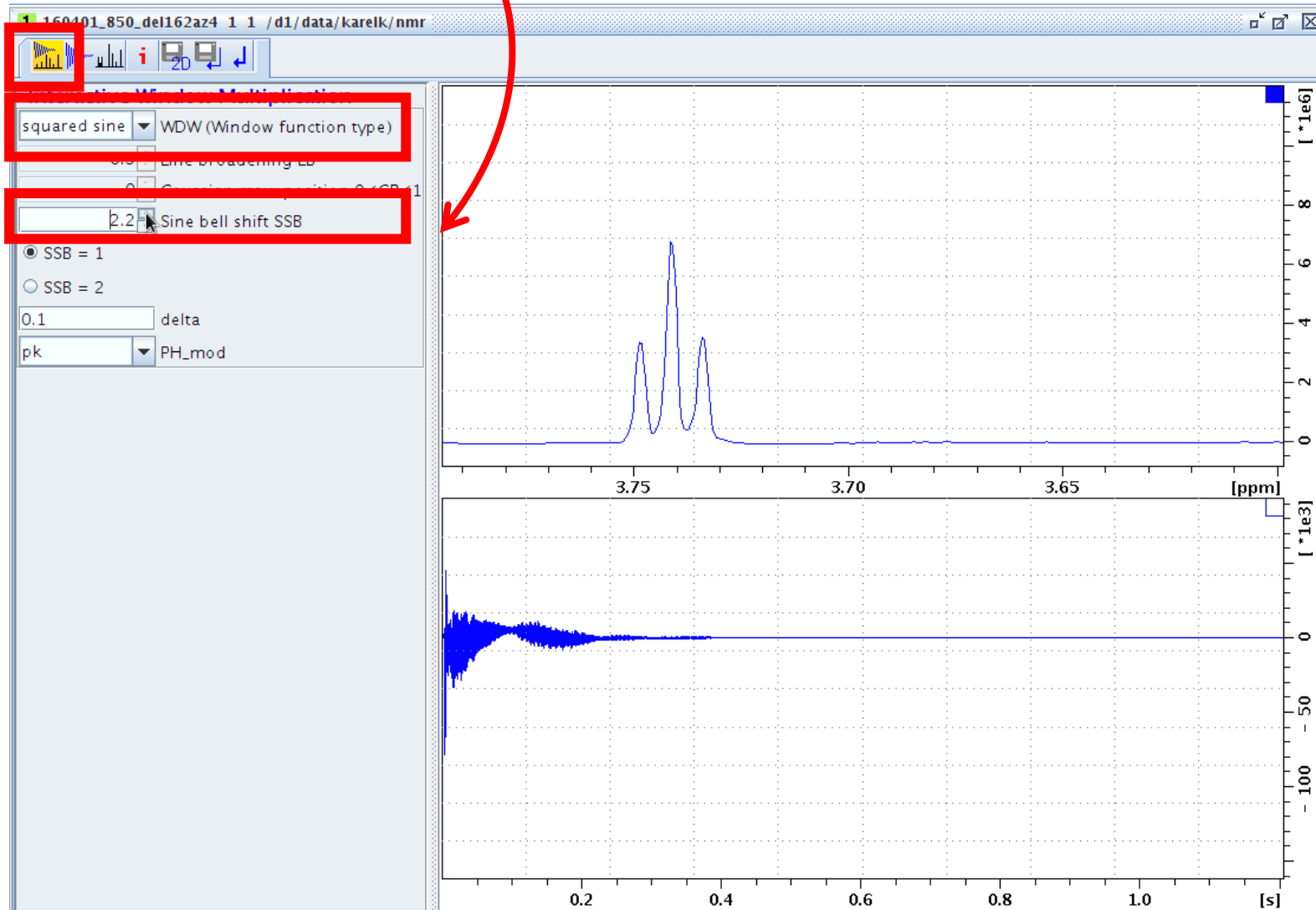
Required parameters

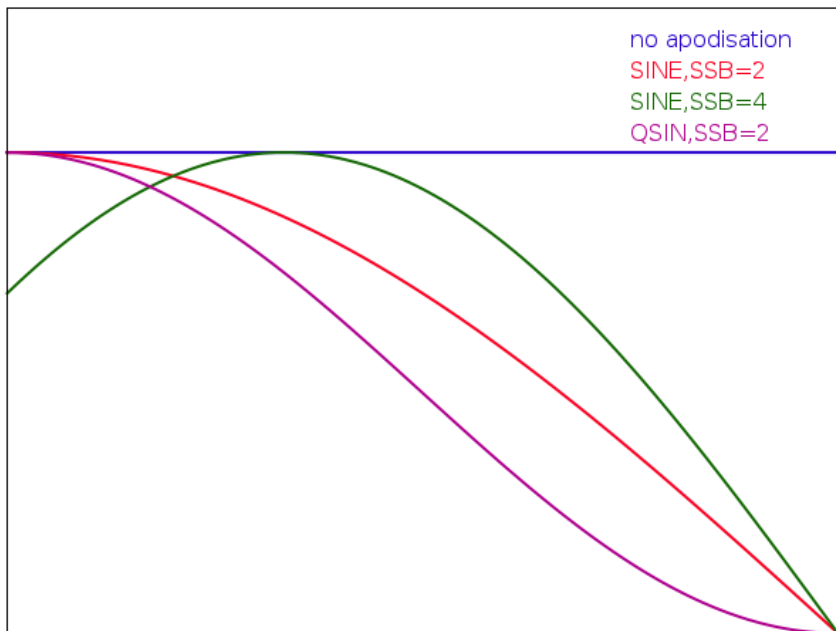
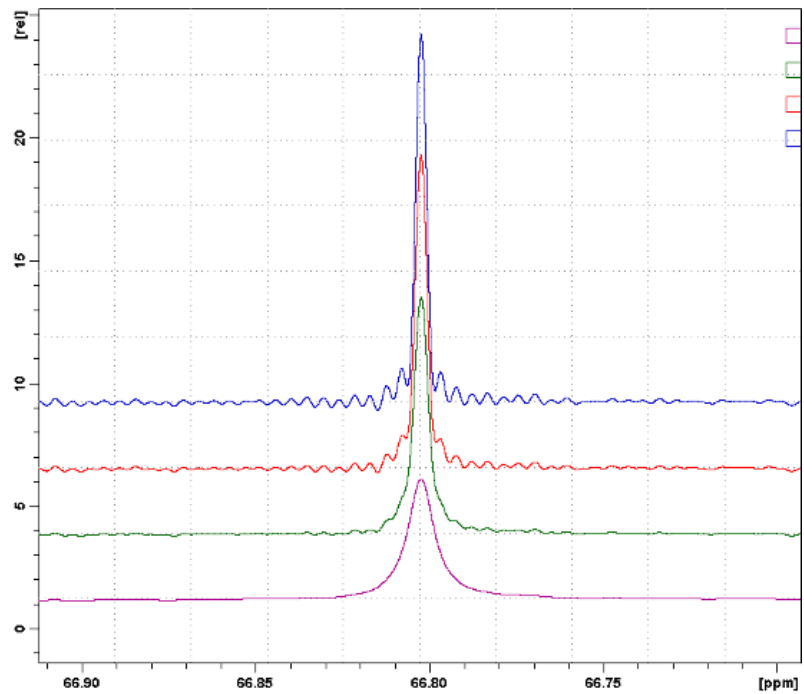
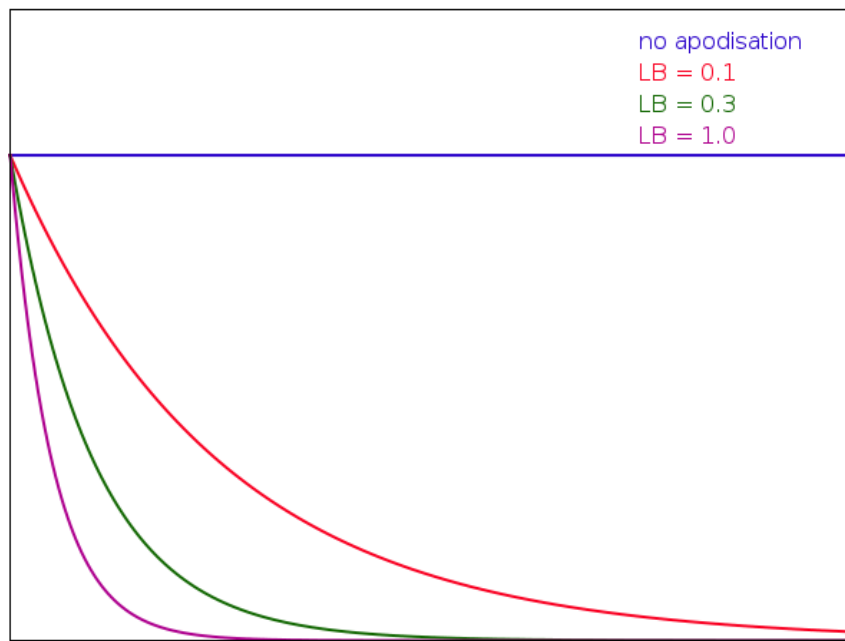
Window function type WDW =	exponential
Line broadening LB [Hz] =	0.3
Gaussian max. position 0<GB<1 =	0
Sine bell shift SSB (0,1,2,..) =	2
Left trapezoid limit 0<TM1<1 =	0
Right trapezoid limit 0<TM2<1 =	0

OK Cancel Help

$$QSIN(t) = \sin[(\pi - \text{PHI}) * (t / \text{AQ} + \text{PHI})]^2$$

$$0 < t < \text{AQ} \text{ and } \text{AQ} = \pi / \text{SSB}$$





Start Process Analyse Publish View Manage

Proc. Spectrum Adjust Phase Calib. Axis Pick Peaks Integrate Advanced

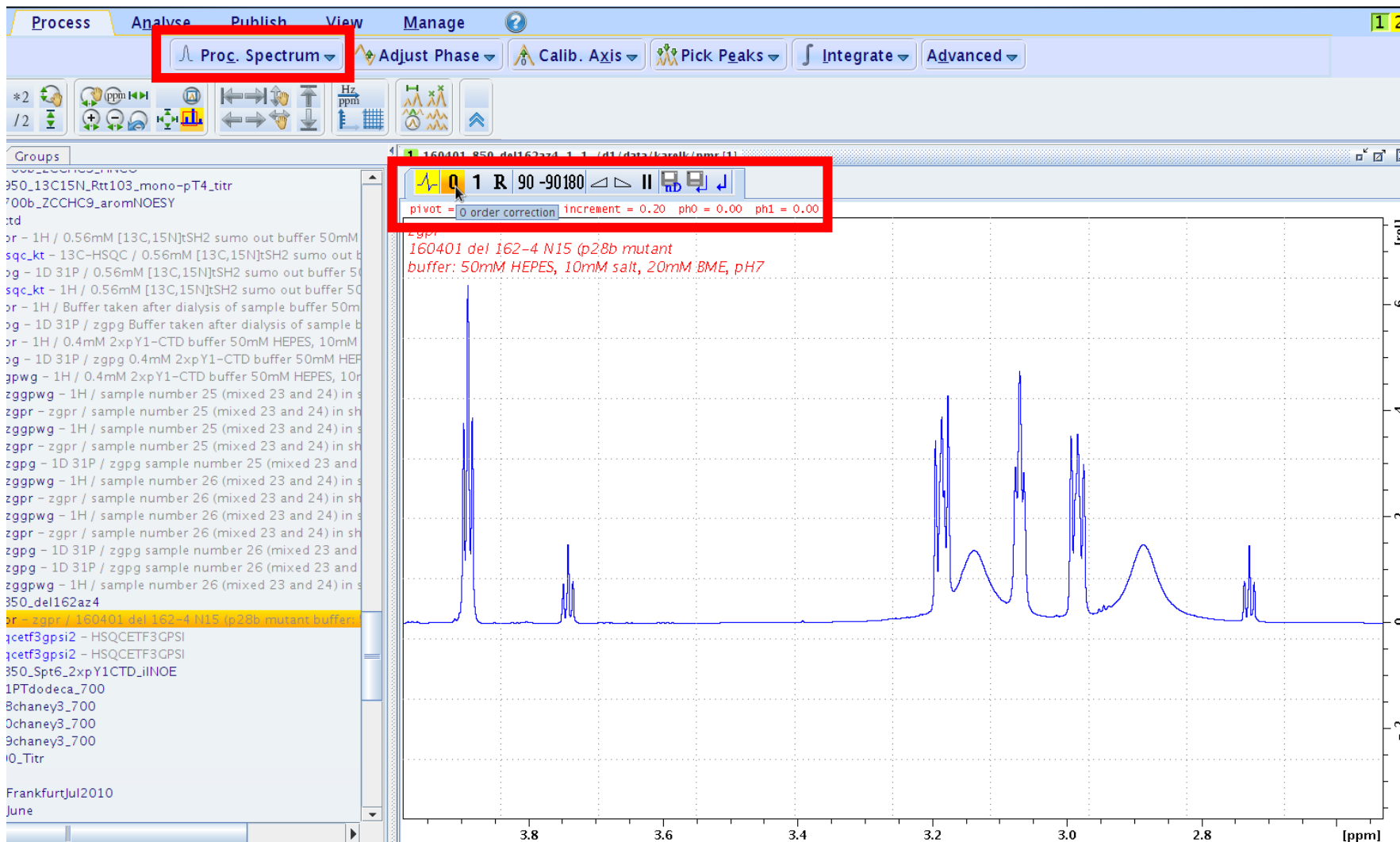
Adjust spectrum phase manually (*ph*)
 Enter manual phasing mode. Allows you to adjust the zero and first order correction terms *PHC0* and *PHC1*.

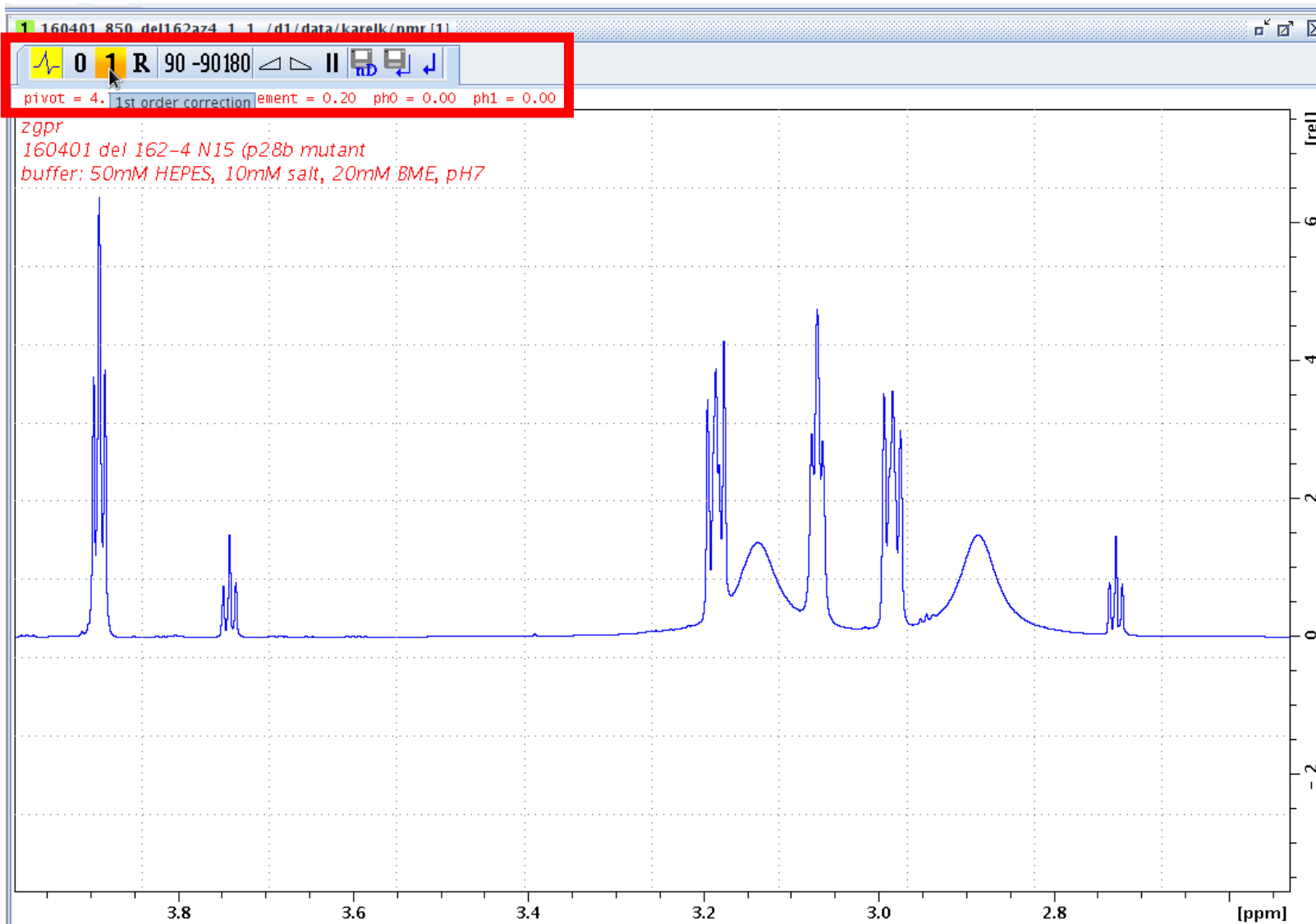
Browser Last50 Groups

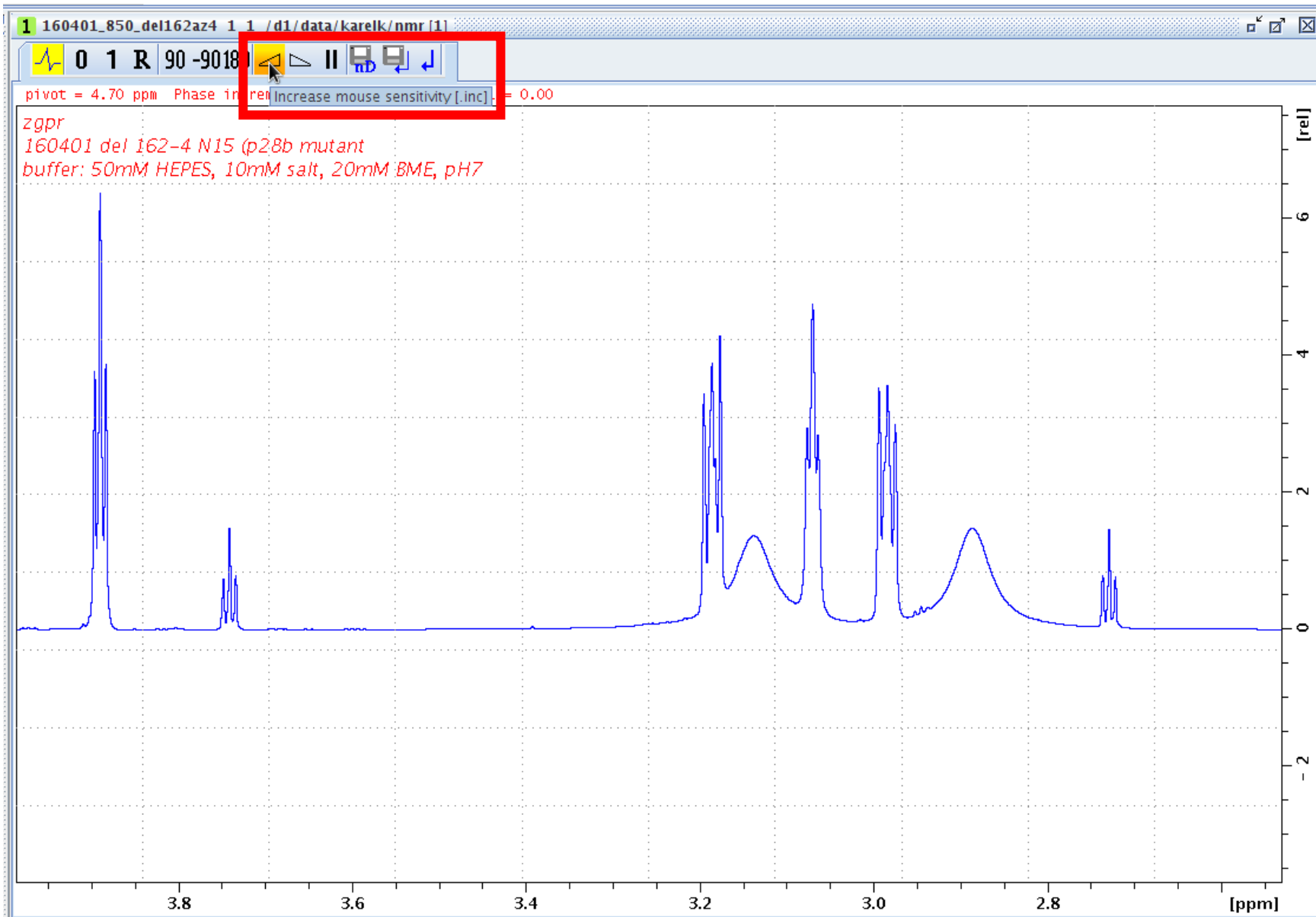
- 160207_950_13C15N_Rtt103_mono-pT4_titr
- 160210_700b_ZCCHC9_aromNOESY
- 160210_ctd
 - 1 - zgpr - 1H / 0.56mM [13C,15N]tSH2 sumo out buffer 50mM
 - 2 - Chsqc_kt - 13C-HSQC / 0.56mM [13C,15N]tSH2 sumo out b
 - 3 - zgpg - 1D 31P / 0.56mM [13C,15N]tSH2 sumo out buffer 50
 - 4 - Chsqc_kt - 1H / 0.56mM [13C,15N]tSH2 sumo out buffer 50
 - 5 - zgpr - 1H / Buffer taken after dialysis of sample buffer 50m
 - 6 - zgpg - 1D 31P / zgpg Buffer taken after dialysis of sample b
 - 7 - zgpr - 1H / 0.4mM 2xpY1-CTD buffer 50mM HEPES, 10mM
 - 8 - zgpg - 1D 31P / zgpg 0.4mM 2xpY1-CTD buffer 50mM HEP
 - 9 - zgppwg - 1H / 0.4mM 2xpY1-CTD buffer 50mM HEPES, 10r
 - 100 - zgppwg - 1H / sample number 25 (mixed 23 and 24) in s
 - 101 - zgpr - zgpr / sample number 25 (mixed 23 and 24) in sh
 - 102 - zgppwg - 1H / sample number 25 (mixed 23 and 24) in s
 - 103 - zgpr - zgpr / sample number 25 (mixed 23 and 24) in sh
 - 104 - zgpg - 1D 31P / zgpg sample number 25 (mixed 23 and
 - 200 - zgppwg - 1H / sample number 26 (mixed 23 and 24) in s
 - 201 - zgpr - zgpr / sample number 26 (mixed 23 and 24) in sh
 - 202 - zgppwg - 1H / sample number 26 (mixed 23 and 24) in s
 - 203 - zgpr - zgpr / sample number 26 (mixed 23 and 24) in sh
 - 204 - zgpg - 1D 31P / zgpg sample number 26 (mixed 23 and
 - 205 - zgpg - 1D 31P / zgpg sample number 26 (mixed 23 and
 - 206 - zgppwg - 1H / sample number 26 (mixed 23 and 24) in s
- 160401_850_del162az4
 - 1 - zgpr - zgpr / 160401 del 162-4 N15 (p28b mutant buffer:
 - 160401_850_del162az4 1 1 / 01/data/karelk/nmr [1]
 - 2 - hsqcetf3gpsi2 - HSQCETf3GPSI
 - 3 - hsqcetf3gpsi2 - HSQCETf3GPSI

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure

zgpr
 160401 del 162-4 N15 (p28b mutant
 buffer: 50mM HEPES, 10mM salt, 20mM BME, pH7







Process

Analyse

Publish

View

Manage

Proc. Spectrum

Adjust Phase

Calib. Axis

Pick Peaks

Integrate

Advanced

1 2



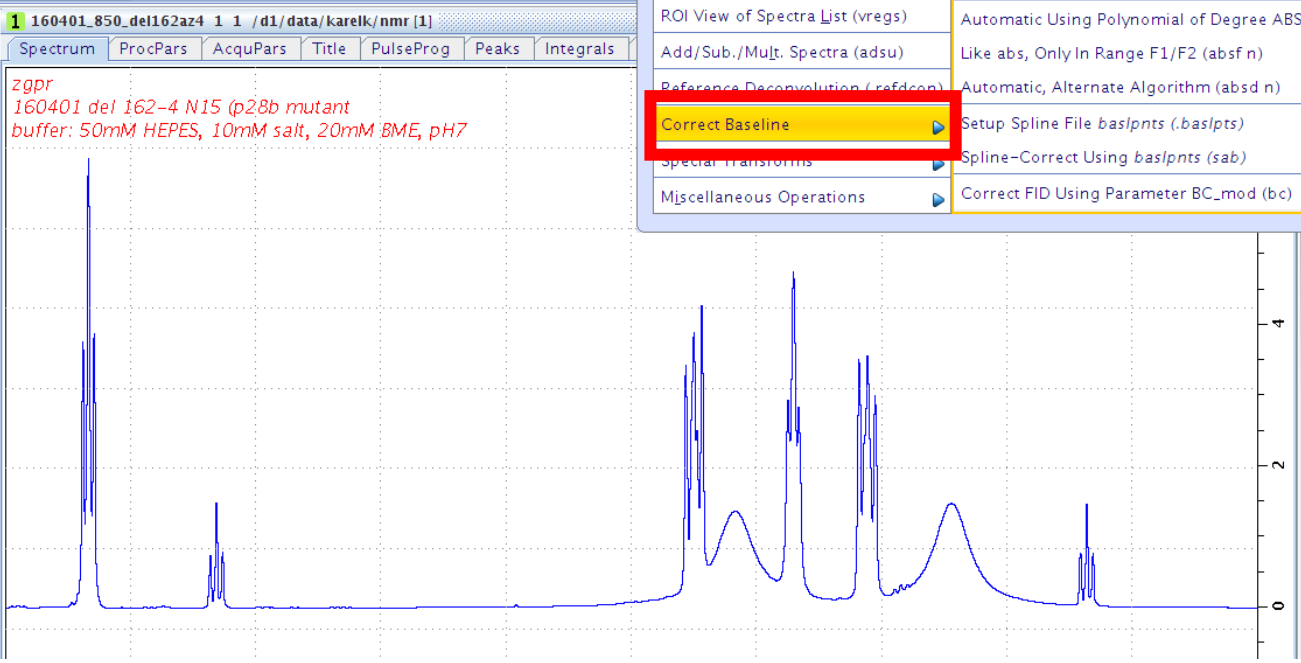
Groups

160401_850_del162az4 1 1 /d1/data/karelk/nmr [1]

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals

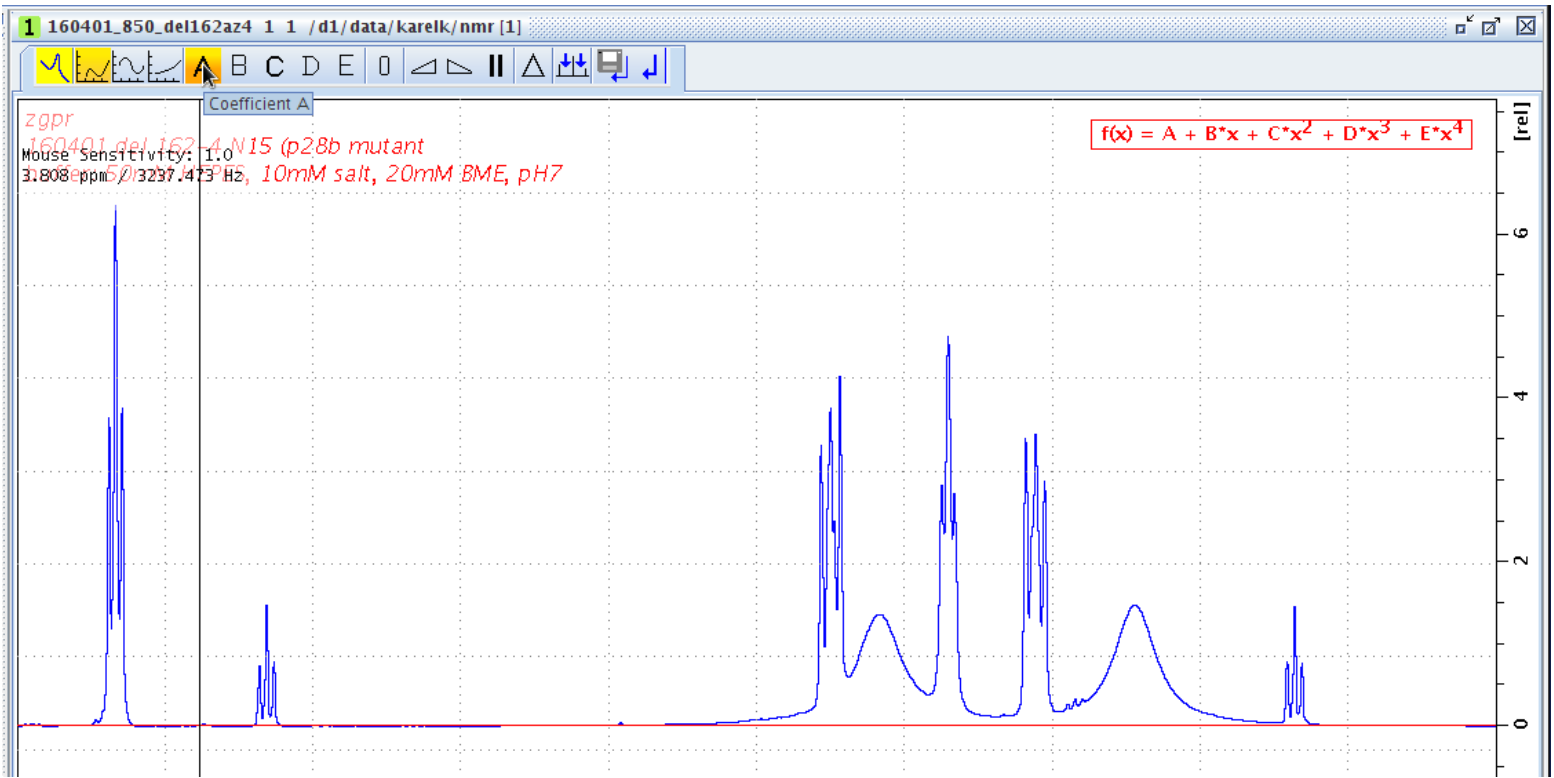
zgpr
160401 del 162-4 N15 (p28b mutant
buffer: 50mM HEPES, 10mM salt, 20mM BME, pH7

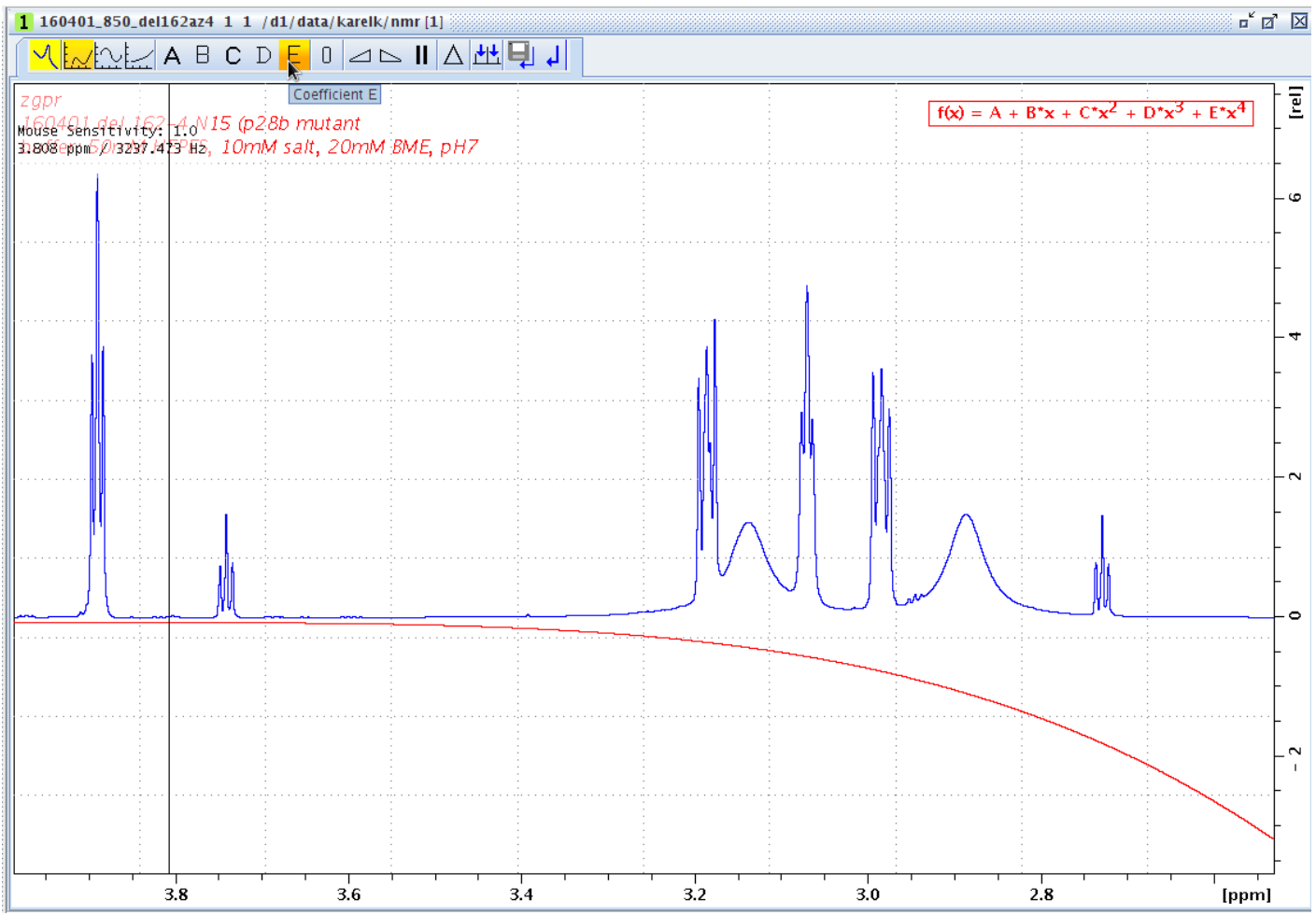
700b_ZCCHC9_aromNOESY
ctd
pr - 1H / 0.56mM [13C,15N]tSH2 sumo out buffer 50mM
isqc_kt - 13C-HSQC / 0.56mM [13C,15N]tSH2 sumo out b
pg - 1D 31P / 0.56mM [13C,15N]tSH2 sumo out buffer 50
isqc_kt - 1H / 0.56mM [13C,15N]tSH2 sumo out buffer 50
pr - 1H / Buffer taken after dialysis of sample buffer 50m
pg - 1D 31P / zgpg Buffer taken after dialysis of sample b
pr - 1H / 0.4mM 2xpY1-CTD buffer 50mM HEPES, 10mM
pg - 1D 31P / zgpg 0.4mM 2xpY1-CTD buffer 50mM HEP
gpwg - 1H / 0.4mM 2xpY1-CTD buffer 50mM HEPES, 10r
zgpgwg - 1H / sample number 25 (mixed 23 and 24) in s
zgpr - zgpr / sample number 25 (mixed 23 and 24) in sh
zgpgwg - 1H / sample number 25 (mixed 23 and 24) in s
zgpr - zgpr / sample number 25 (mixed 23 and 24) in sh
zgpg - 1D 31P / zgpg sample number 25 (mixed 23 and
zgpgwg - 1H / sample number 26 (mixed 23 and 24) in s
zgpr - zgpr / sample number 26 (mixed 23 and 24) in sh
zgpgwg - 1H / sample number 26 (mixed 23 and 24) in s
zgpr - zgpr / sample number 26 (mixed 23 and 24) in sh
zgpg - 1D 31P / zgpg sample number 26 (mixed 23 and
zgpgwg - 1H / sample number 26 (mixed 23 and 24) in s
zgpr - zgpr / 160401 del 162-4 N15 (p28b mutant buffer:
qcetf3gpsi2 - HSQCETf3GPSI
qcetf3gpsi2 - HSQCETf3GPSI



- Process Dataset List (serial)
- Integrate Spectra List (intser)
- ROI View of Spectra List (vregs)
- Add/Sub./Mult. Spectra (adsu)
- Reference Deconvolution (refdecon)
- Special Transforms
- Miscellaneous Operations
- Manual correction mode (.basl)
- Repeat Correction Using File baselms (bcm)
- Automatic Using Polynomial of Degree ABSG (abs n)
- Like abs, Only In Range F1/F2 (absf n)
- Automatic, Alternate Algorithm (absd n)
- Setup Spline File baslpnts (.baslpnts)
- Spline-Correct Using baslpnts (sab)
- Correct FID Using Parameter BC_mod (bc)

Correct Baseline





Process

Analyse

Publish

View

Manage

Proc. Spectrum

Adjust Phase

Calib. Axis

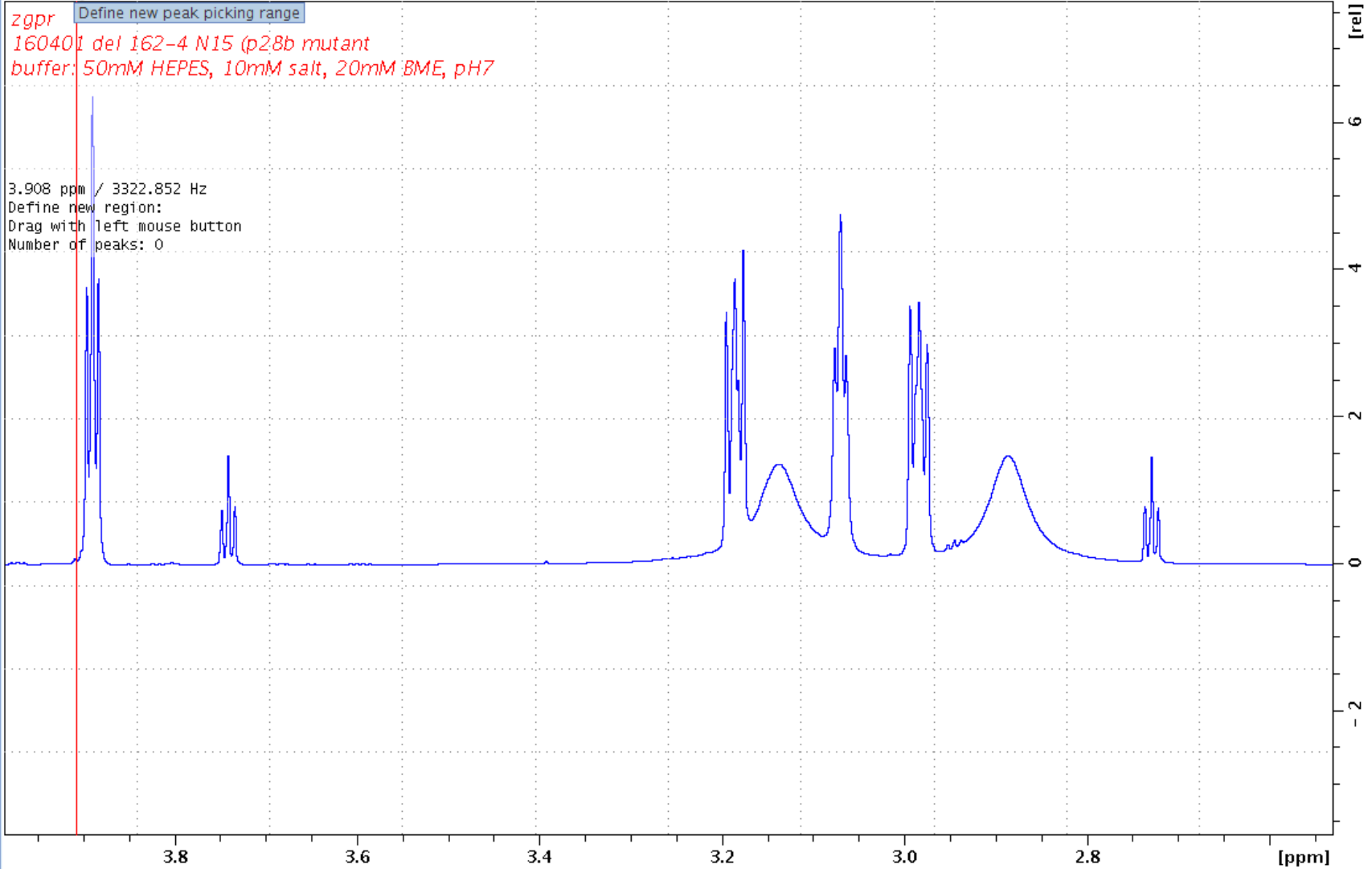
Pick Peaks

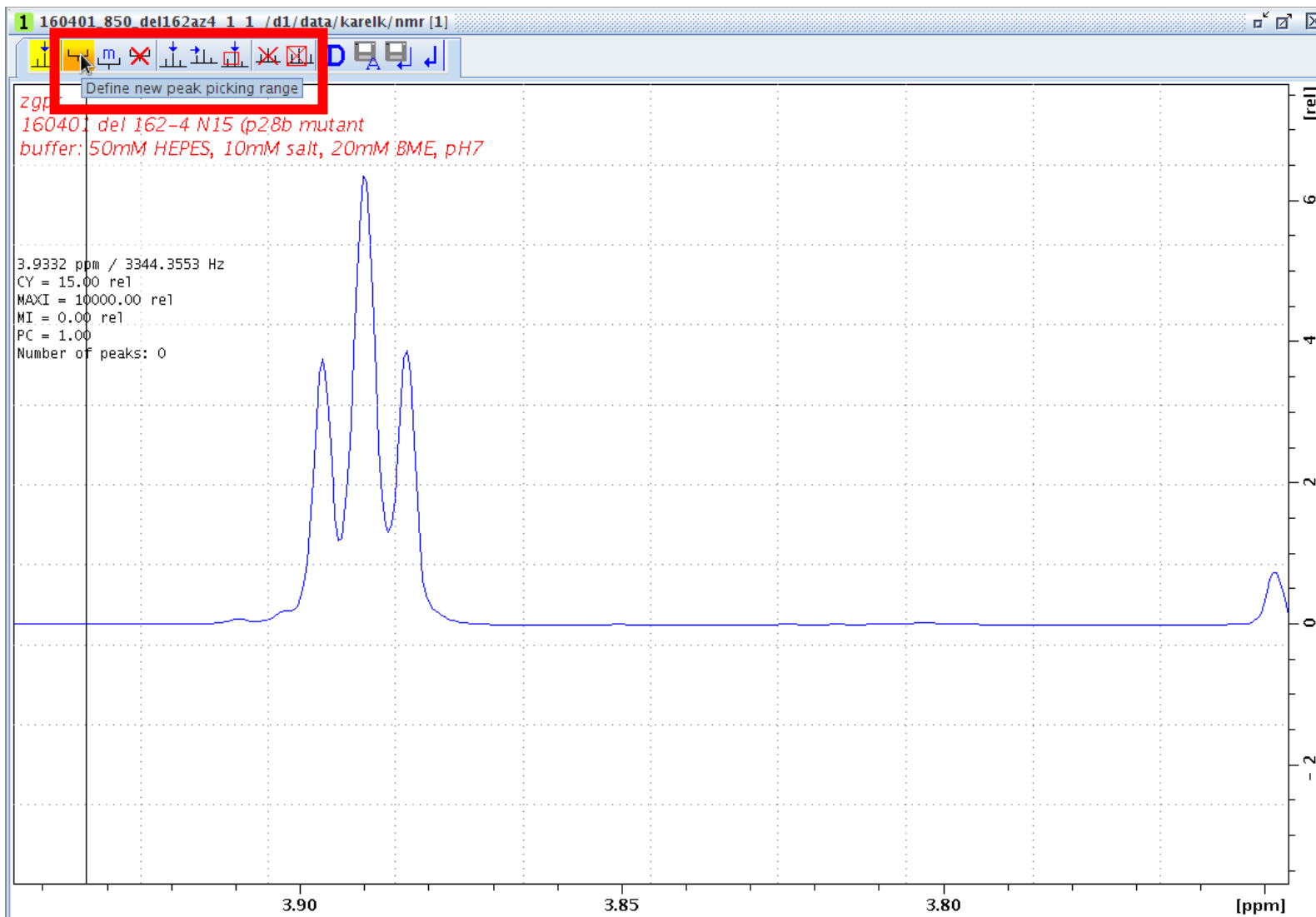
1 160401_850_del162az4 1 1 /d1/data/karelk/nmr [1]

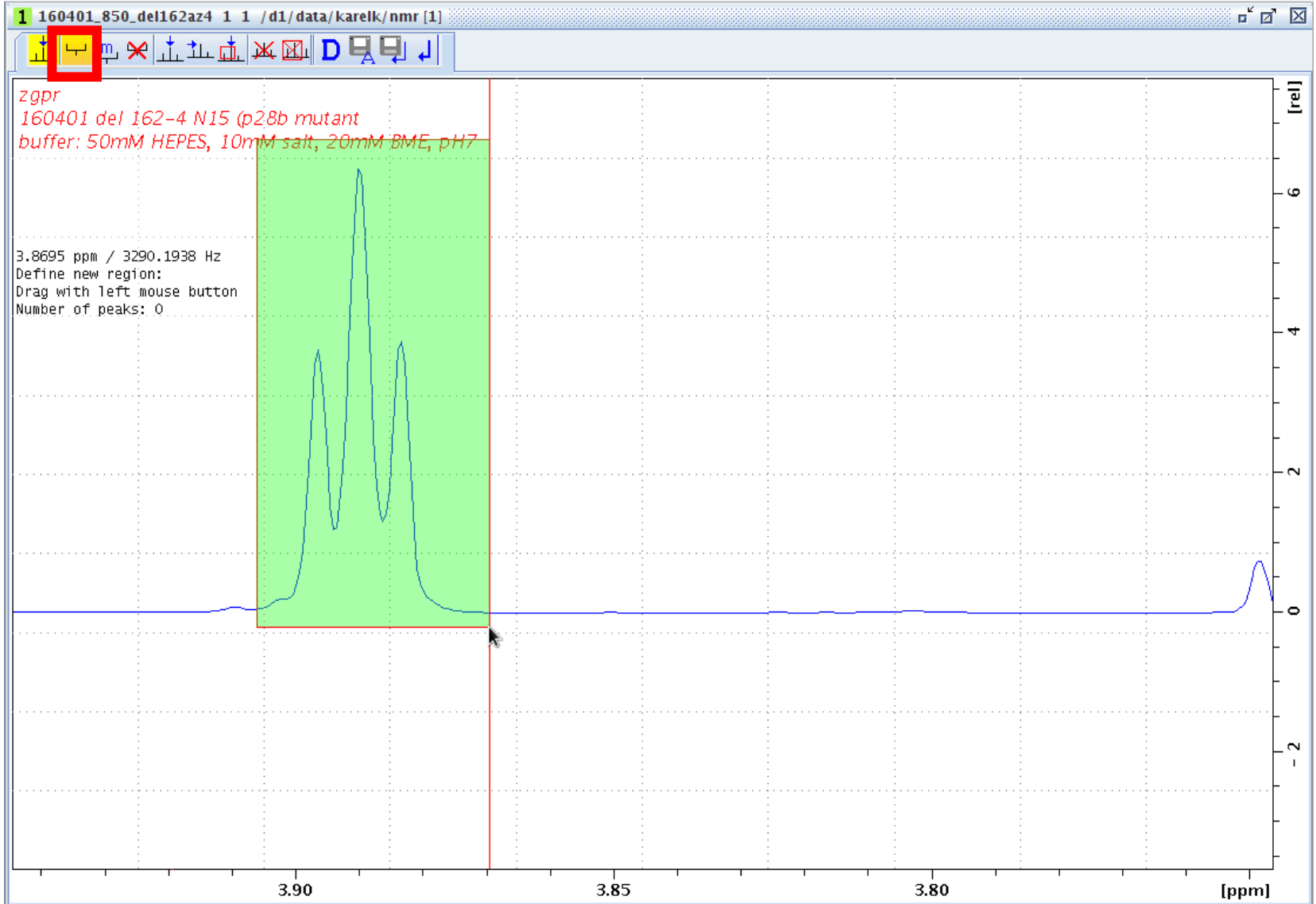


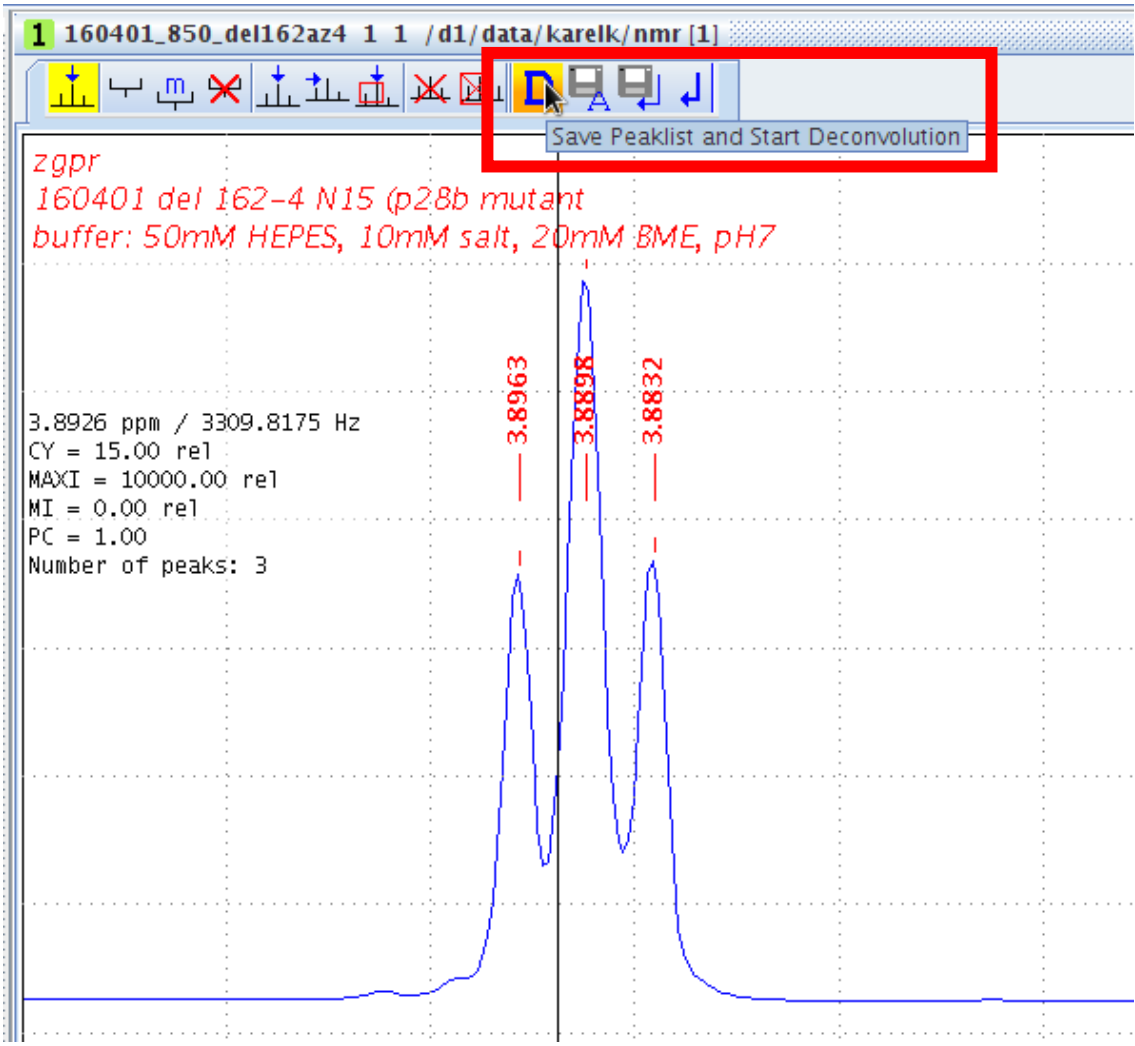
zgpr Define new peak picking range
160401 del i62-4 N15 (p28b mutant
buffer: 50mM HEPES, 10mM salt, 20mM BME, pH7

3.908 ppm / 3322.852 Hz
Define new region:
Drag with left mouse button
Number of peaks: 0











160207_950_13C15N_Rtt103_mono-pT4_titr
 160210_700b_ZCCHC9_aronNOESY
 160210_ctd

- 1 - zgpr - 1H / 0.56mM [13C,15N]tSH2 sumo out buffer 50mM
- 2 - Chsqc_kt - 13C-HSQC / 0.56mM [13C,15N]tSH2 sumo out b
- 3 - zgpg - 1D 31P / 0.56mM [13C,15N]tSH2 sumo out buffer 50
- 4 - Chsqc_kt - 1H / 0.56mM [13C,15N]tSH2 sumo out buffer 50
- 5 - zgpr - 1H / Buffer taken after dialysis of sample buffer 50m
- 6 - zgpg - 1D 31P / zgpg Buffer taken after dialysis of sample b
- 7 - zgpr - 1H / 0.4mM 2xpY1-CTD buffer 50mM HEPES, 10mM
- 8 - zgpg - 1D 31P / zgpg 0.4mM 2xpY1-CTD buffer 50mM HEP
- 9 - zgpgwg - 1H / 0.4mM 2xpY1-CTD buffer 50mM HEPES, 10r
- 100 - zgpgwg - 1H / sample number 25 (mixed 23 and 24) in s
- 101 - zgpr - zgpr / sample number 25 (mixed 23 and 24) in sh
- 102 - zgpgwg - 1H / sample number 25 (mixed 23 and 24) in s
- 103 - zgpr - zgpr / sample number 25 (mixed 23 and 24) in sh
- 104 - zgpg - 1D 31P / zgpg sample number 25 (mixed 23 and
- 200 - zgpgwg - 1H / sample number 26 (mixed 23 and 24) in s
- 201 - zgpr - zgpr / sample number 26 (mixed 23 and 24) in sh
- 202 - zgpgwg - 1H / sample number 26 (mixed 23 and 24) in s
- 203 - zgpr - zgpr / sample number 26 (mixed 23 and 24) in sh
- 204 - zgpg - 1D 31P / zgpg sample number 26 (mixed 23 and
- 205 - zgpg - 1D 31P / zgpg sample number 26 (mixed 23 and
- 206 - zgpgwg - 1H / sample number 26 (mixed 23 and 24) in s

160401_850_del162az4 1 1 /d1/data/karelk/nmr [1]

Data List

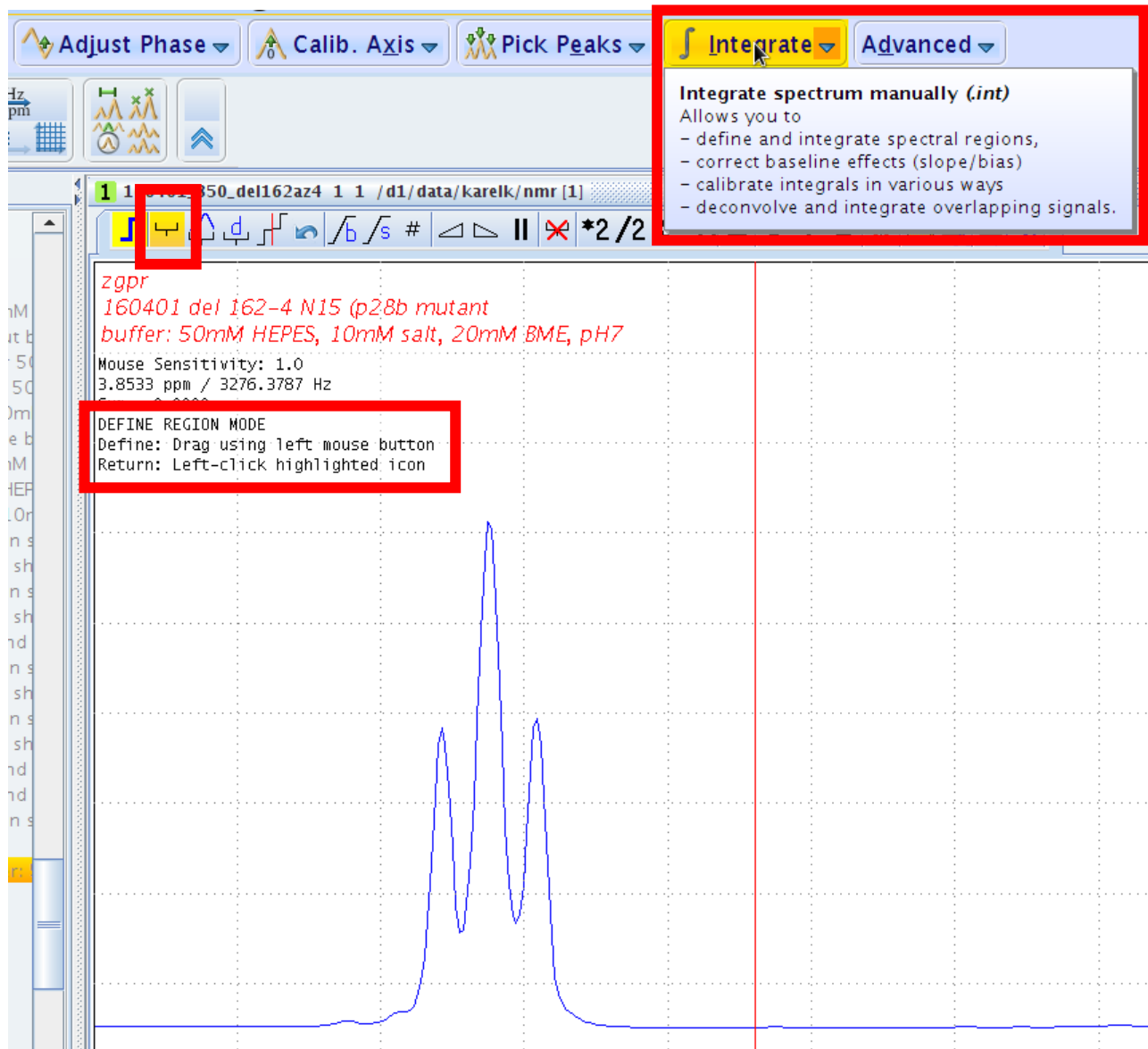
- 2: 160401_850_del162az4 1 999 /d1/data/karelk/nmr
- 1: 160401_850_del162az4 1 1 /d1/data/karelk/nmr

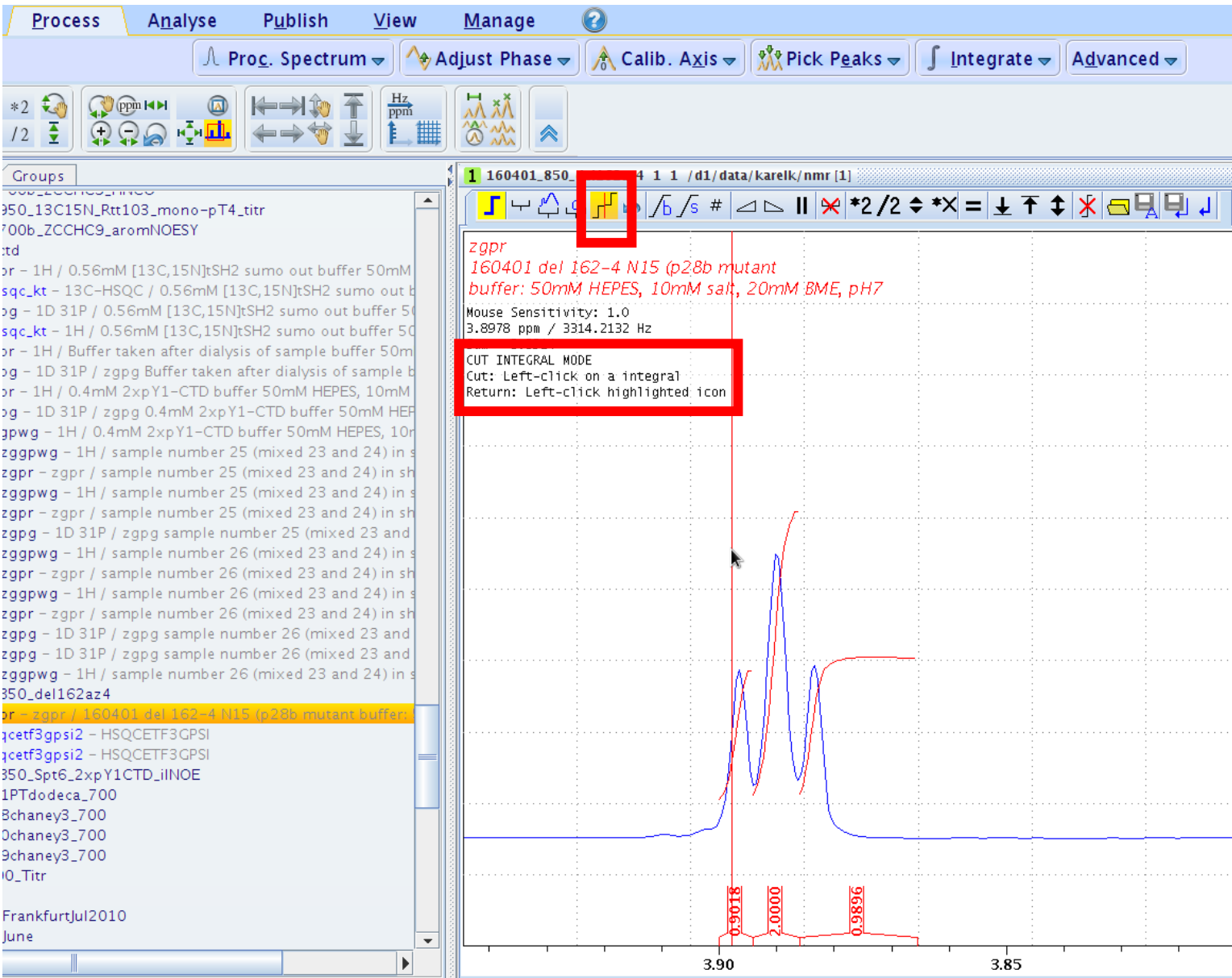
Deconvolution result (dconpeaks.txt)

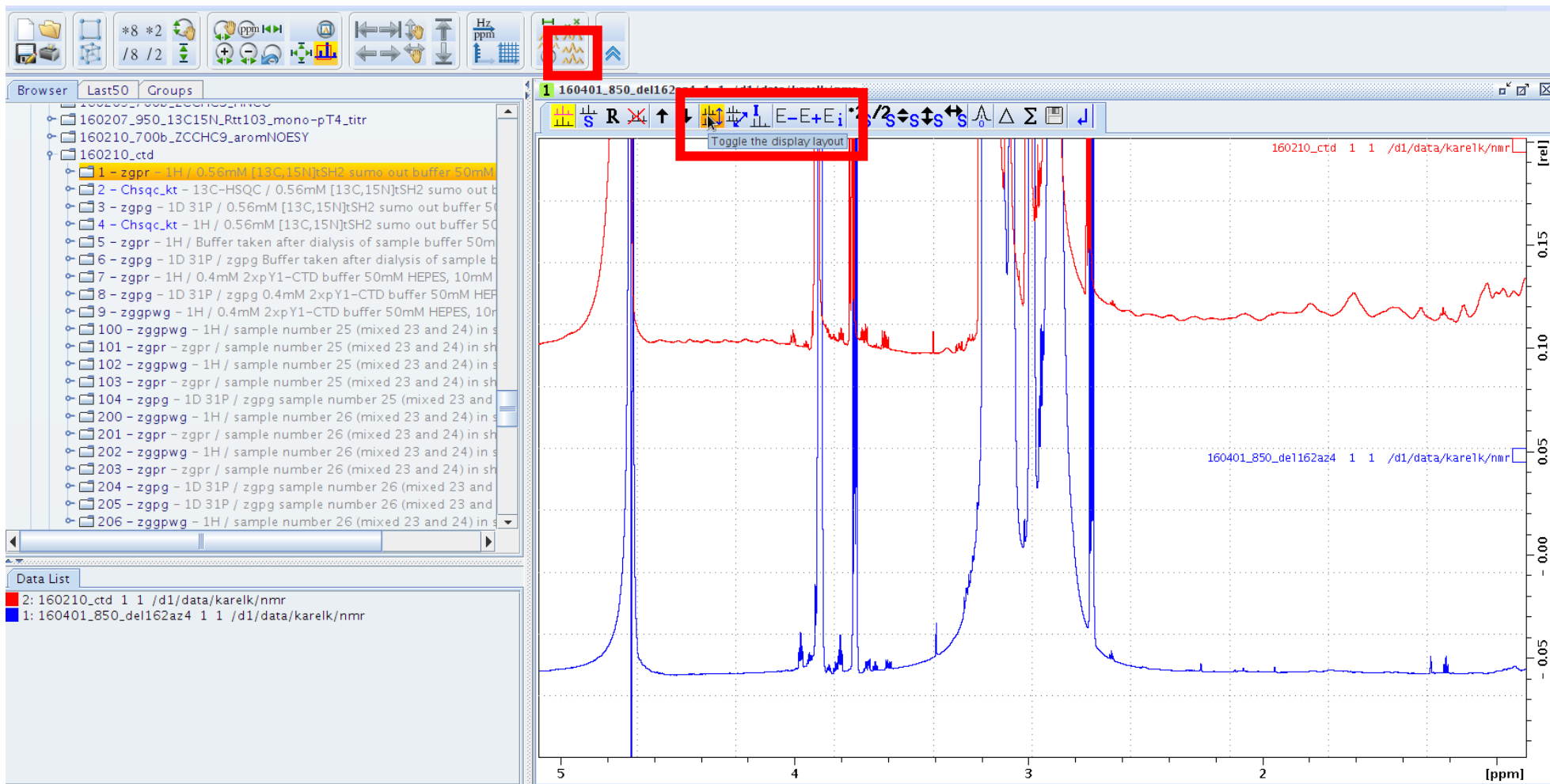
File Edit Search

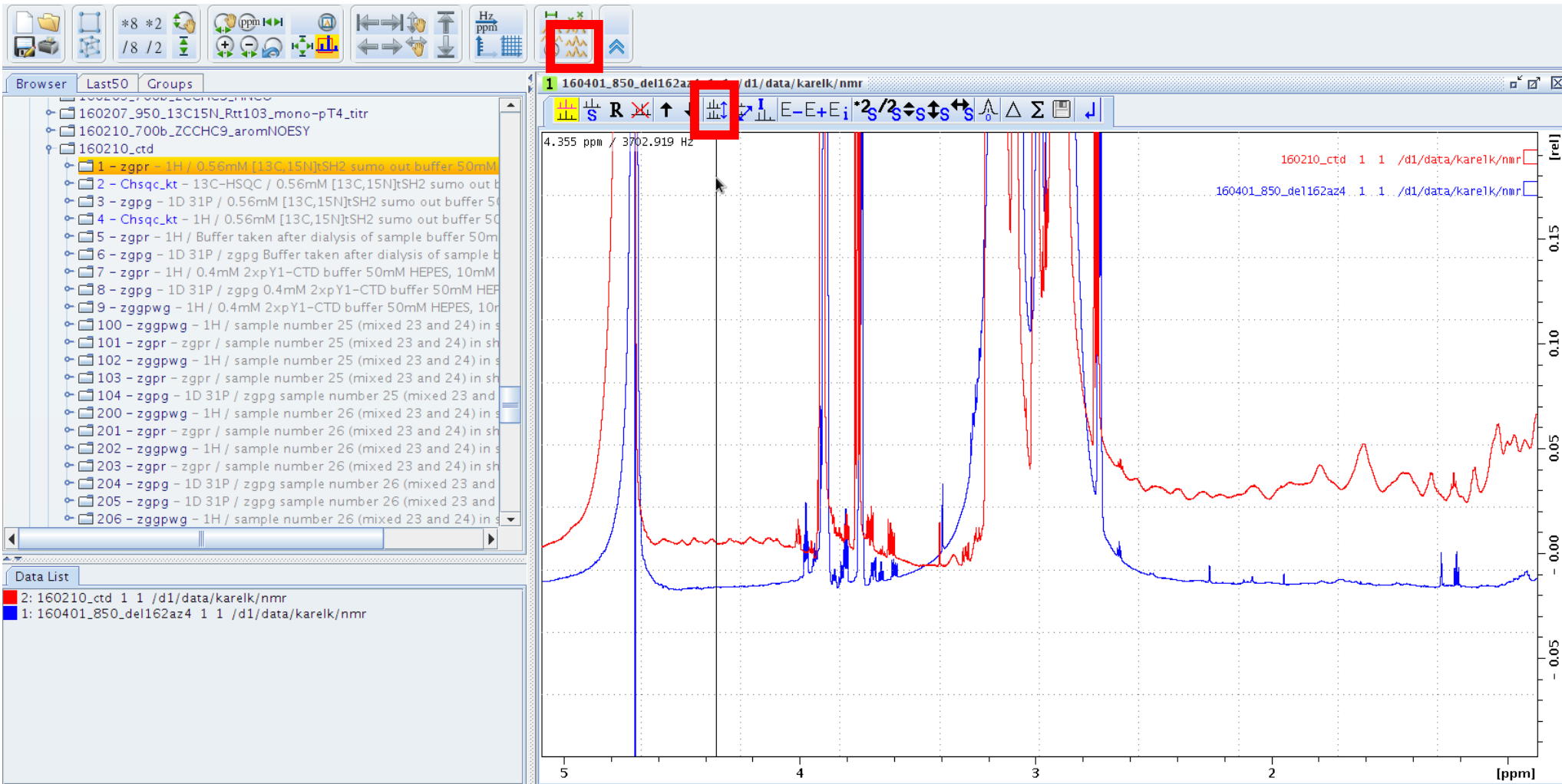
1 Data set: /d1/data/karelk/nmr/160401_850_del162az4/1/pdata/1/
 2
 3 Fit type: Mixed Lorentzian and Gaussian
 4
 5 Fit

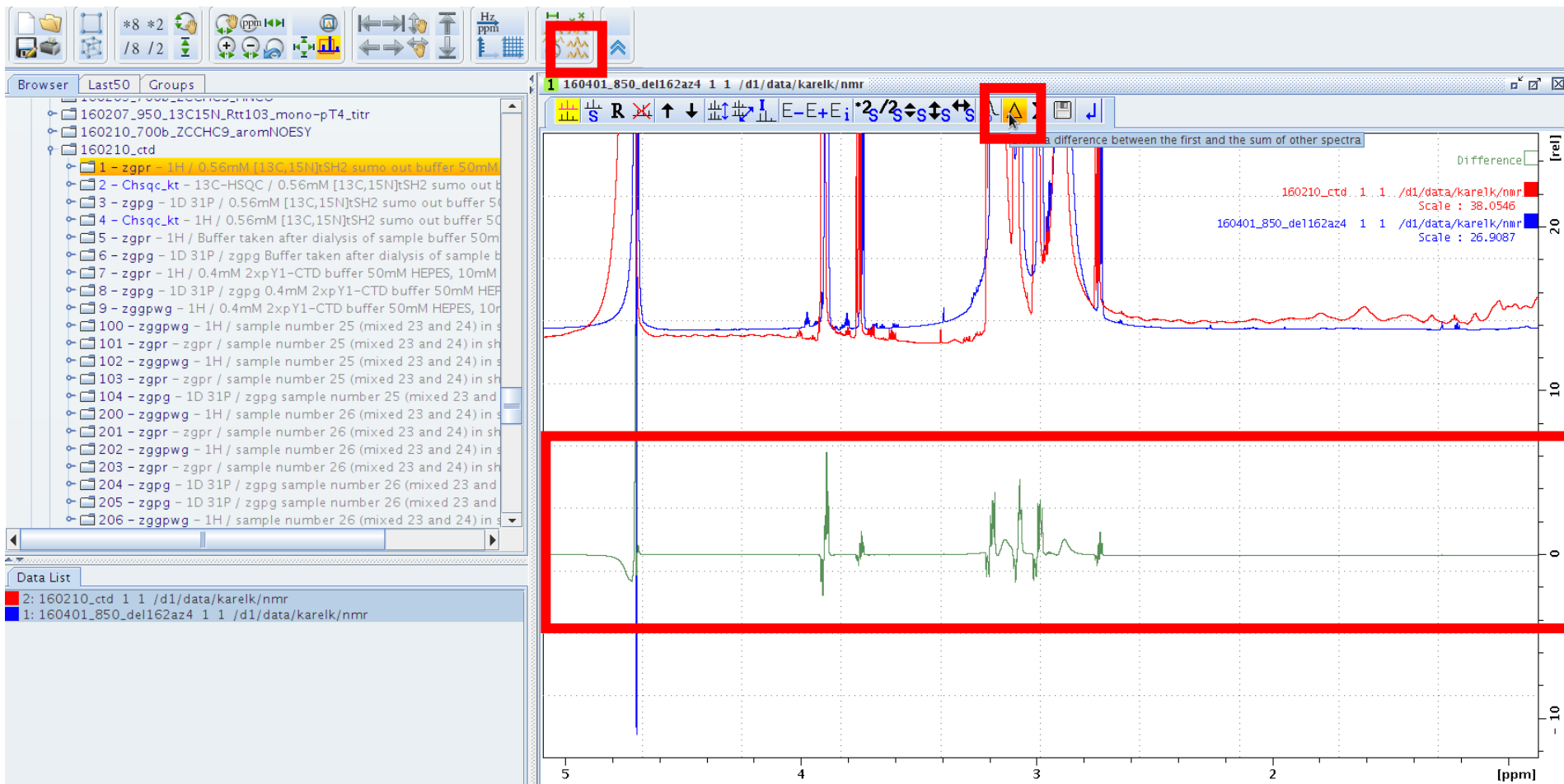
	Frequency ppm	Hz	Width ppm	Intensity Hz	Area	%Lor. chisq
6						
7						
8	1					1.1e+15
9						
10	3.897	3313.20	0.00239	2.034	3.621	27.901
11	STD:	0.000	0.06	0.00022	0.189	0.217
12						
13	3.890	3307.60	0.00326	2.773	6.507	68.365
14	STD:	0.000	0.04	0.00016	0.135	0.187
15						
16	3.883	3301.98	0.00237	2.015	3.778	28.846
17	STD:	0.000	0.06	0.00021	0.179	0.218
18						
19						

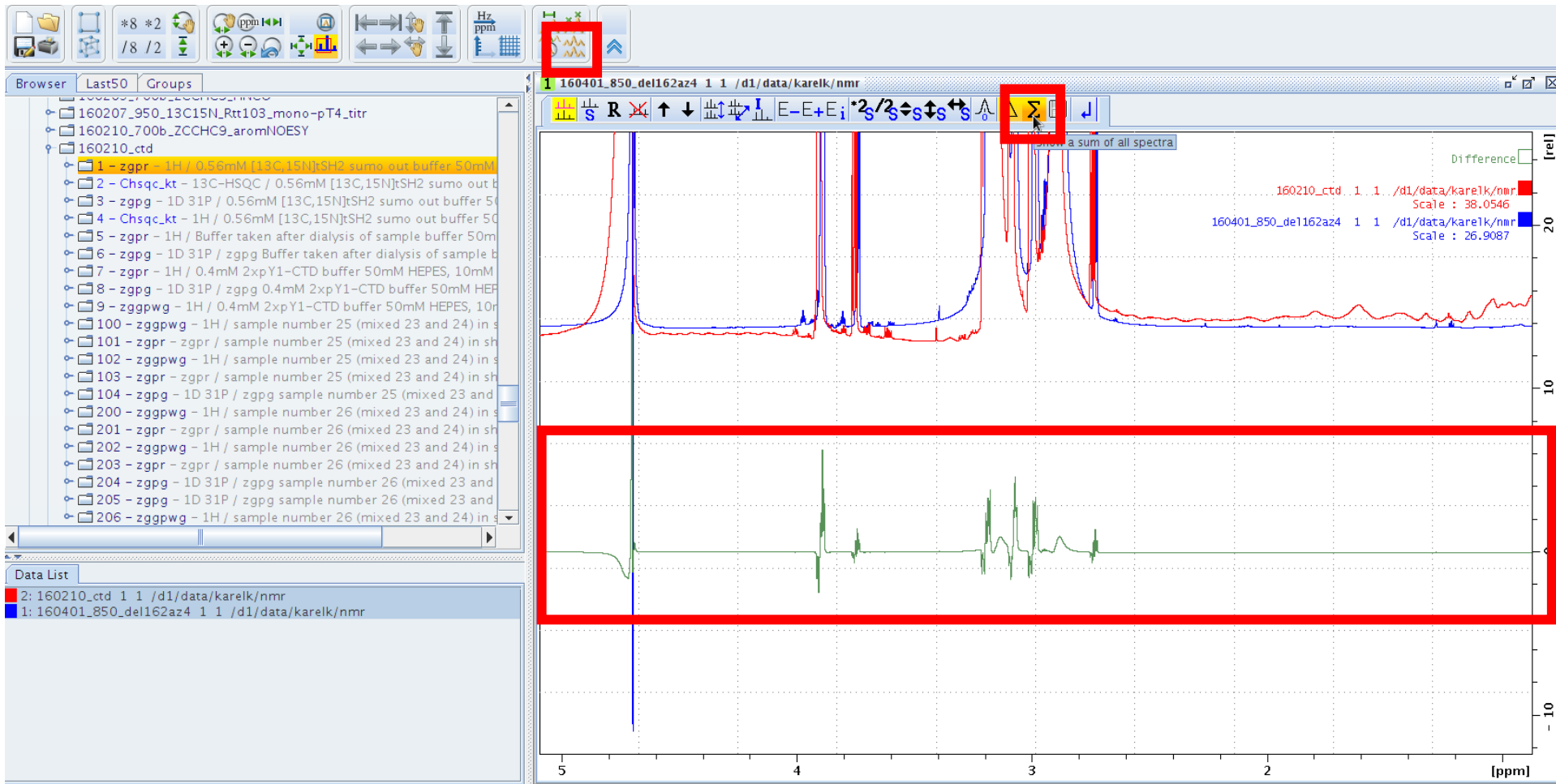


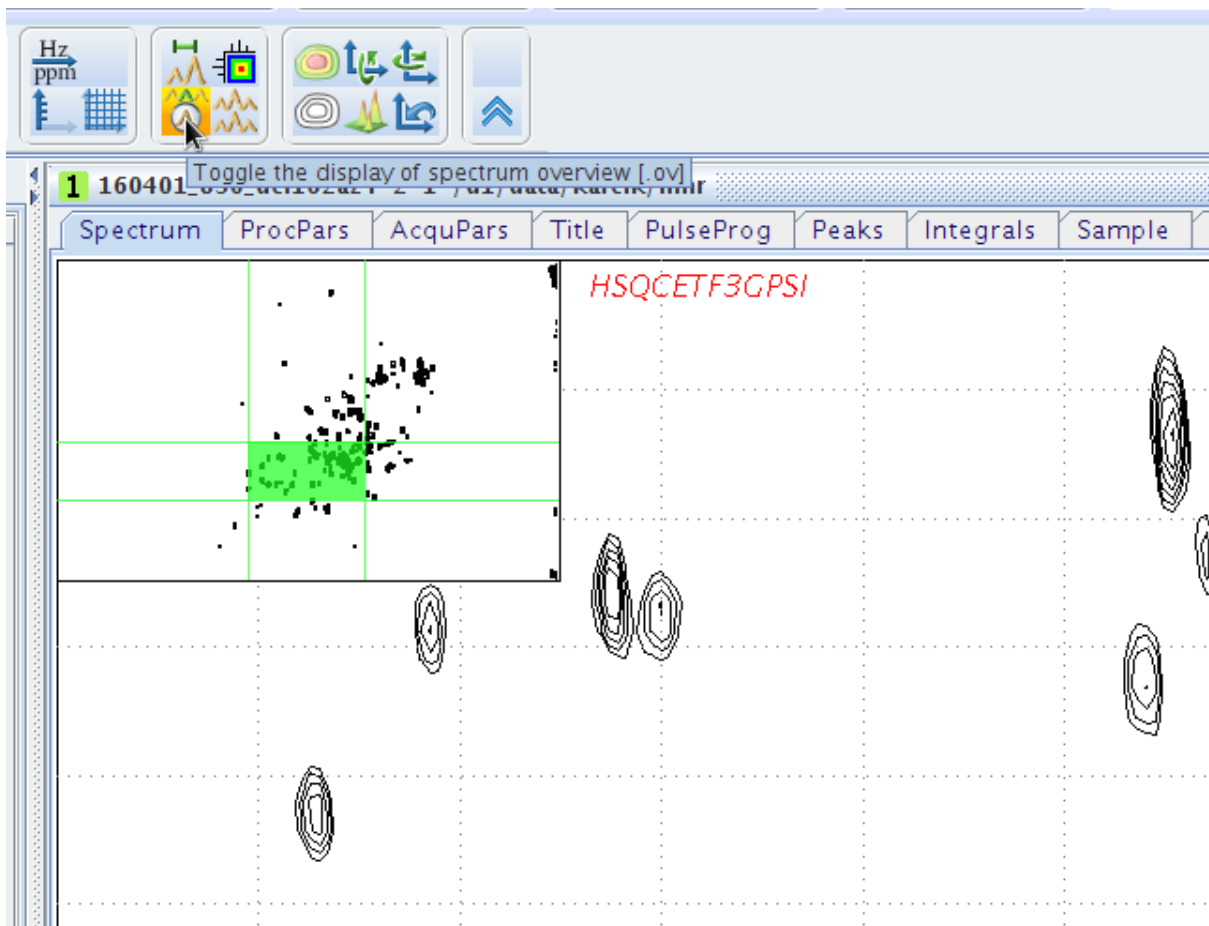


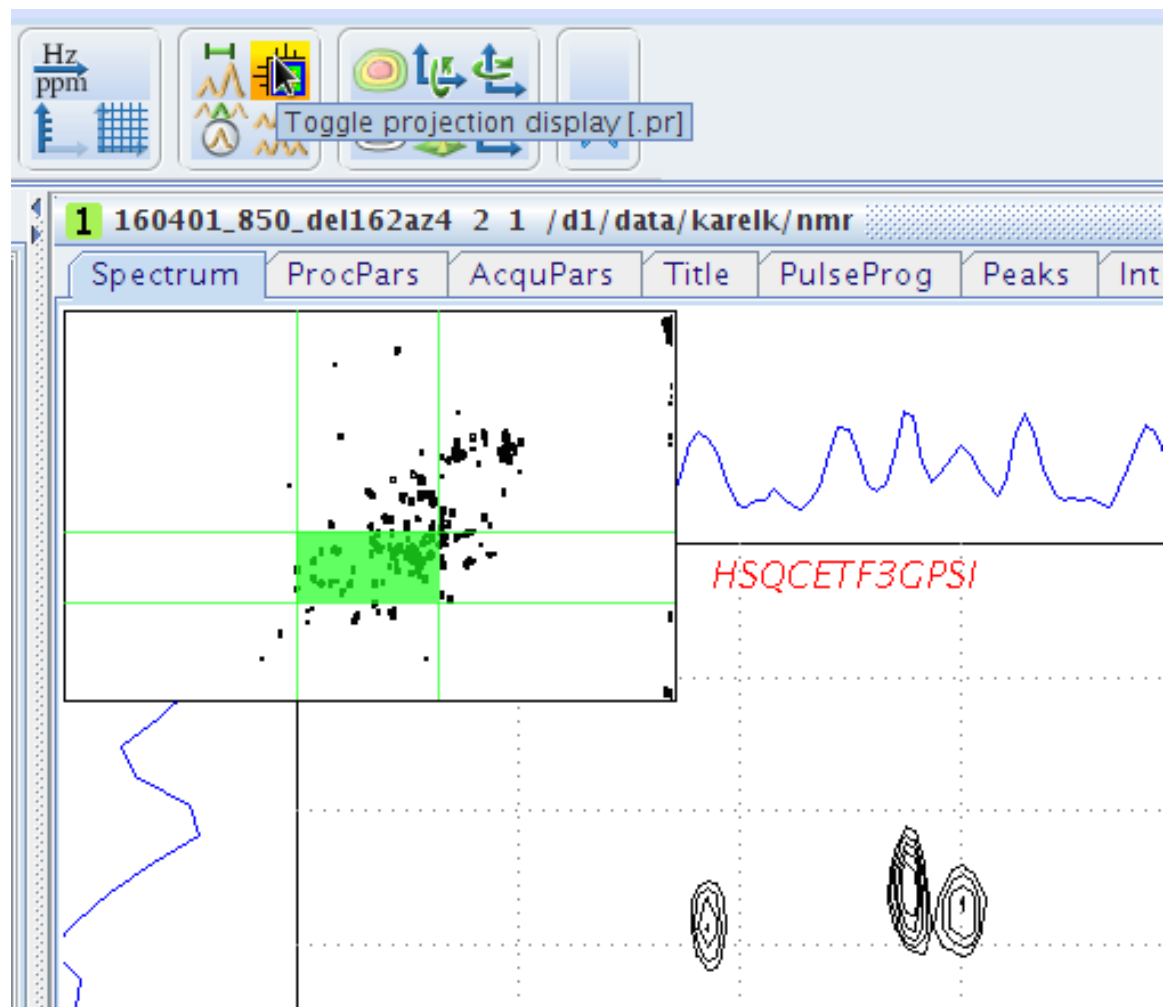


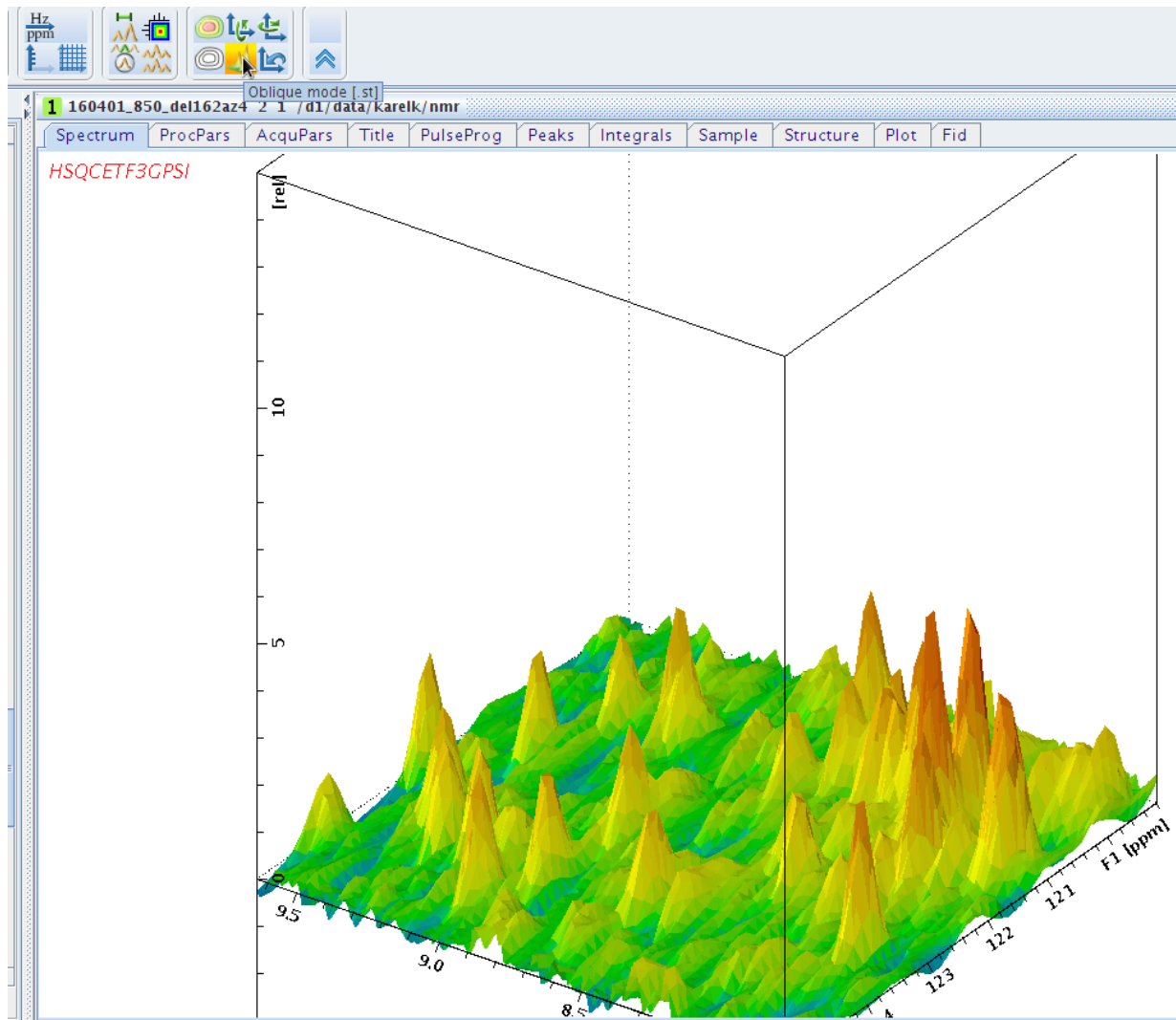












160401_850_del162az4 2 1 /d1/data/karek/nmr

15N_Rtt103_mono-pT4_titr
 CHC9_aromNOESY

0.56mM [13C,15N]tSH2 sumo out buff
 13C-HSQC / 0.56mM [13C,15N]tSH2 s
 1P / 0.56mM [13C,15N]tSH2 sumo ou
 1H / 0.56mM [13C,15N]tSH2 sumo out
 Buffer taken after dialysis of sample bu
 1P / zgpg Buffer taken after dialysis of
 0.4mM 2xpY1-CTD buffer 50mM HEPB
 1P / zgpg 0.4mM 2xpY1-CTD buffer 5
 1H / 0.4mM 2xpY1-CTD buffer 50mM H
 1H / sample number 25 (mixed 23 ar
 pr / sample number 25 (mixed 23 and
 1H / sample number 25 (mixed 23 ar
 pr / sample number 25 (mixed 23 and
 31P / zgpg sample number 25 (mixe
 1H / sample number 26 (mixed 23 ar
 pr / sample number 26 (mixed 23 and
 1H / sample number 26 (mixed 23 ar
 pr / sample number 26 (mixed 23 and
 31P / zgpg sample number 26 (mixe
 31P / zgpg sample number 26 (mixe
 1H / sample number 26 (mixed 23 ar
 62az4
 / 160401 del 162-4 N15 (p28b mutar
i2 - HSQCETf3GPSI
 i2 - HSQCETf3GPSI
 _2xpY1CTD_iINOE
 a_700
 _700
 _700

160401_850_del162az4 2 1 /d1/data/karek/nmr

1	3789.2	0.0
2	4547.0	0.0
3	5456.4	0.0
4	6547.6	0.0
5	7857.2	0.0
6	9428.6	0.0
7	11314.3	0.0
8	13577.3	0.0
9	16292.7	0.0
10	19551.3	0.0

Required parameters

Calculation method

Multiply by increment
 Add increment

Contour level sign

Positive & Negative
 Positive
 Negative

	Positive	Negative
Base level	3789.2	-3789.2
Level increment	1.200	1.800
Number of levels	25	

Fill Clear Apply

OK Cancel

Process Analyse Publish View Manage

Proc. Spectrum Adjust Phase Calib. Axis Pick Peaks Integrate Advanced

8 * 2 8 / 2

Groups

- 160401_850_del162az4 2 1 /d1/data/karelk/nmr
- 700b_ZCCHC9_aromNOESY
- _950_13C15N_Rtt103_mono-pT4_titr
- _700b_ZCCHC9_aromNOESY
- _ctd
- gpr - 1H / 0.56mM [13C,15N]tSH2 sumo out buffer 50mM
- hsqc_kt - 13C-HSQC / 0.56mM [13C,15N]tSH2 sumo out b
- gpg - 1D 31P / 0.56mM [13C,15N]tSH2 sumo out buffer 50
- hsqc_kt - 1H / 0.56mM [13C,15N]tSH2 sumo out buffer 50
- gpr - 1H / Buffer taken after dialysis of sample buffer 50m
- gpg - 1D 31P / zgpg Buffer taken after dialysis of sample b
- gpr - 1H / 0.4mM 2xpY1-CTD buffer 50mM HEPES, 10mM
- gpg - 1D 31P / zgpg 0.4mM 2xpY1-CTD buffer 50mM HEP
- gpgwg - 1H / 0.4mM 2xpY1-CTD buffer 50mM HEPES, 10r
- zgpgwg - 1H / sample number 25 (mixed 23 and 24) in s
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- zgpr - zgpr / sample number 25 (mixed 23 and 24) in sh
- zgpg - 1D 31P / zgpg sample number 25 (mixed 23 and
- zgpgwg - 1H / sample number 26 (mixed 23 and 24) in s
- zgpr - zgpr / sample number 26 (mixed 23 and 24) in sh
- zgpgwg - 1H / sample number 26 (mixed 23 and 24) in s
- zgpr - zgpr / sample number 26 (mixed 23 and 24) in sh
- zgpg - 1D 31P / zgpg sample number 26 (mixed 23 and
- zgpgwg - 1H / sample number 26 (mixed 23 and 24) in s

160401_850_del162az4 2 1 /d1/data/karelk/nmr

Spectrum ProcParams AcqParams Title PulseProg Peaks Integrals Sample Structure

HSQCETFGPSI

Phase correction requires at least one imaginary data part:

Processed data file '2ir' not found: No such file or directory
 160401_850_del162az4 2 1 /d1/data/karelk/nmr
 Processed data file '2ri' not found: No such file or directory
 160401_850_del162az4 2 1 /d1/data/karelk/nmr

Close Details...

Process Analyse Publish View Manage

Proc. Spectrum Adjust Phase Calib. Axis Pick Peaks

*2 /2

Groups

1 160401_850_del162az4 2 1 /d1/data/karelk/nmr

Click the right mouse button to select the peaks for phase correction

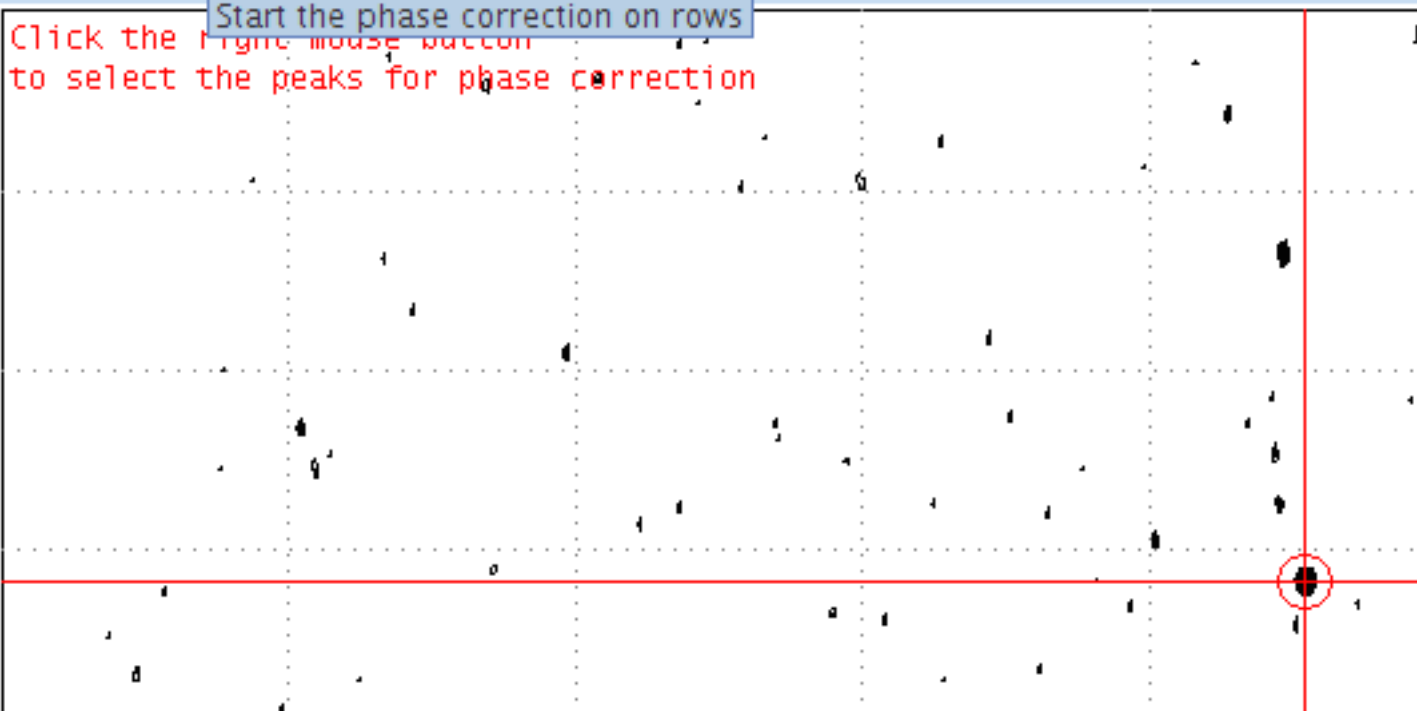
col : 9.922 ppm / 8436.552 Hz Index = 355
row : 112.08 ppm / 9656.45 Hz Index = 165
Value = -433.6

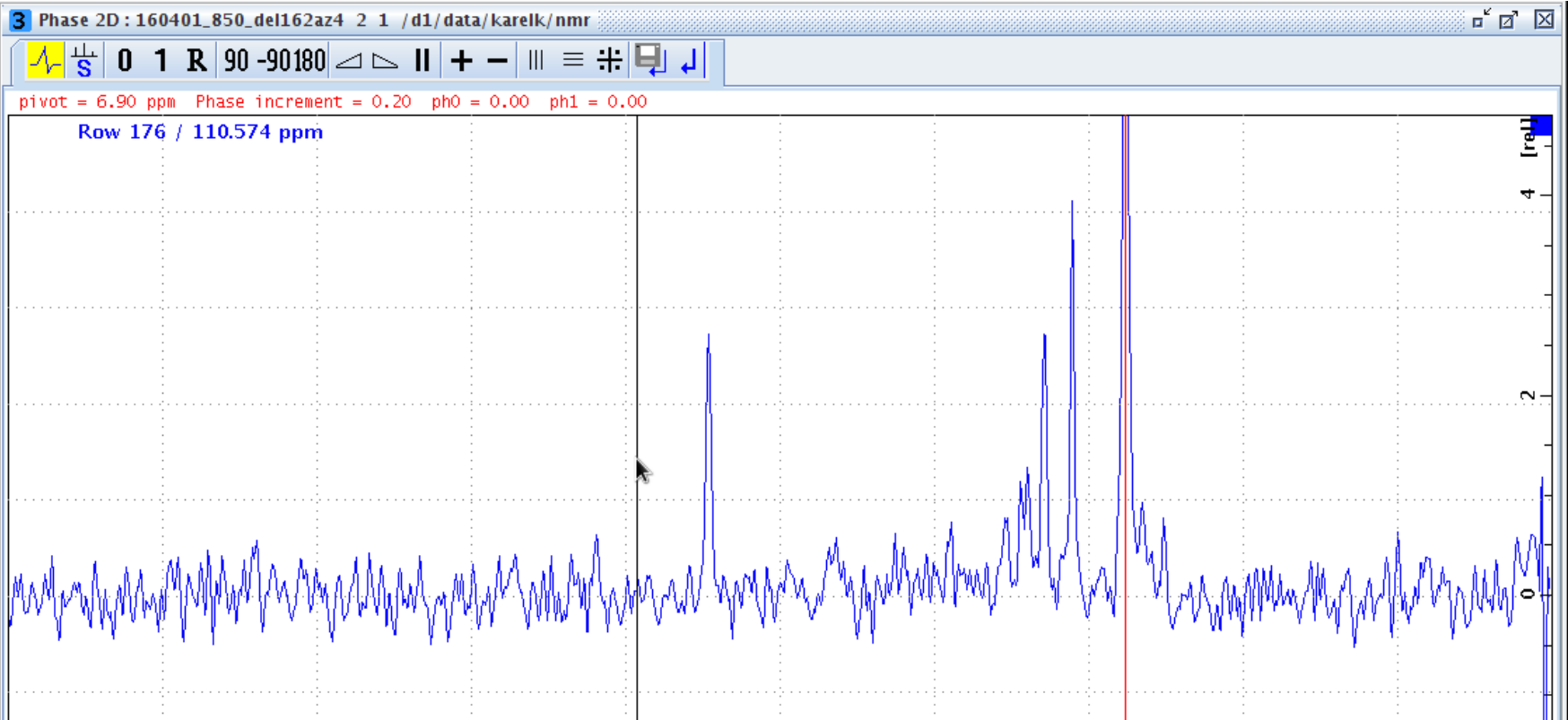
1 160401_850_del162az4 2 1 /d1/data/karelk/nmr



Start the phase correction on rows

Click the right mouse button
to select the peaks for phase correction





Quick reference:

- 1) edp – open Processing tab
- 2) qsin – multiply FID with qsin window function
- 3) qfp – qsine+ft+phase correction
- 4) efp – exponential w. f'tion+ft+phase corr.
- 5) 1 td – display number of set TD points in F1
- 6) 1s td – display really acquired # TD pts in F1
- 7) 1s te – display temperature @ which was experiment measured
- 8) fp – Fourier transformation+phase correction
- 9) .ph – start phase menu
- 10) .md – spectra overlay window
- 11) re 1 – go to ExpNo 1 of current dataset
- 12) rep 1 – go to ProcNo of current ExpNo
- 13) levcalc – calculate contour levels
- 14) edlev – edit contour levels
- 15) xf1 – process 2D data in F1
- 16) xf2 – process 2D data in F2
- 17) xfb – process 2D
- 18) xfb n – process 2D and remove 2ri, 2ir, 2ii
- 19) abs1, abs2 – baseline correction in 2D
- 20) ft3d – 3D data processing
- 21) ft3d n - process 3D and remove imaginary part
- 22) tabs1, tabs2, tabs3 – baseline correction in 3D
- 23) ftnd 0 – processing of 3D acquired with NUS
- 24) edmac *name* – create or edit macro *name*
- 25) wrp 2 y – write processed data to ProcNo 2 and if exists, overwrite
- 26) rser 1 – extract first FID of an nD experiment
- 27) apk – automatic phase correction
- 28) show – show active processes
- 29) curplot – set up printer
- 30) print – print spectrum

