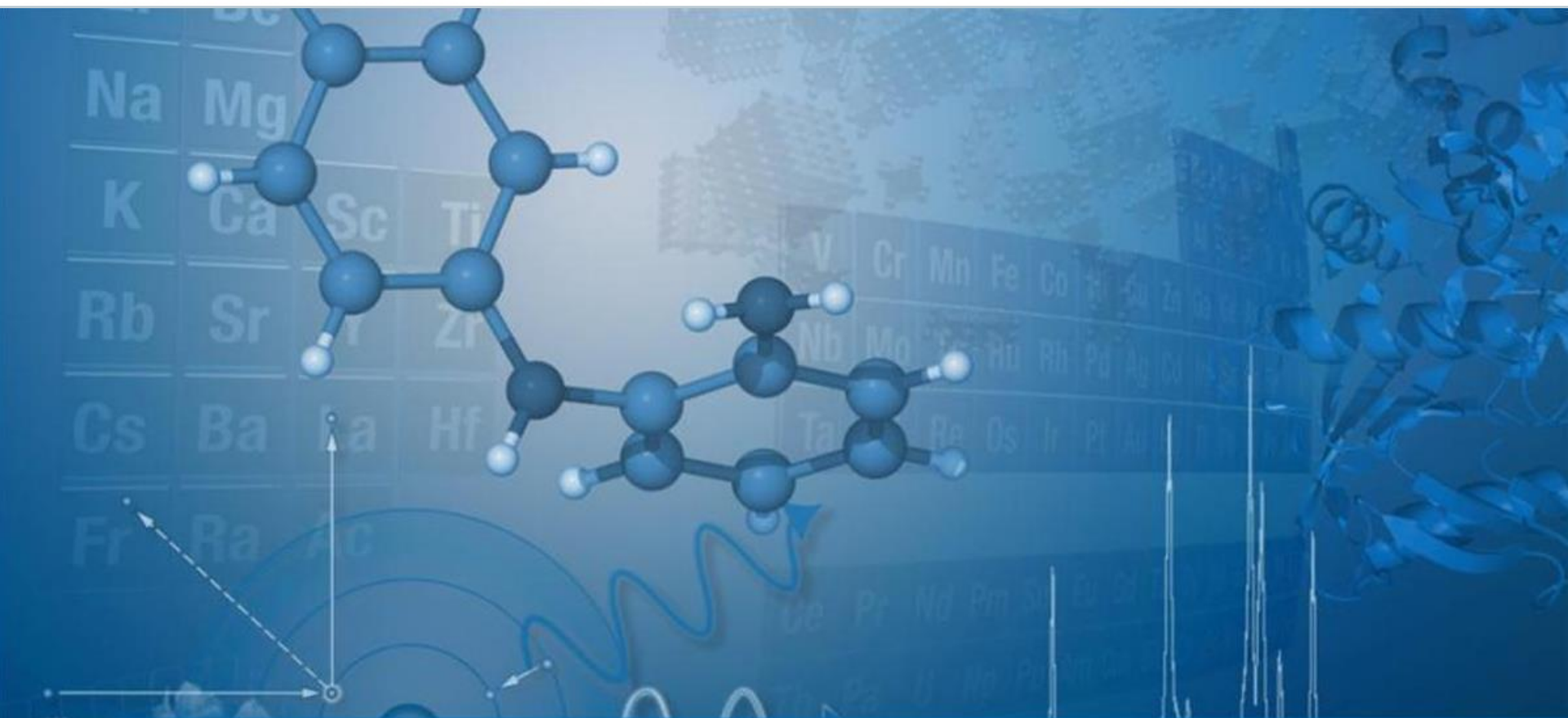
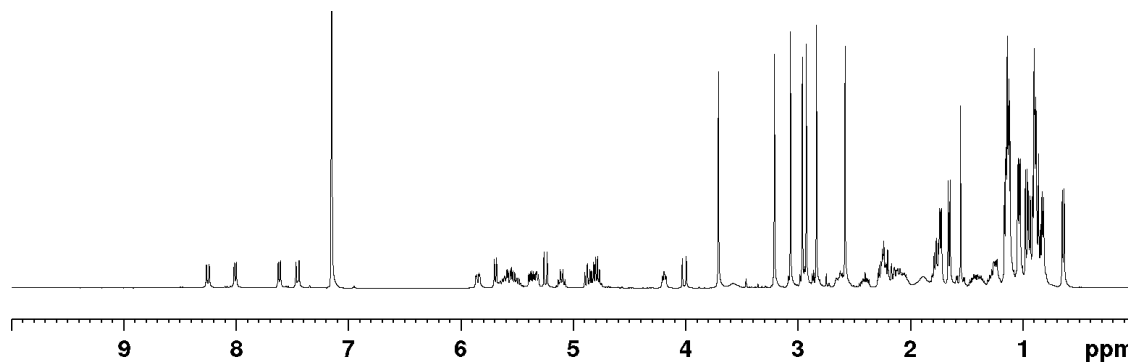
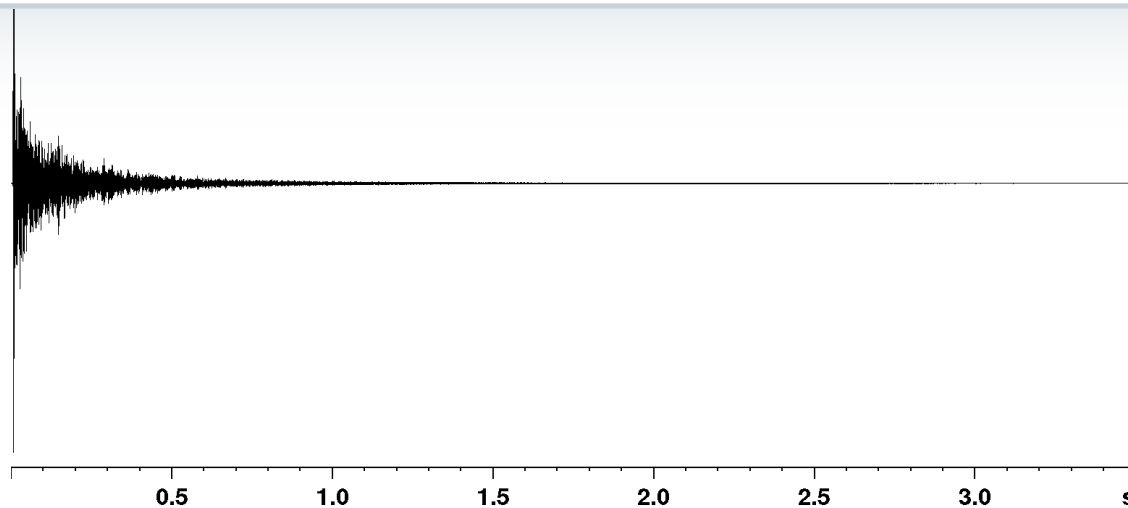


1D Processing

Dr. Benjamin Görling



How to get a good spectrum?



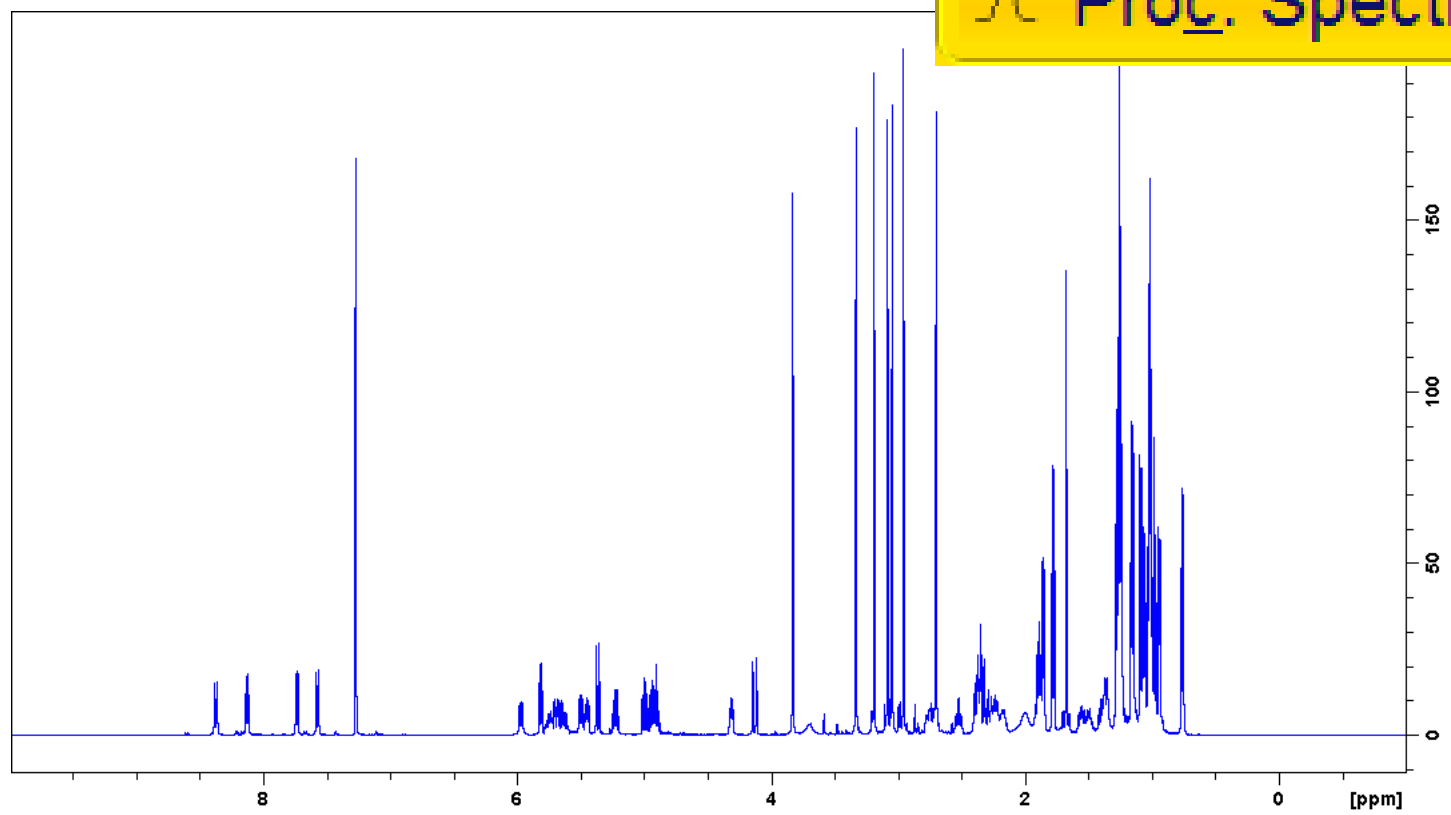
1-Click processing



File Start **Process** Analyse Publish View Manage ?

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

Proc. Spectrum



1-Click processing options



File Start **Process** Analyse Publish View Manage ?

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

- Configure Standard Processing (proc1d)
- Window Multiplication (wm)
- Fourier Transform (ft)
- Fourier Transform Options ... (ftf)
- Start Automation AU Program (xaup)

Proc. Spectrum

proc1d

Press 'Execute' to process the current dataset.
Press 'Save' to just change the processing options.
Changed options will be effective when pressing the one-click 'Proc. Spectrum' button.

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

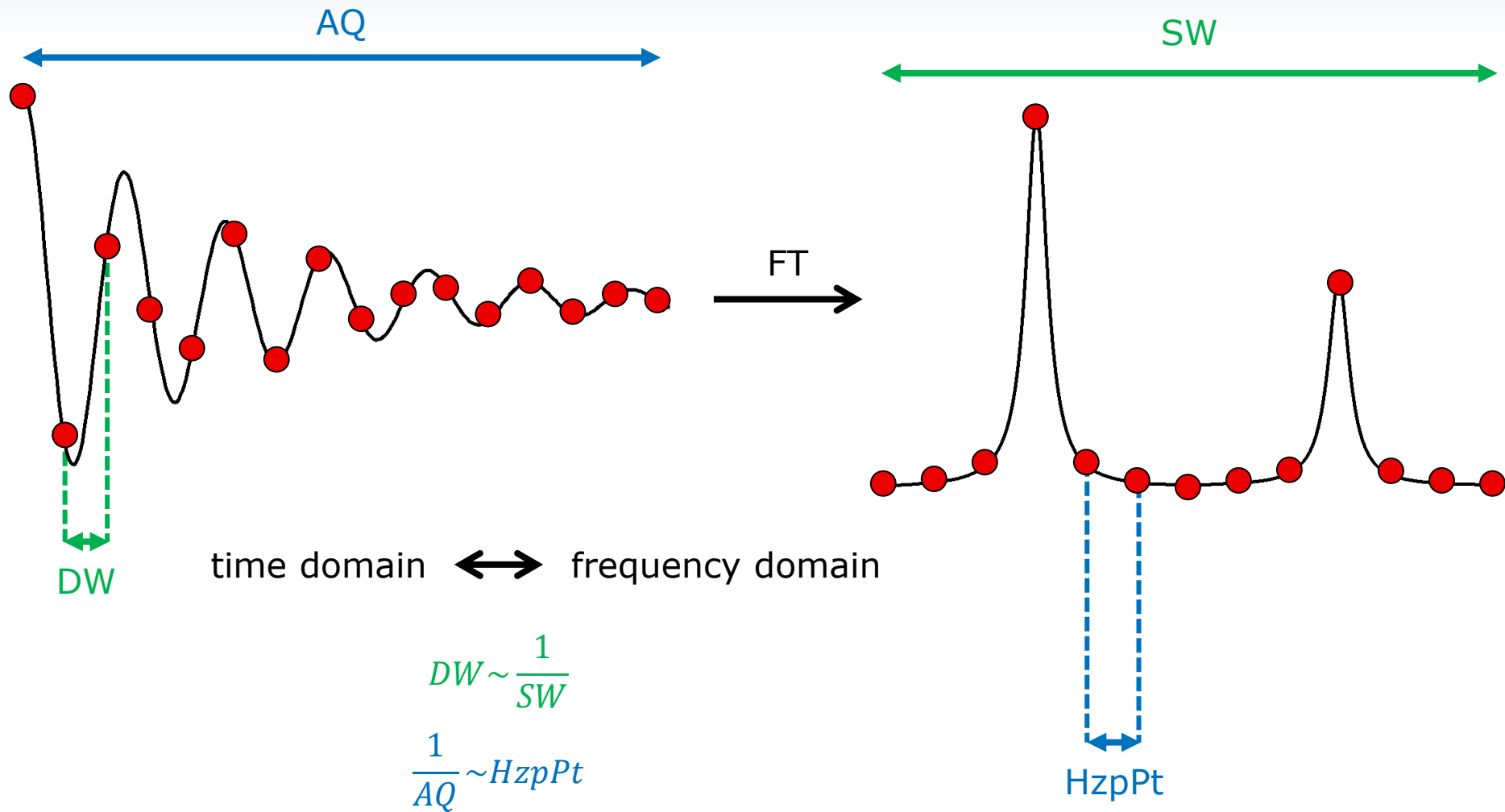
Save Execute Cancel

Processing commands



- **[ft]** Fourier transformation
- **[em]** multiplication with exponential window function
- **[pk]** phase spectrum
- **[fp]** **[ft]** + **[pk]**
- **[ef]** **[em]** + **[ft]**
- **[efp]** **[em]** + **[ft]** + **[pk]**

Fourier transformation

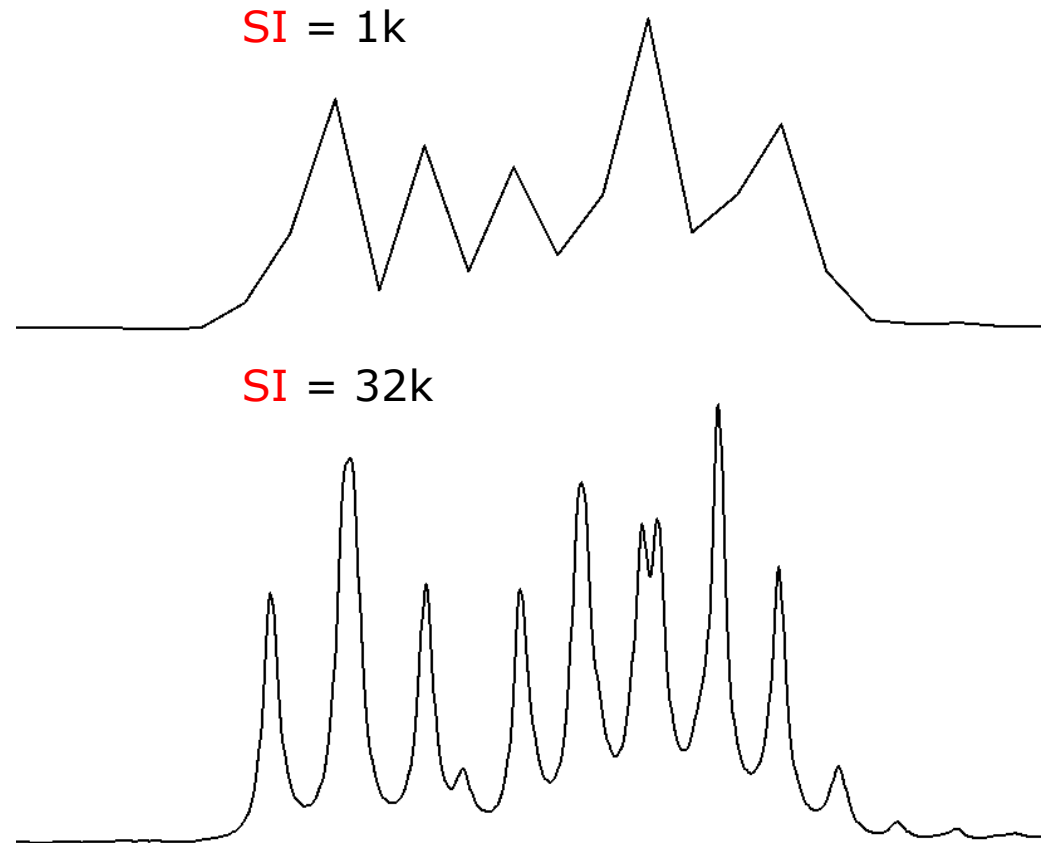


Resolution



- To get a good resolution you need enough data points **TD** (acquisition) and **SI** (processing).

- $SI = \frac{TD}{2}$

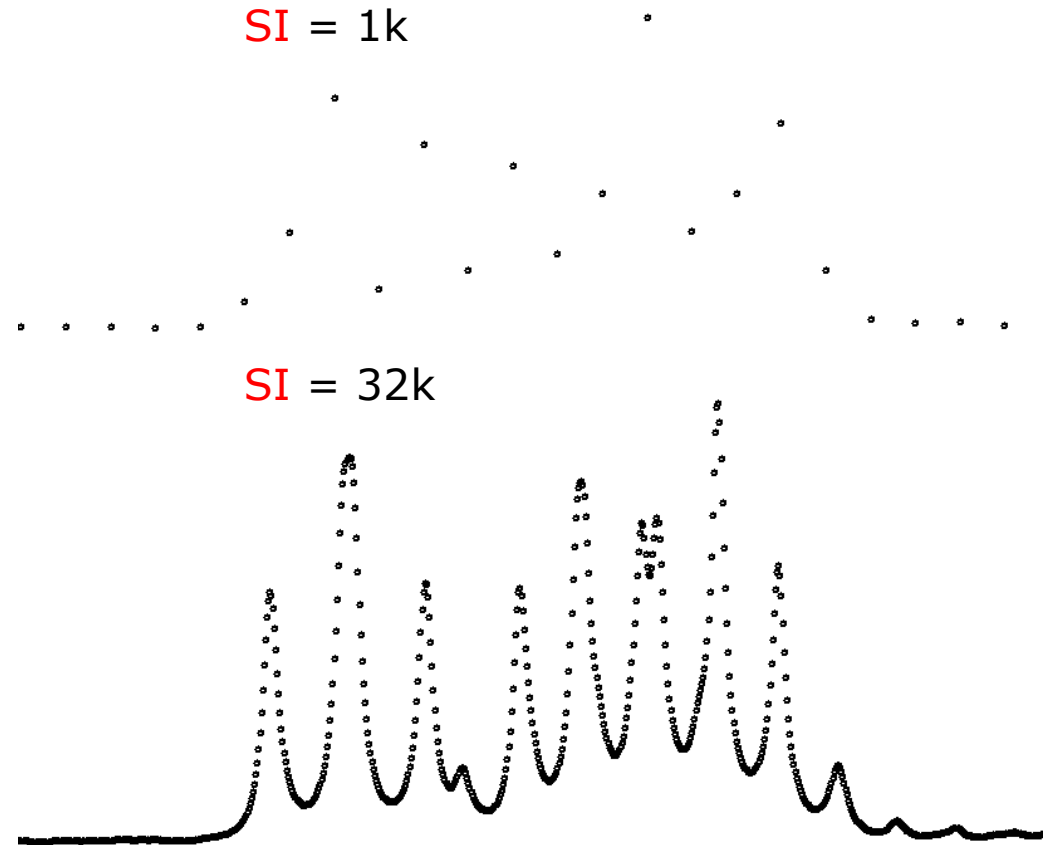


Resolution

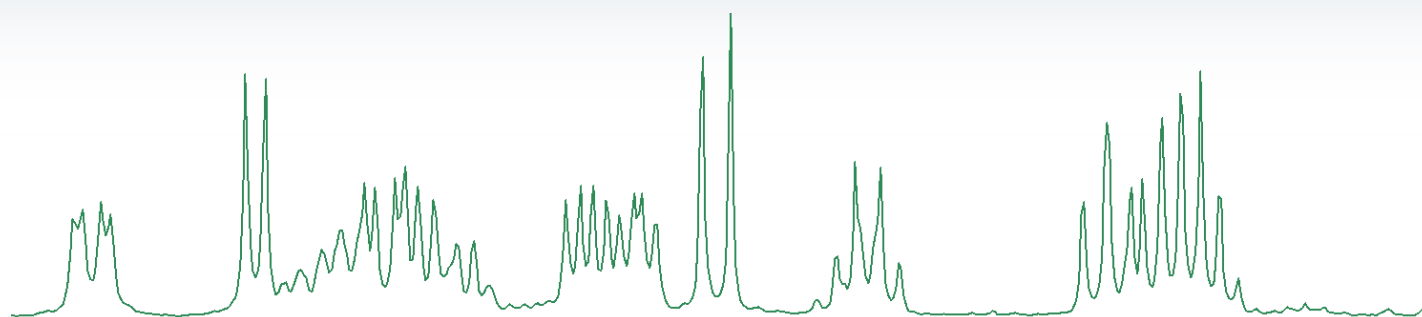


- To get a good resolution you need enough data points **TD** (acquisition) and **SI** (processing).

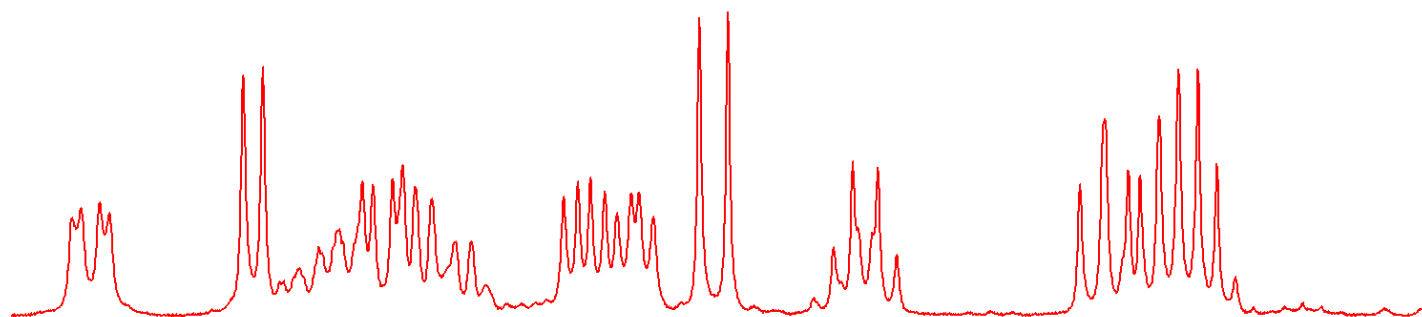
- $SI = \frac{TD}{2}$



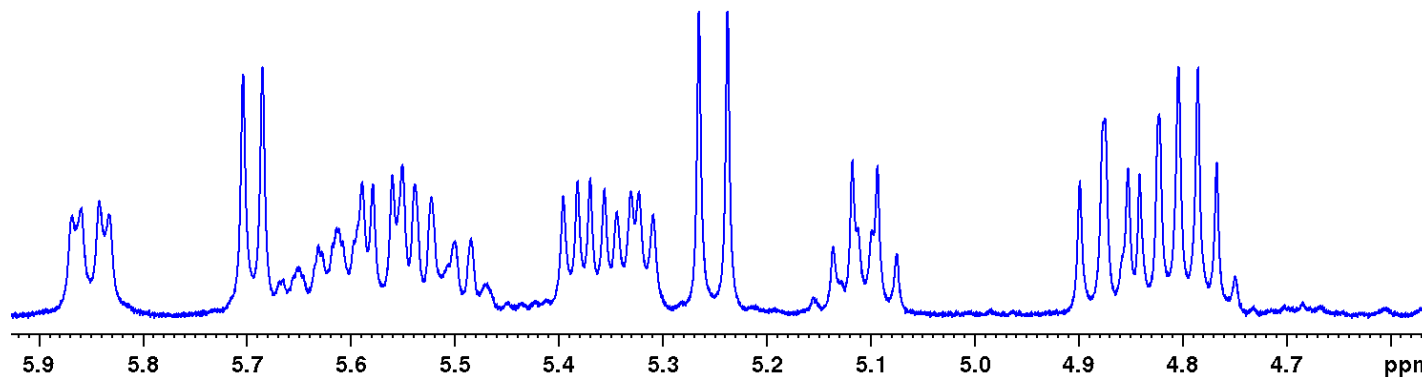
Zero filling



AQ: 1s
TD: 16k
SI: 8k
Res.: 0.97Hz

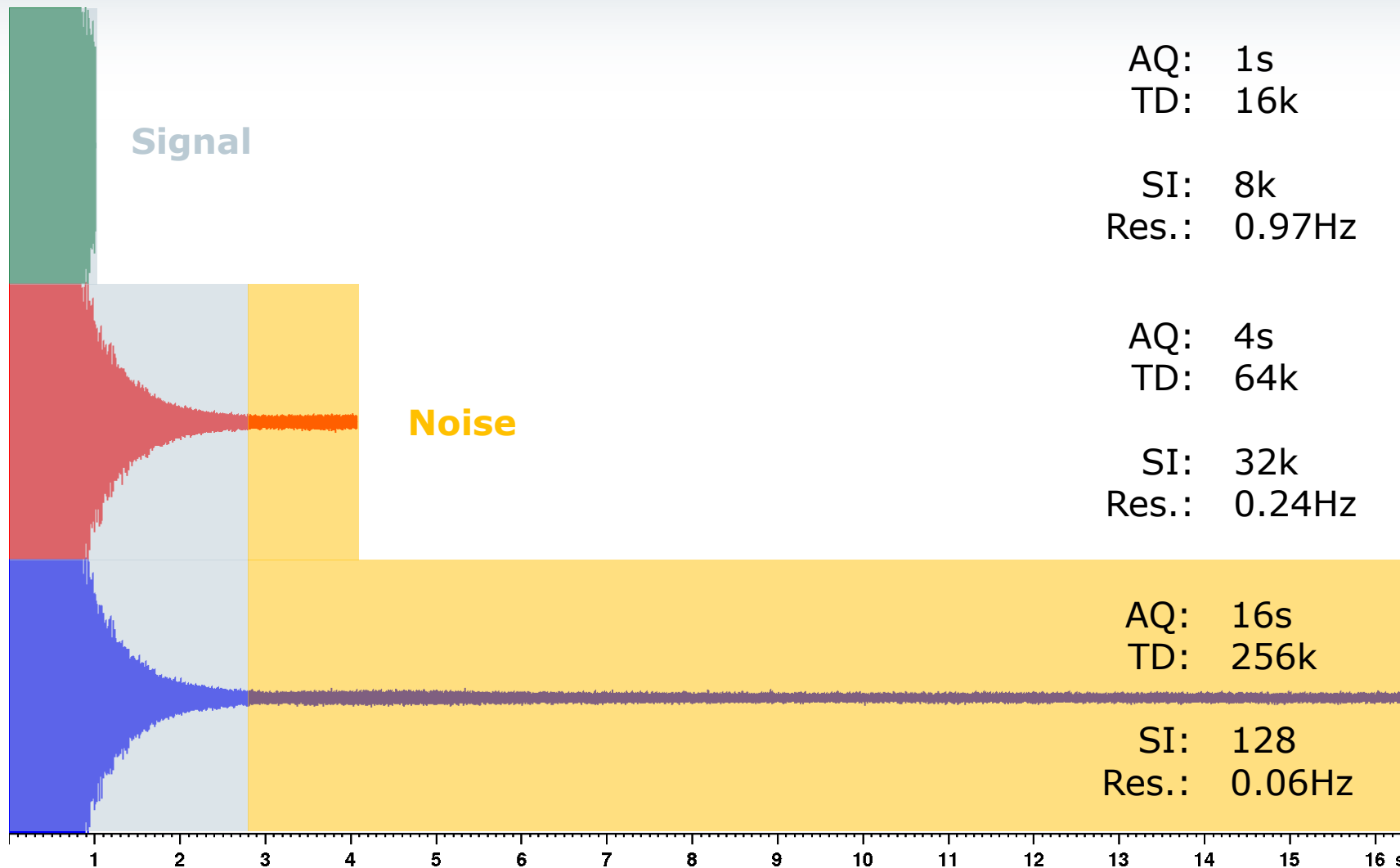


AQ: 4s
TD: 64k
SI: 32k
Res.: 0.24Hz

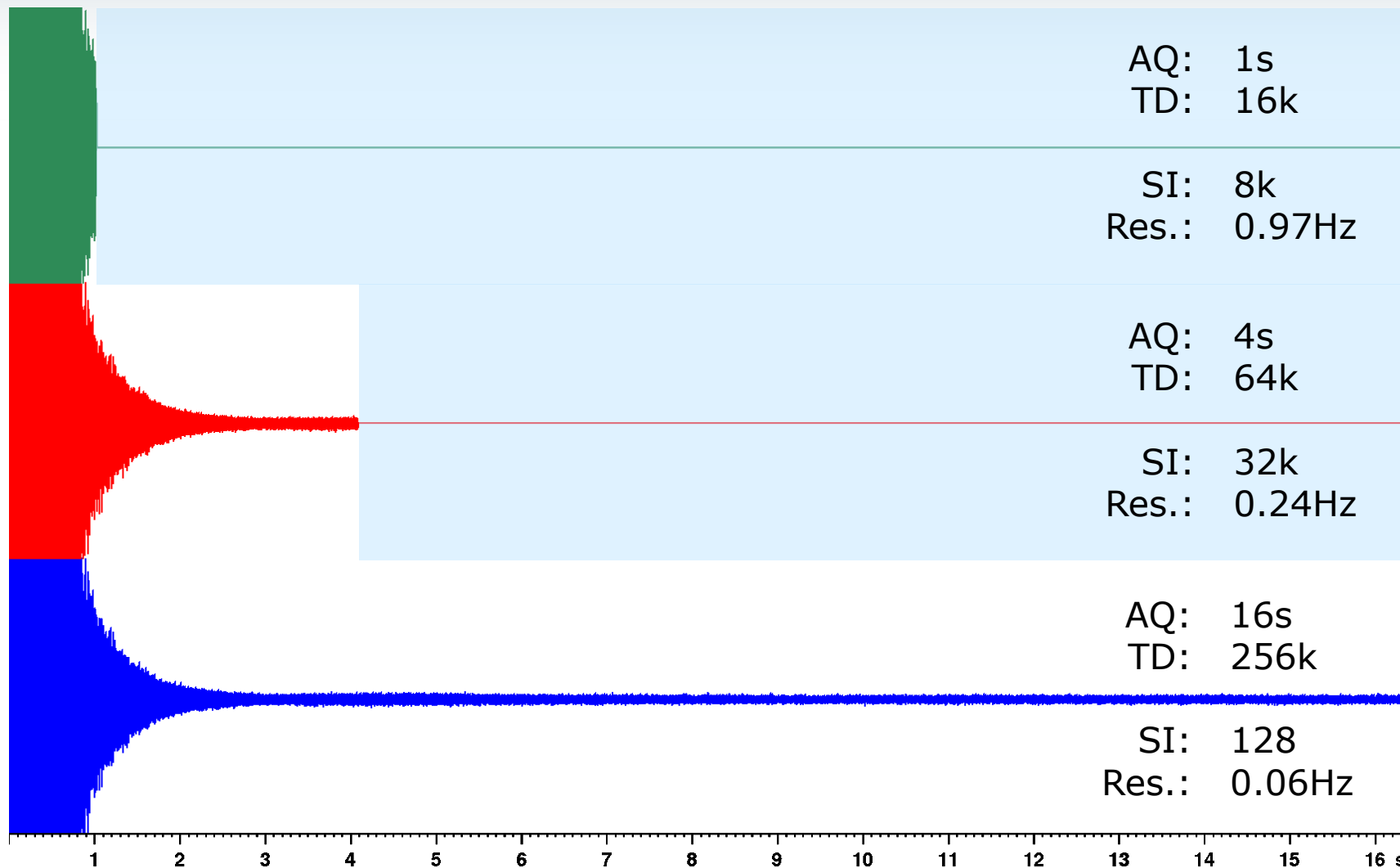


AQ: 16s
TD: 256k
SI: 128k
Res.: 0.06Hz

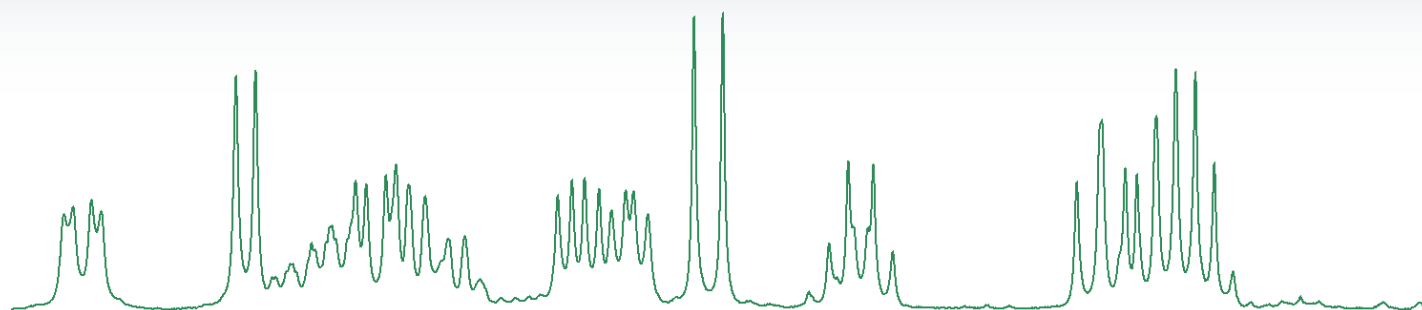
Zero filling



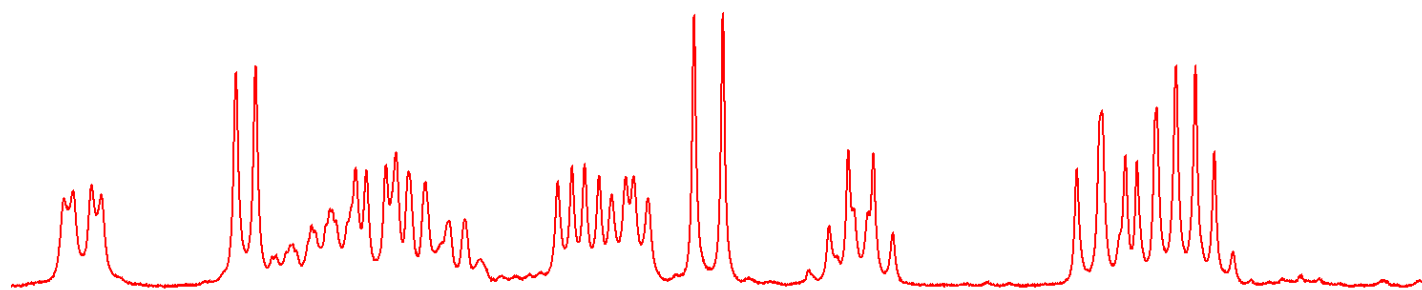
Zero filling



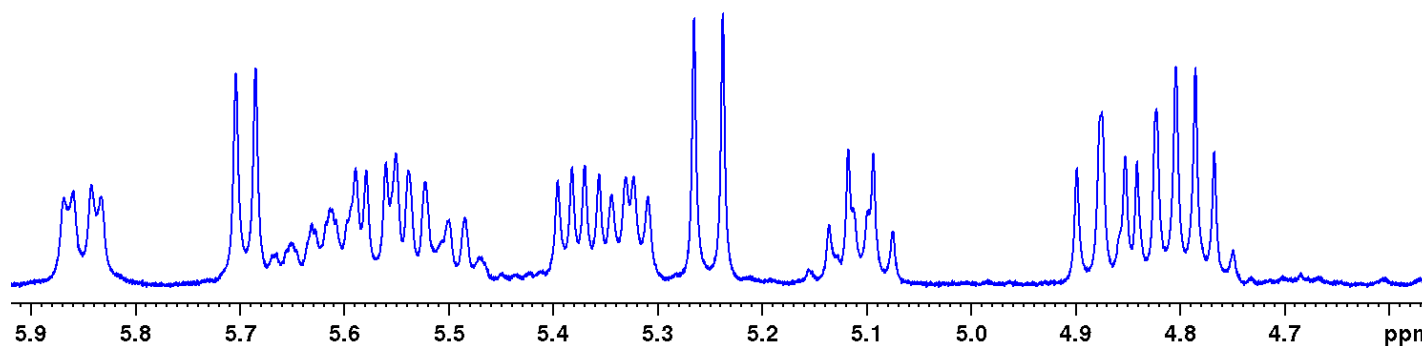
Zero filling



AQ: 1s
TD: 16k
SI: 128k



AQ: 4s
TD: 64k
SI: 128k



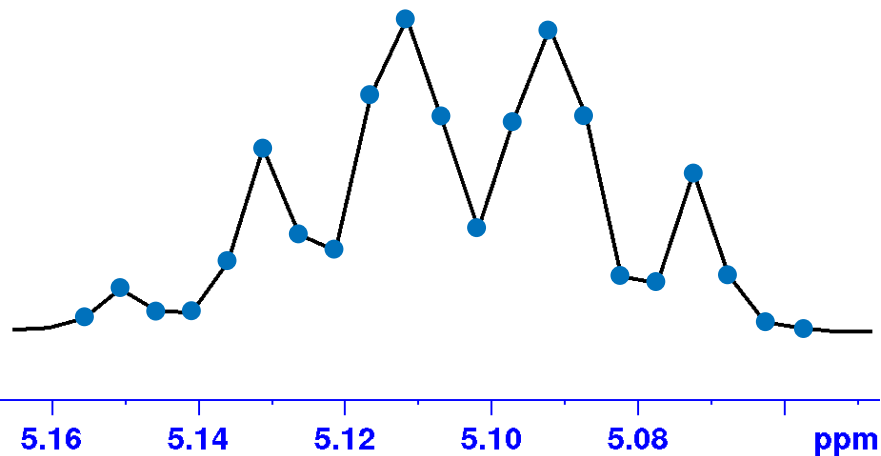
AQ: 16s
TD: 256k
SI: 128k

5.9 5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 ppm

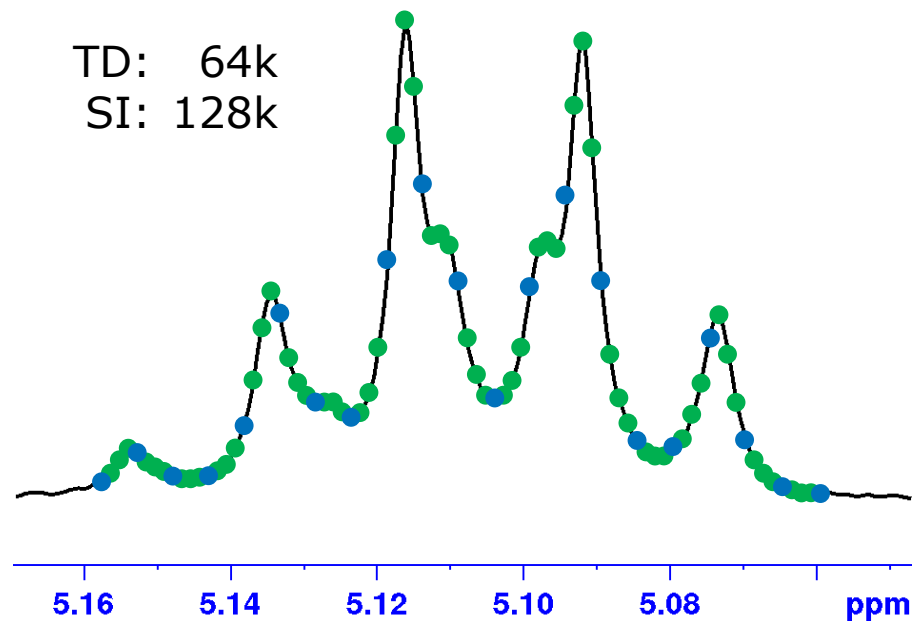
Zero filling



TD: 64k
SI: 32k



TD: 64k
SI: 128k



Parameters



- Parameters are :
 - size **SI**
 - spectrum reference frequency **SR**
 - spectral resolution **HzpPt**
- SI** is the amount of data points of the processed data. Typically **TD/2**. You can use the same value as for **TD** to get a better resolution. This is called zero filling.
- SR** is the shift for referencing the spectrum; interpreted by plot routines for generating the axis (scale) calibration
- HzpPt** is the spectral resolution, signals that are closer together than **HzpPt /2** cannot be resolved;

Window function [wm]



File Start **Process** Analyse Publish View Manage ?

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

- Configure Standard Processing (proc1d)
- Window Multiplication (wm)**
- Fourier Transform (ft)
- Fourier Transform Options ... (ftf)
- Start Automation AU Program (xaup)

Proc. Spectrum

Window function - em

Options

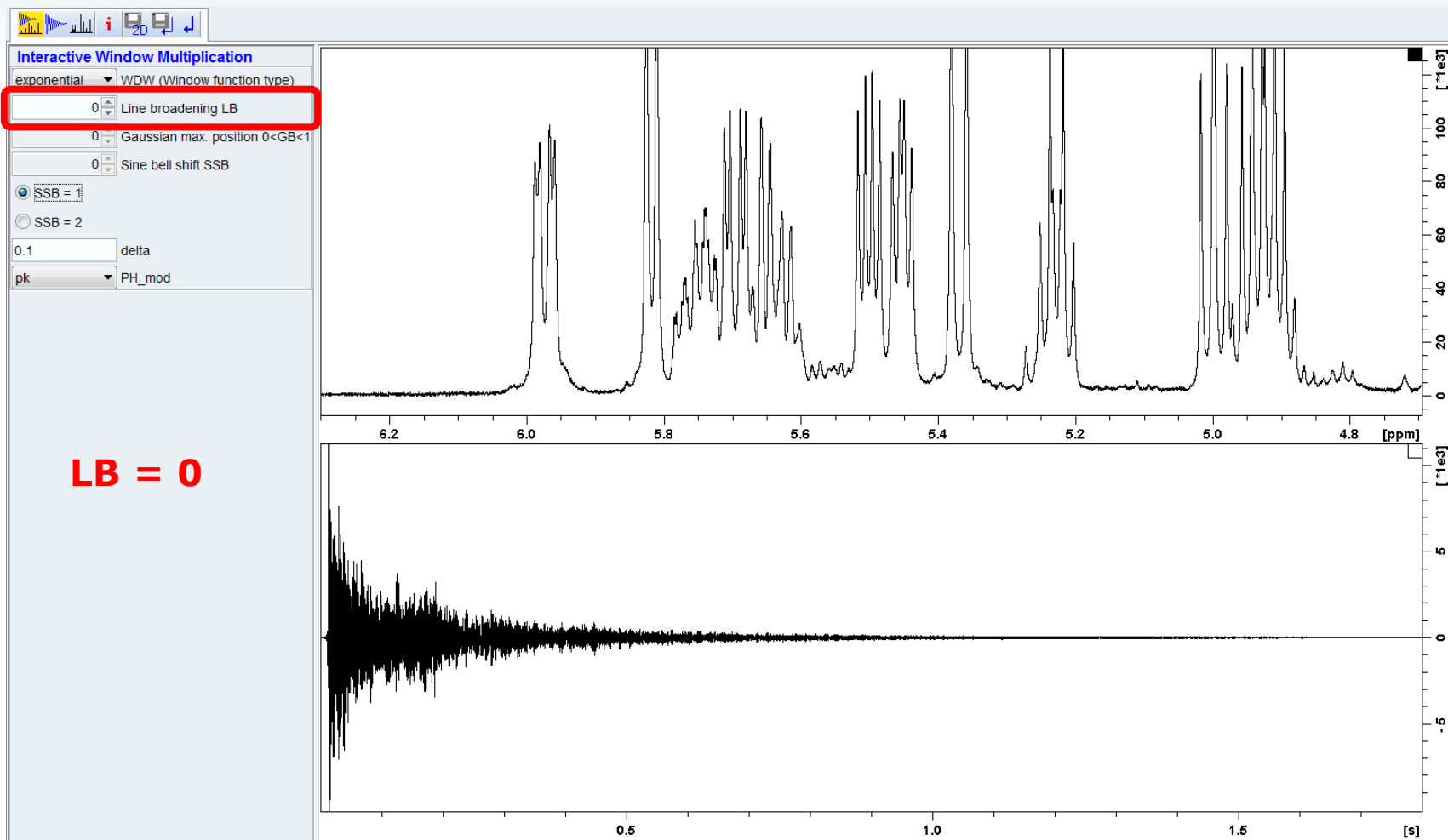
Manual window adjustment

Required parameters

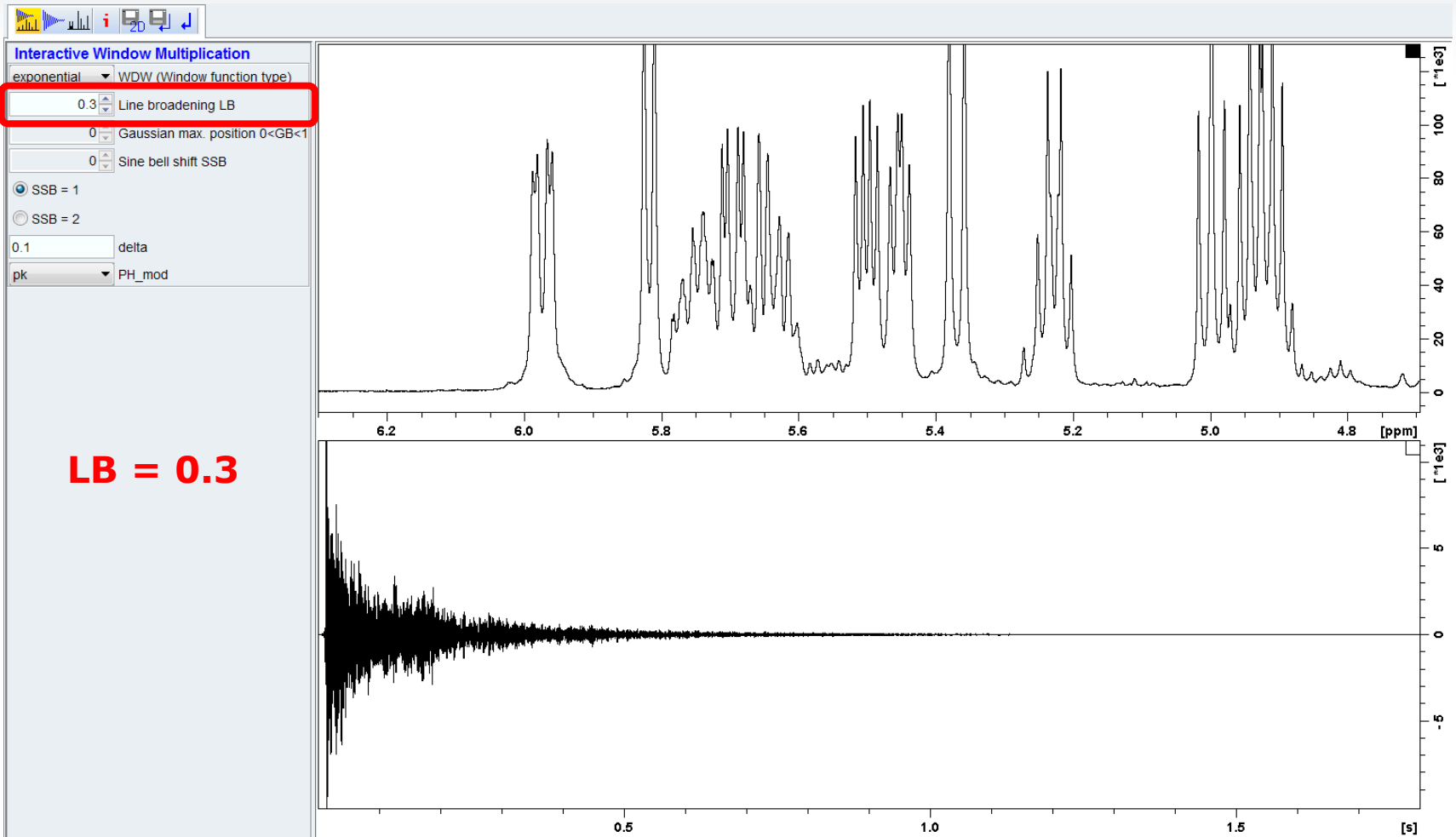
Window function type WDW =	exponential
Line broadening LB [Hz] =	0.3
Gaussian max. position 0<GB<1 =	0
Sine bell shift SSB (0,1,2,..) =	2
Left trapezoid limit 0<TM1<1 =	0
Right trapezoid limit 0<TM2<1 =	0

OK Cancel Help

Exponential window function

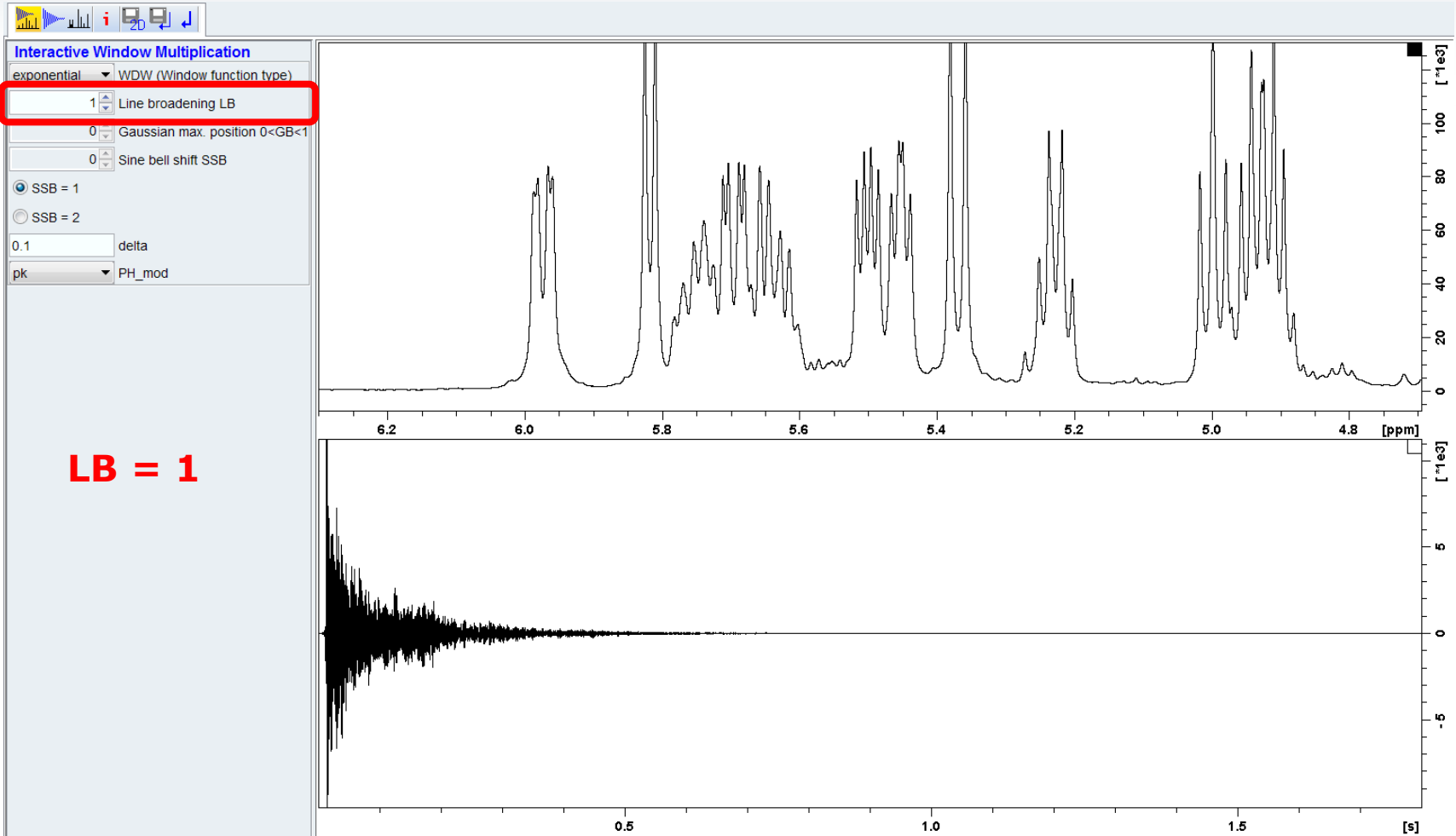


Exponential window function

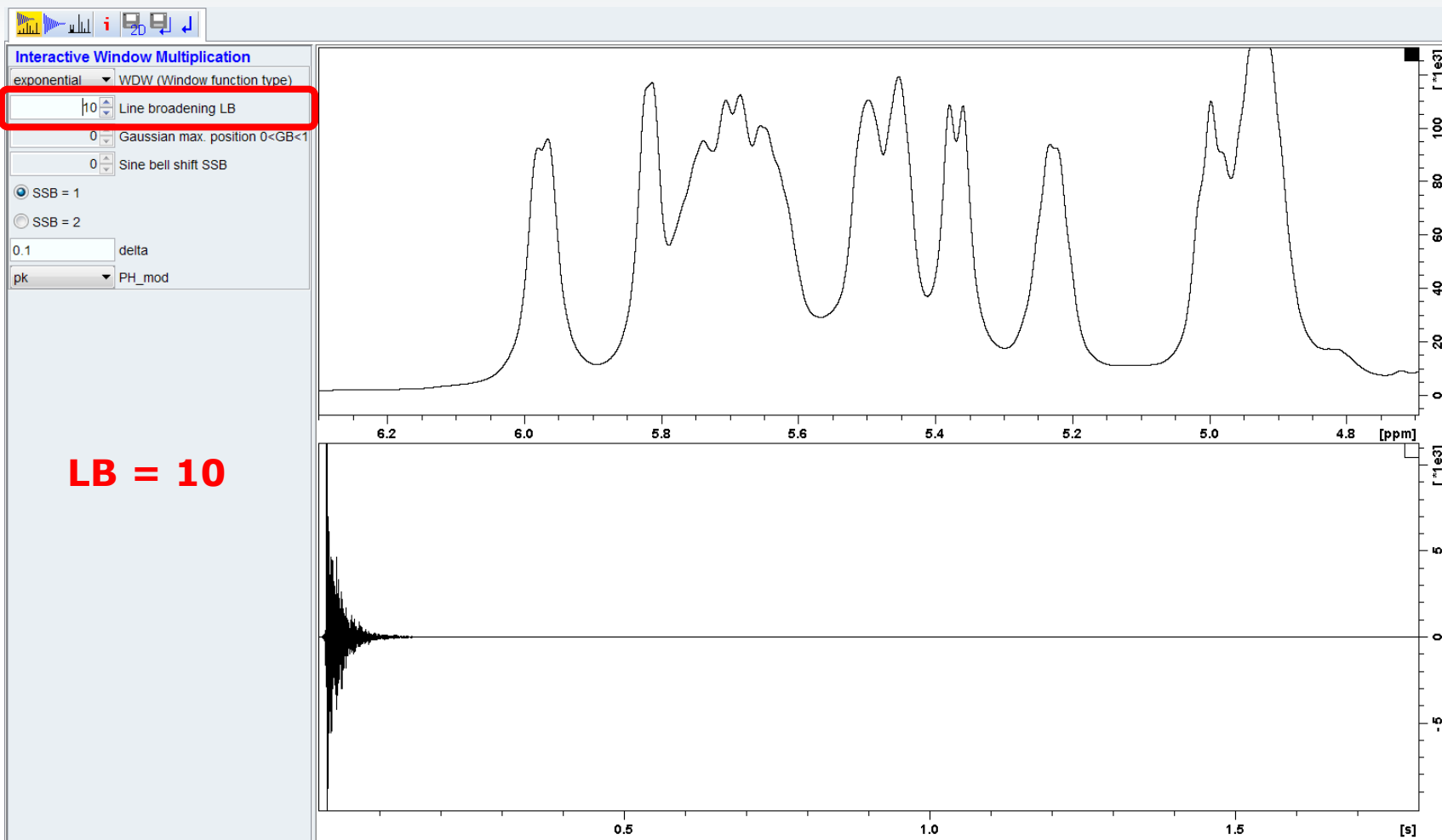


LB = 0.3

Exponential window function



Exponential window function

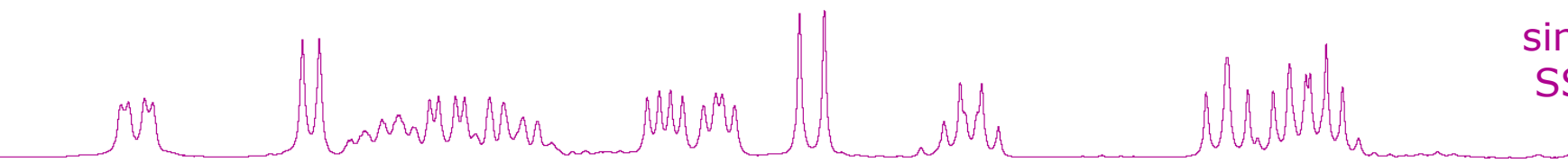


- Digital Filtering [em], [gm]
- There are several window functions, which can be used to optimize the spectrum.

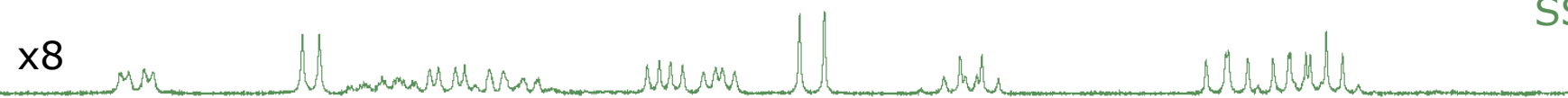
Function	Command	Factor	Range
Exponential	em	LB	>0
Gaussian	gm	LB and GB	LB<0, 0<GB<1
Sine bell	sinm	SSB	0, 1, 2, ...
Squared sine	qsine	SSB	0, 1, 2, ...

- Sine bell and squared sine need to be used for 2D spectra!

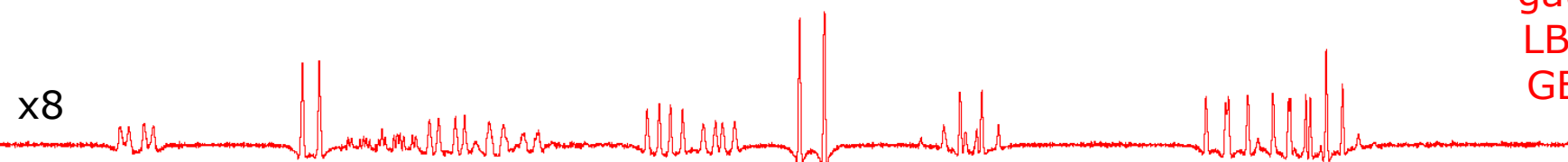
Effect of window functions



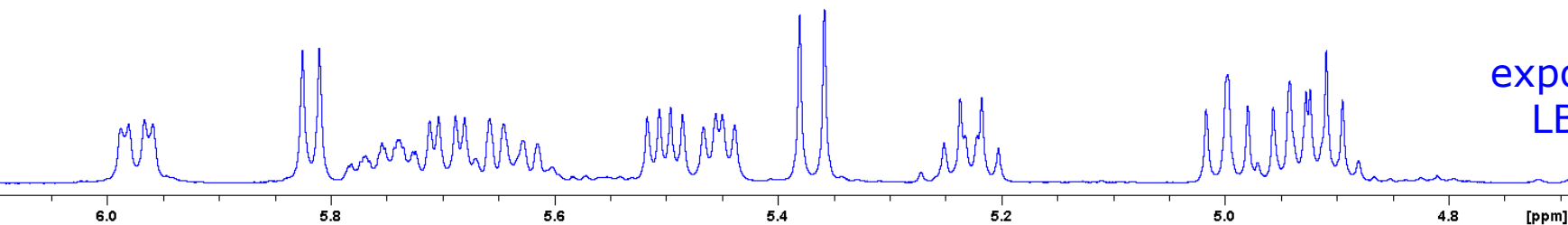
sine bell
SSB: 2



sine bell
SSB: 0



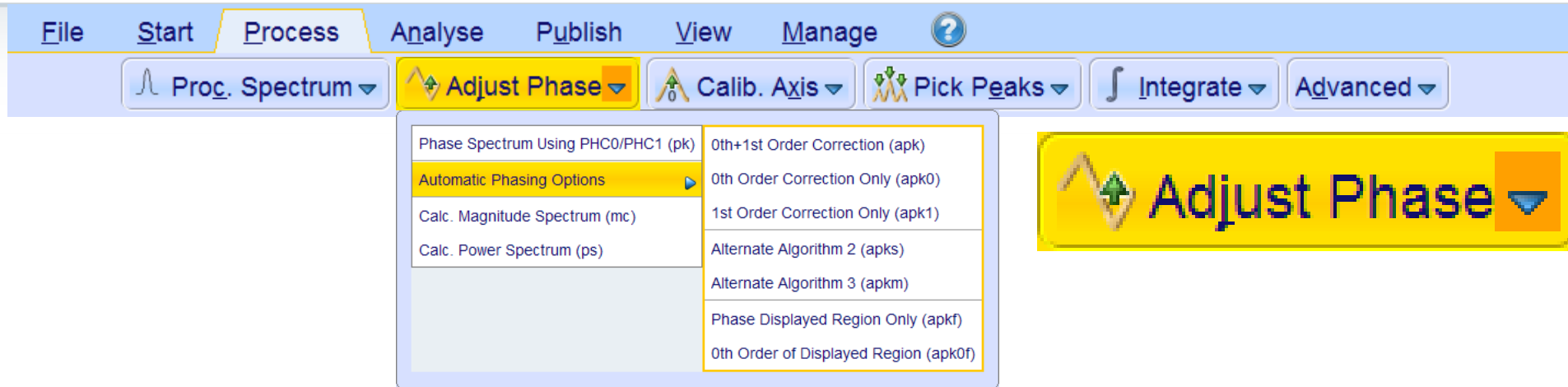
gaussian
LB: -0.7
GB: 0.5



exponential
LB: 0.3

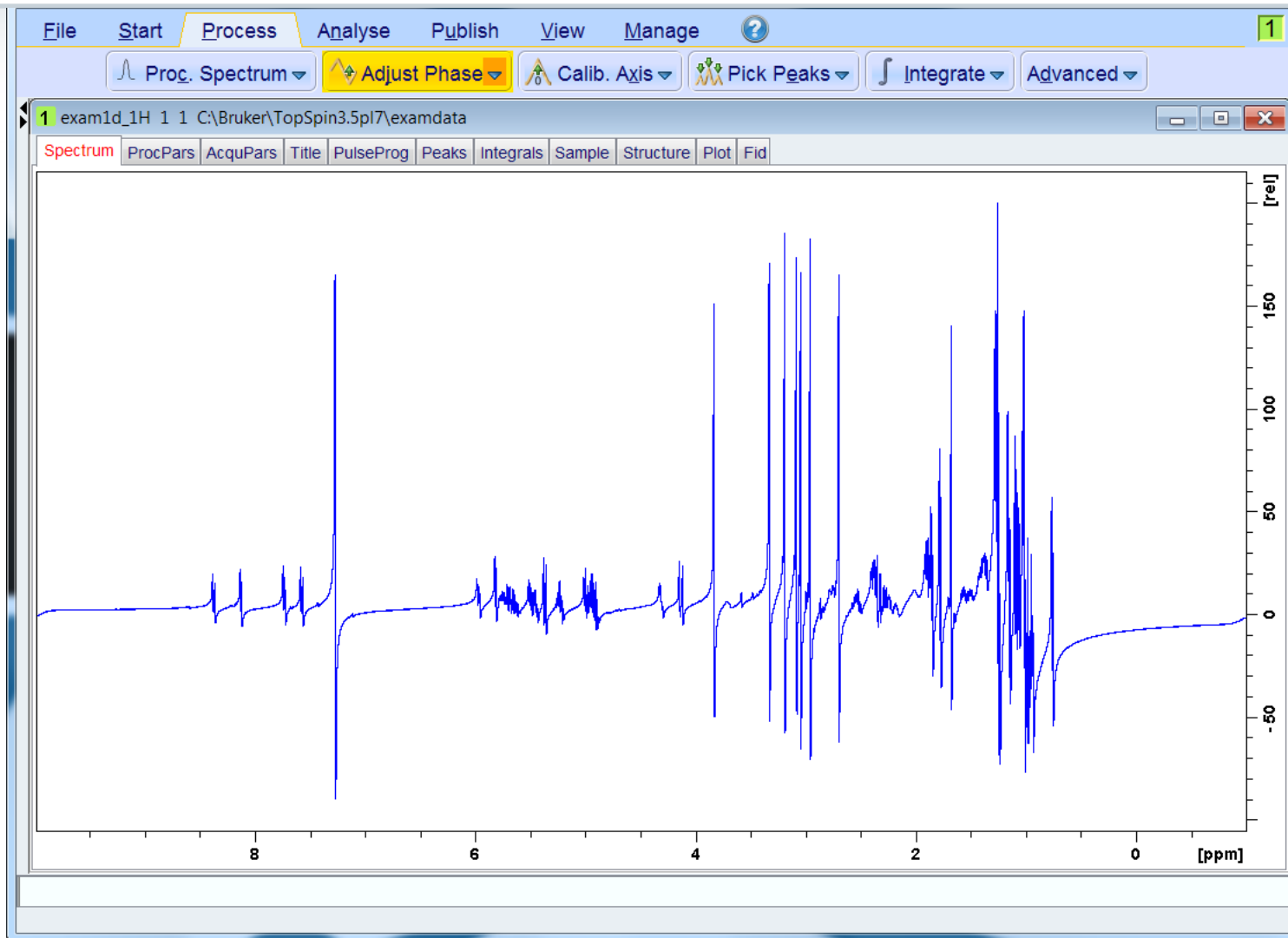
6.0 5.8 5.6 5.4 5.2 5.0 4.8 [ppm]

Adjust Phase

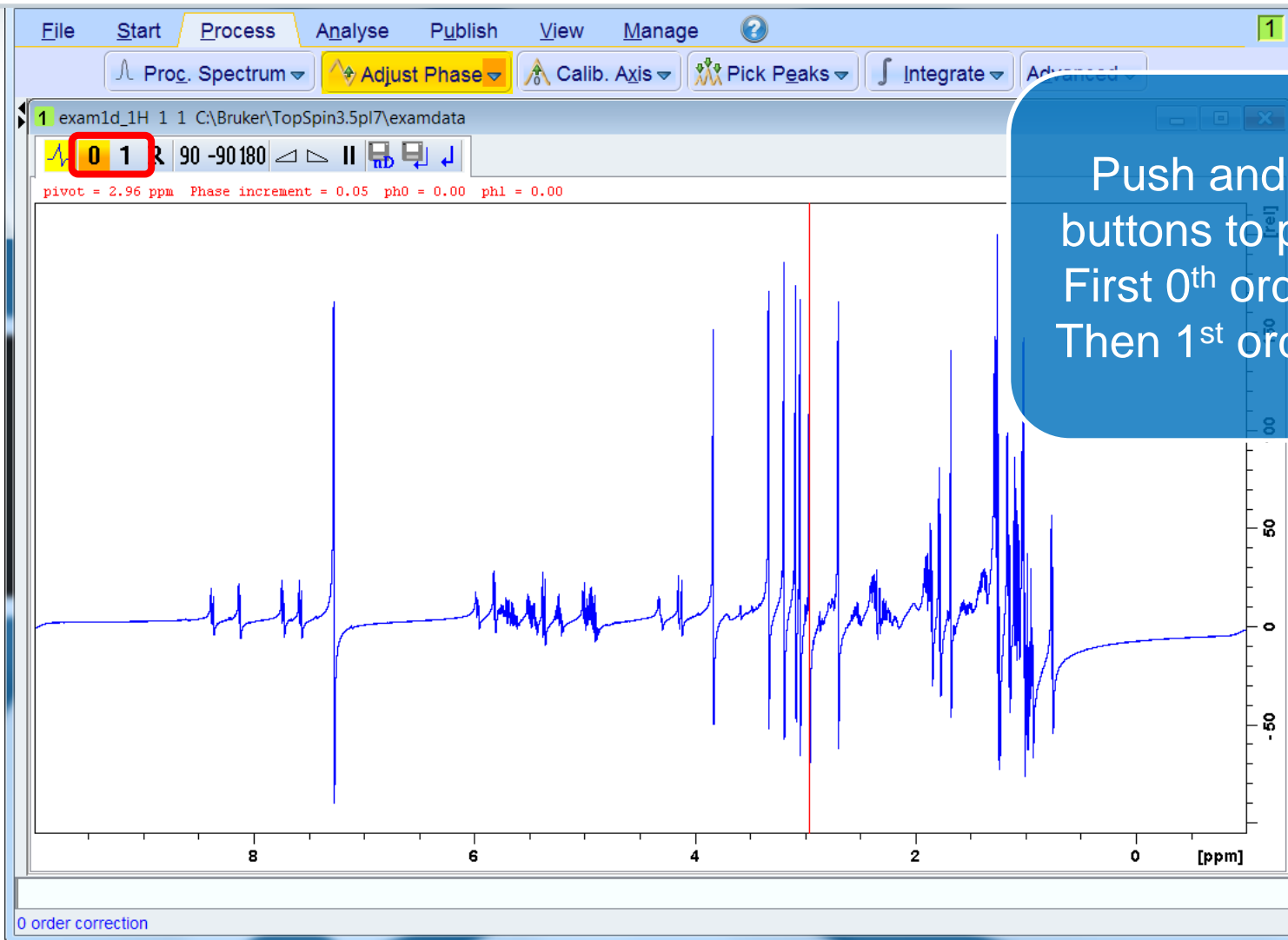


- Manual phase correction with **[.ph]**
- Automatic phase correction with **[apk]/[apk0]**
- Uses previously defined phase correction values **[pk]**

Phasing

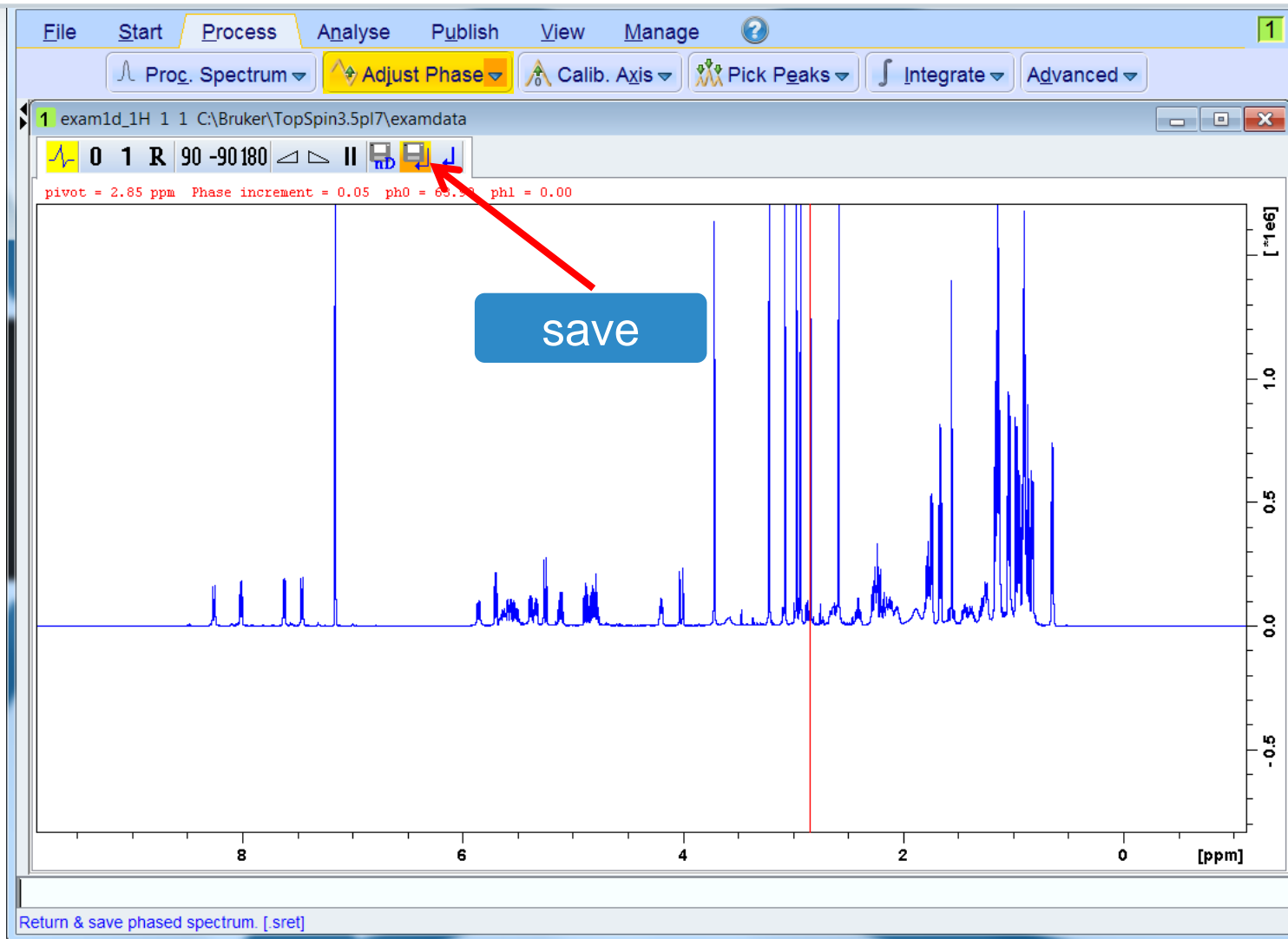


Phasing



Push and hold buttons to phase. First 0th order **0**. Then 1st order **1**.

Phasing



Phasing



The screenshot shows the Bruker software interface with the 'Process' tab selected. The 'Adjust Phase' button is highlighted in yellow. The 'Phase correction' section is highlighted with a red box, showing the following parameters:

Parameter	Value	Description
PHC0 [degrees]	63.900	0th order correction for pk
PHC1 [degrees]	0	1st order correction for pk
PH_mod	no	Phasing modes for trf, xfb, ...

Other sections visible in the interface include:

- Baseline correction:** ABSG (5), ABSF1 [ppm] (10.00000), ABSF2 [ppm] (0), BCFW [ppm] (1.00000), COROFFS [Hz] (0), BC_mod (quad).
- Fourier transform:** TDef (0), STSR (0), STSI (0), ME_mod (no), NCOEF (0), LPBIN (0), TDoff (0).

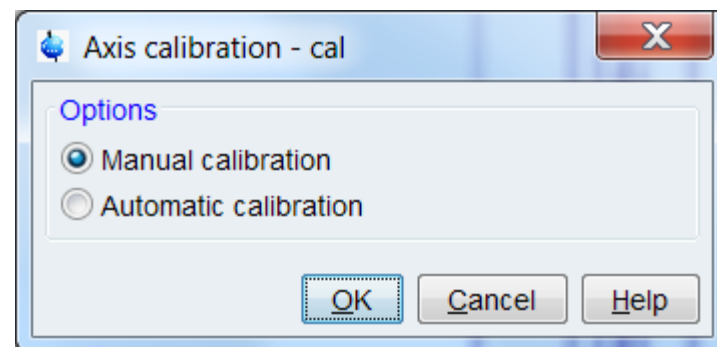
- Use previously defined phase correction values [**pk**]

Calibrate Axis



Set TMS To 0 ppm (sref)
Requires edlock setup!

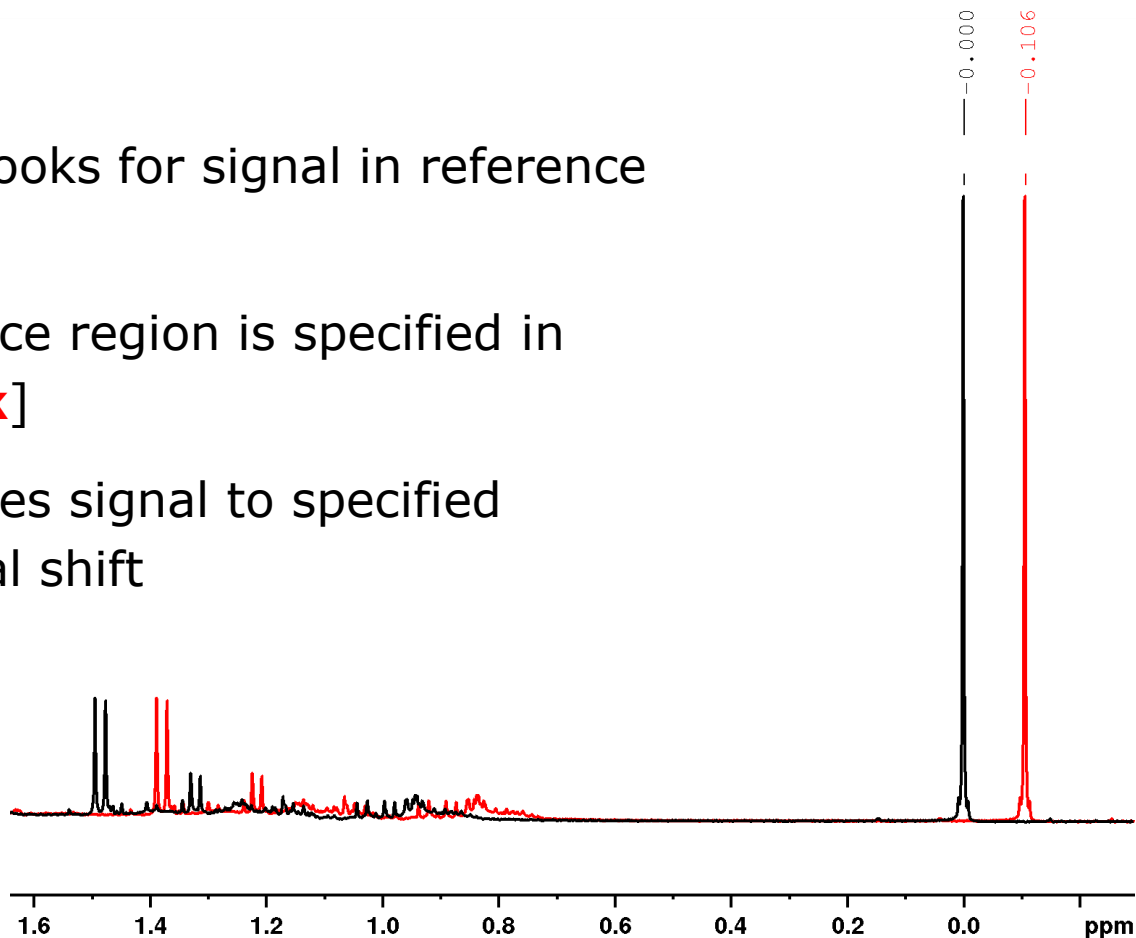
- Open reference dialog with [**cal**]
- Automatic referencing [**sref**]
- Reference manually [**.cal**]



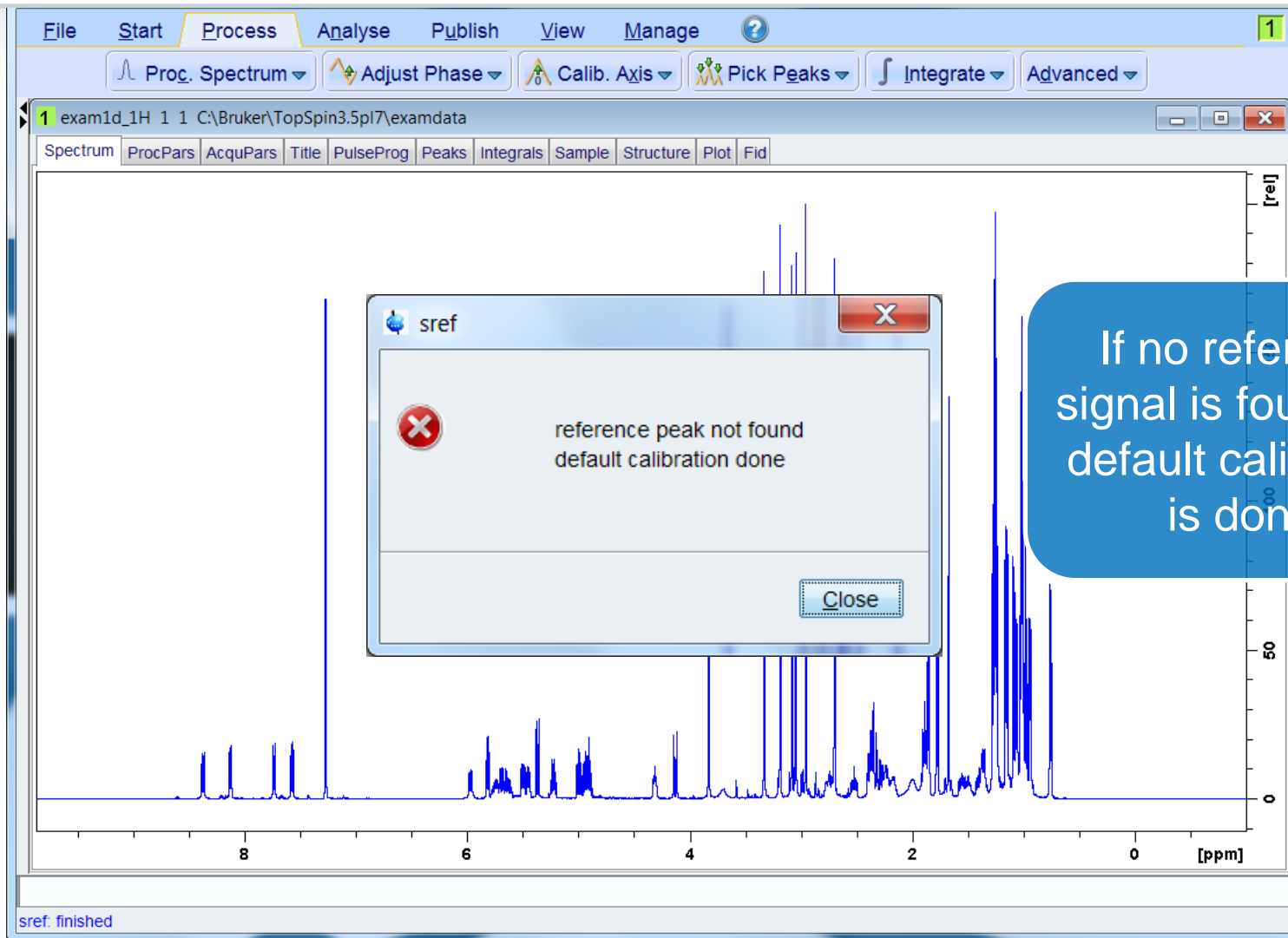
Automatic calibration



- [**sref**] looks for signal in reference region
- Reference region is specified in [**edlock**]
- Calibrates signal to specified chemical shift

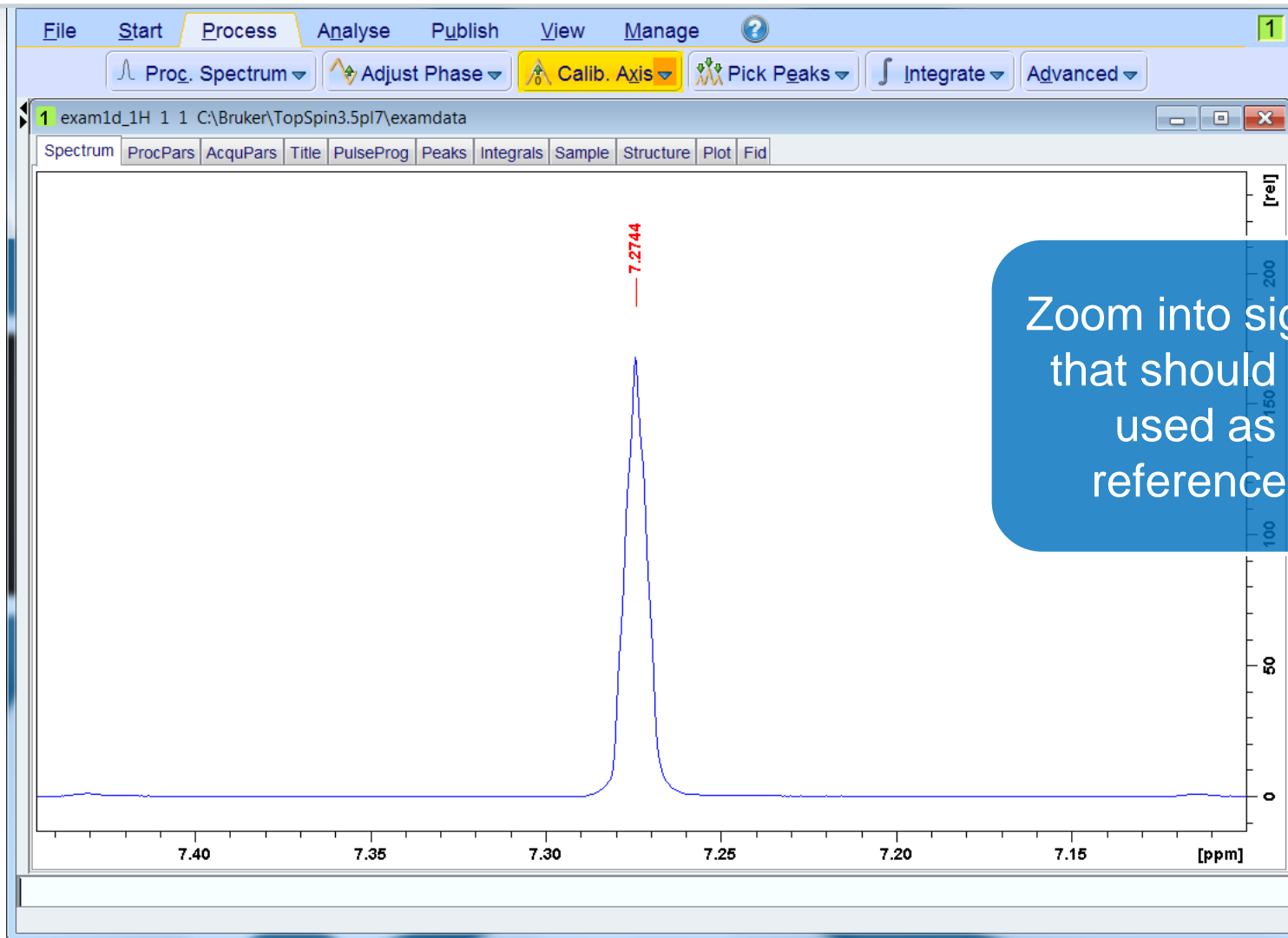


Automatic calibration



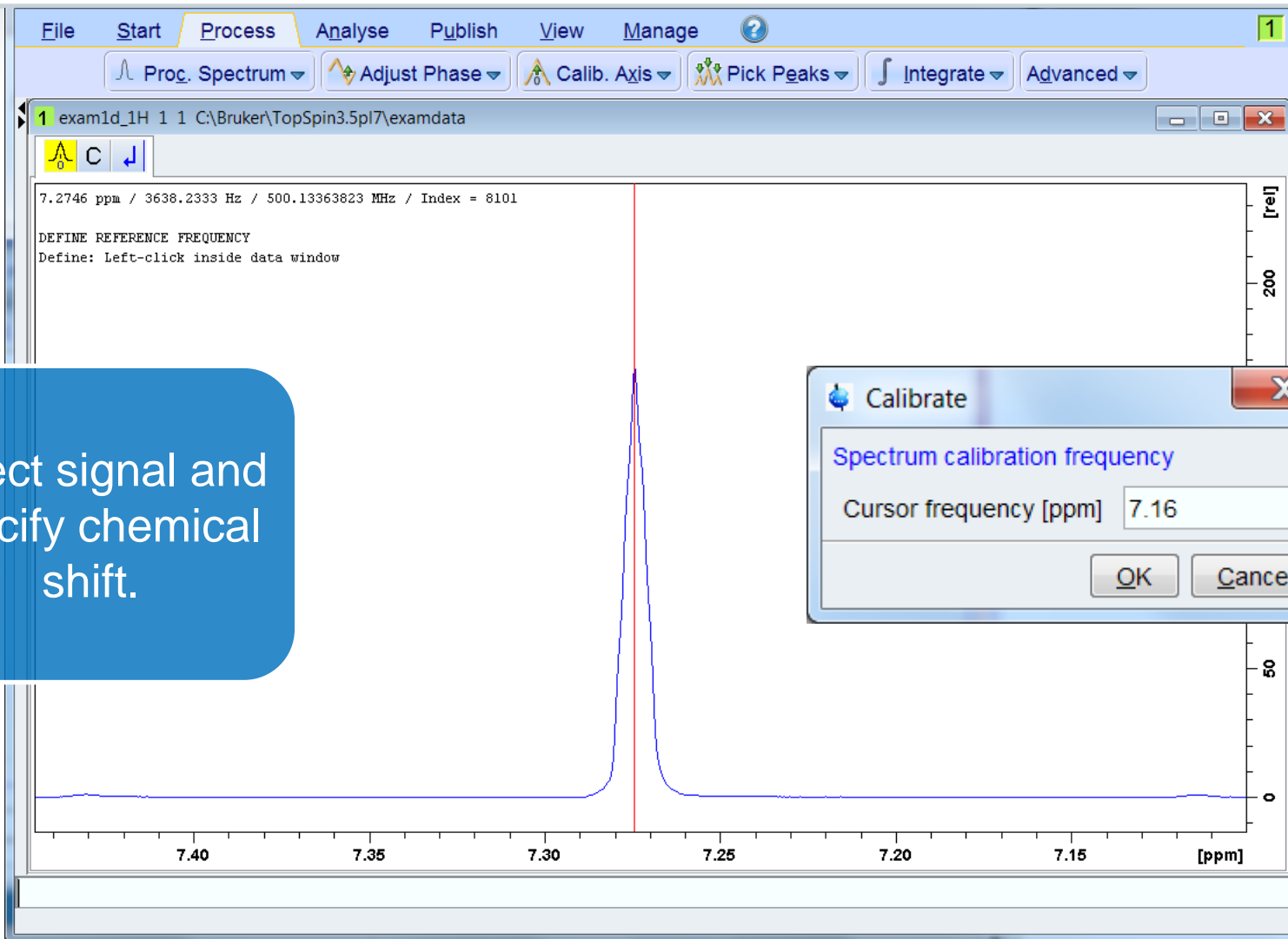
If no reference signal is found, the default calibration is done.

Manual calibration



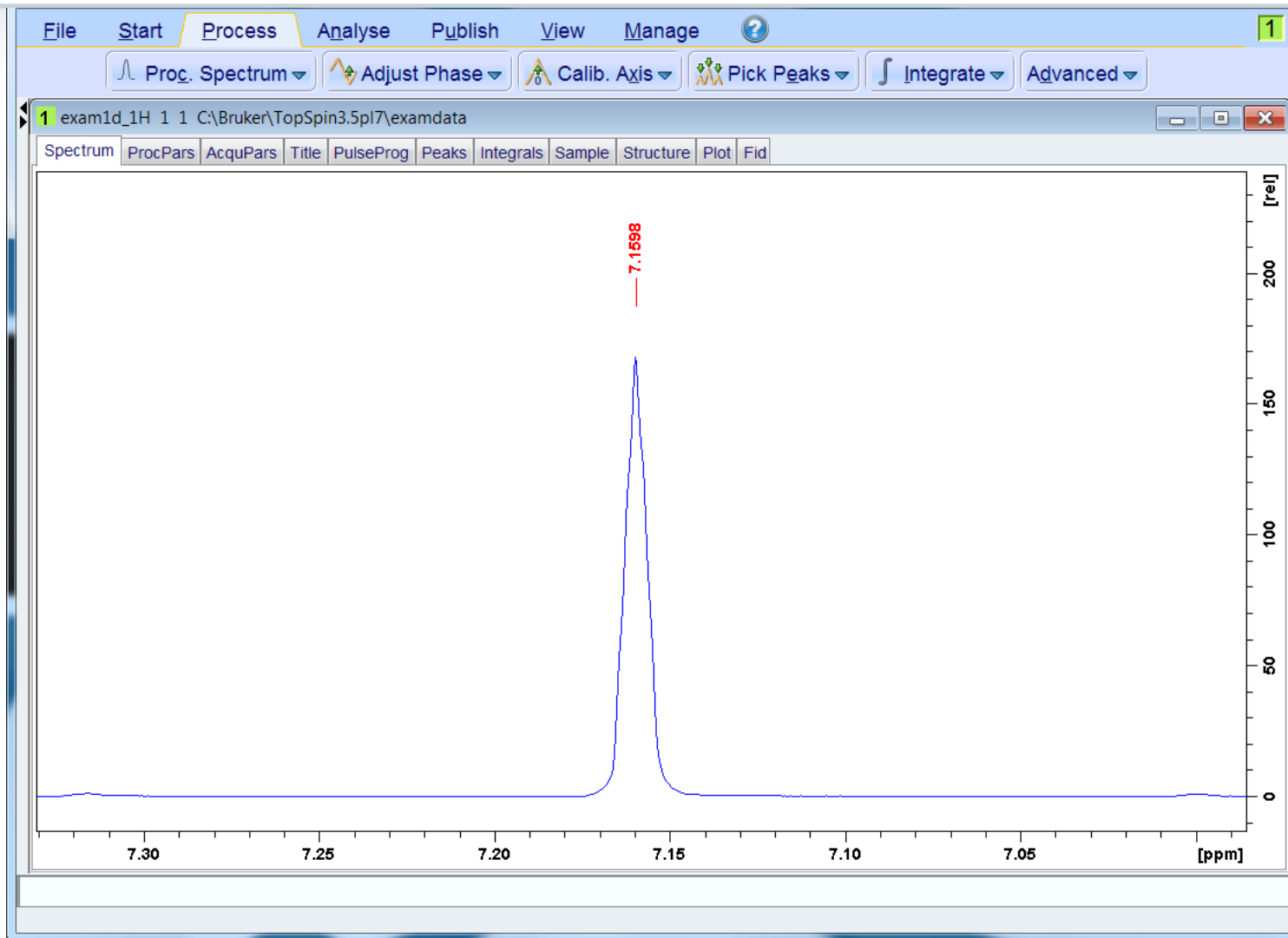
Zoom into signal that should be used as reference.

Manual calibration



Select signal and
specify chemical
shift.

Manual calibration



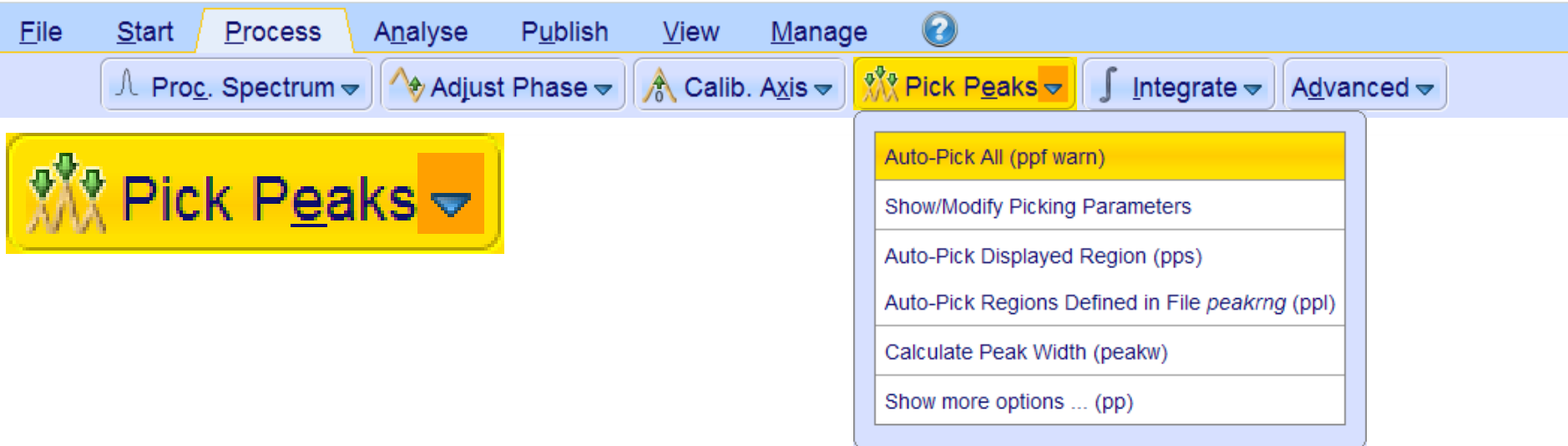
Caution!

If you want to determine a frequency for
selective experiments

SR needs to be set to 0!

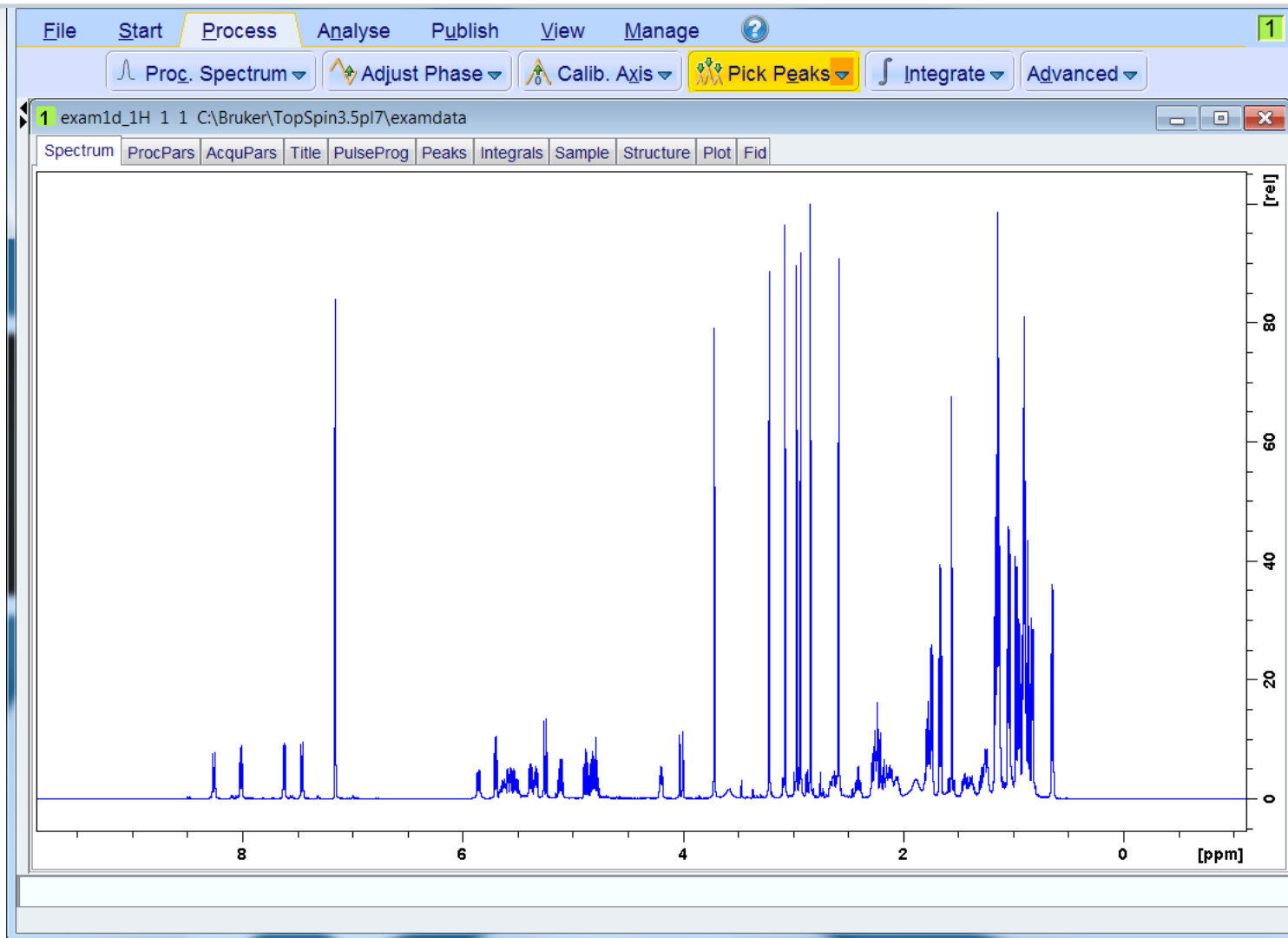
SR is only used for visualisation!

Pick Peaks

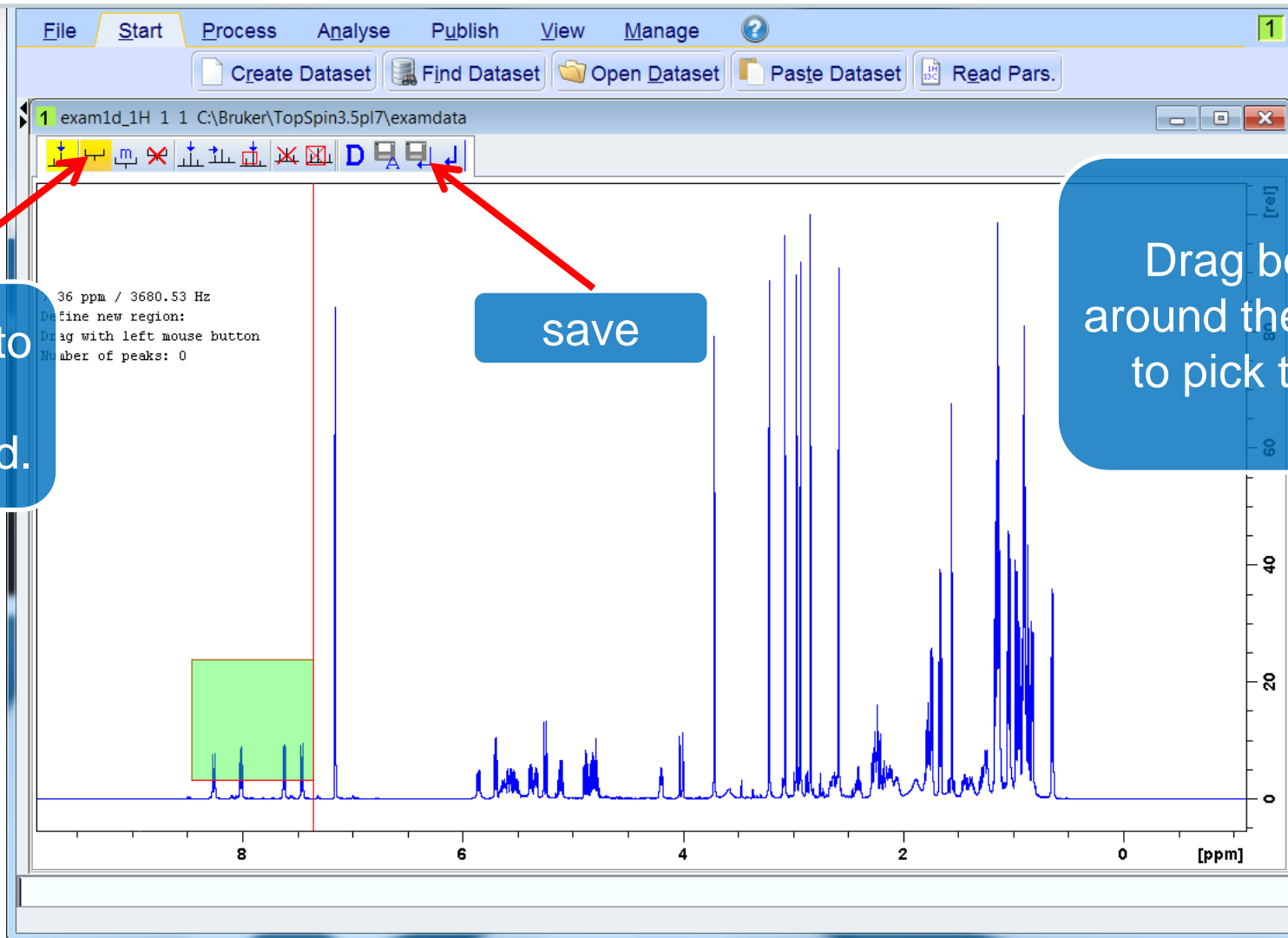


- Automatic peak picking of full spectrum [**ppf warn**]
- Automatic peak picking of displayed region [**pps**]
- [**.pp**] open manual peak picking

Pick Peaks



Pick Peaks

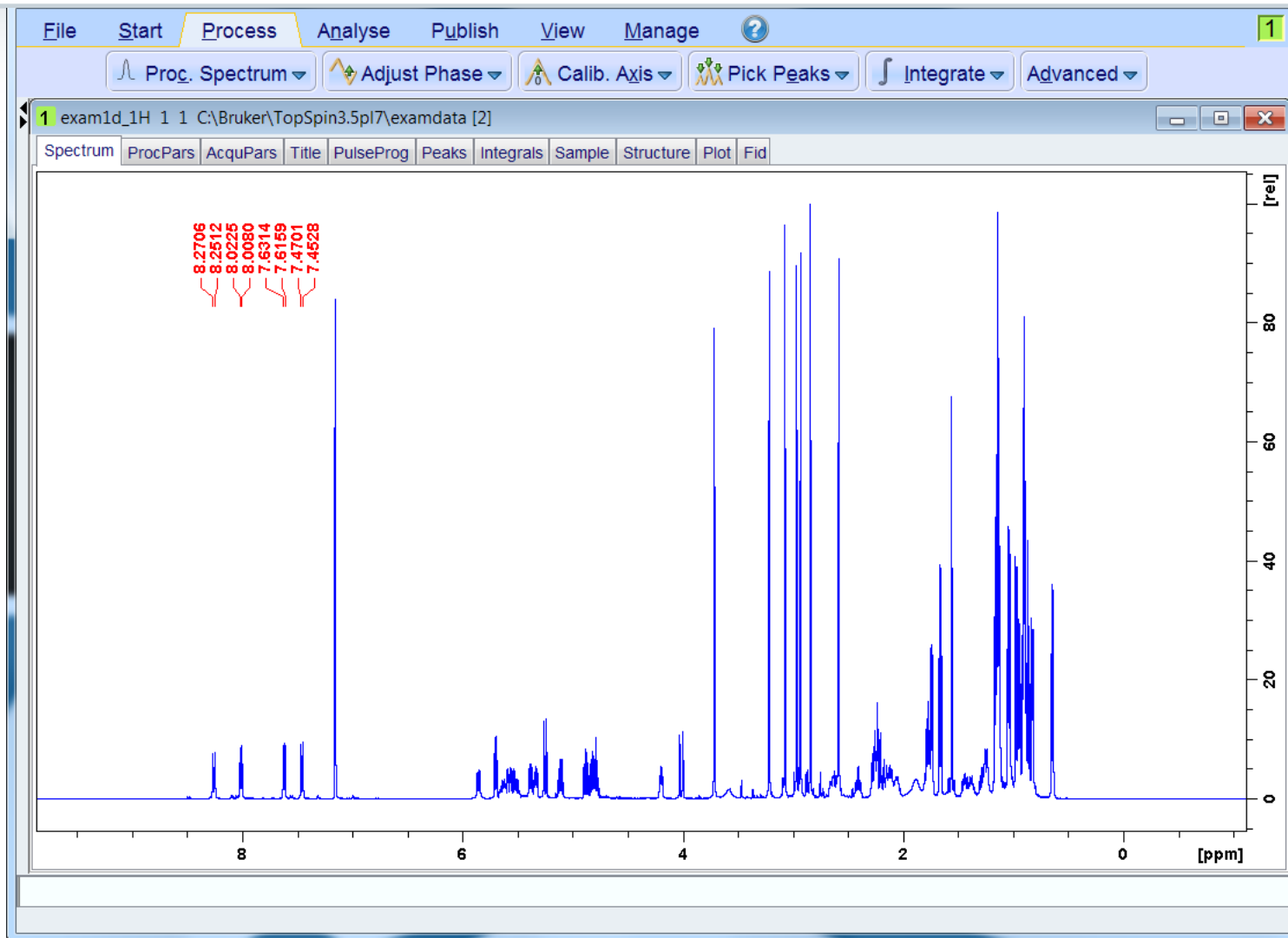


Needs to be selected.

save

Drag boxes around the peaks to pick them.

Pick Peaks



Pick Peaks



File Start **Process** Analyse Publish View Manage ? 1

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

exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata

Spectrum ProcPars AcqPars Title PulseProg **Peaks** Integrals Sample Structure Plot Fid

Peak	v(F1) [ppm]	Intensity [abs]	Annotation
1	8.2706	157292.88	
2	8.2512	161750.83	
3	8.0225	178332.21	
4	8.0080	183574.56	
5	7.6314	185004.26	
6	7.6159	193454.27	
7	7.4701	190291.50	
8	7.4528	197267.36	

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

Pick Peaks



File Start **Process** Analyse Publish View Manage ? 1

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

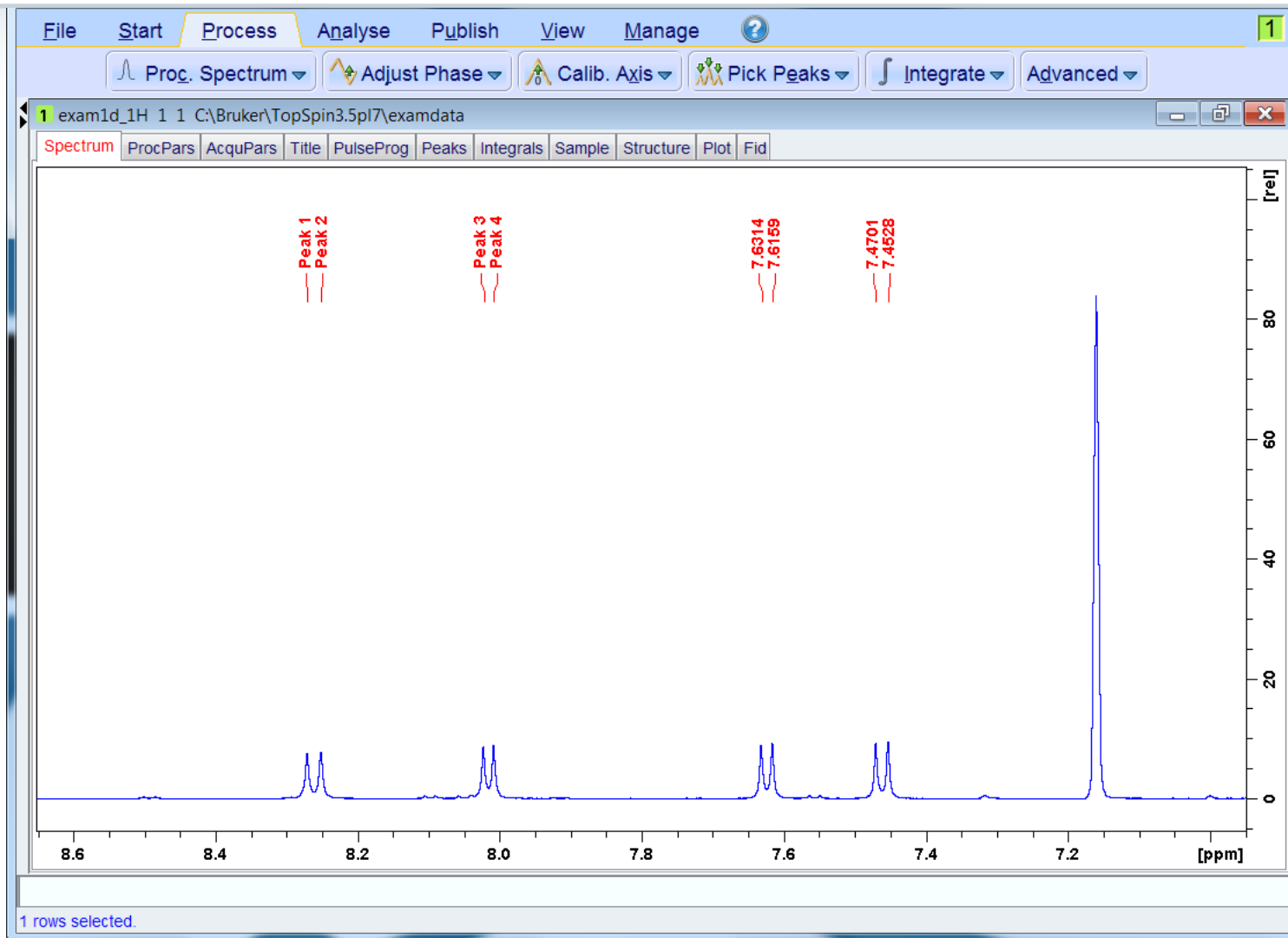
exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata

Spectrum ProcPars AcqPars Title PulseProg **Peaks** Integrals Sample Structure Plot Fid

Peak	v(F1) [ppm]	Intensity [abs]	Annotation
1	8.2706	157292.88	Peak 1
2	8.2512	161750.83	Peak 2
3	8.0225	178332.21	Peak 3
4	8.0080	183574.56	Peak 4
5	7.6314	185004.26	
6	7.6159	193454.27	
7	7.4701	190291.50	
8	7.4528	197267.36	

1 rows selected.

Pick Peaks



Parameters



- Parameters are :
 - intensity of reference peak (**CY**)
 - minimum relative intensity (**MI**)
 - maximum relative intensity (**MAXI**)
 - peak picking sensitivity (**PC**)
 - peak sign (**PSIGN**)
- **CY** defines the relative intensity of reference peak, also used for plotting (in cm).
- **MI** and **MAXI** must be chosen relative to **CY**, they define the smallest and largest peak that is picked.
- **PC** is the sensitivity for peak picking, only peaks that are larger than noise \times **PC** are picked.
- **PSIGN** defines if only positive or negative peaks or both are picked

Automatic Peak Picking Options

[pp]



Peak picking - pps

Options

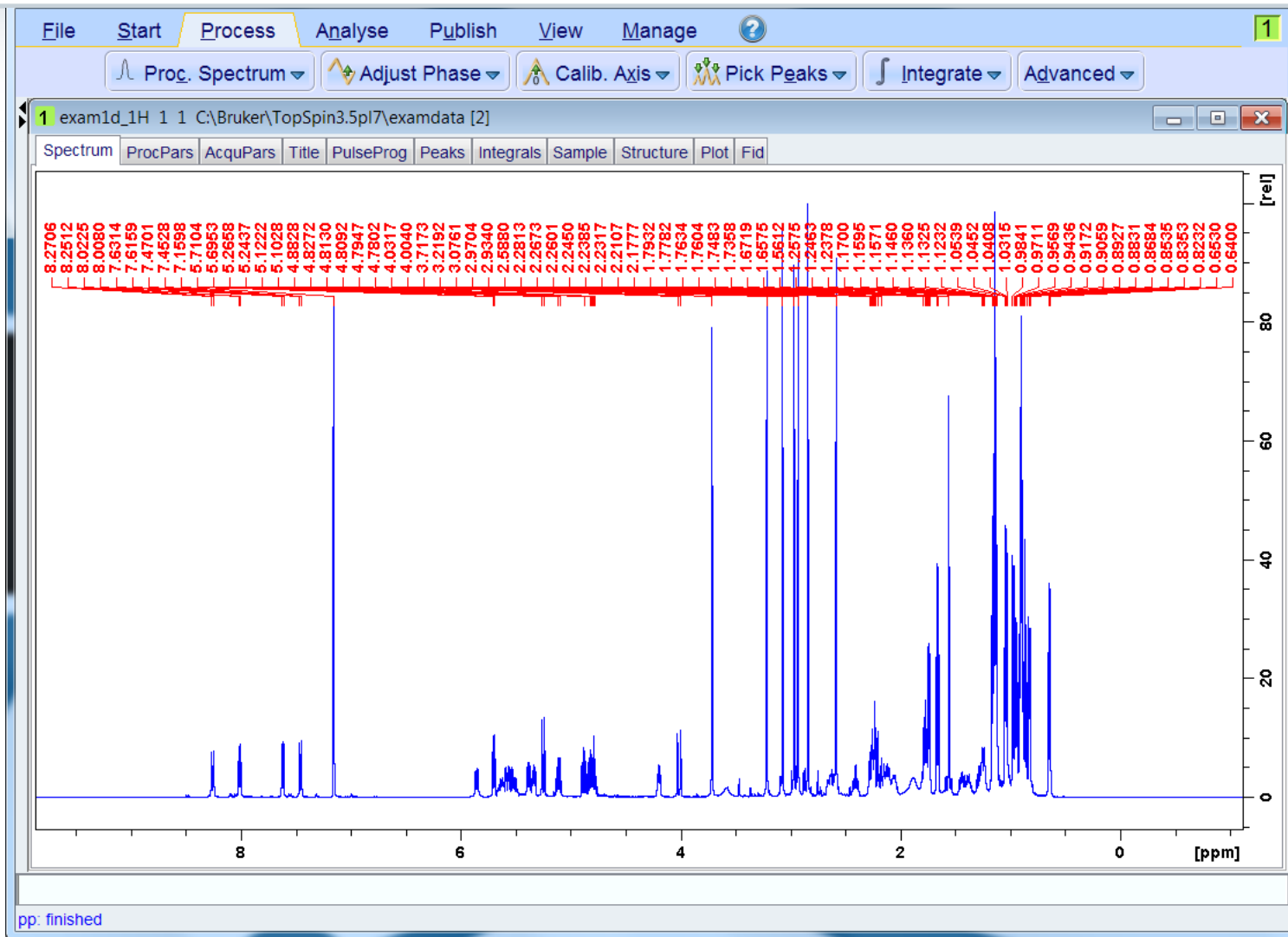
- Auto-Pick peaks on displayed spectrum region
- Auto-Pick peaks on full spectrum
- Define regions / peaks manually, adjust MI, MAXI
- Auto-Pick peaks in predefined regions (file 'peakrng')
- Calculate width of currently displayed peak

Required parameters

Left picking limit F1P =	9.8757
Right picking limit F2P =	-1.1104
Intensity of reference peak CY [rel] =	100
Minimum intensity MI [rel] =	0.001
Maximum intensity MAXI [rel] =	100
Detection sensitivity PC =	5
Fraction of peak height for width calc. [0...1] =	0.5
Pick peaks of sign PSIGN =	both
Reference peak selection mode PSCAL =	global
Region file for PSCAL = sreg/psreg: SREGLST =	1H.CDCI3

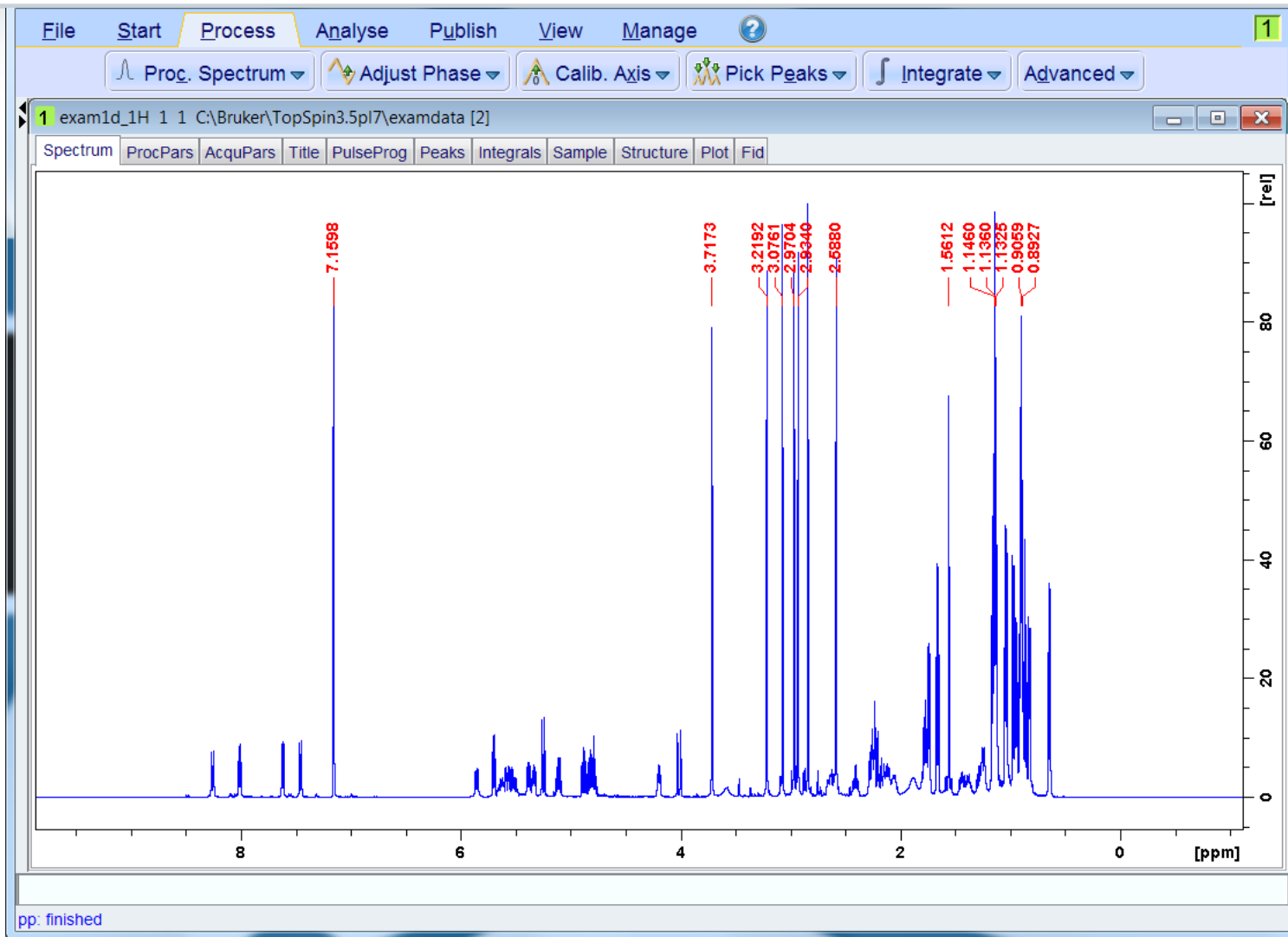
OK Cancel Help

Automatic Peak Picking



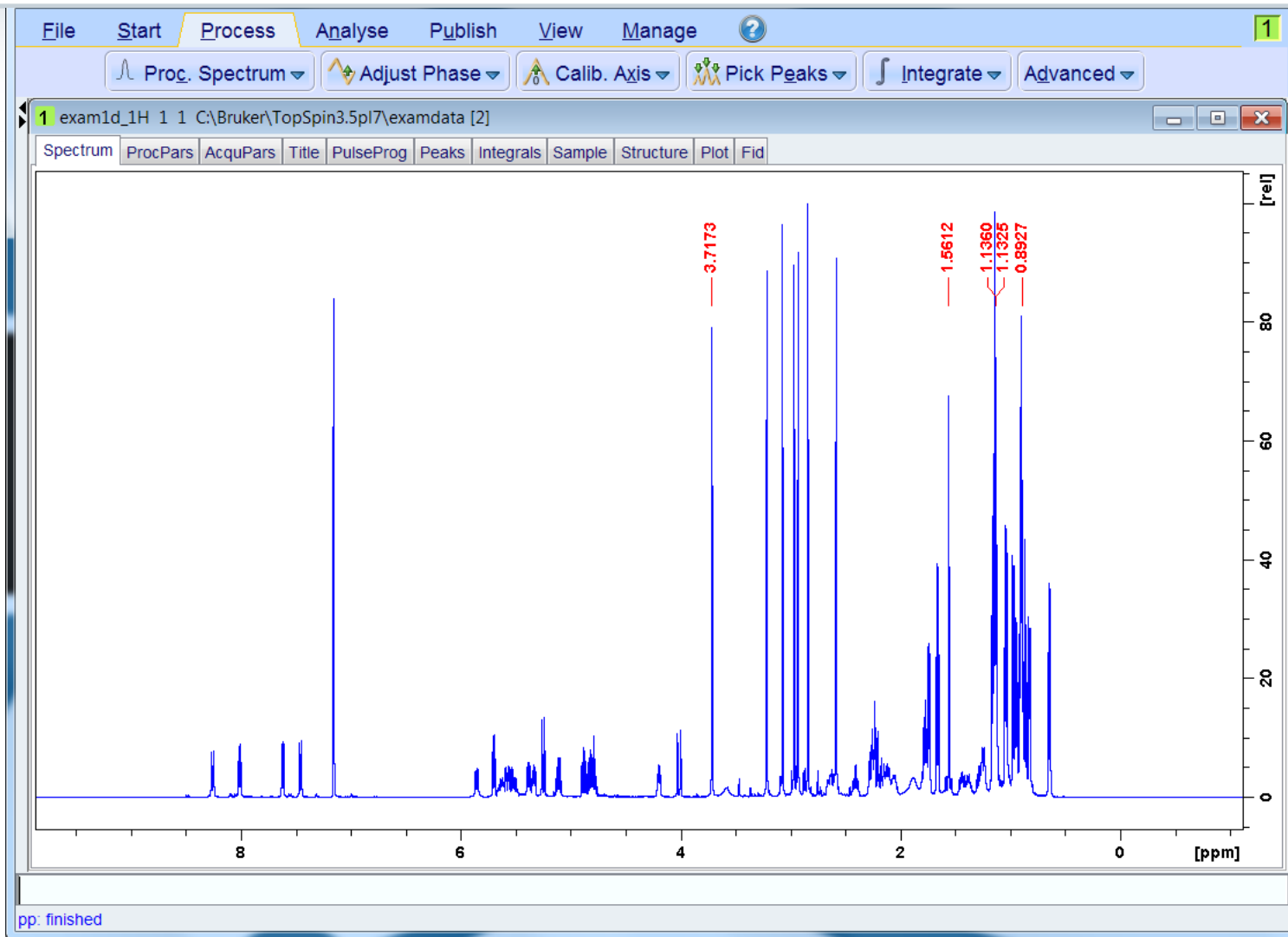
MI: 0.001
MAXI: 100
CY: 100
PC: 1

Automatic Peak Picking



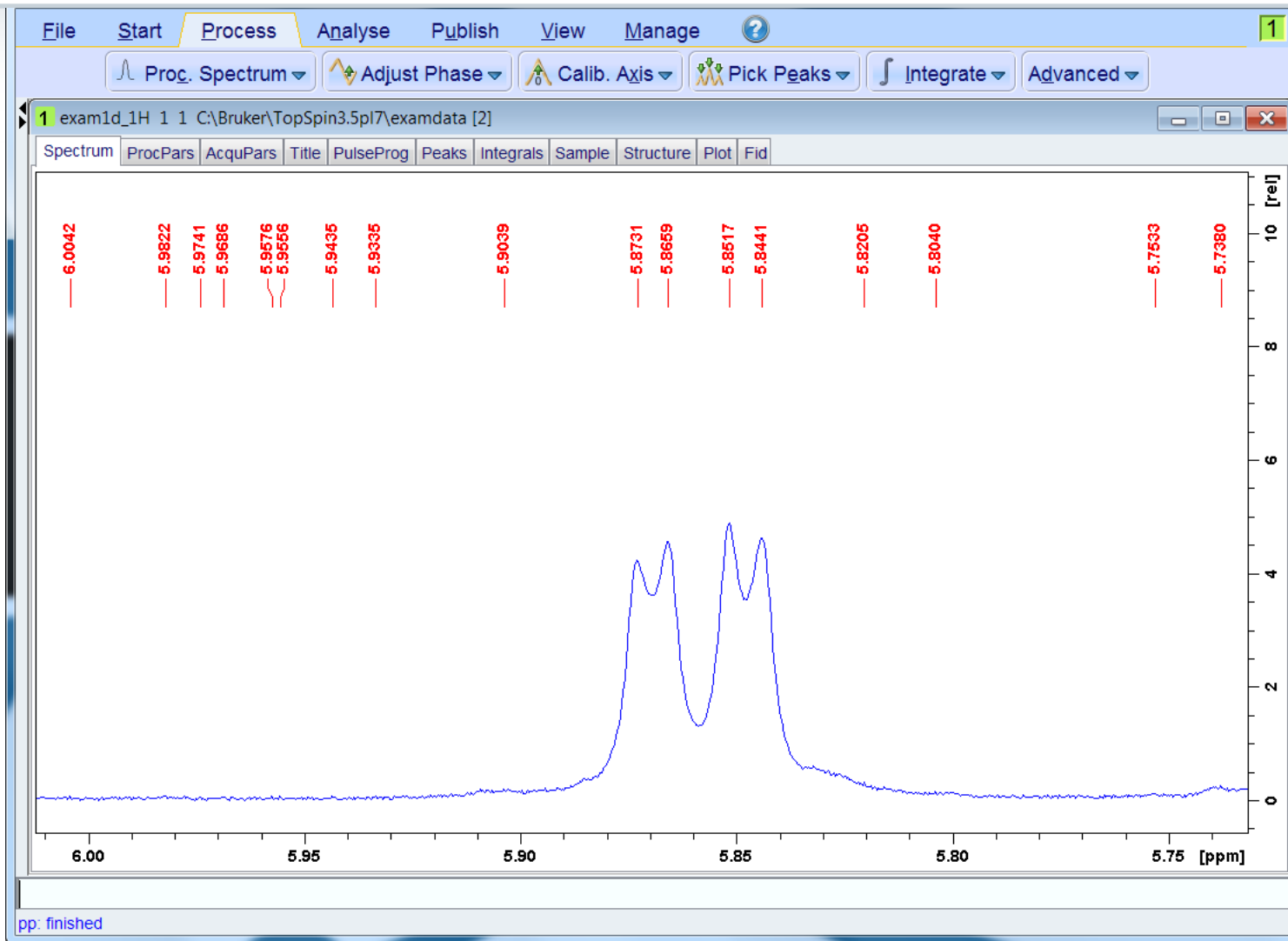
MI: 50
MAXI: 100
CY: 100
PC: 1

Automatic Peak Picking



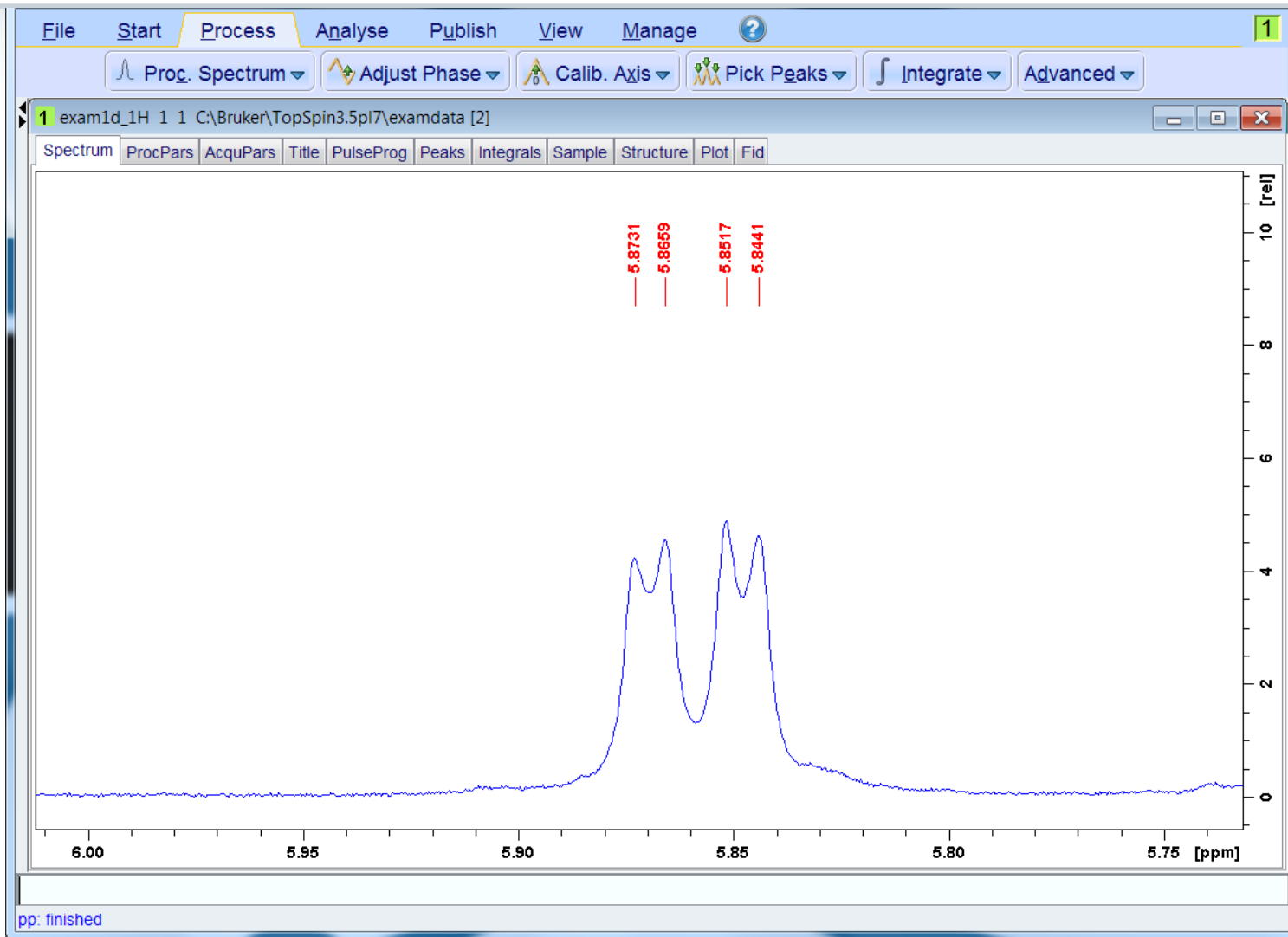
MI: 50
MAXI: 80
CY: 100
PC: 1

Automatic Peak Picking



MI: 0.001
MAXI: 100
CY: 100
PC: 1

Automatic Peak Picking



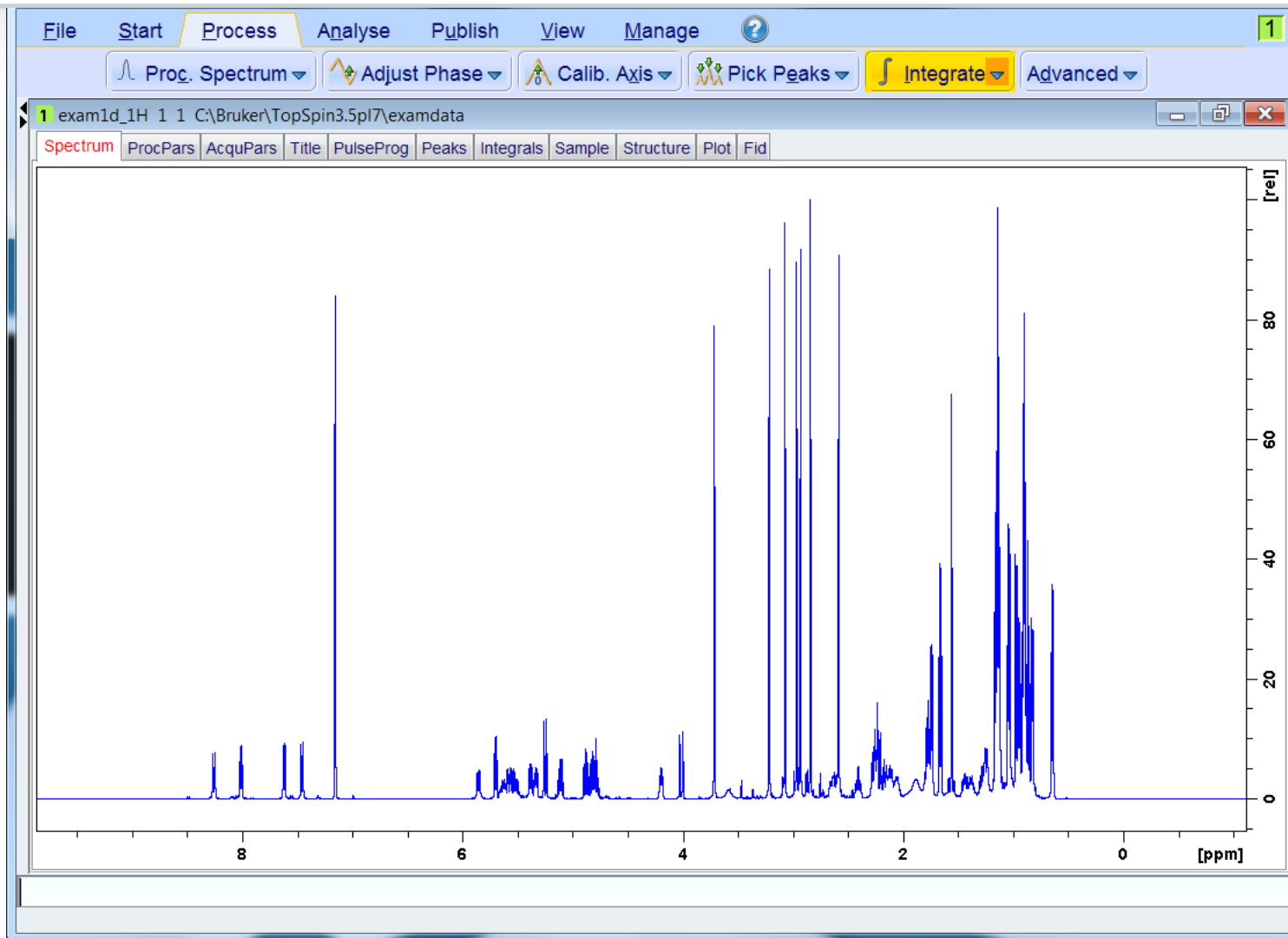
MI: 0.001
MAXI: 100
CY: 100
PC: 5

Integrate

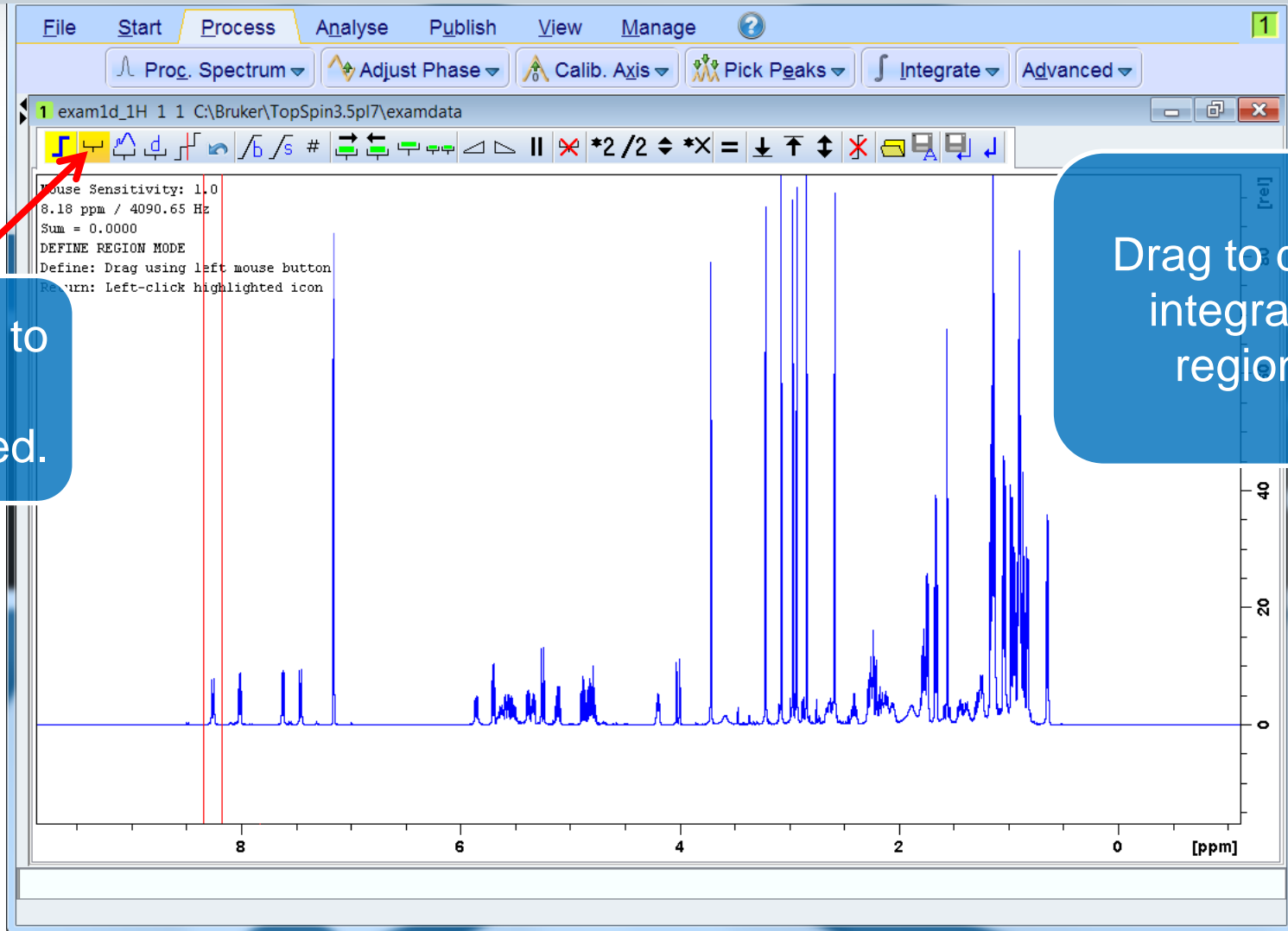


- Automatic integration [**int auto**]
- Automatic integration with baseline correction [**abs**]
- [**.int**] open manual integration mode

Manual Integration



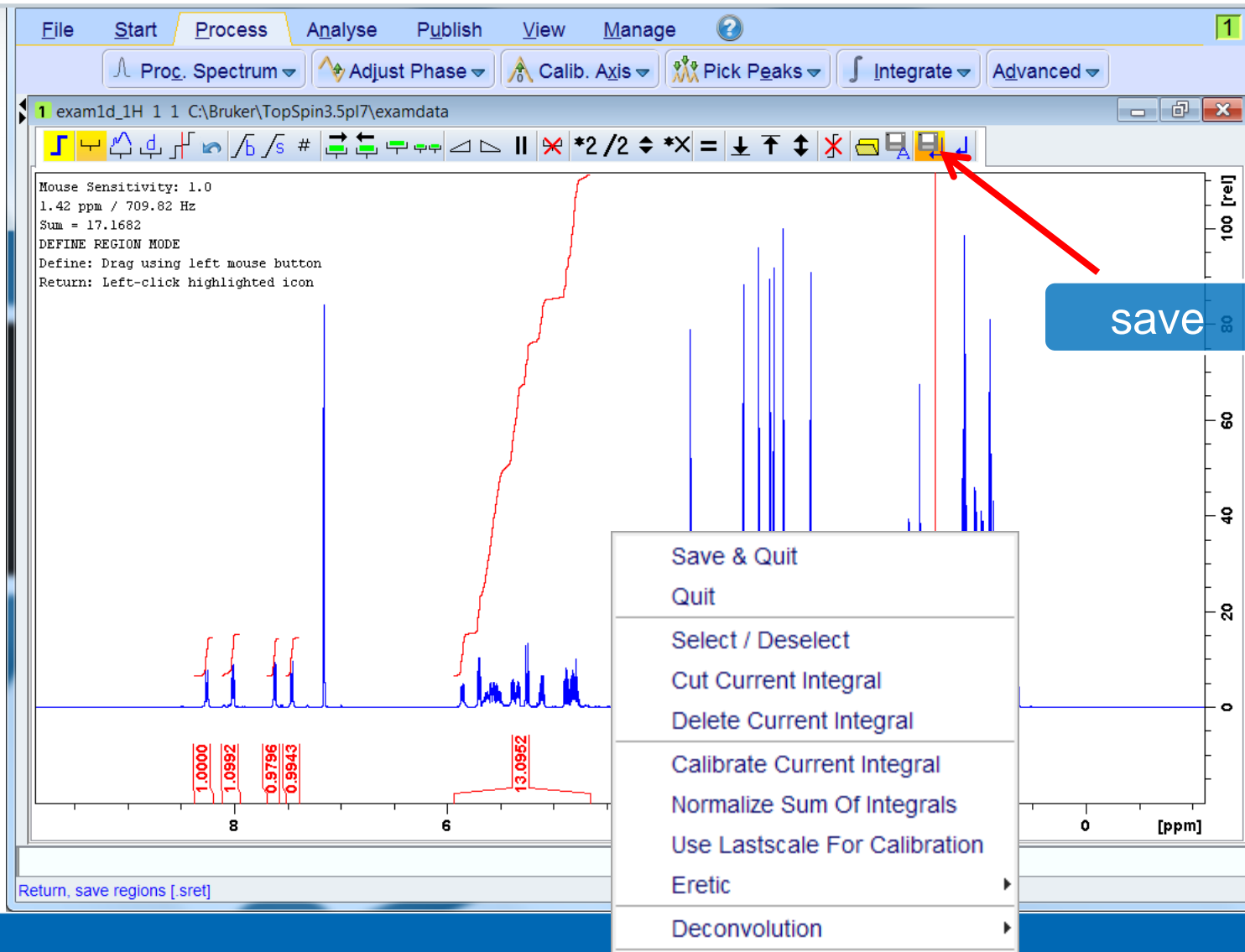
Manual Integration



Needs to be selected.

Drag to define integration regions.

Manual Integration



Integrals



File Start **Process** Analyse Publish View Manage

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

exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata

Object	Integral [abs]	Integral [rel]	Peaks	v(F1) [ppm]
Integral 1	7952946.33	1.0000	0	8.2896
Integral 2	8741599.39	1.0992	0	8.0320
Integral 3	7790588.66	0.9796	0	7.6377
Integral 4	7907330.26	0.9943	0	7.4538
Integral 5	104145465.43	13.0952	0	5.2986

- Expand
- Show spectrum
- Expand spectrum**
- Delete
- Define as reference
- Calibrate by reference
- Copy
- Export...
- Import...
- Print...
- Print preview...
- Table properties...

Parameters



- Parameters are :
 - integral extension factor (**AZFE**)
 - minimum distance between peaks (**AZFW**)
 - integral sensitivity factor (**ISEN**)
 - integral sensitivity factor (**ABSL**)
- Integral regions are extended at both sides by **AZFE** ppm. If this extension causes adjacent regions to overlap, the center of the overlap is used as the limit of the two regions.
- If peaks are more than **AZFW** apart, they are treated independently.
- Only the regions of integrals which are larger (area) than the largest integral divided by **ISEN** are stored.
- Data points greater than **ABSL** × (standard deviation) are considered spectral information

Automatic Integration

[int]



Integration - abs+li

Options

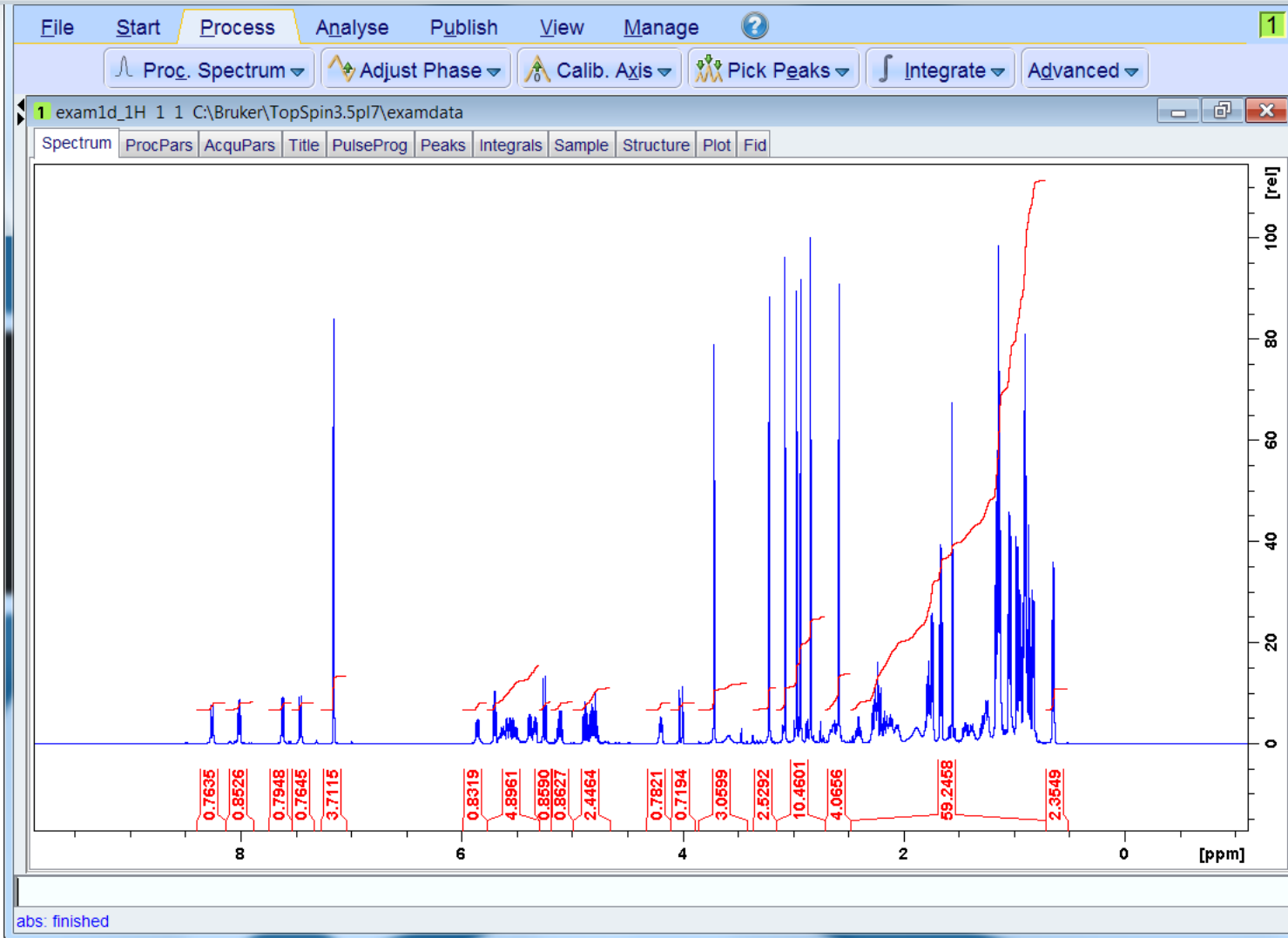
- Define integral regions manually
- Auto-find regions, integrate & display result
- Integrate existing regions (file 'intrng') & display result
- List peaks and integrals (using regions file 'intrng') within the displayed region
- List peaks and integrals (using regions file 'intrng') of the entire spectrum
- Integrate a list of spectra

Required parameters

Integration sensitivity factor ABSL (0..100) =	20
Minimum separation between independent integral regions AZFW [ppm] =	0.05
Integral region extension factor AZFE [ppm] =	0.1
Integral sensitivity factor with reference to the largest integral ISEN (>0) =	1024
Degree of polynomial ABSG (0..5) =	5
Left spectral range limit F1P [ppm] =	9.87574863433837
Right spectral range limit F2P [ppm] =	-1.1104046957893
Scale 1D integrals relative to a reference dataset INTSCL (-1, 0, >0) =	1
Automatic baseline correction of integrals (if regions auto-detected!) INTBC =	yes

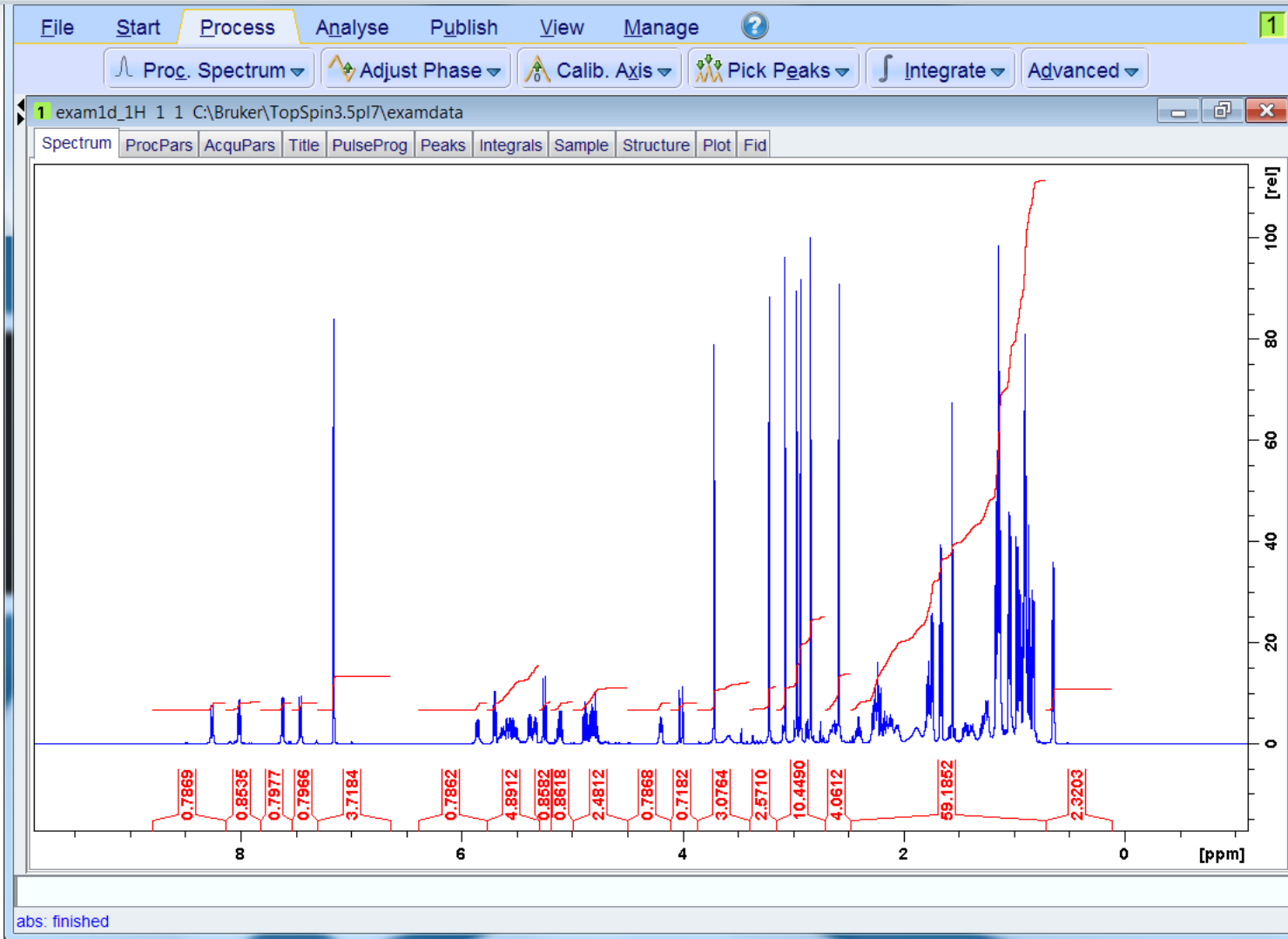
OK Cancel Help

Automatic Integration



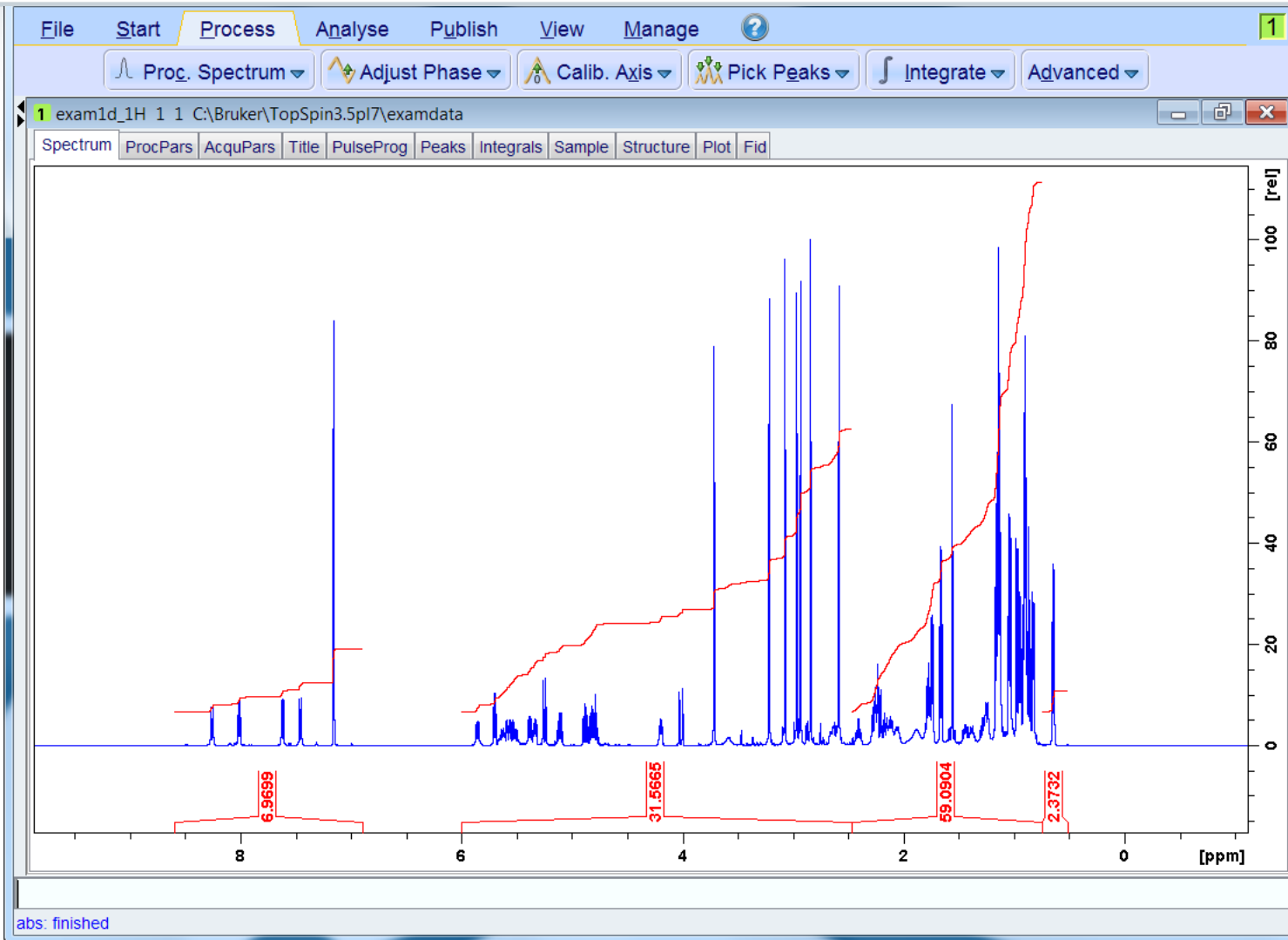
ISEN: 128
AZFE: 0.1
AZFW: 0.05
ABSL: 20

Automatic Integration



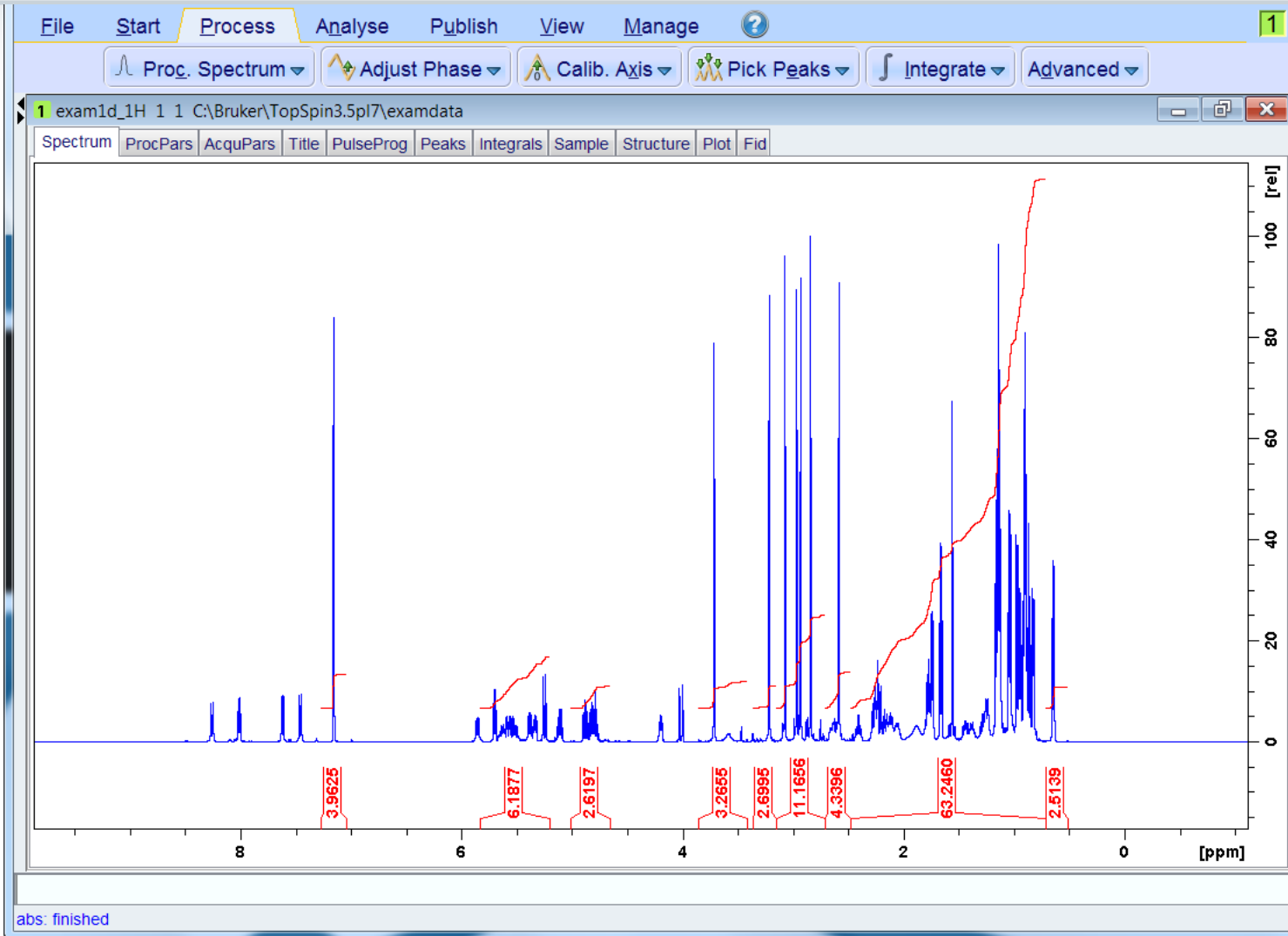
ISEN: 128
AZFE: 0.5
AZFW: 0.05
ABSL: 20

Automatic Integration



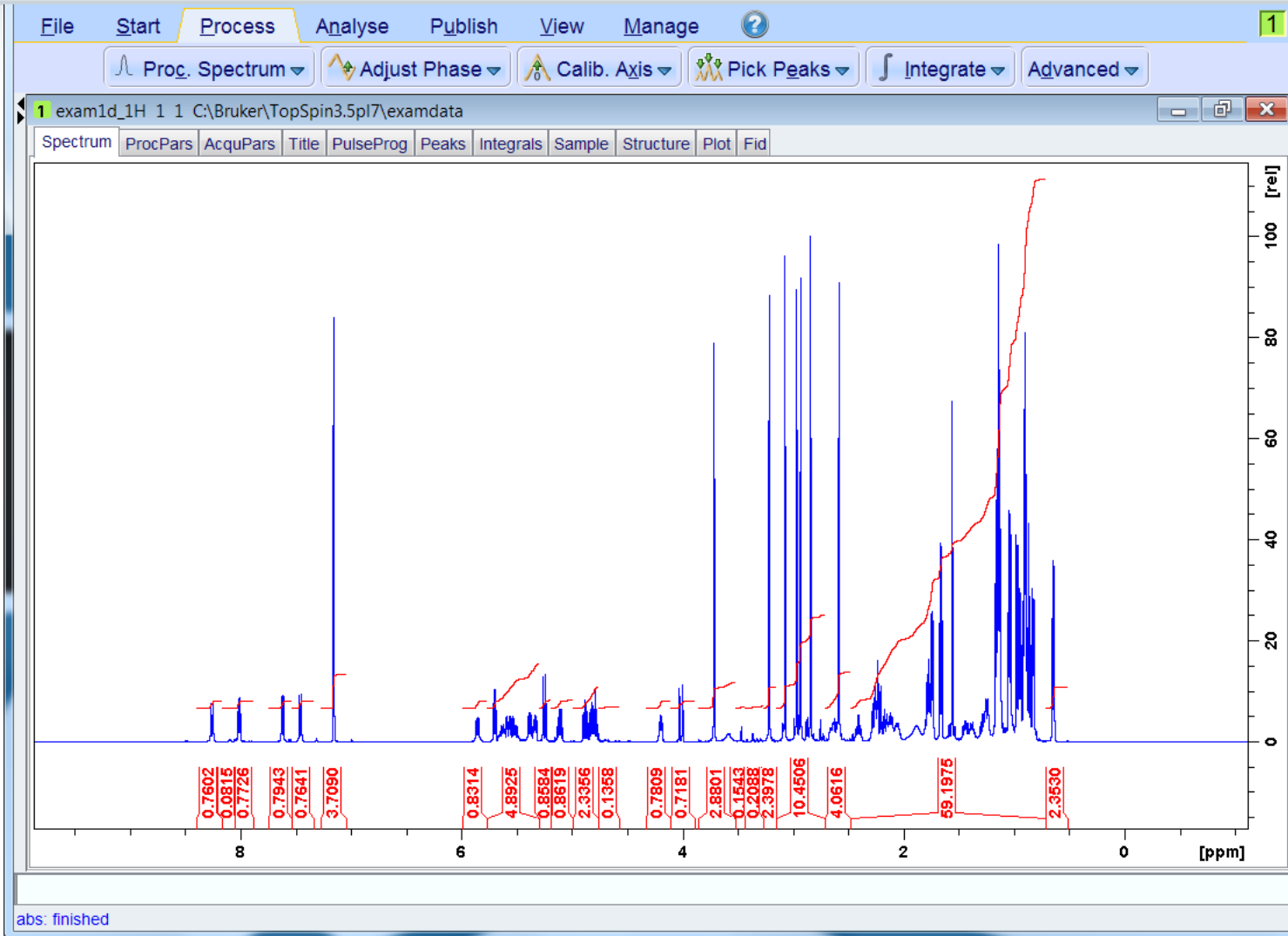
ISEN: 128
AZFE: 0.1
AZFW: 0.5
ABSL: 20

Automatic Integration



ISEN: 64
AZFE: 0.1
AZFW: 0.05
ABSL: 20

Automatic Integration



ISEN: 1k
AZFE: 0.1
AZFW: 0.05
ABSL: 20

Advanced

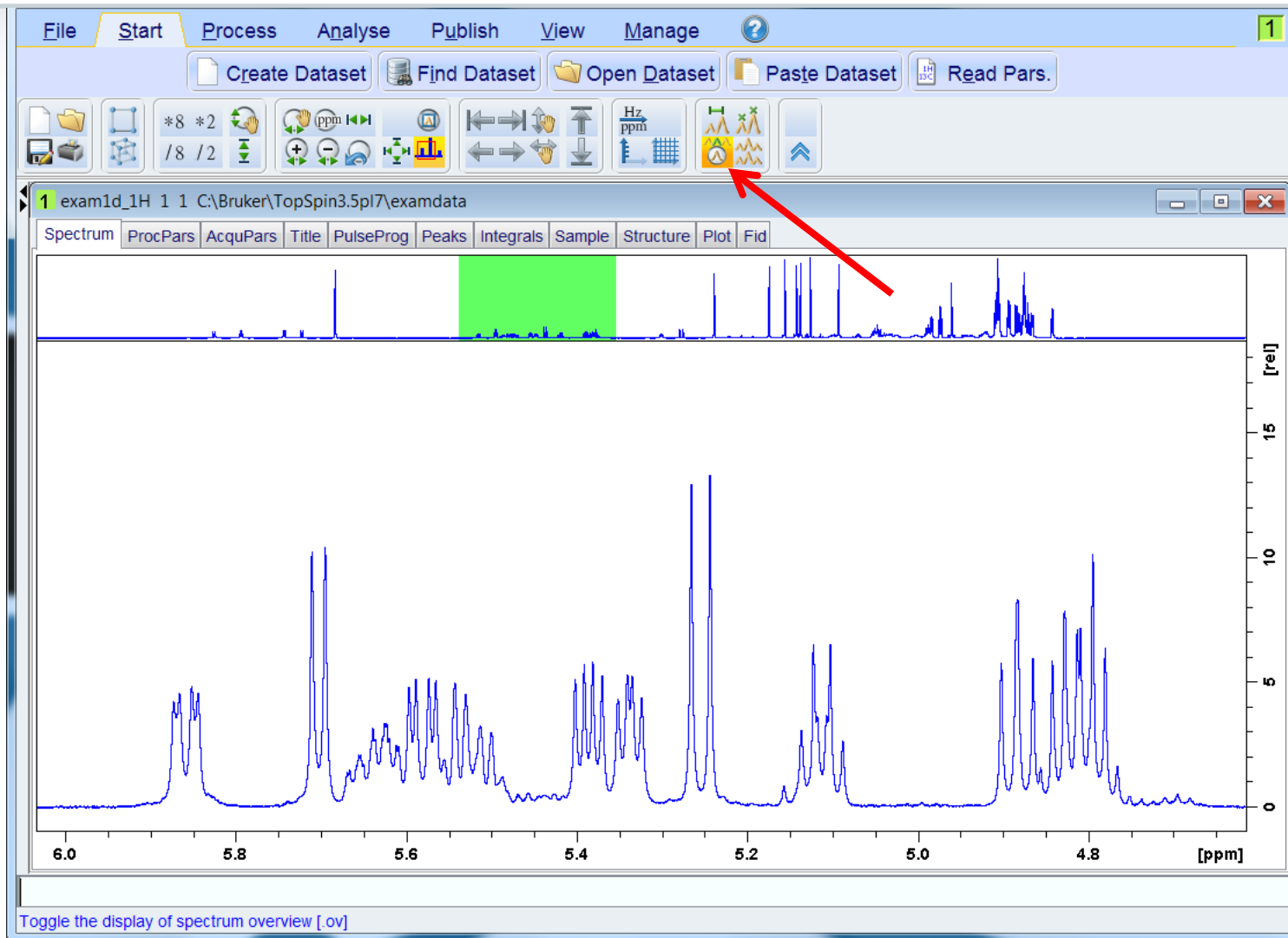


The screenshot shows the Bruker software interface with the 'Advanced' menu open. The menu items are:

Process Dataset <u>L</u> ist (serial)	Manual correction mode (.basl)
Integrate Spectra <u>L</u> ist (intser)	Repeat Correction Using File <i>base_info</i> (bcm)
ROI View of Spectra <u>L</u> ist (vregs)	Automatic Using Polynomial of Degree ABSG (abs n)
Add/Sub./Mujt. Spectra (adsu)	Like abs, Only In Range F1/F2 (absf n)
Reference <u>D</u> econvolution (.refdcon)	Automatic, Alternate Algorithm (absd n)
Correct Baseline	Setup Spline File <i>baslpts</i> (.baslpts)
Special Transforms	Spline-Correct Using <i>baslpts</i> (sab)
Mjiscellaneous Operations	Correct FID Using Parameter BC_mod (bc)

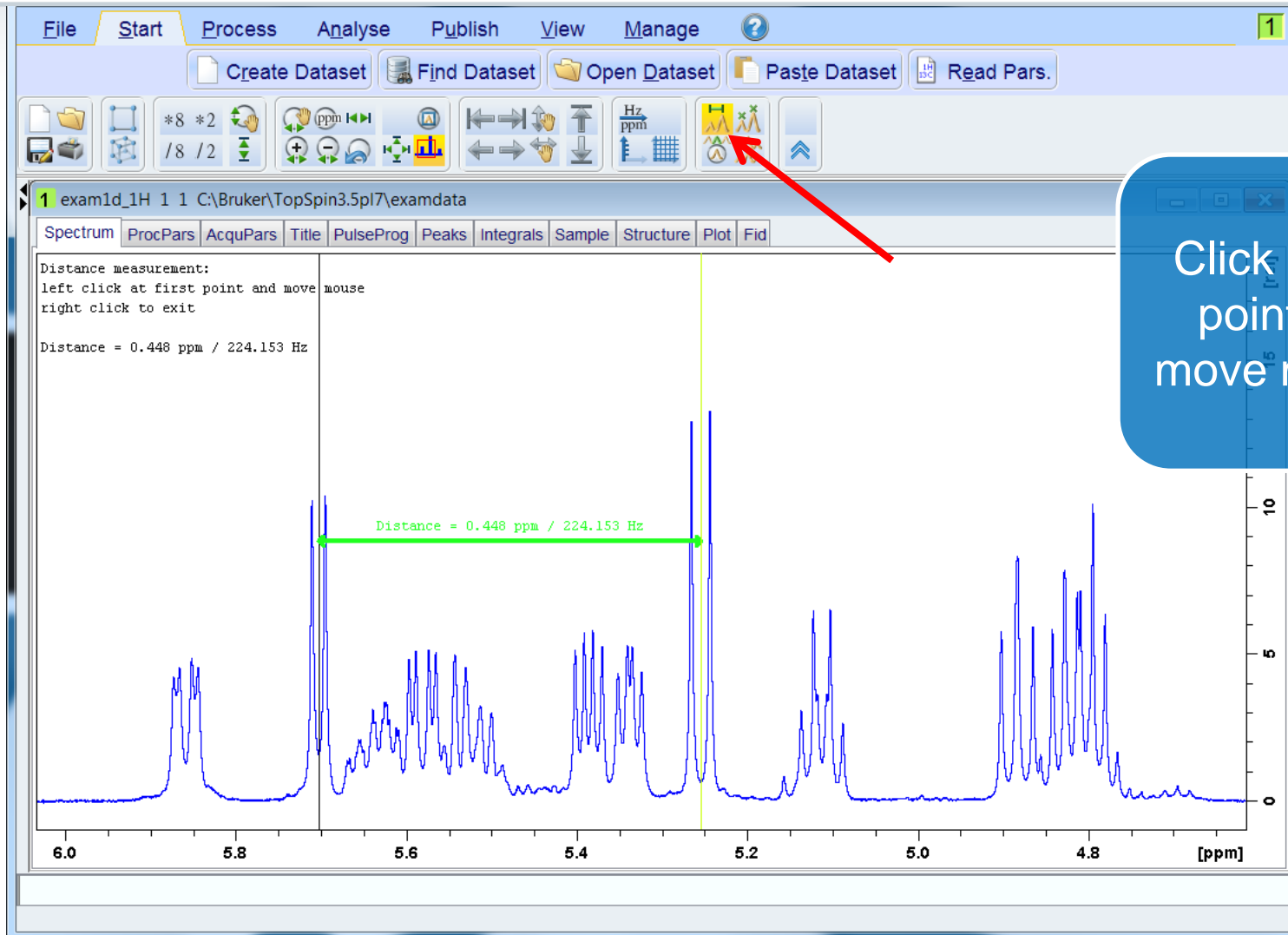
- [**abs**] performs automatic baseline correction and integration
- [**abs n**] performs automatic baseline correction (no integration)
- [**.basl**] manual baseline correction mode
- [**bas**] opens dialog for baseline correction

Toggle spectrum overlay



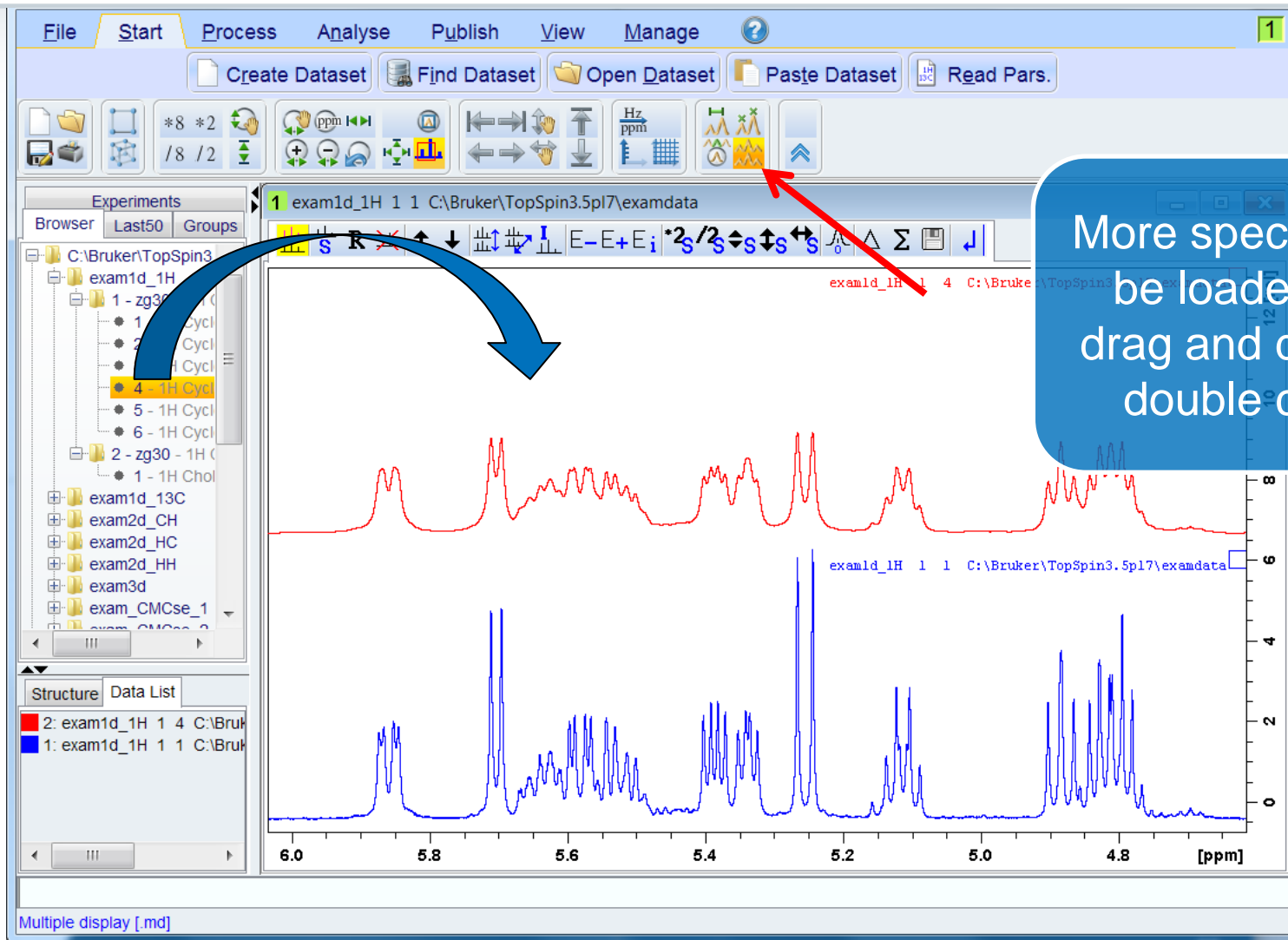
Toggle the display of spectrum overview [ov]

Measure distances



Click at first point and move mouse.

Dual display



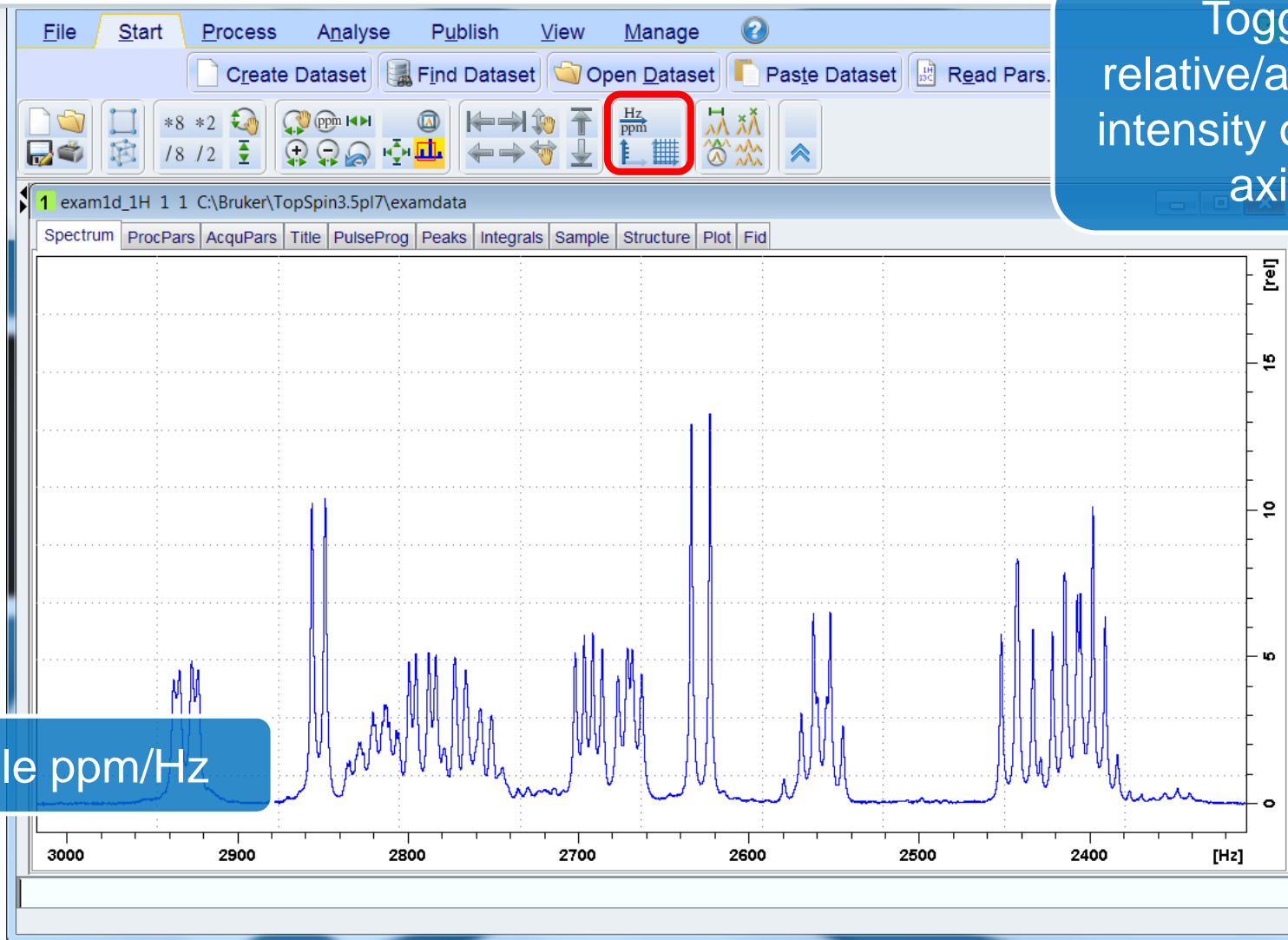
More spectra can be loaded via drag and drop or double click.

Multiple display [.md]

Toggle axis units and grid

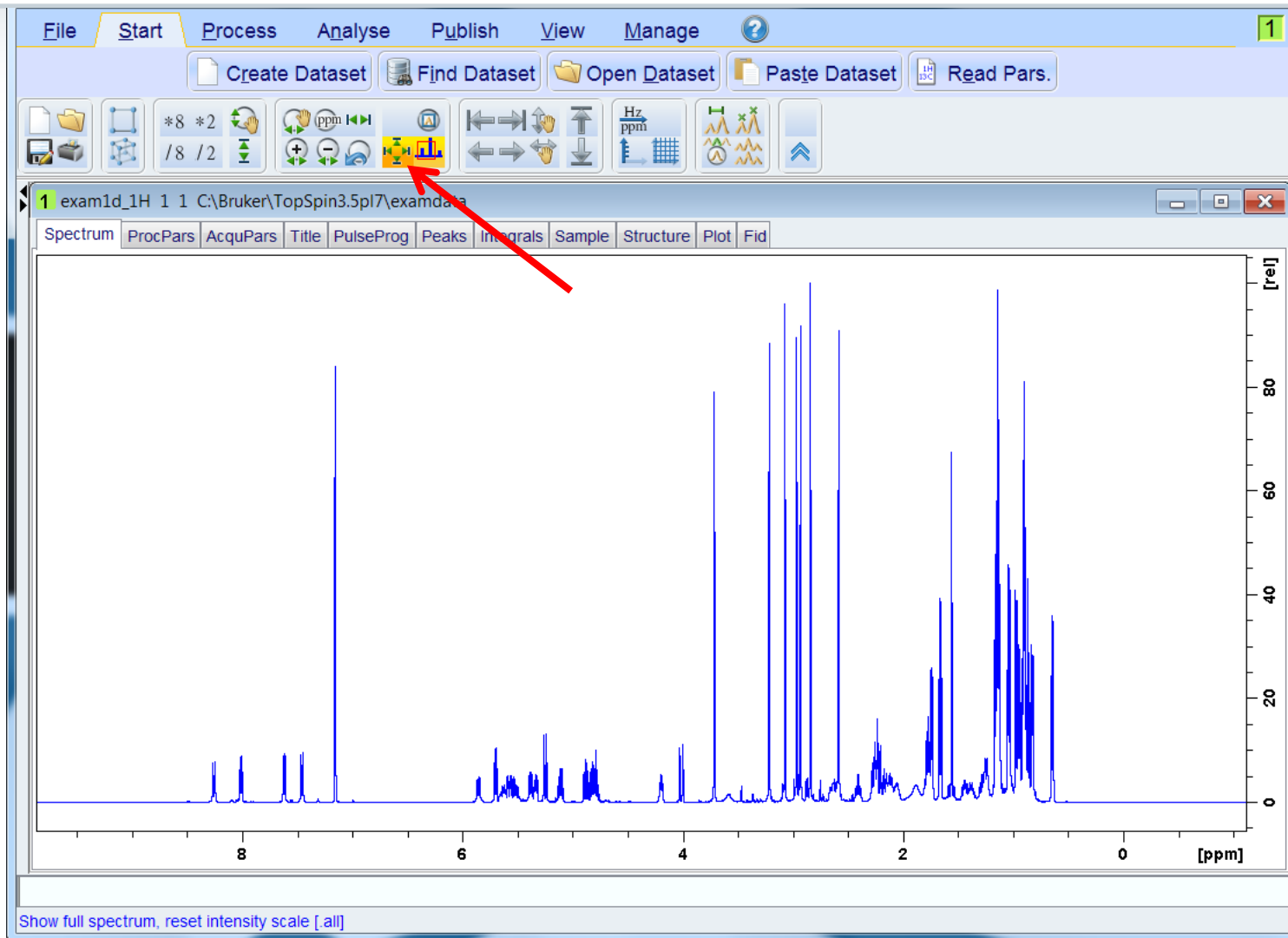


Toggle relative/absolute intensity or hides axis

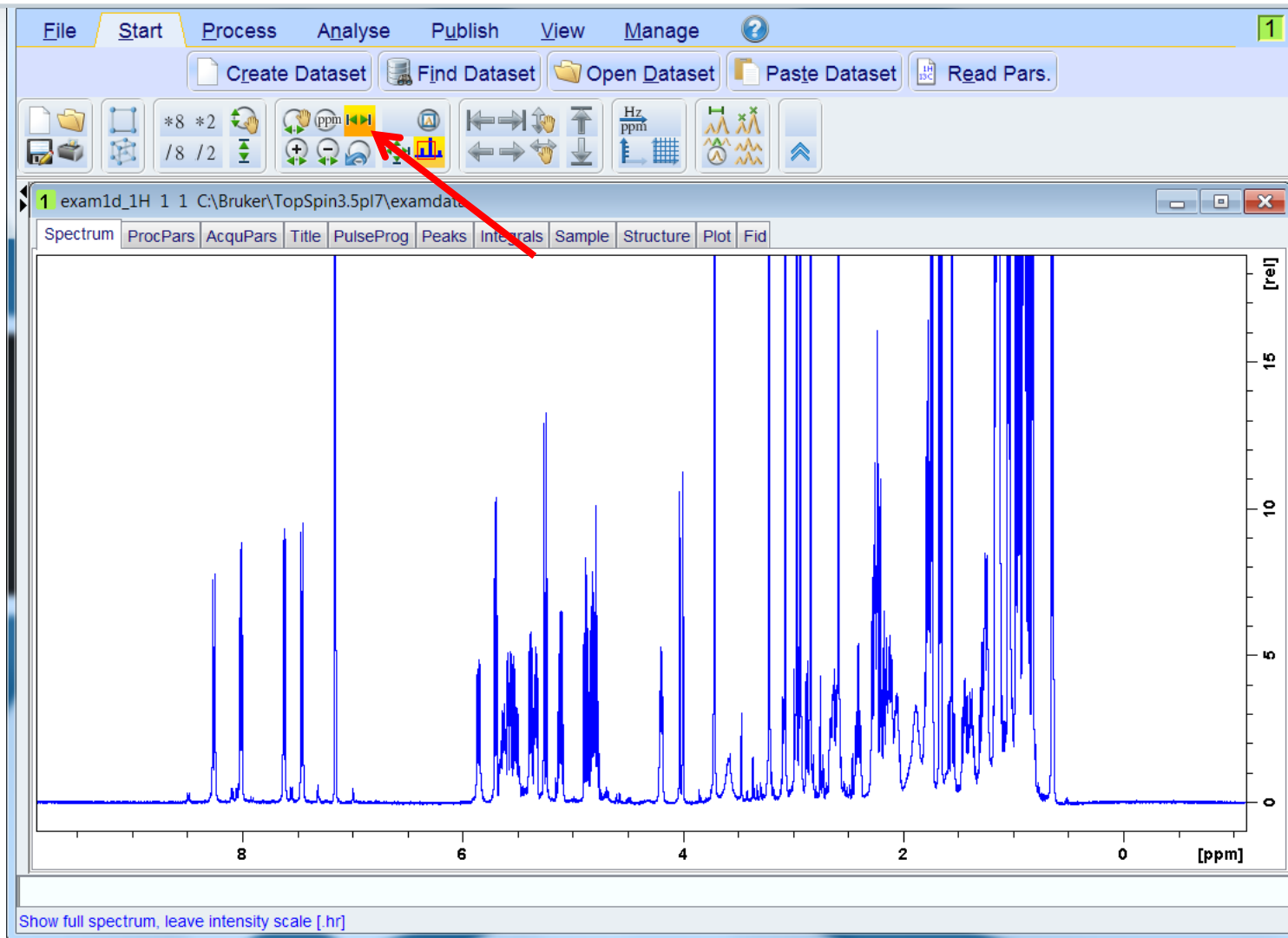


Toggle ppm/Hz

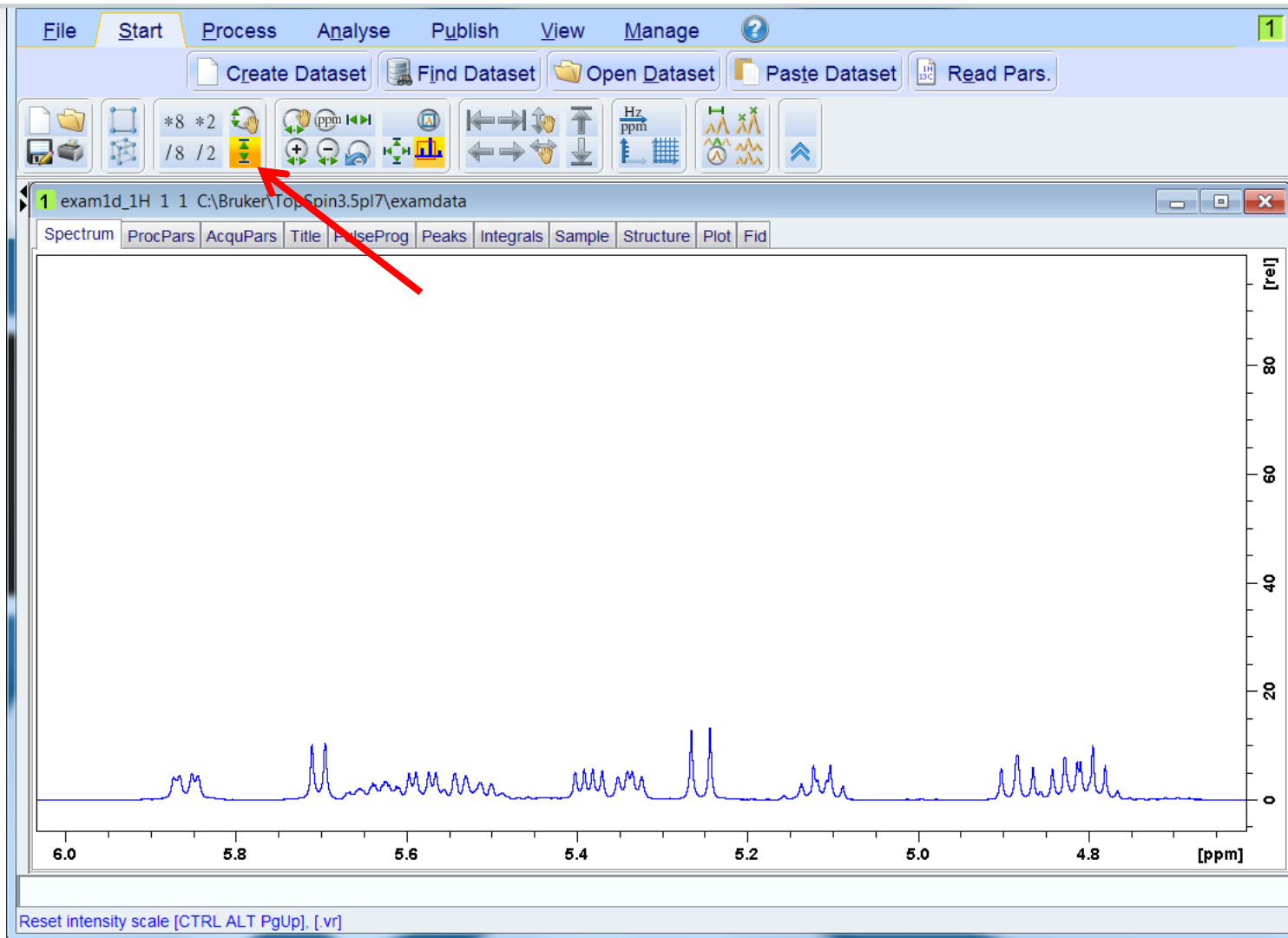
Show full spectrum, reset intensity



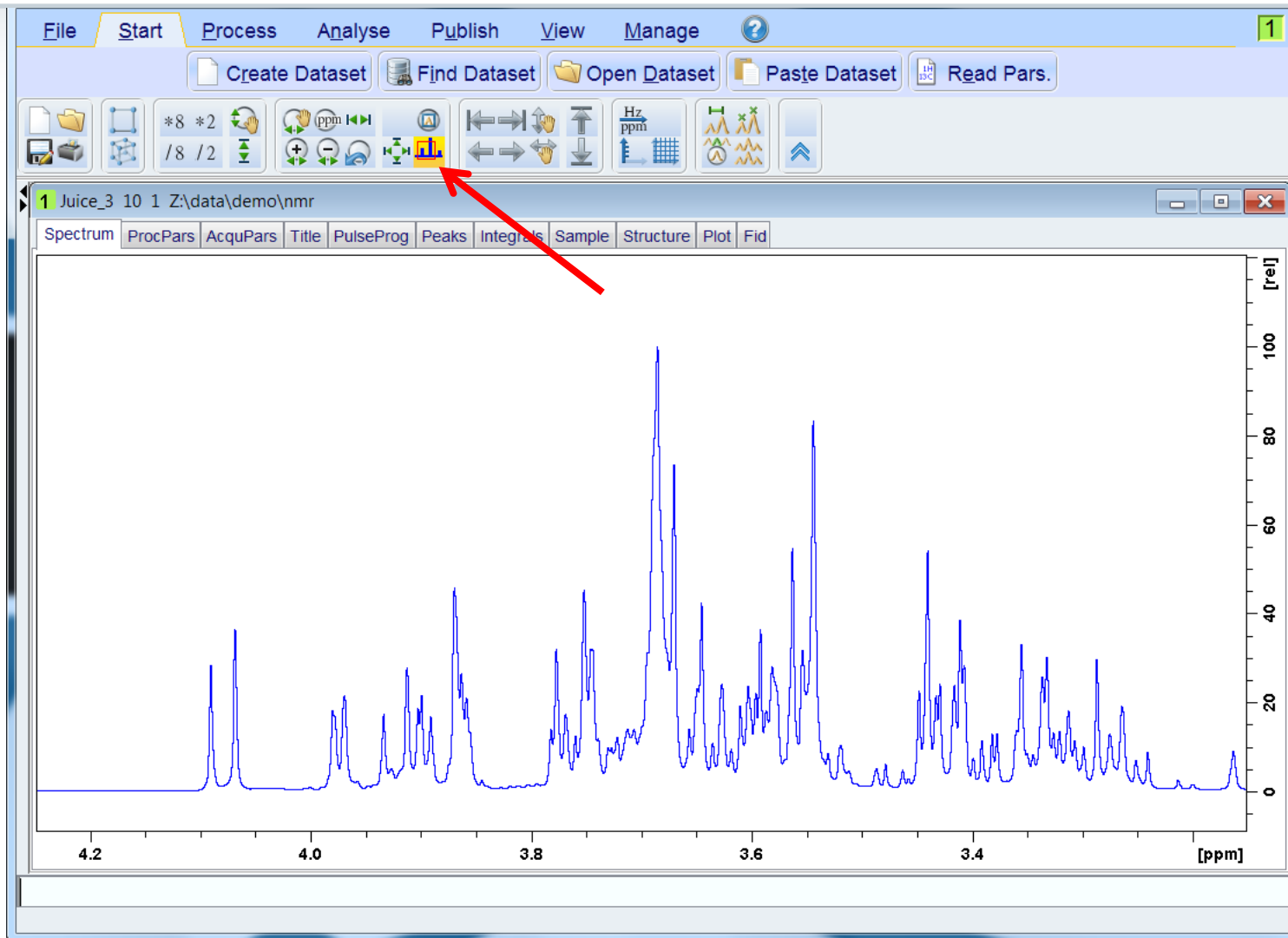
Show full spectrum, do not reset intensity



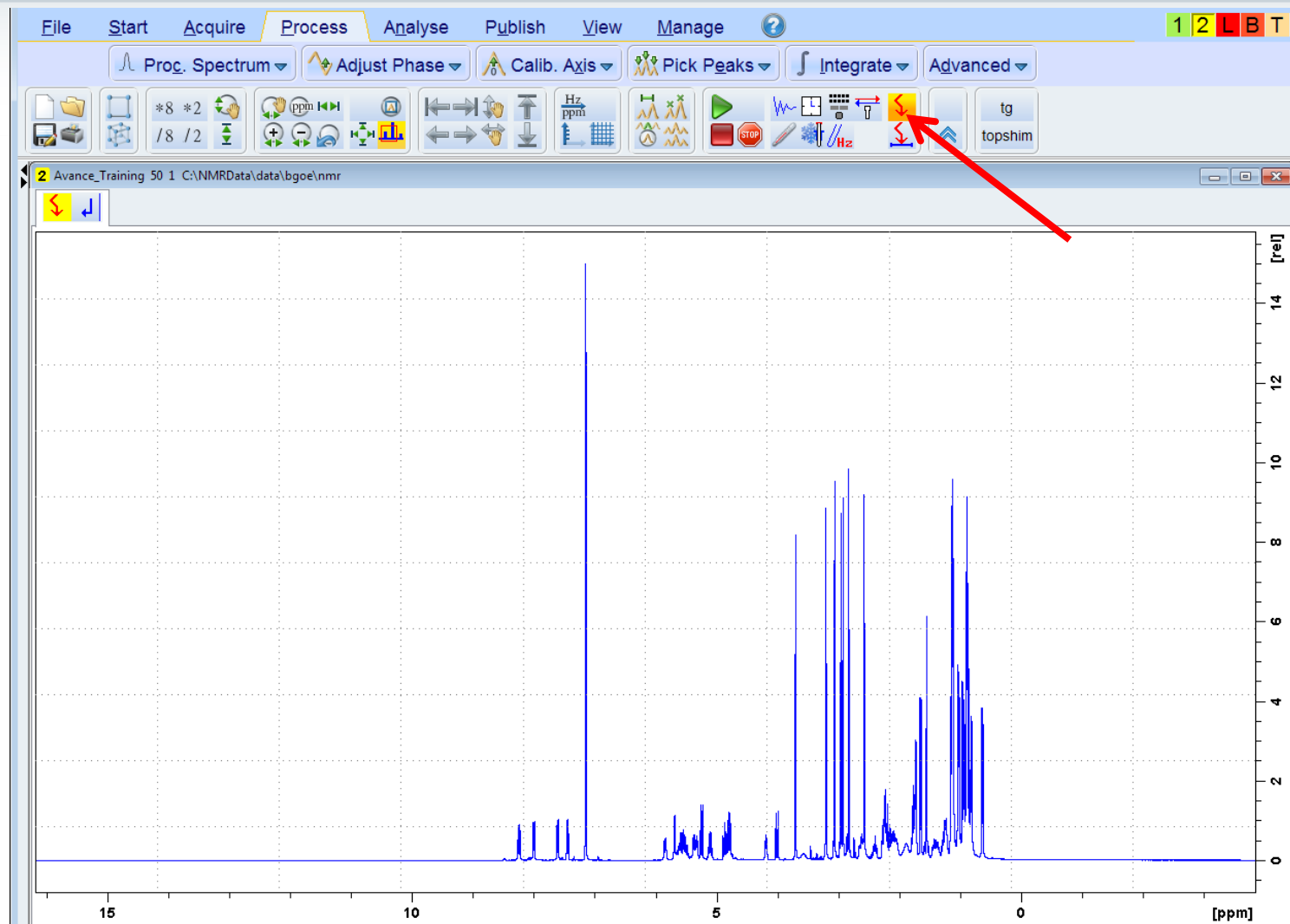
Reset intensity



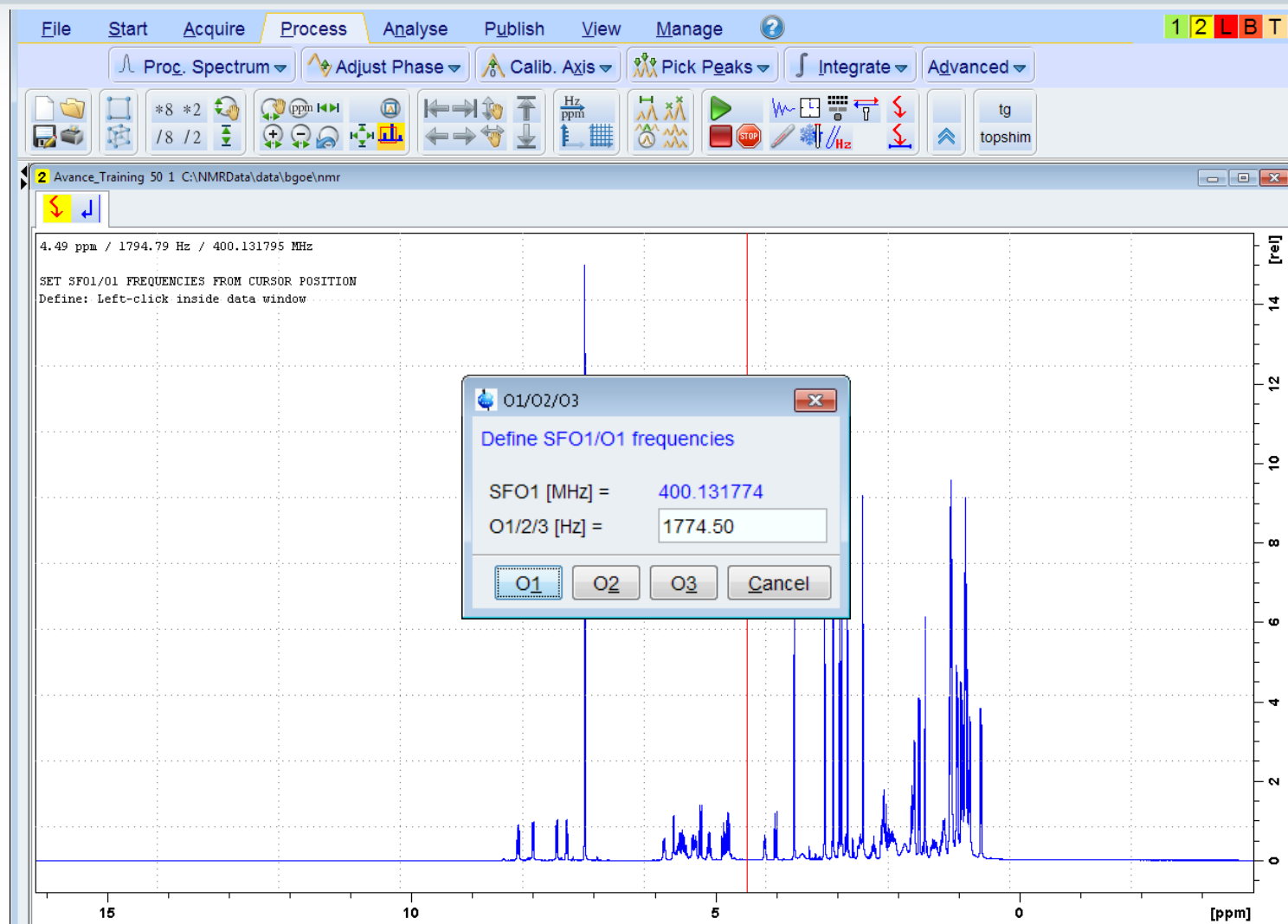
Retain scale and intensity



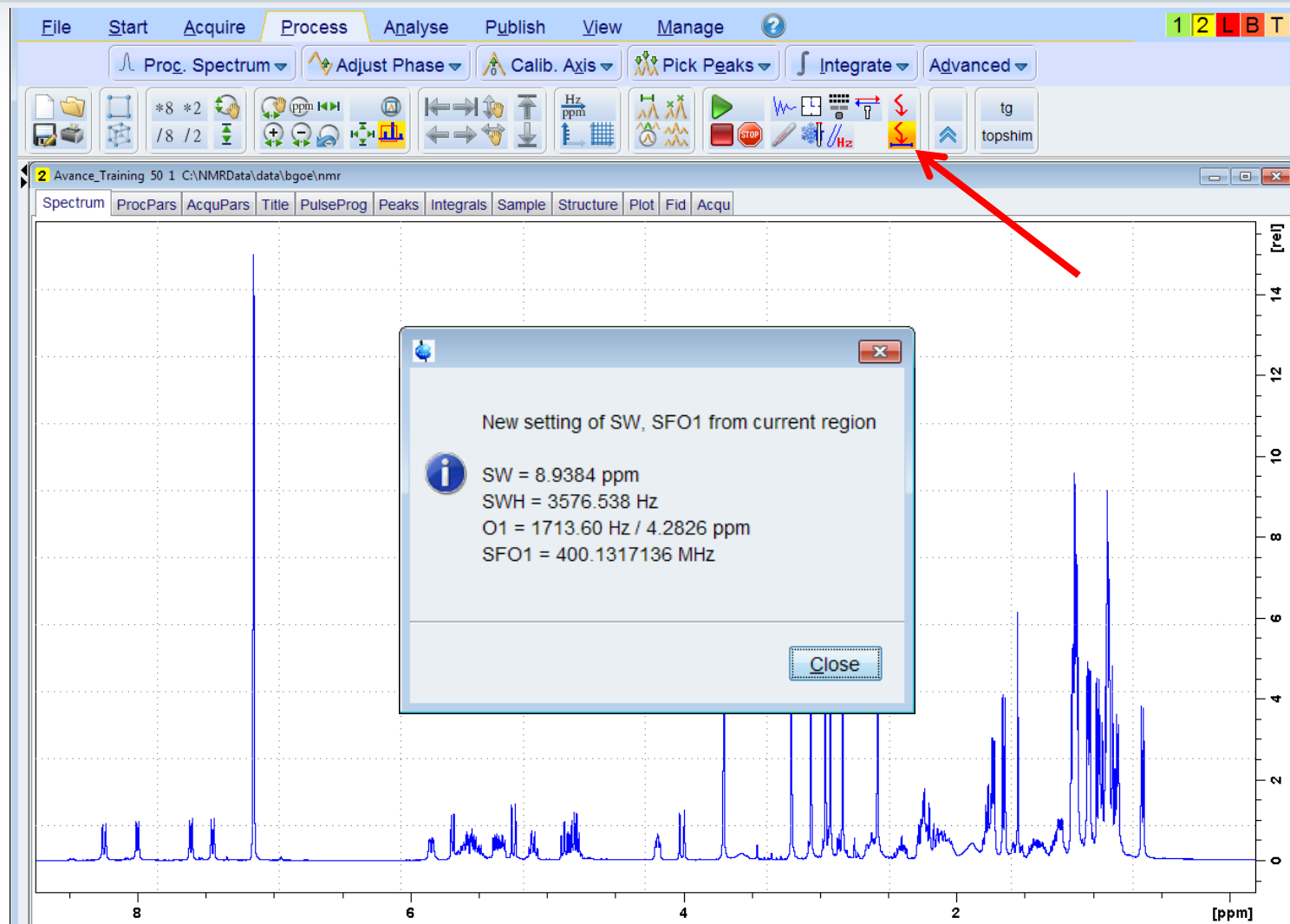
Set transmitter frequency by cursor

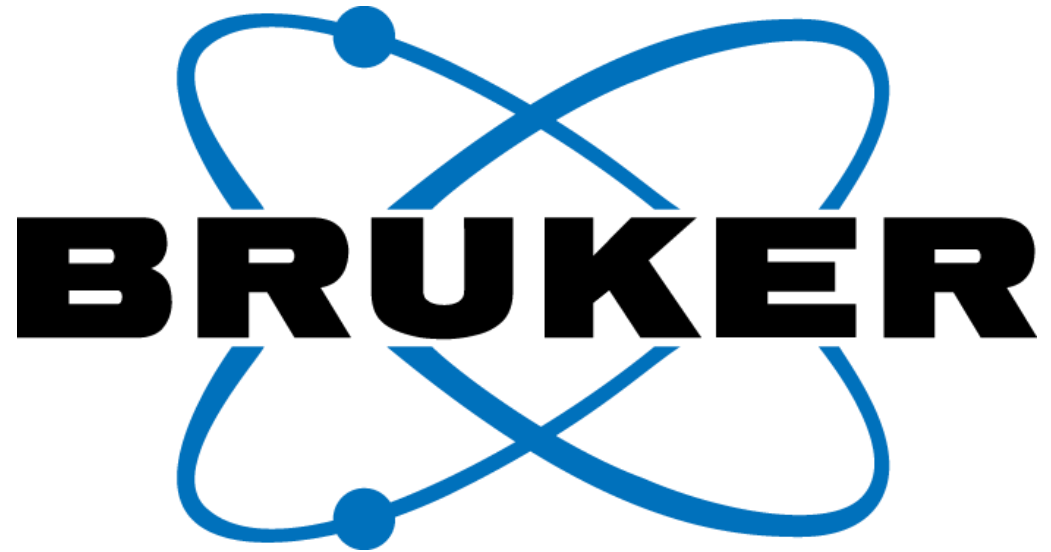


Set transmitter frequency by cursor



Set SW to current region and O1 in center





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