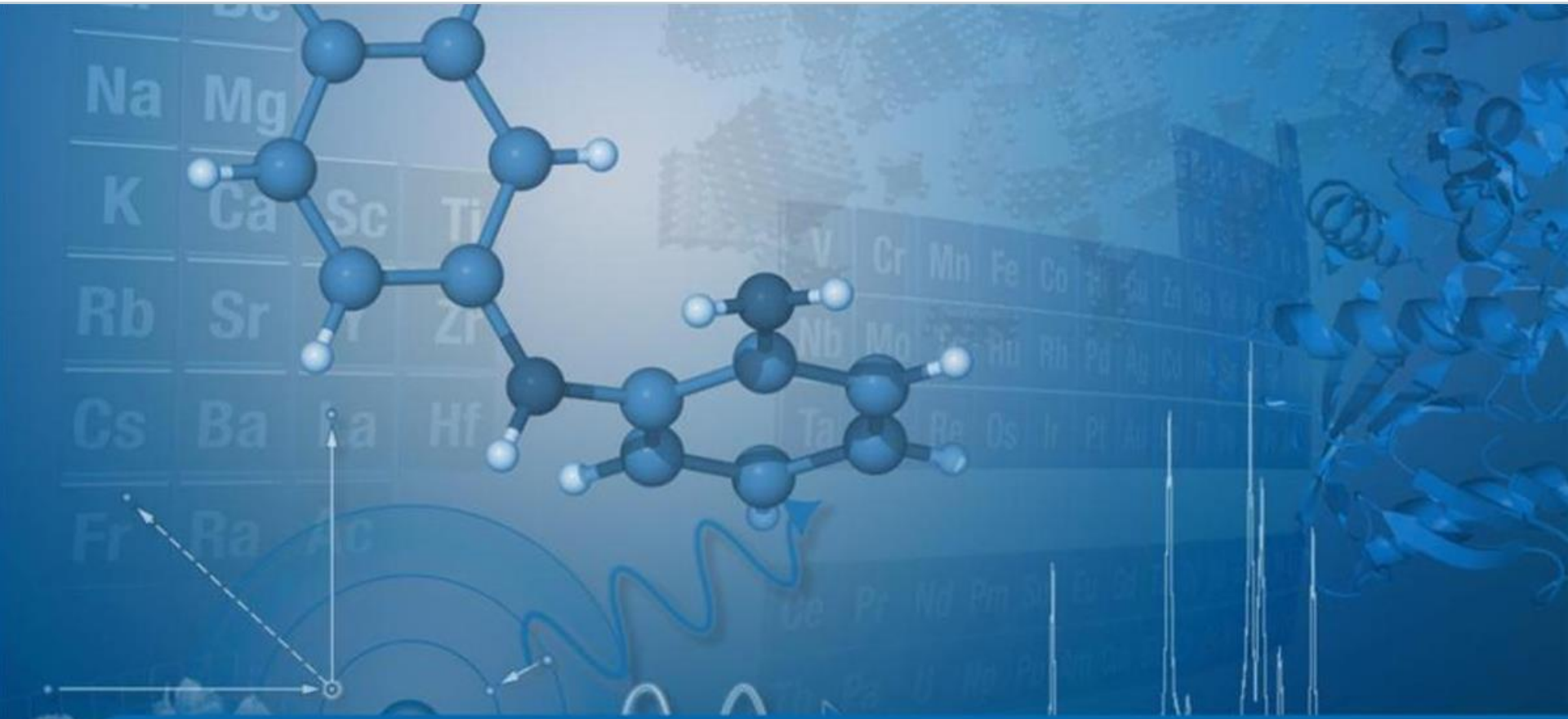
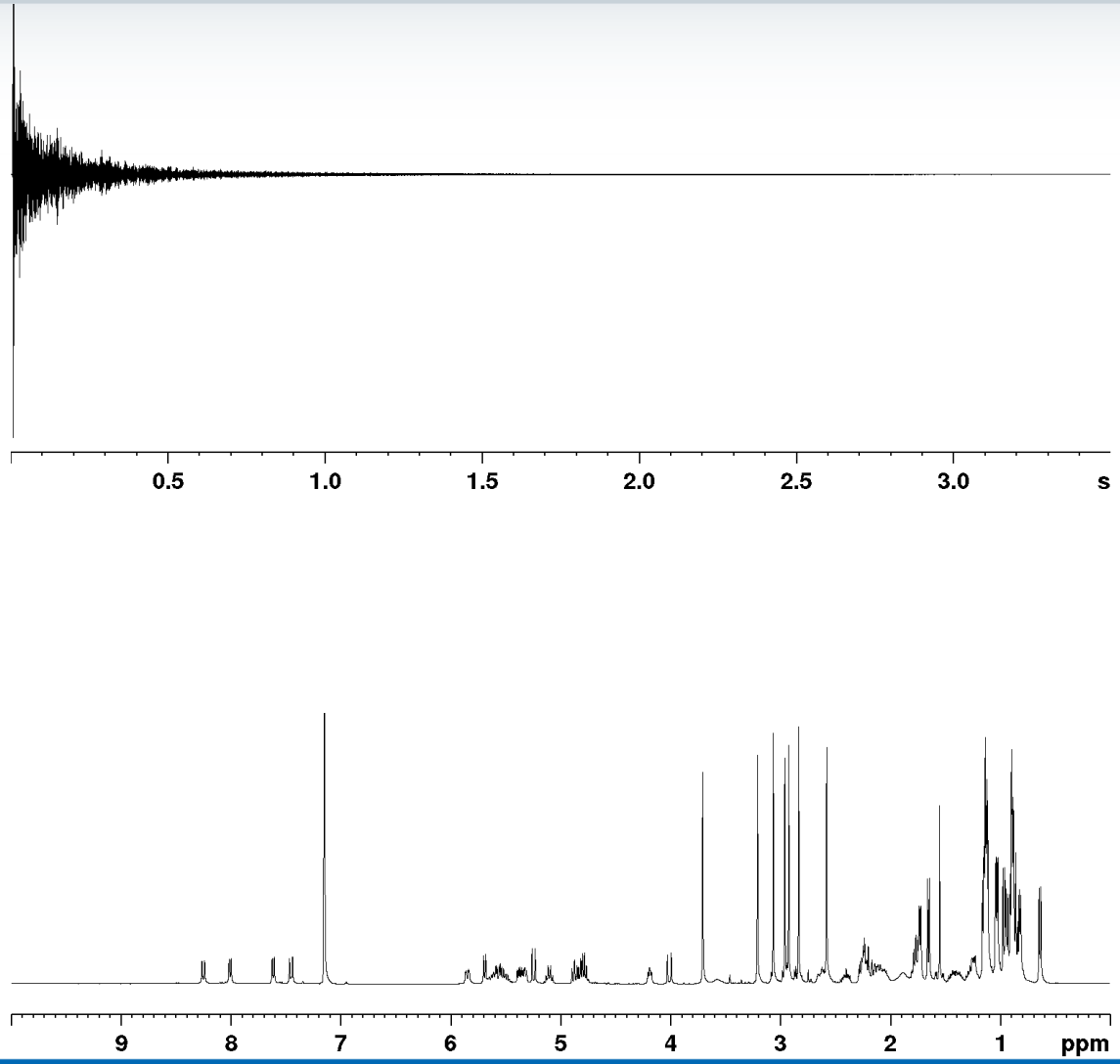
1D Processing

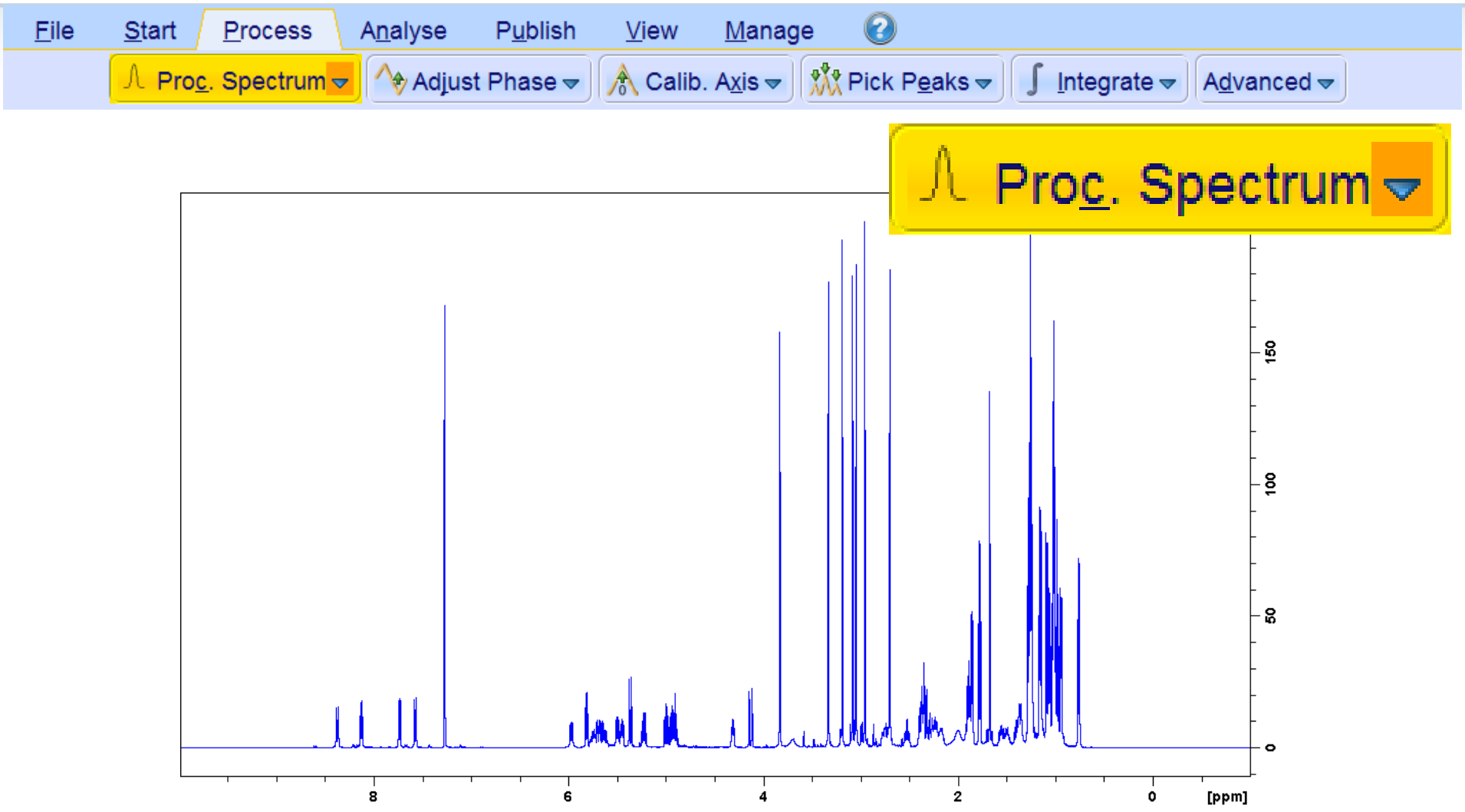
Dr. Benjamin Görling



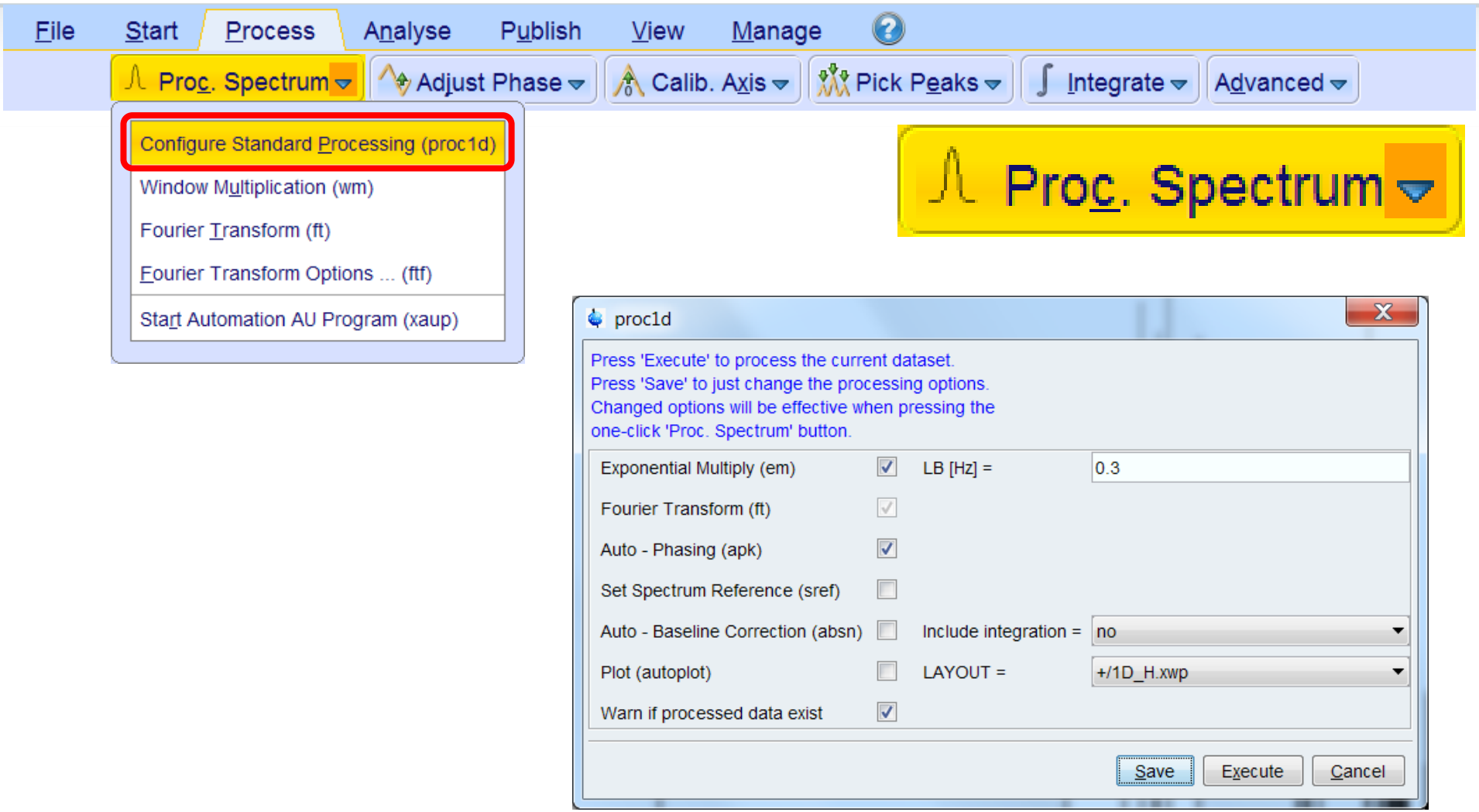
How to get a good spectrum?



1-Click processing



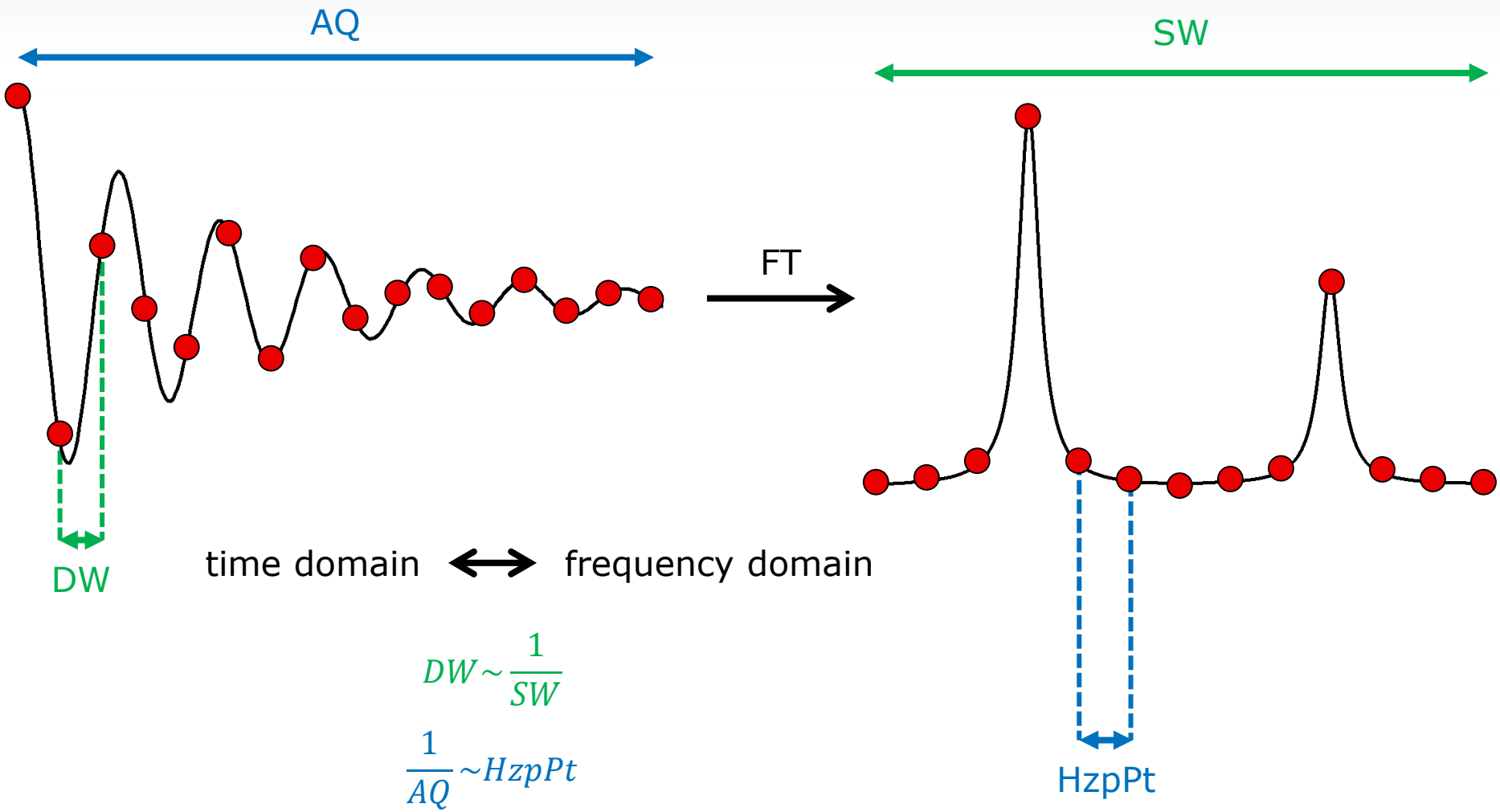
1-Click processing options



Processing commands

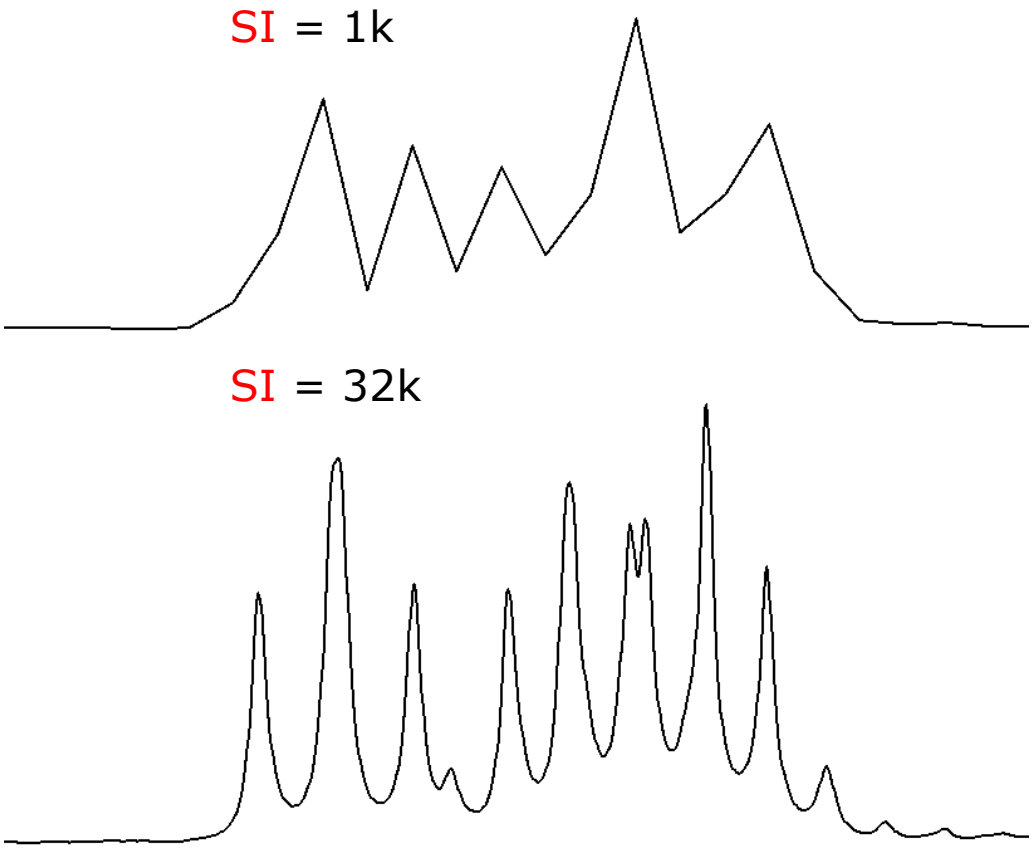
- [**ft**] Fourier transformation
- [**em**] multiplication with exponential window function
- [**pk**] phase spectrum
- [**fp**] [**ft**] + [**pk**]
- [**ef**] [**em**] + [**ft**]
- [**efp**] [**em**] + [**ft**] + [**pk**]

Fourier transformation



Resolution

- To get a good resolution you need enough data points TD (acquisition) and SI (processing).
- $SI = \frac{TD}{2}$



Resolution

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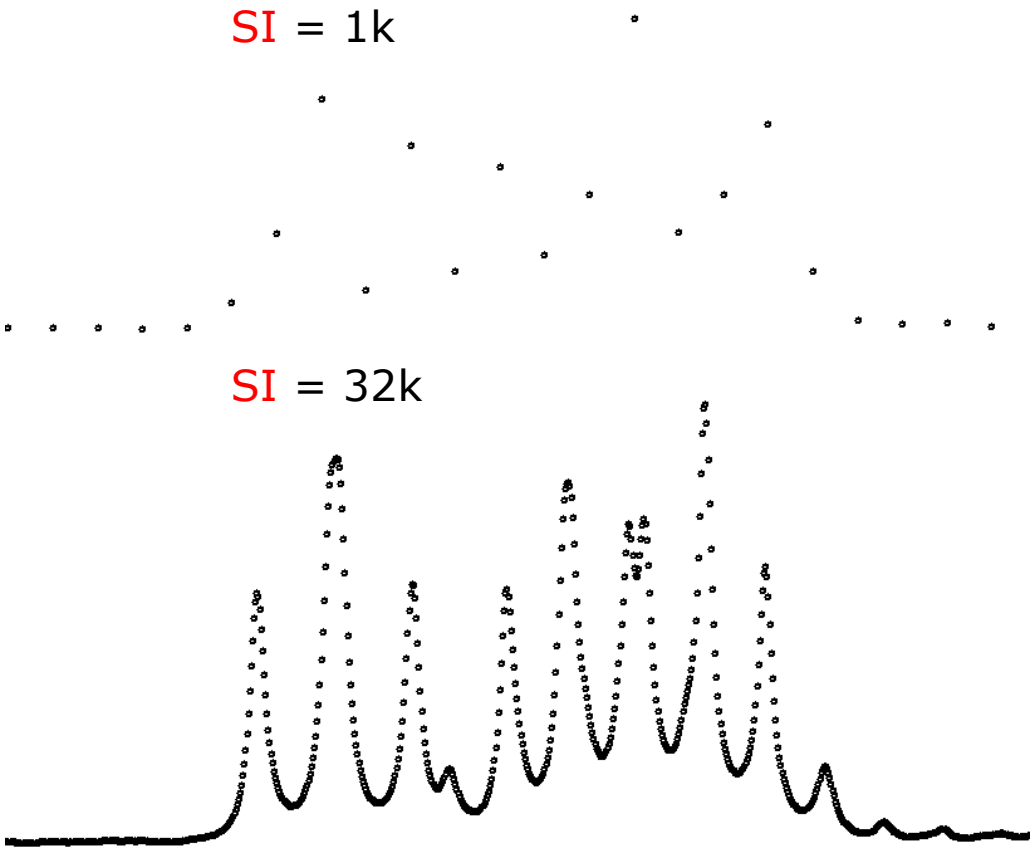
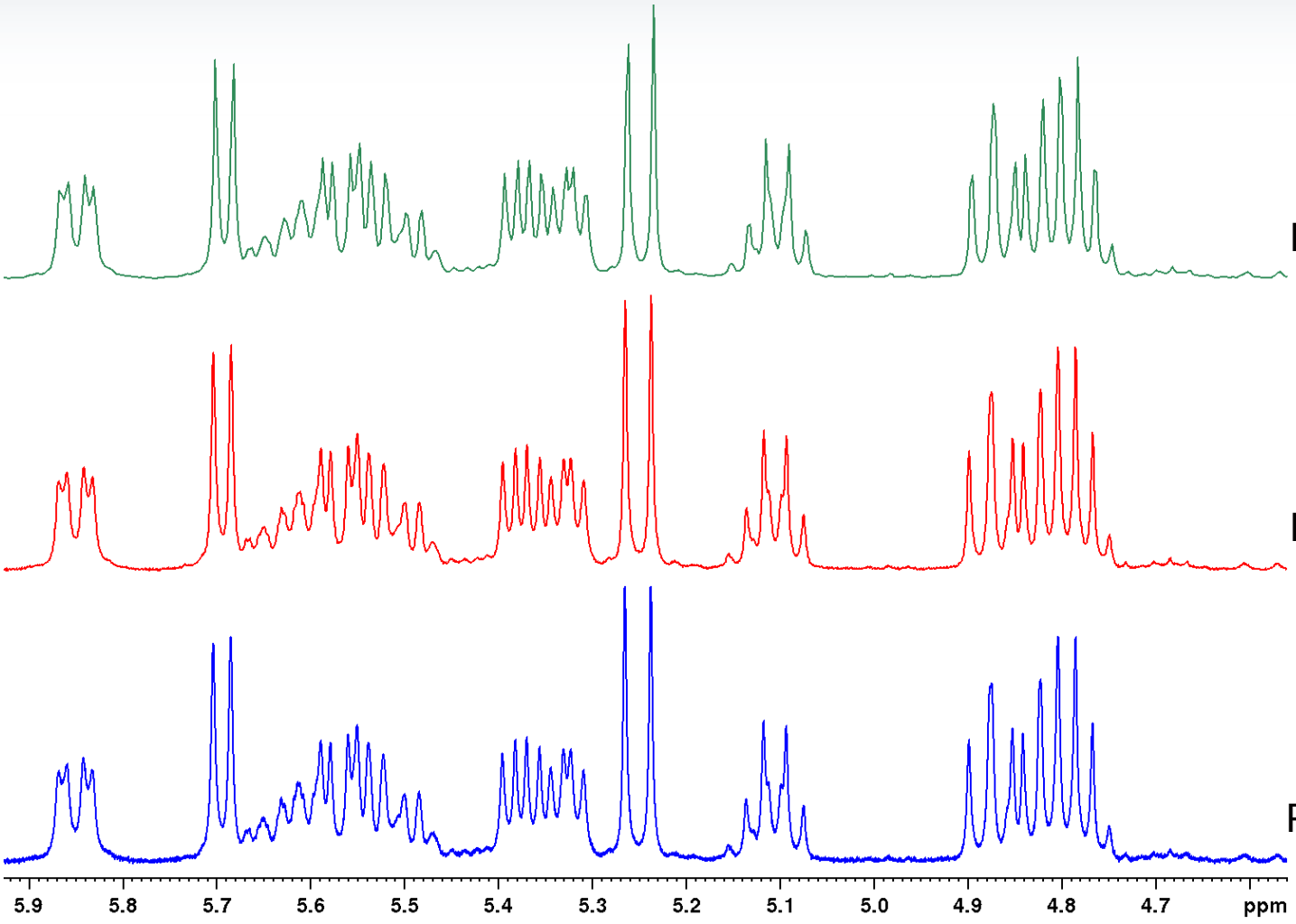


Zero filling

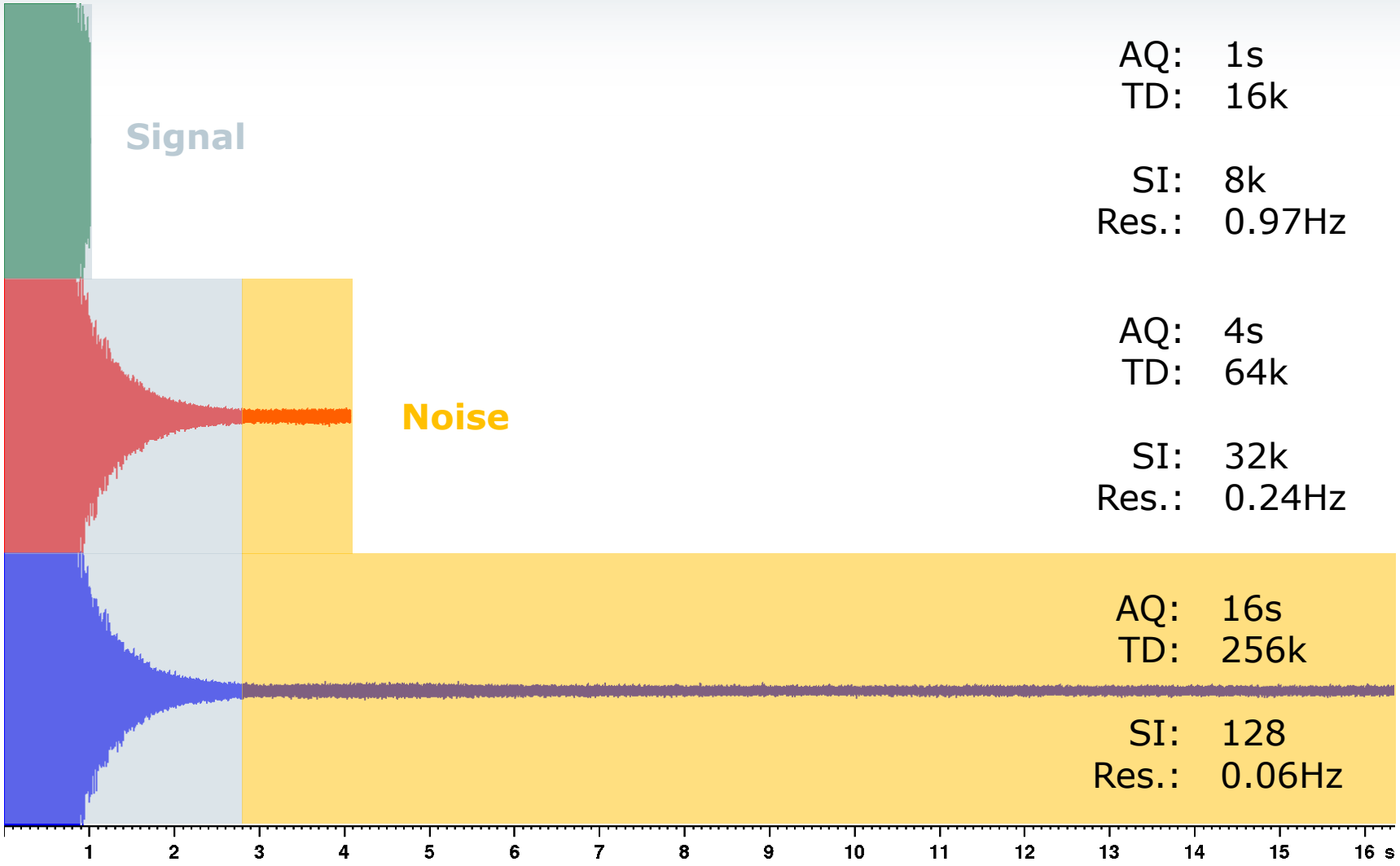


AQ: 1s
TD: 16k
SI: 8k
Res.: 0.97Hz

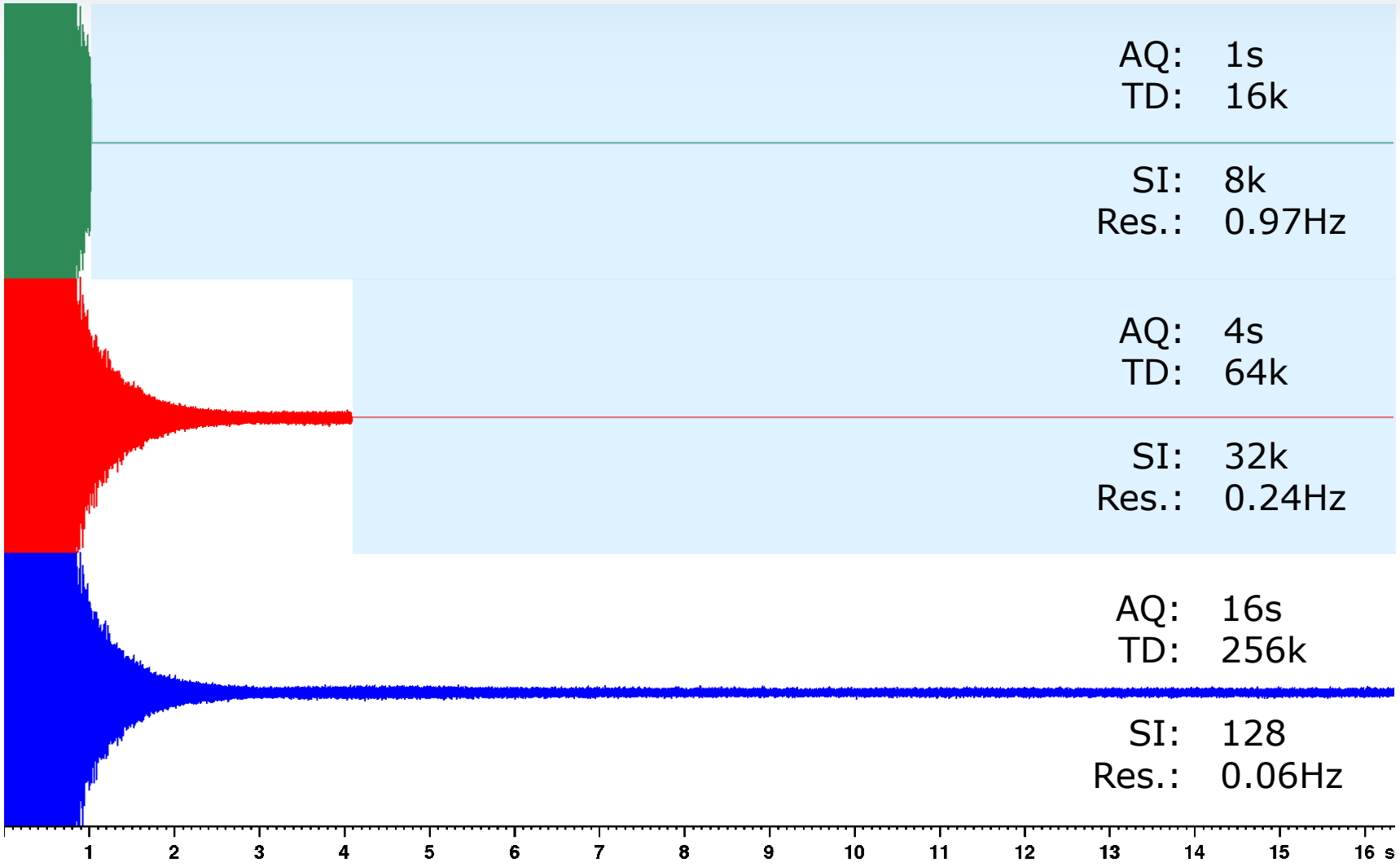
AQ: 4s
TD: 64k
SI: 32k
Res.: 0.24Hz

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

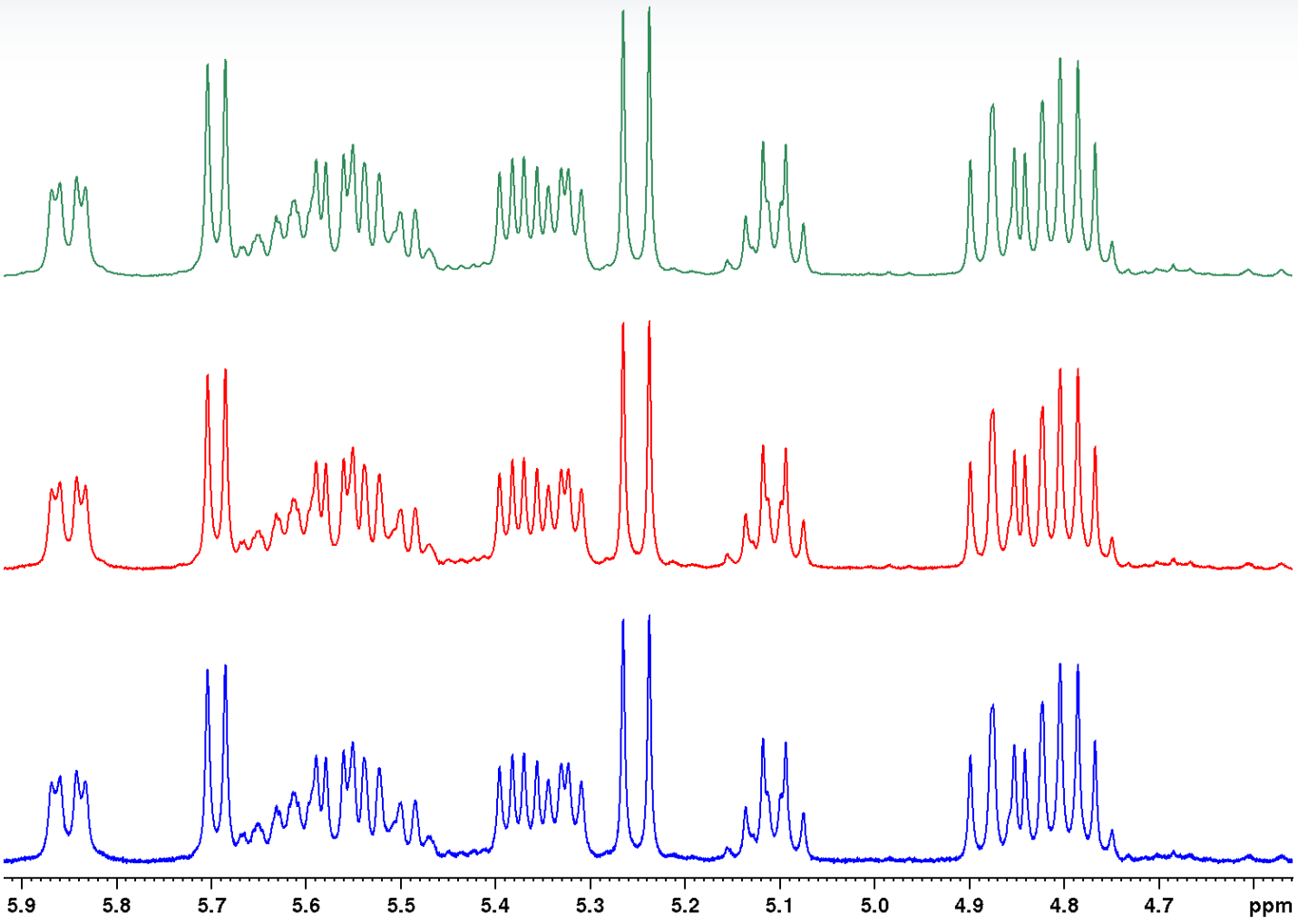
Zero filling



Zero filling



Zero filling

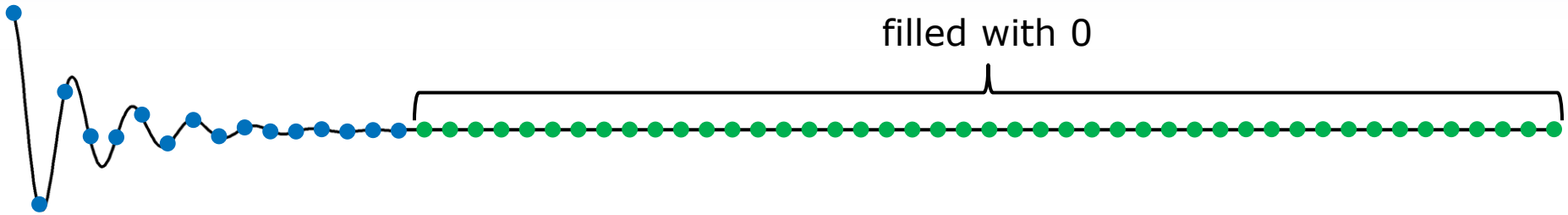


AQ: 1s
TD: 16k
SI: 128k

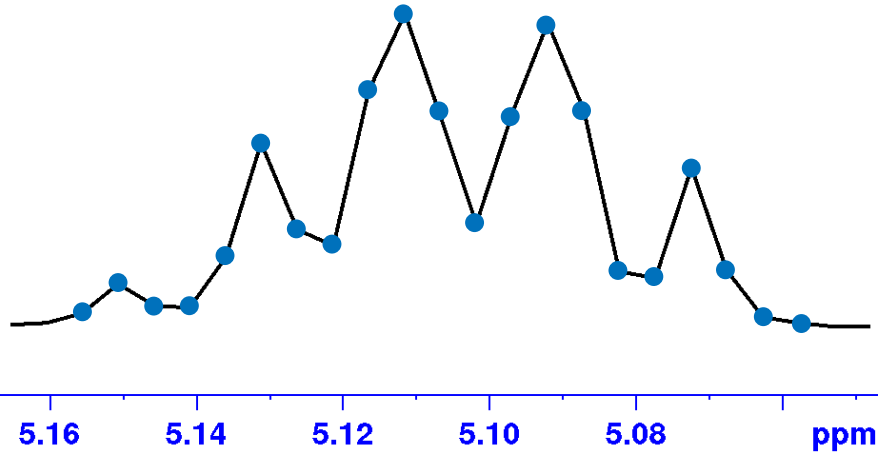
AQ: 4s
TD: 64k
SI: 128k

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

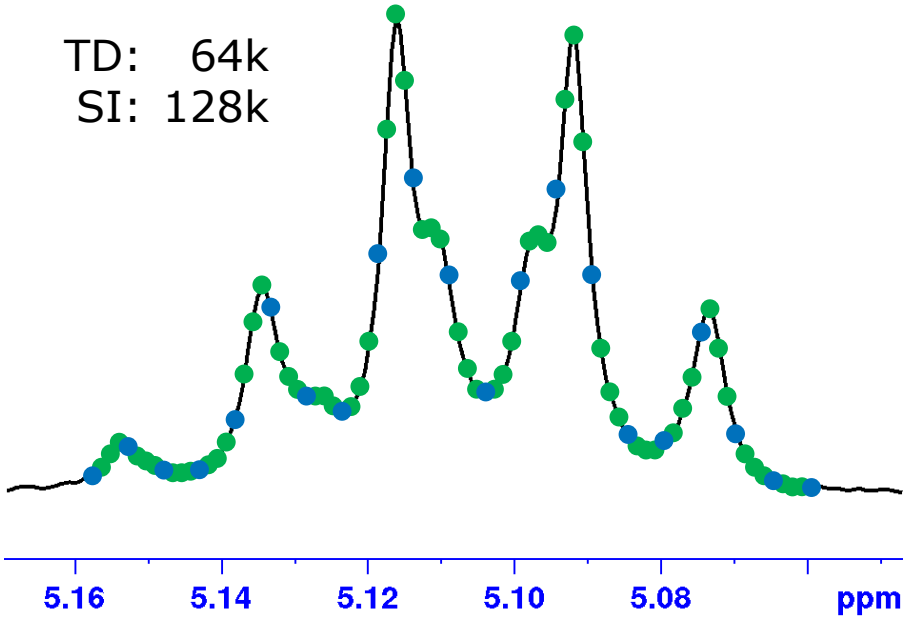
Zero filling



TD: 64k
SI: 32k



TD: 64k
SI: 128k

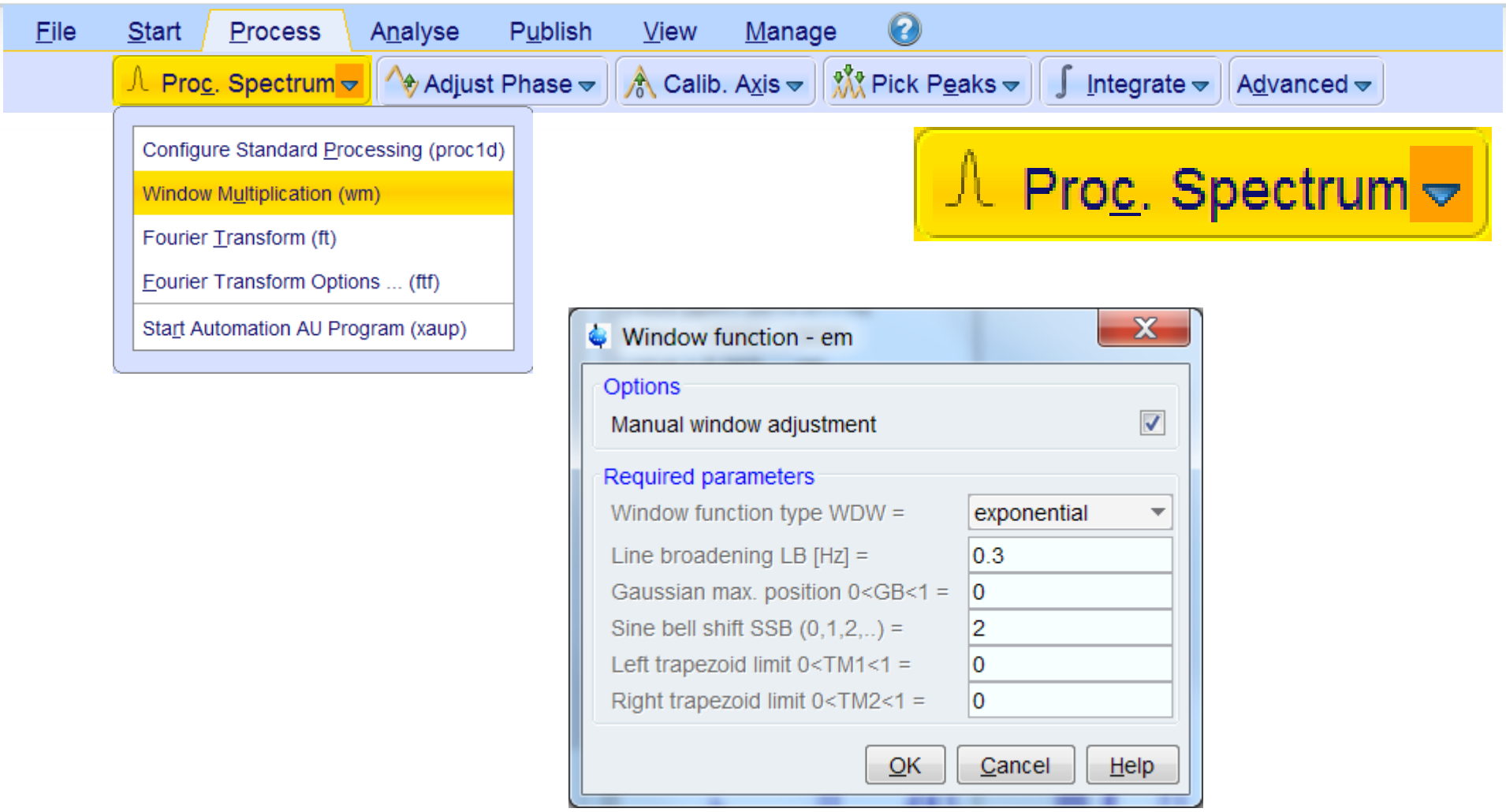


Parameters

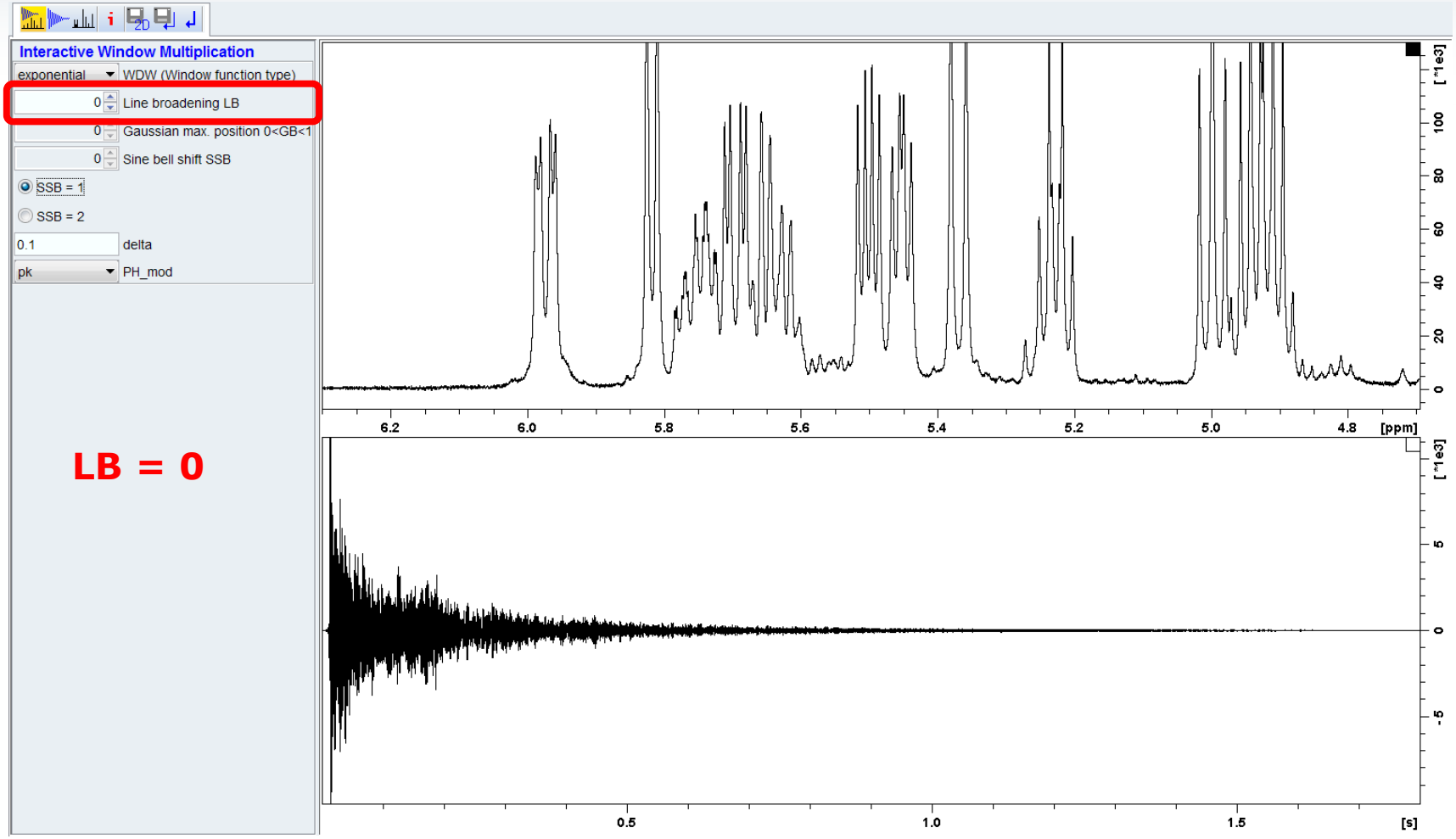
- Parameters are : size SI
  spectrum reference frequency SR
  spectral resolution HzpPt

- 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;

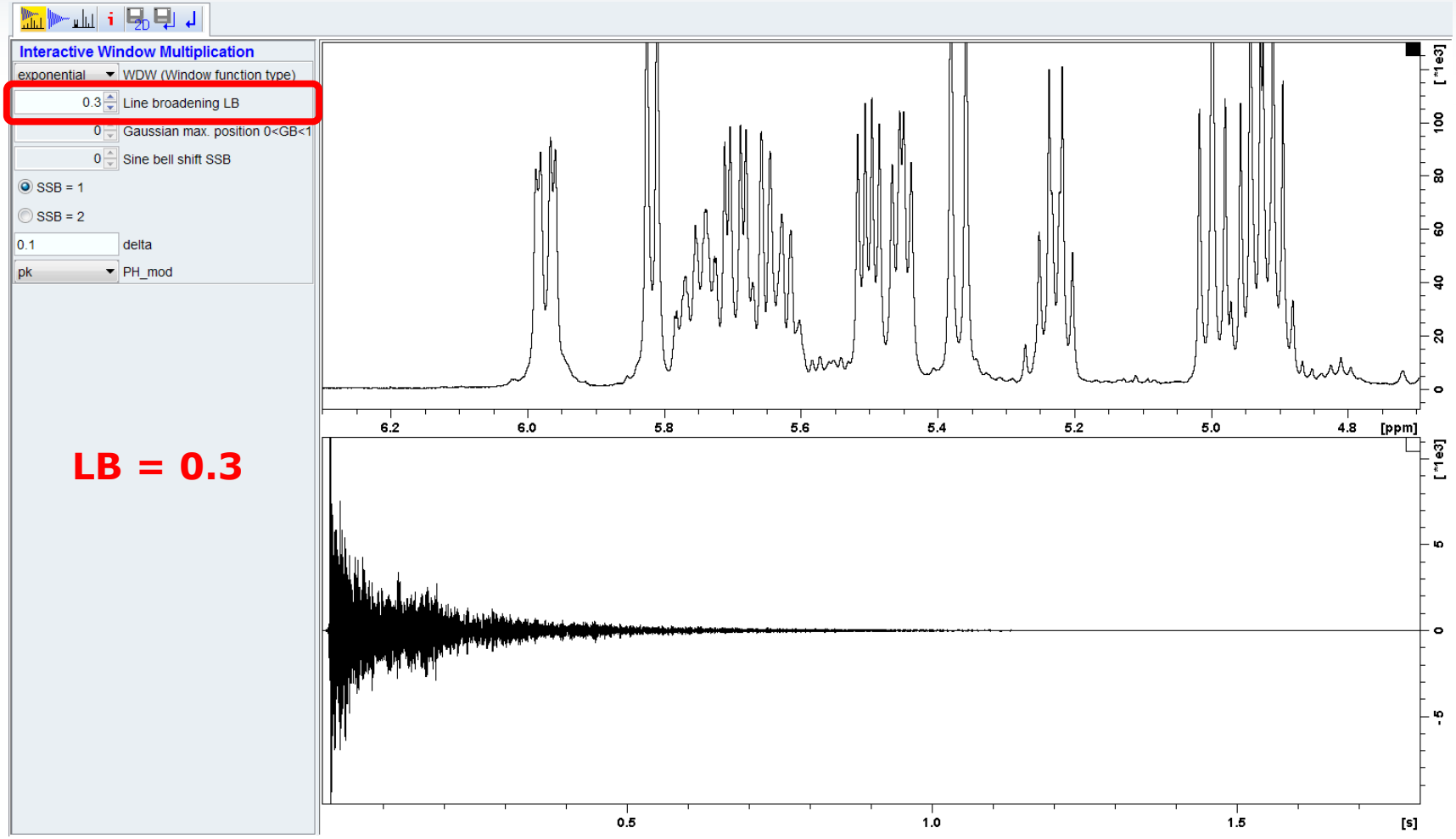
Window function [**wm**]



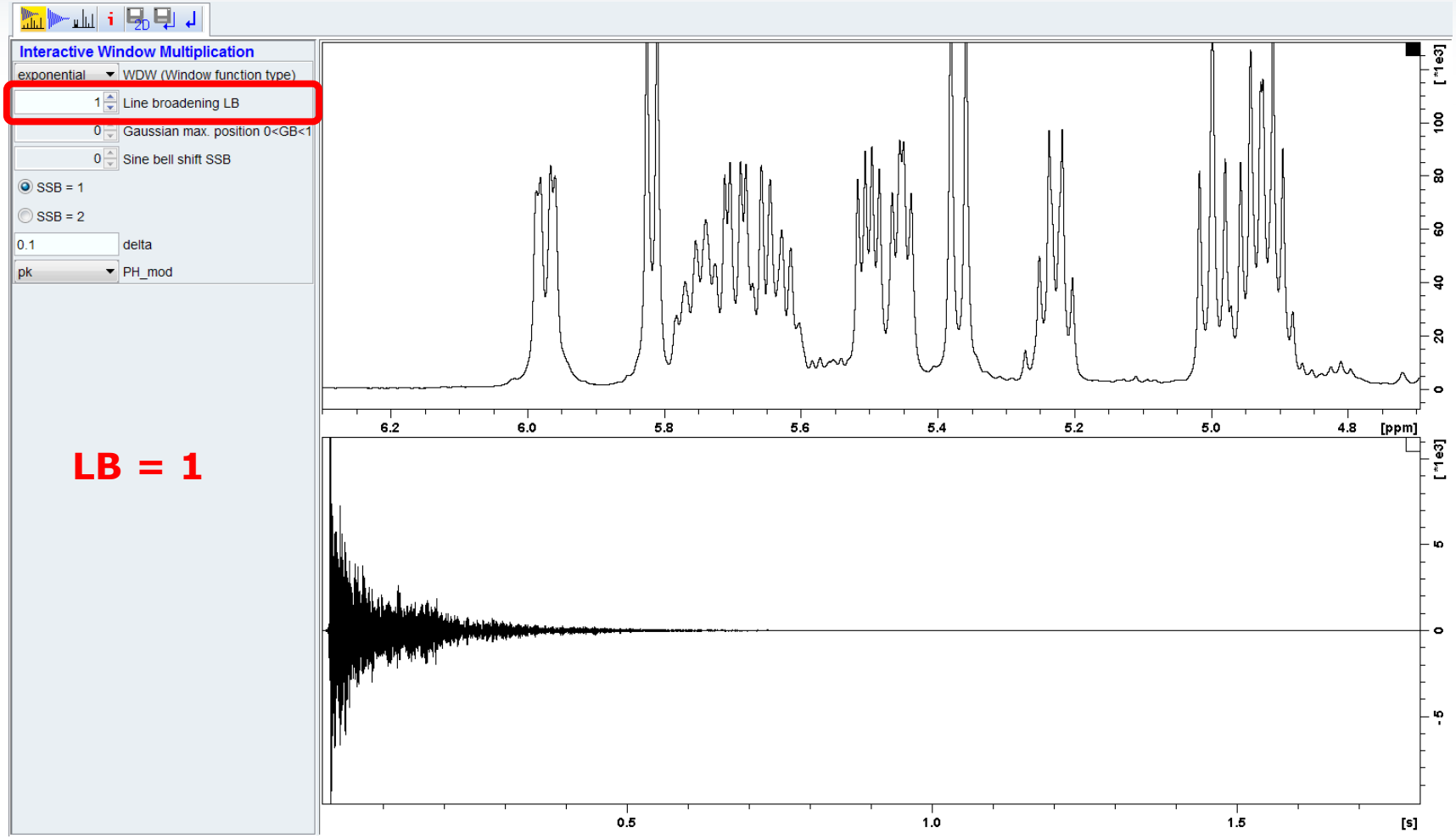
Exponential window function



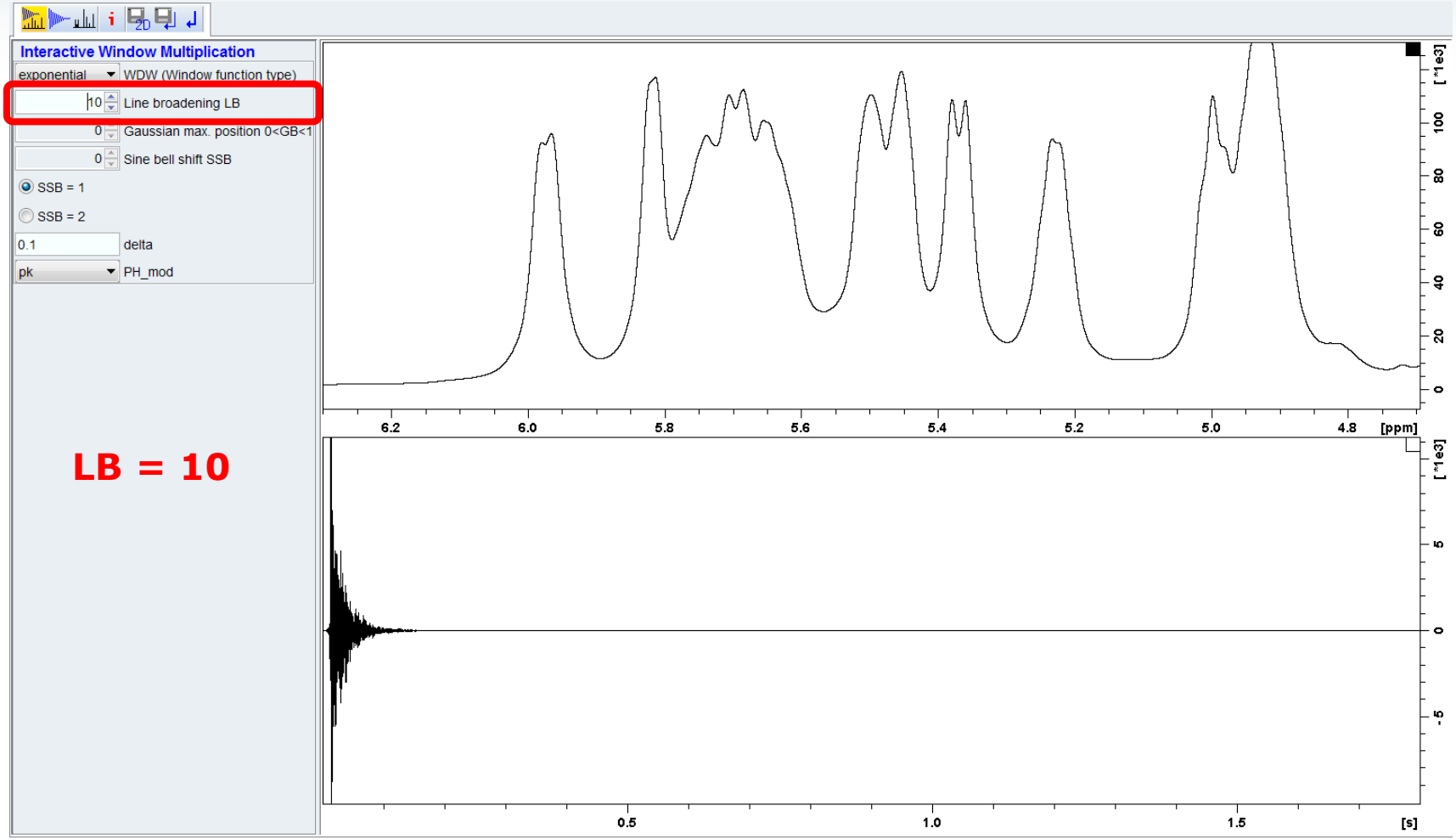
Exponential window function



Exponential window function



Exponential window function



Window functions

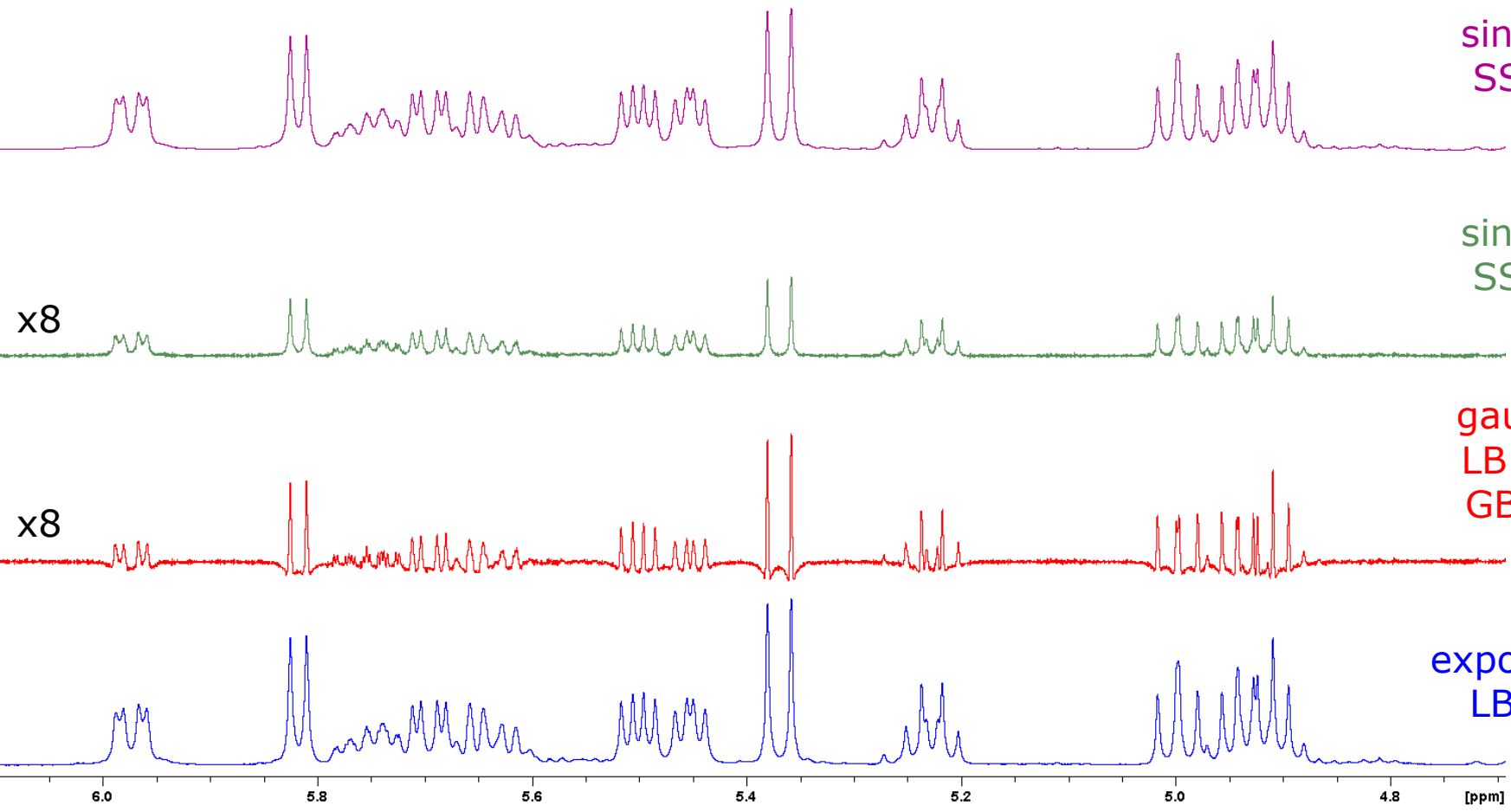
- Digital Filtering [**em**], [**gm**]

- There are several window functions, which can be used to optimize the spectrum.

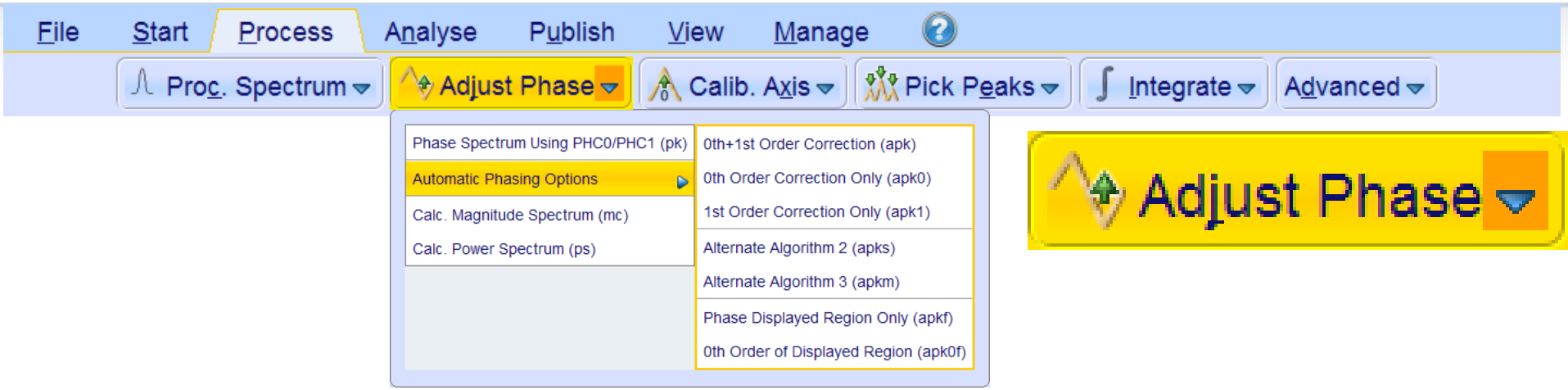
Function	Command	Factor	Range
Exponential	em	LB	>0
Gaussian	gm	LB and GB	LB<0, 0<GB<1
Sine bell	sinm	SSB	0, 1, 2, …
Squared sine	qsin	SSB	0, 1, 2, …

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

Effect of window functions

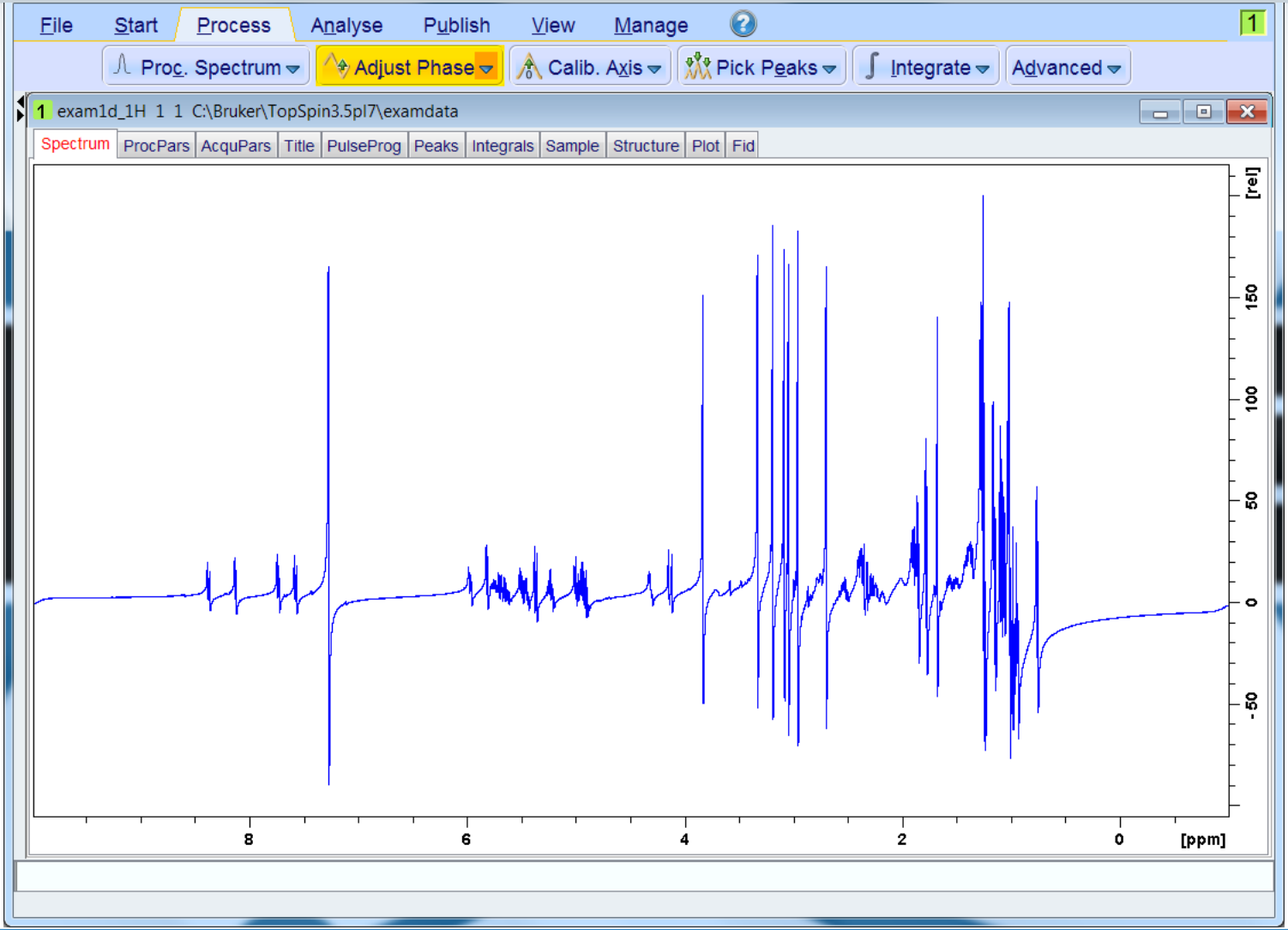


Adjust Phase

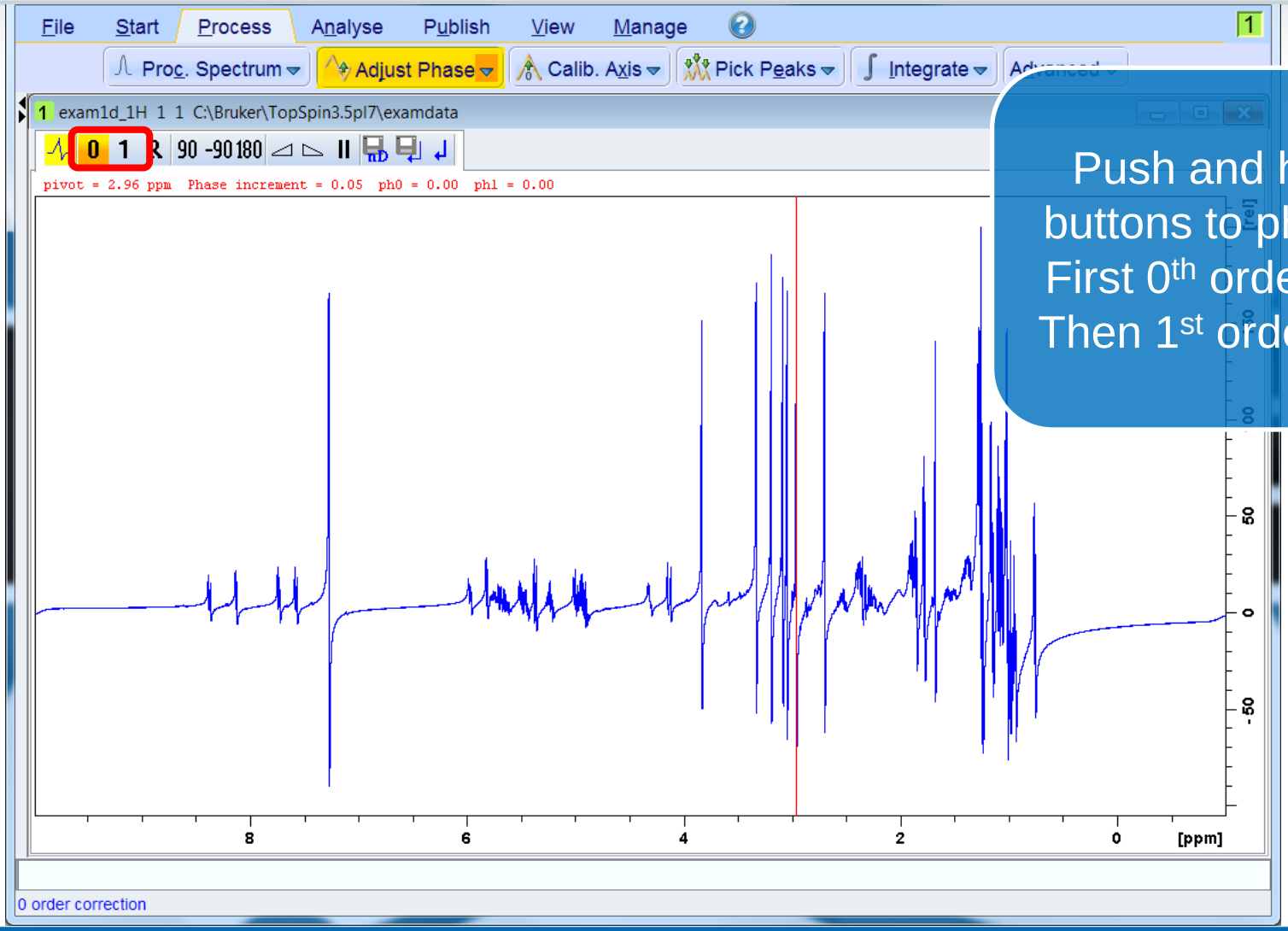


- Manual phase correction with [**.ph**]
- Automatic phase correction with [**apk**]/[**apk0**]
- Uses previously defined phase correction values [**pk**]

Phasing

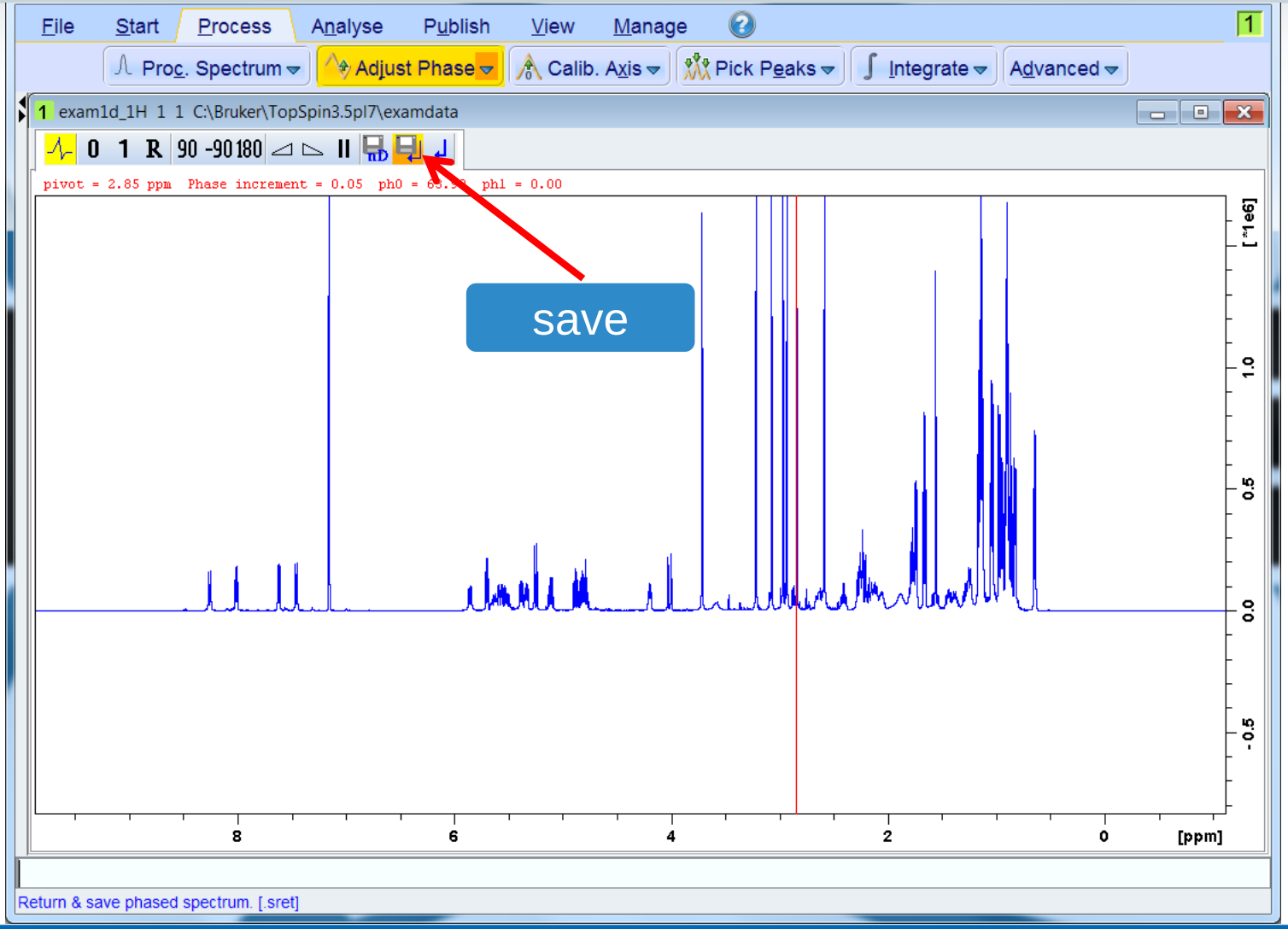

File
Start
Process
Analyse
Publish
View
Manage
1
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata
Spectrum
ProcPars
AcquPars
Title
PulseProg
Peaks
Integrals
Sample
Structure
Plot
Fid
[rel]
150
100
50
0
-50
8
6
4
2
0
[ppm]

Phasing

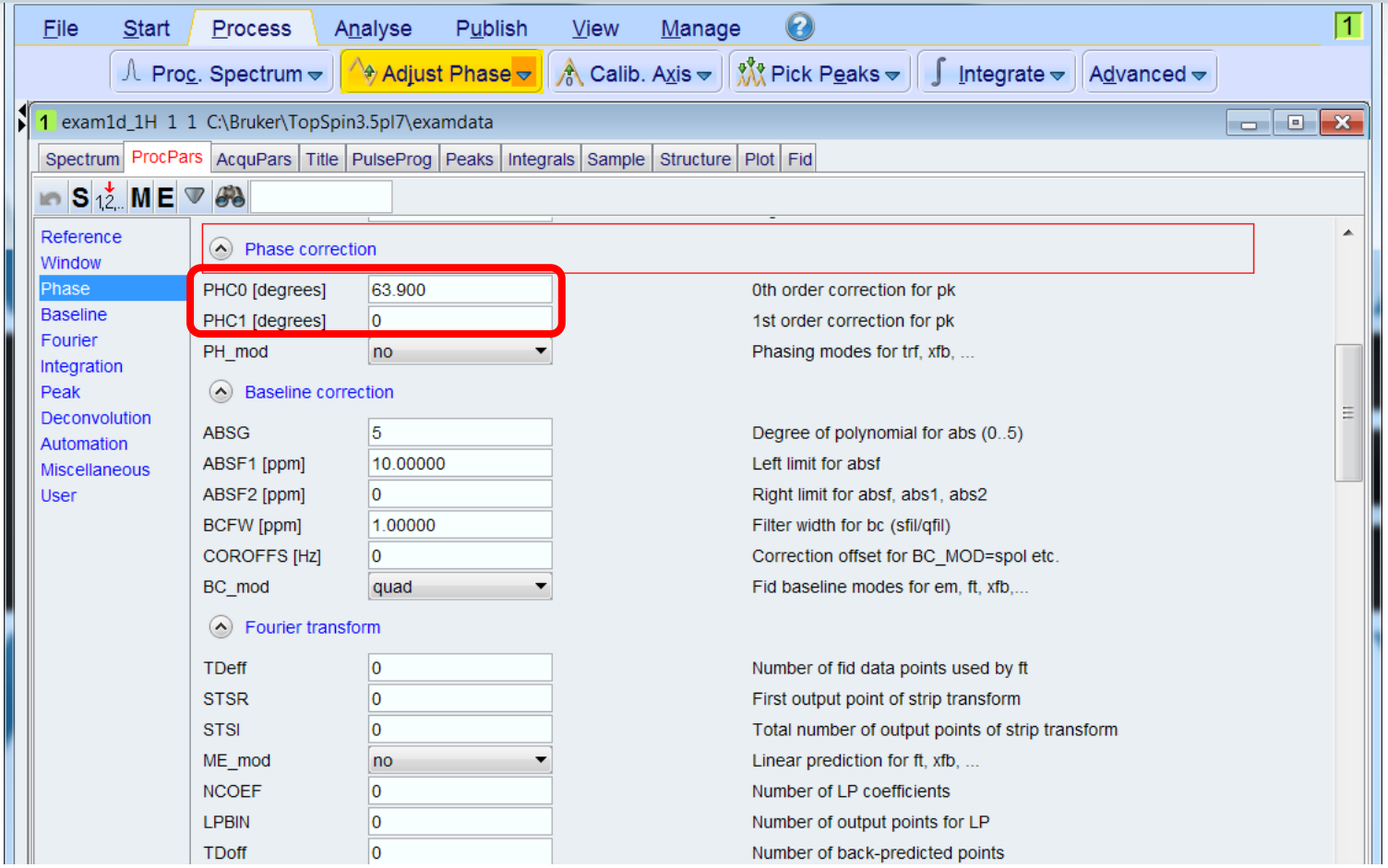


Push and hold buttons to phase.
First 0th order **0**.
Then 1st order **1**.

Phasing

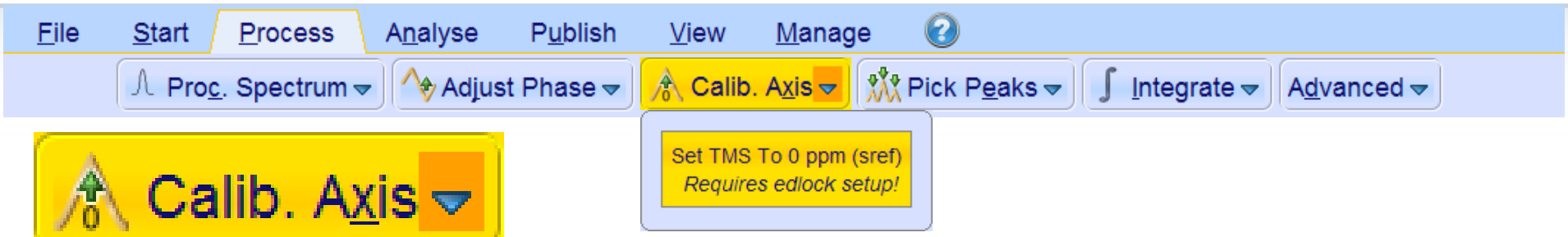

File
Start
Process
Analyse
Publish
View
Manage
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata
pivot = 2.85 ppm Phase increment = 0.05 ph0 = 65.30 ph1 = 0.00
save
[*1e6]
1.0
0.5
0.0
-0.5
8
6
4
2
0
[ppm]
Return & save phased spectrum. [.sret]

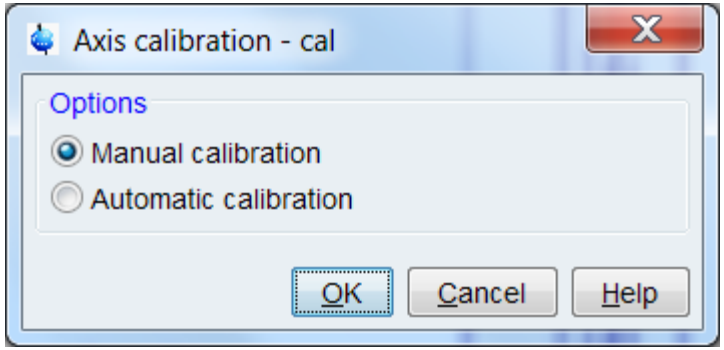
Phasing



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

Calibrate Axis

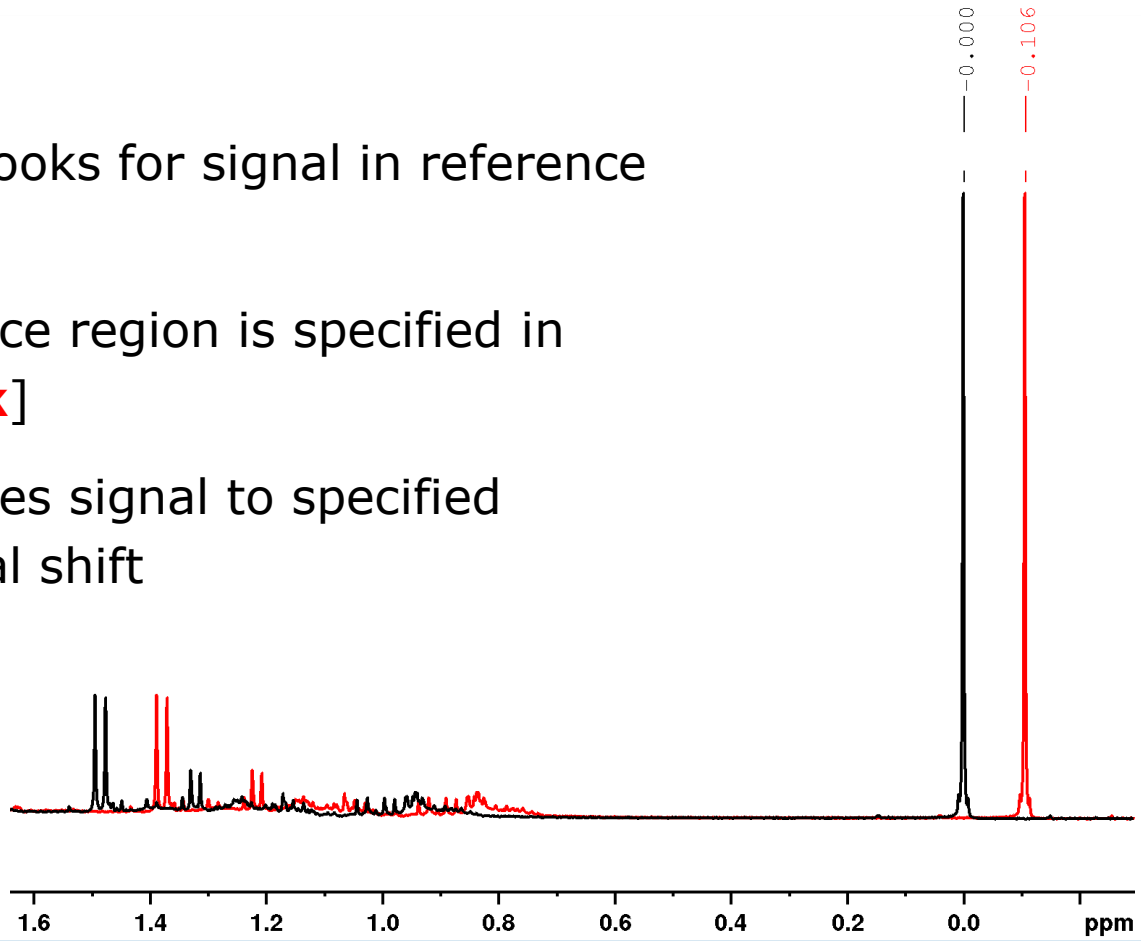




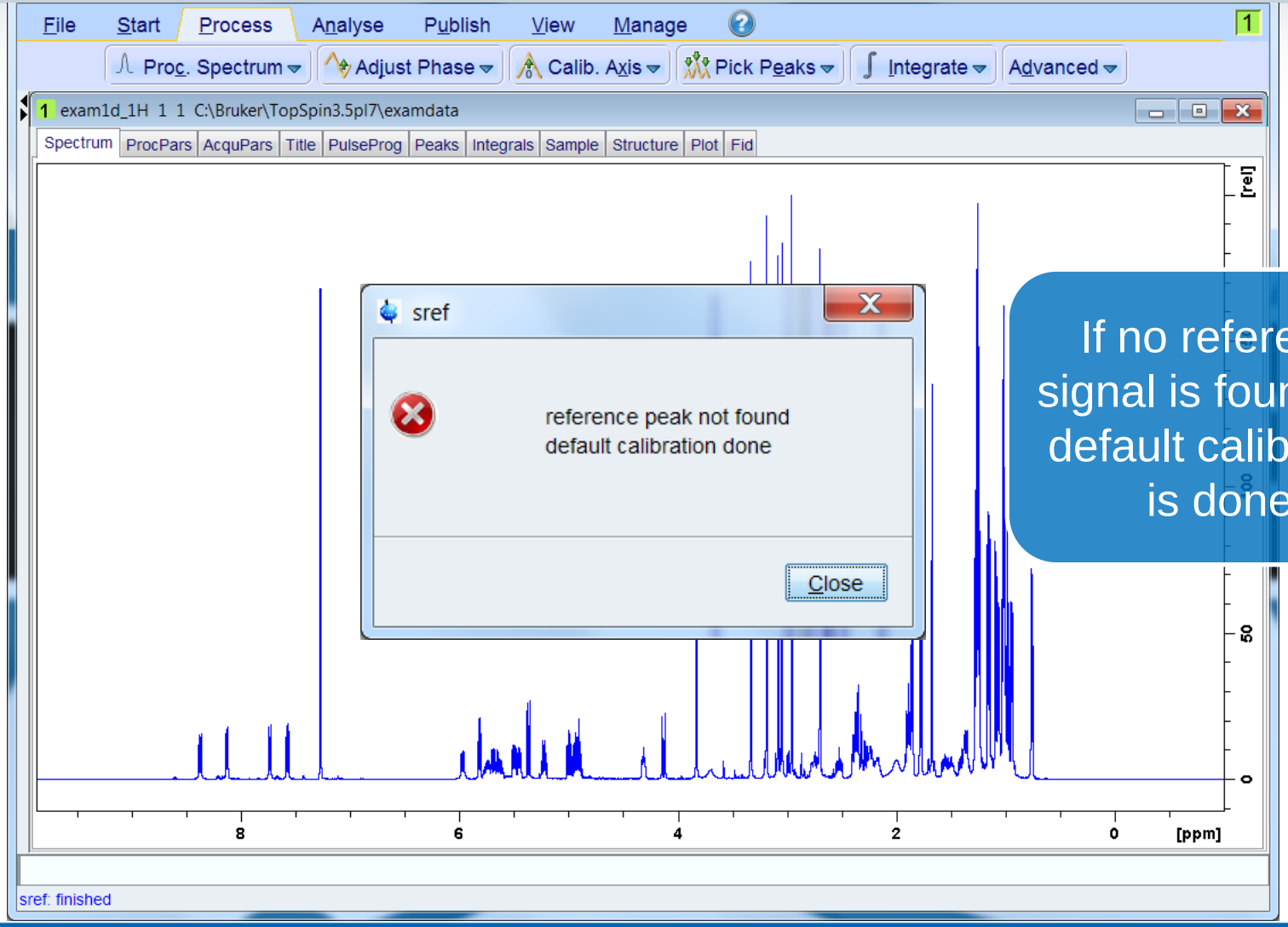
- Open reference dialog with [**cal**]
- Automatic referencing [**sref**]
- Reference manually [**.cal**]

Automatic calibration

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

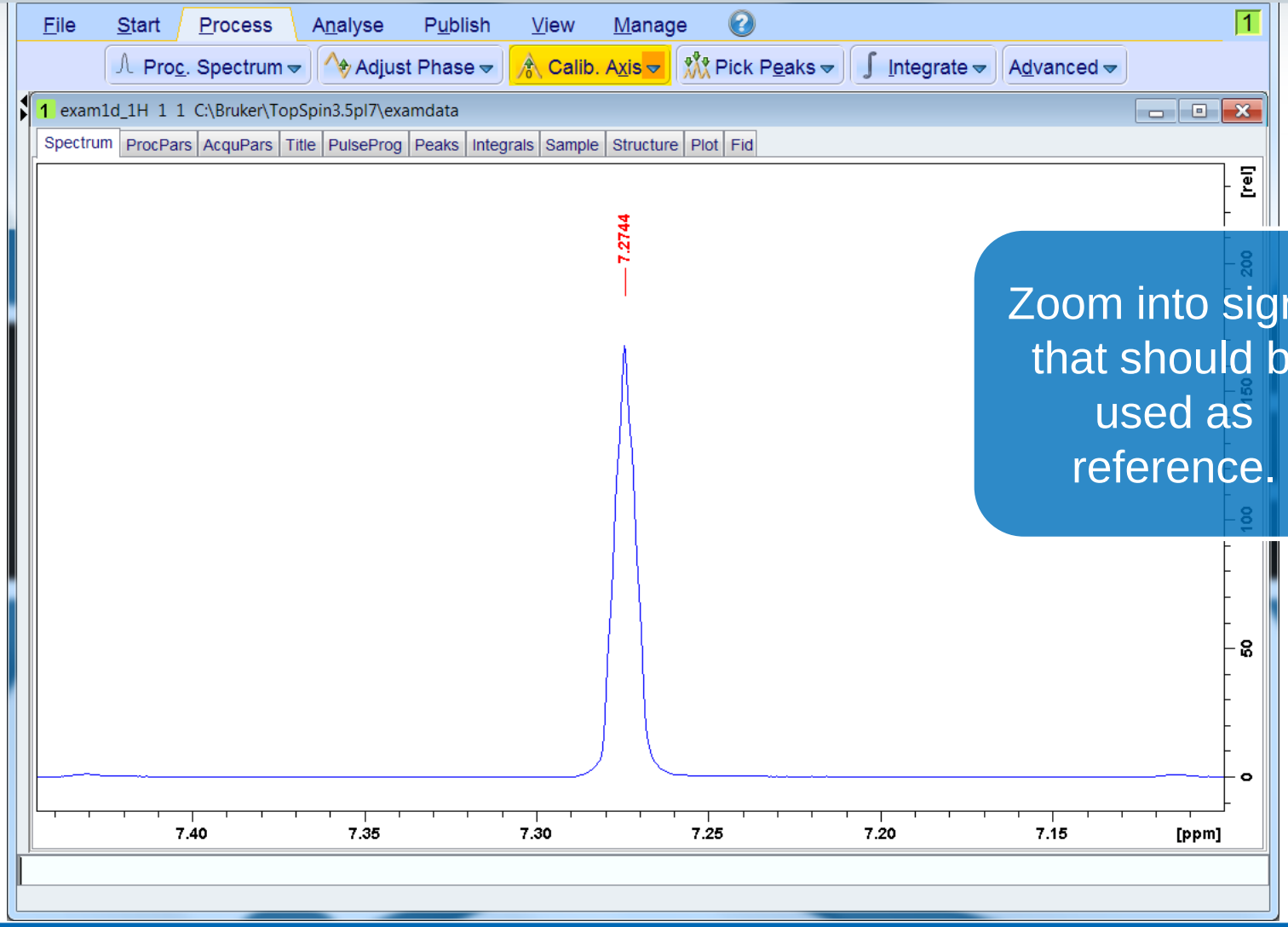


Automatic calibration

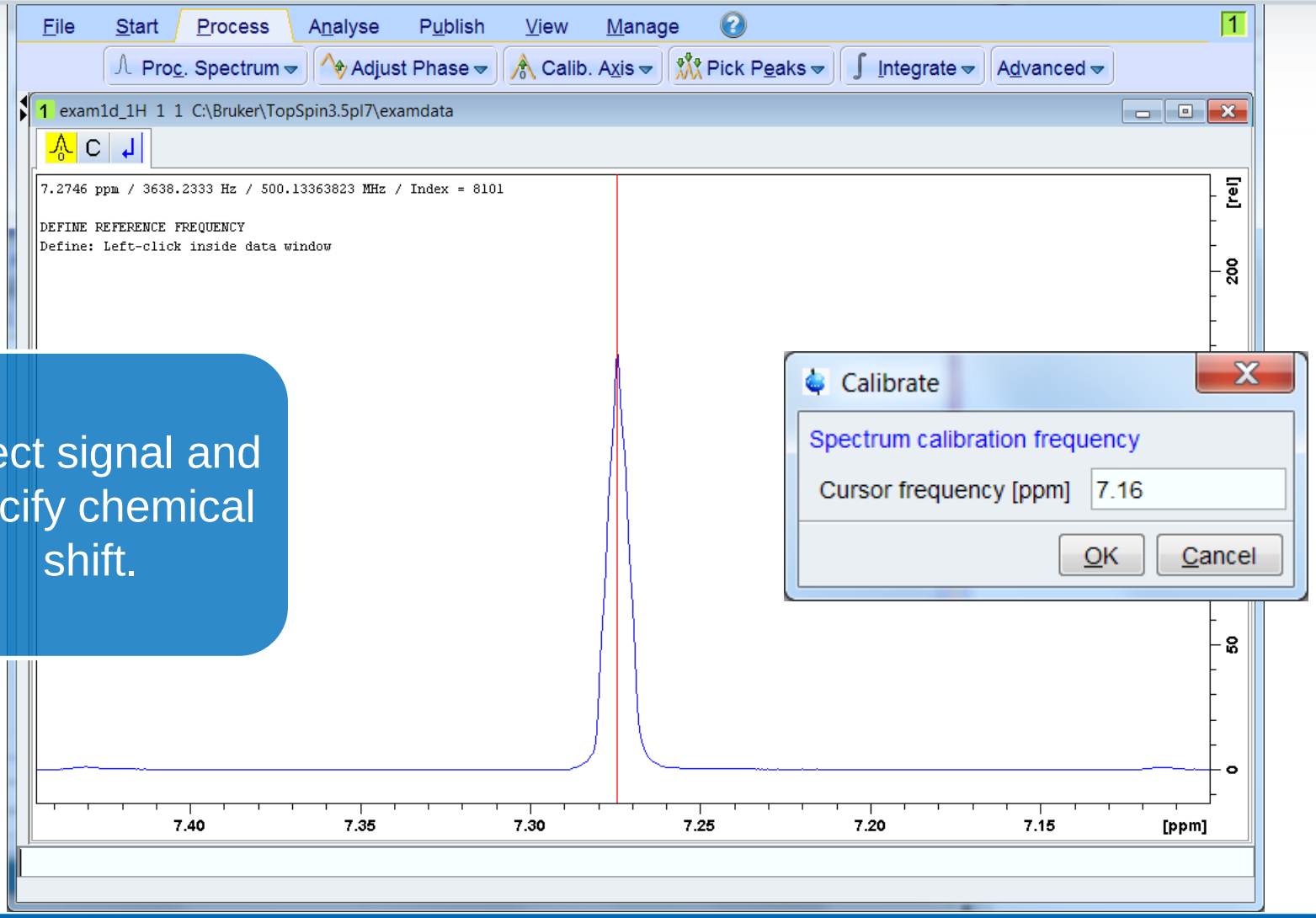


If no reference signal is found, the default calibration is done.

Manual calibration

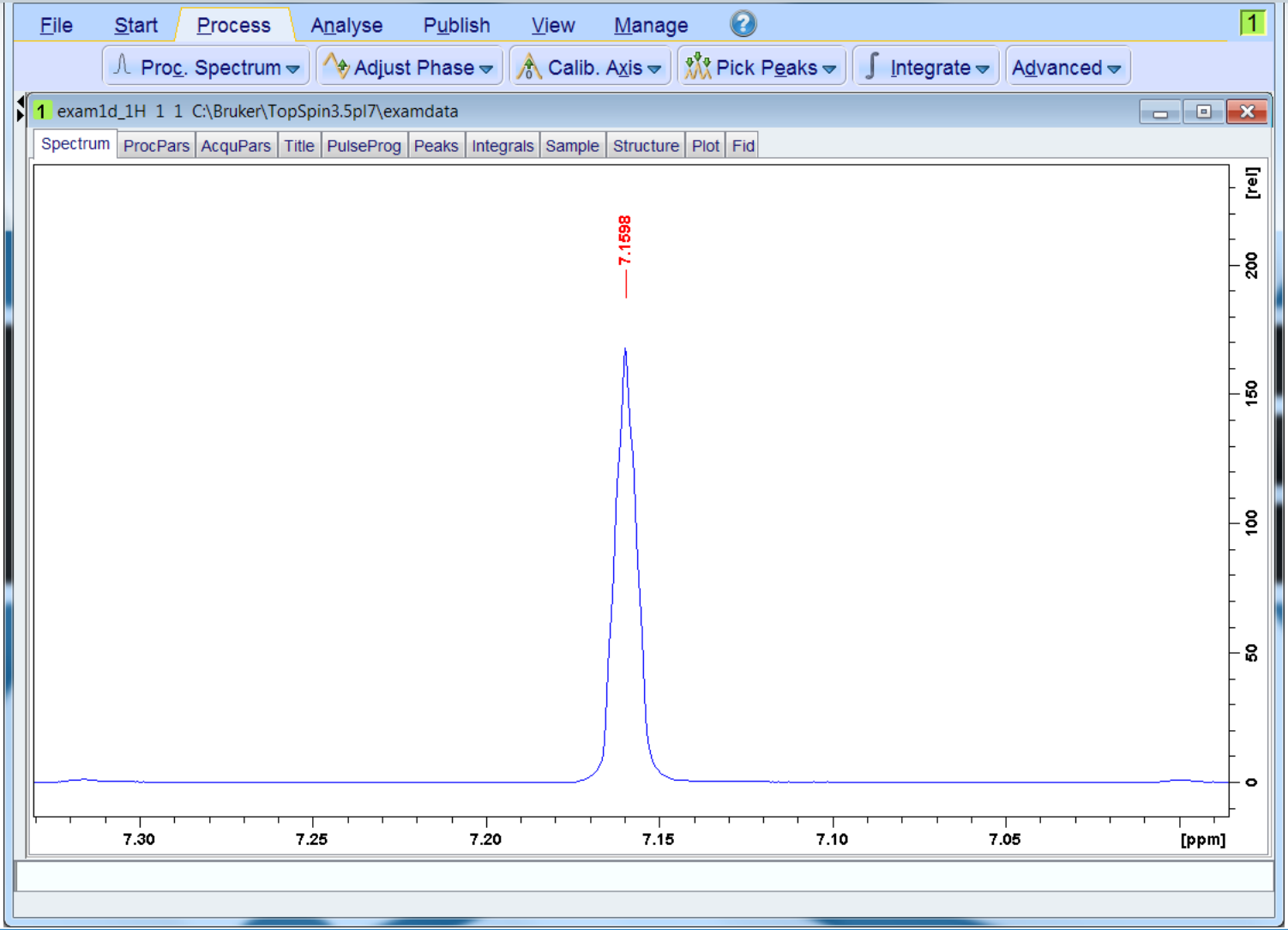


Manual calibration



Select signal and specify chemical shift.

Manual calibration



Calibrate Axis

Caution!

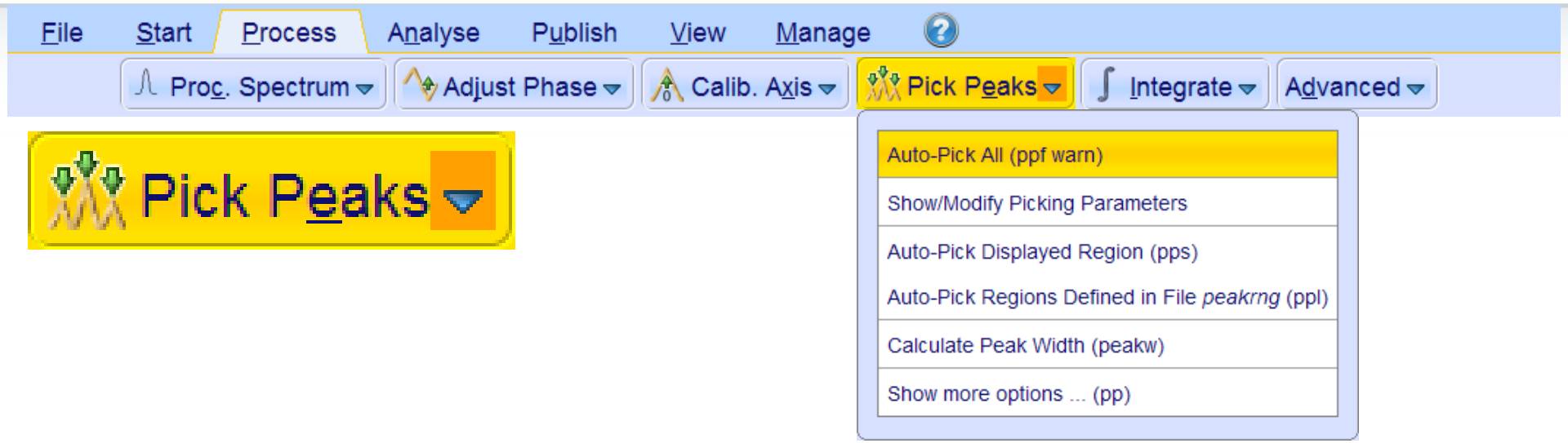
If you want to determine a frequency for

selective experiments

SR needs to be set to 0!

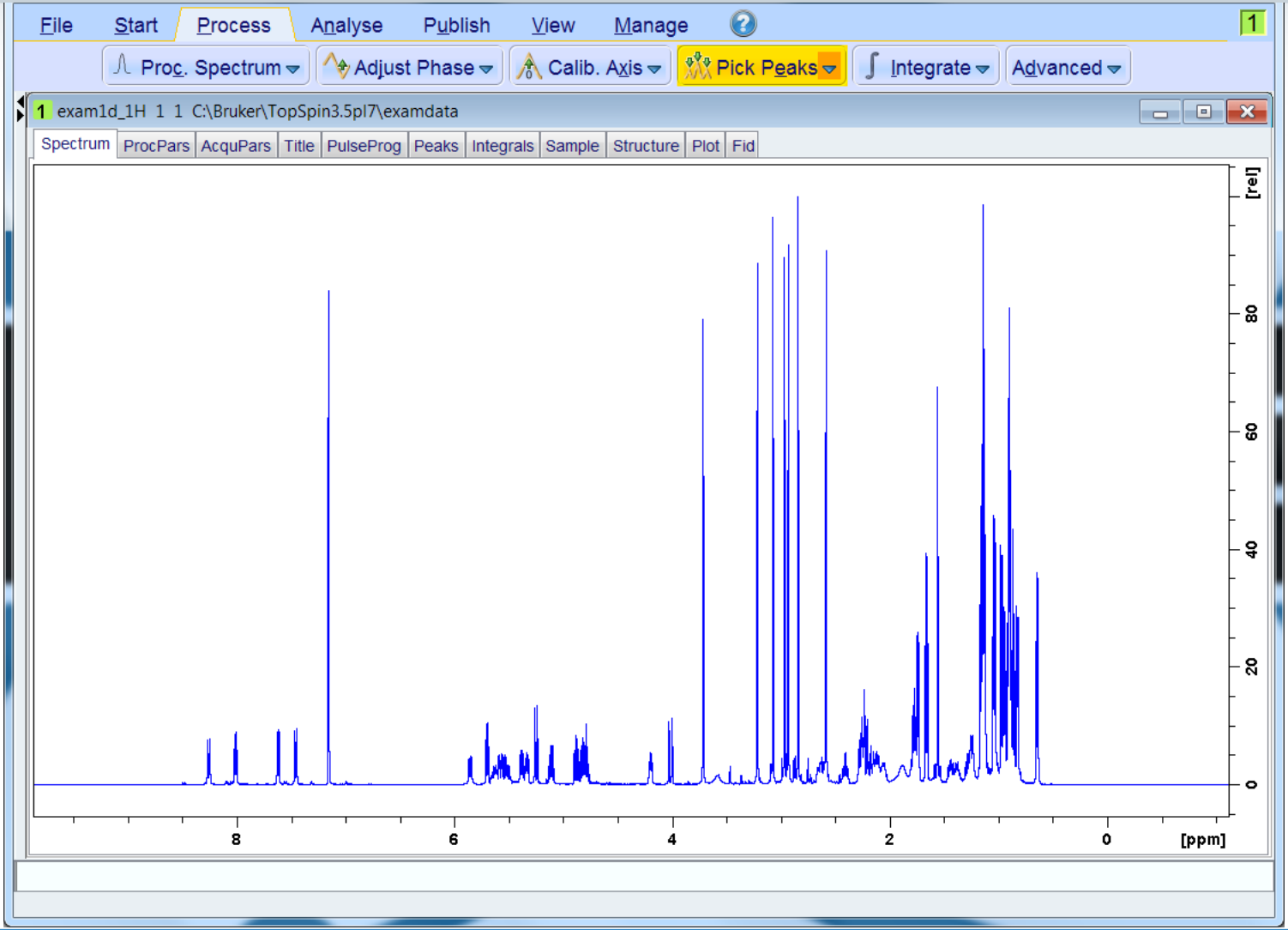
SR is only used for visualisation!

Pick Peaks

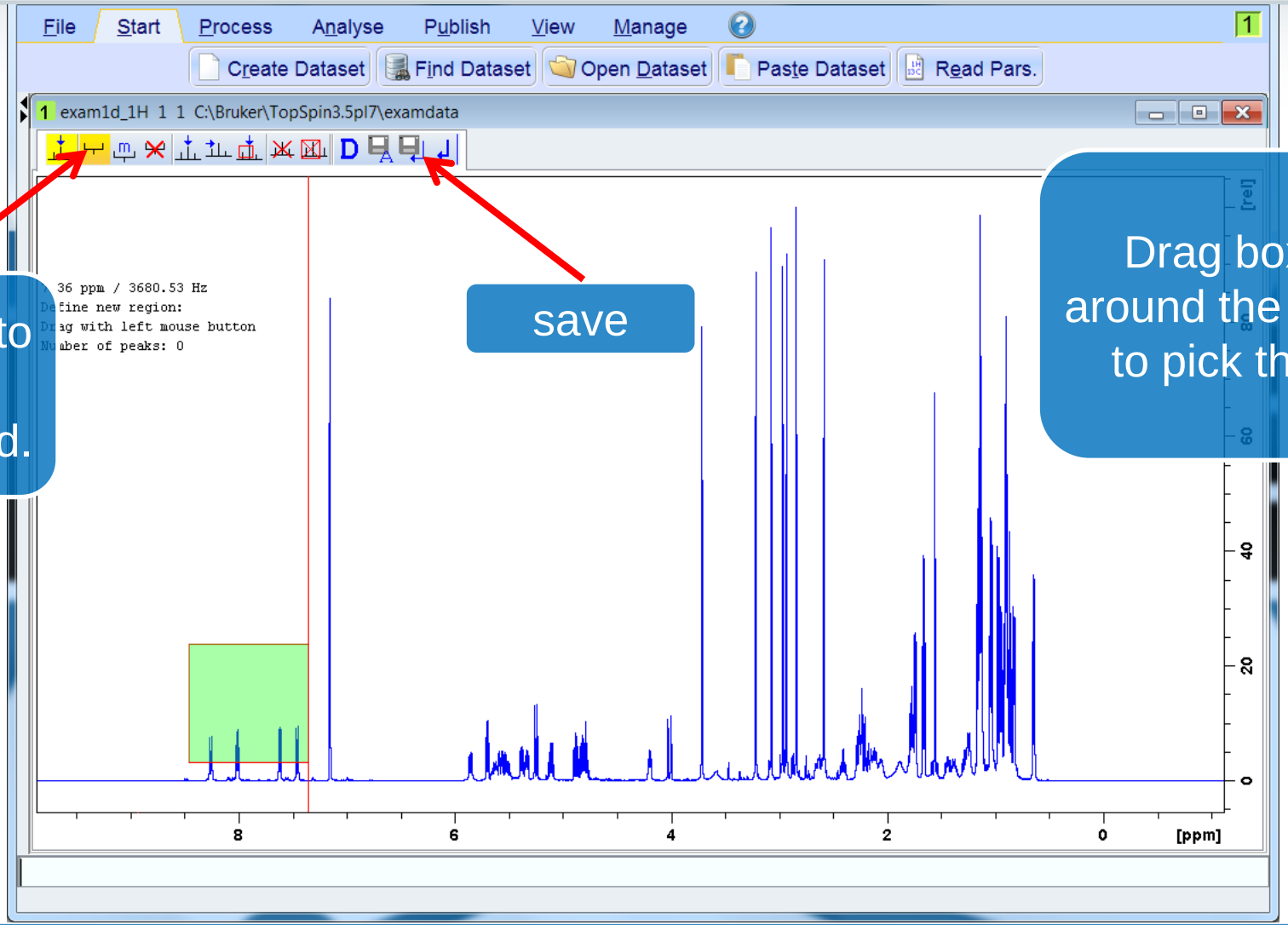


- Automatic peak picking of full spectrum [**ppf warn**]
- Automatic peak picking of displayed region [**pps**]
- [**.pp**] open manual peak picking

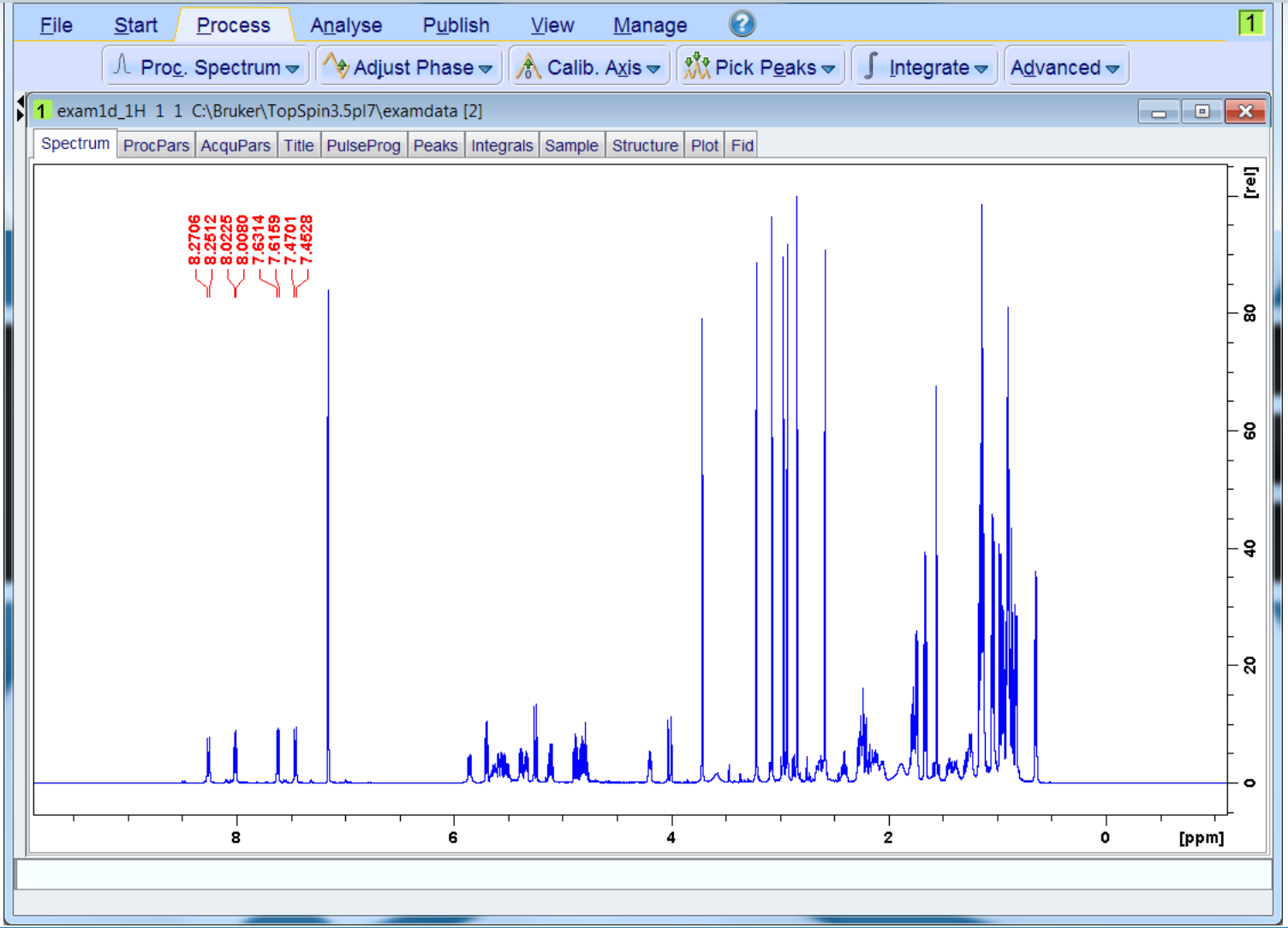
Pick Peaks


File
Start
Process
Analyse
Publish
View
Manage
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata
Spectrum
ProcPars
AcquPars
Title
PulseProg
Peaks
Integrals
Sample
Structure
Plot
Fid
[rel]
0
20
40
60
80
8
6
4
2
0
[ppm]

Pick Peaks


File
Start
Process
Analyse
Publish
View
Manage
Create Dataset
Find Dataset
Open Dataset
Paste Dataset
Read Pars.
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata
36 ppm / 3680.53 Hz
Define new region:
Drag with left mouse button
Number of peaks: 0
8
6
4
2
0
[ppm]
[rel]
Needs to be selected.
save
Drag boxes around the peaks to pick them.

Pick Peaks


File
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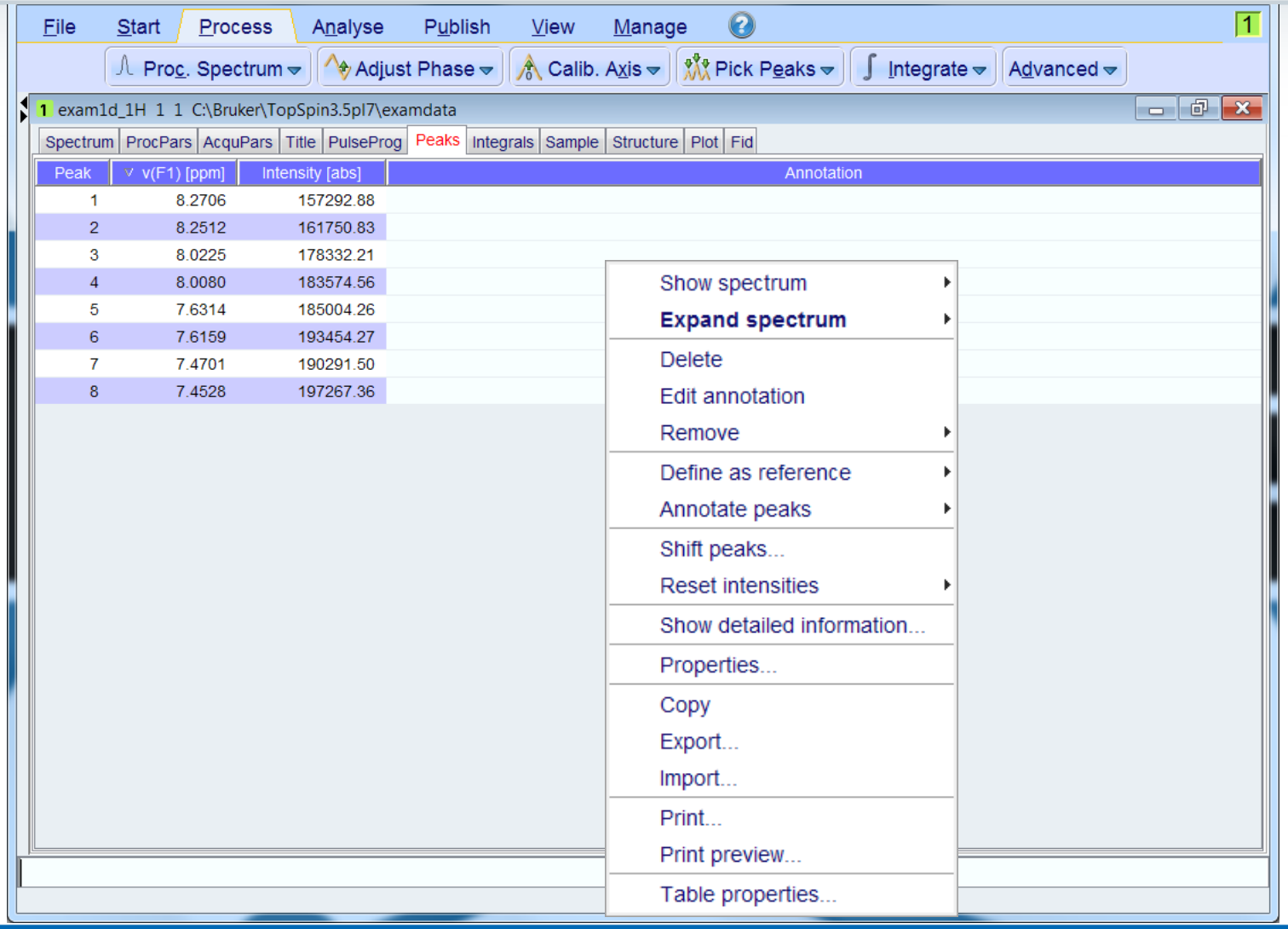
Analyse
Publish
View
Manage
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata [2]
Spectrum
ProcPars
AcquPars
Title
PulseProg
Peaks
Integrals
Sample
Structure
Plot
Fid
8.2706
8.2512
8.0225
8.0080
7.6314
7.6159
7.4701
7.4528
[rel]
0
20
40
60
80
8
6
4
2
0
[ppm]

Pick Peaks


File
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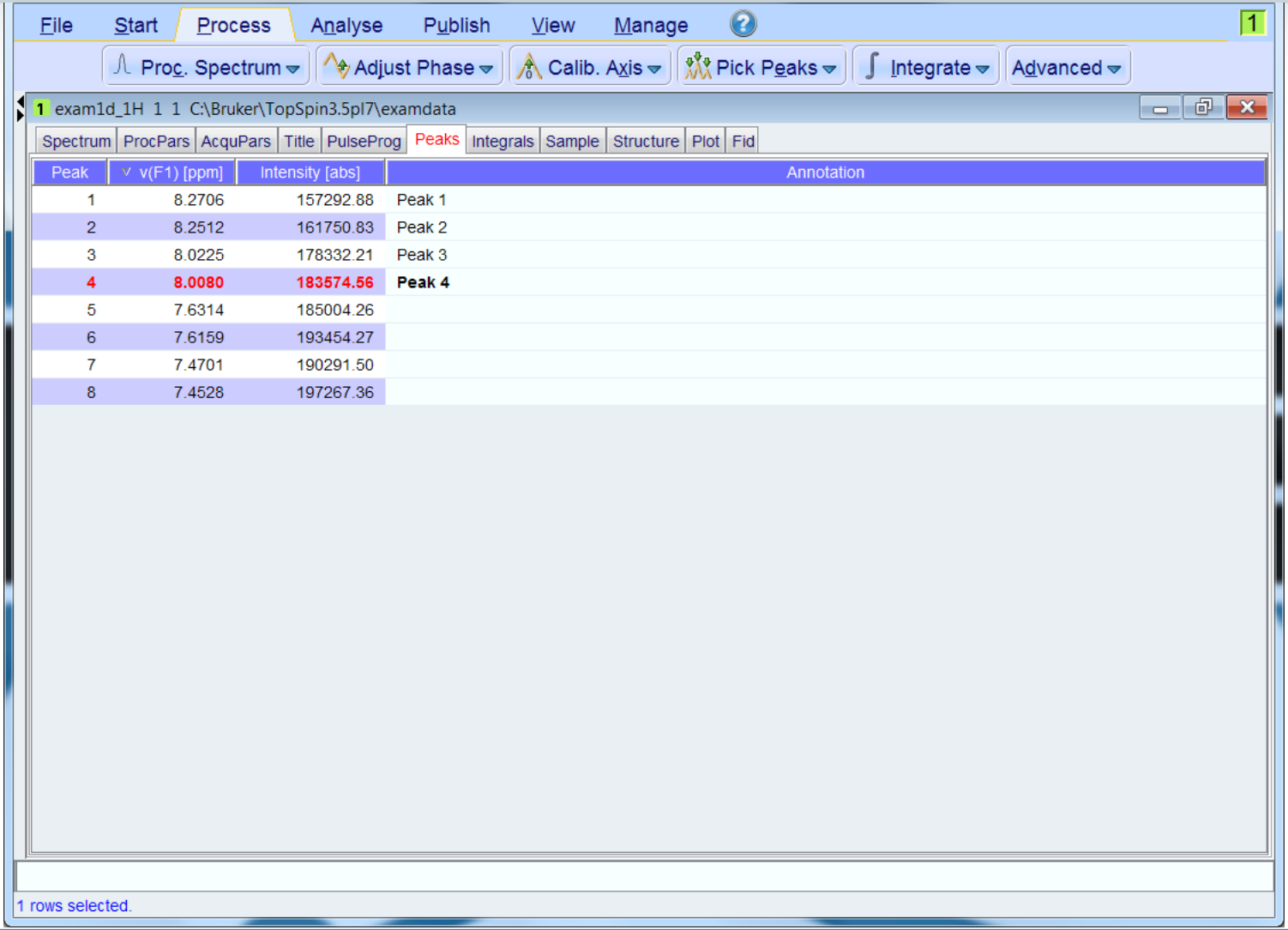
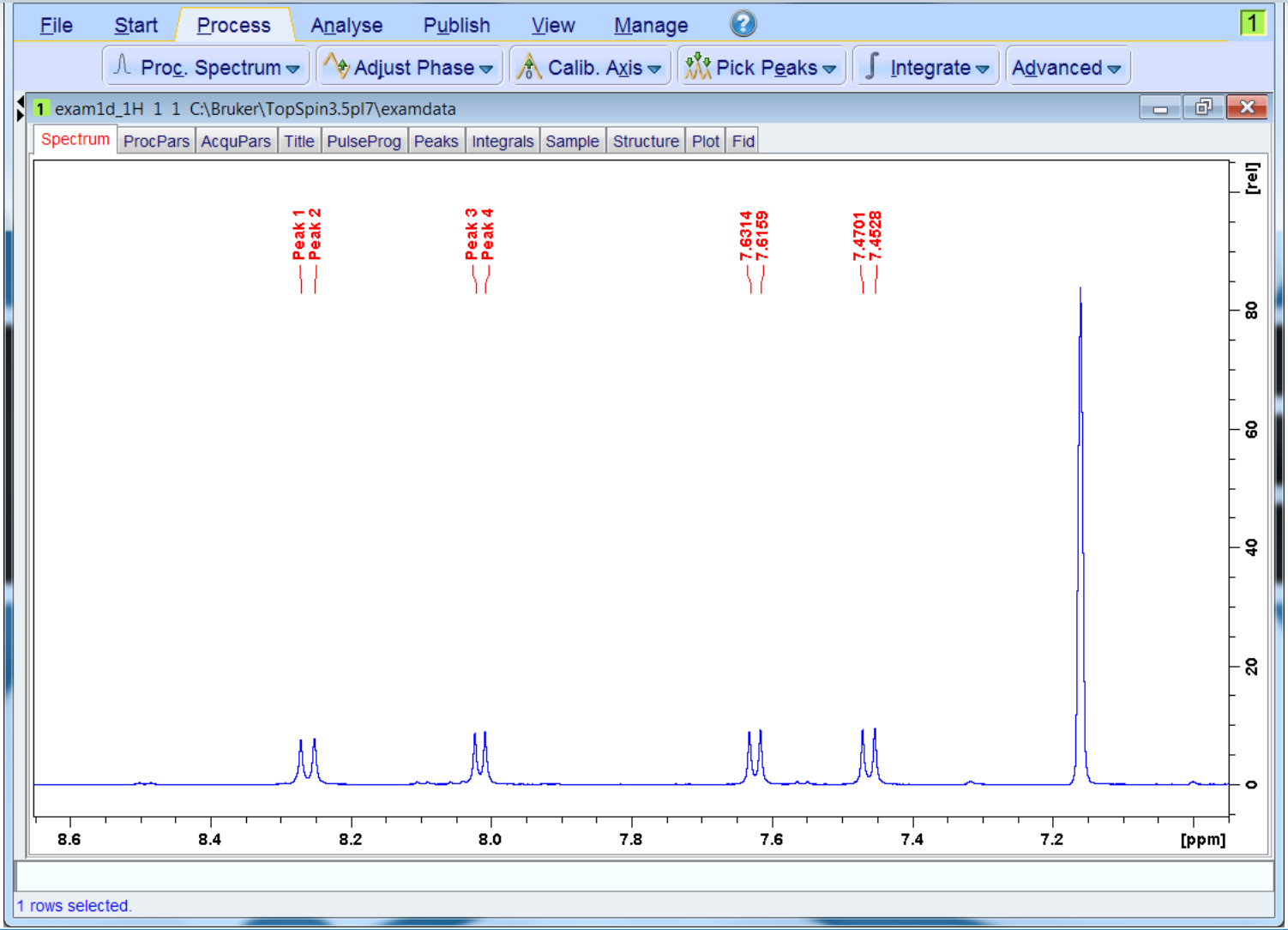
Publish
View
Manage
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata
Spectrum
ProcPars
AcquPars
Title
PulseProg
Peaks
Integrals
Sample
Structure
Plot
Fid
Peak
v(F1) [ppm]
Intensity [abs]
Annotation
1 8.2706 157292.88
2 8.2512 161750.83
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
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata
Spectrum
ProcPars
AcquPars
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.

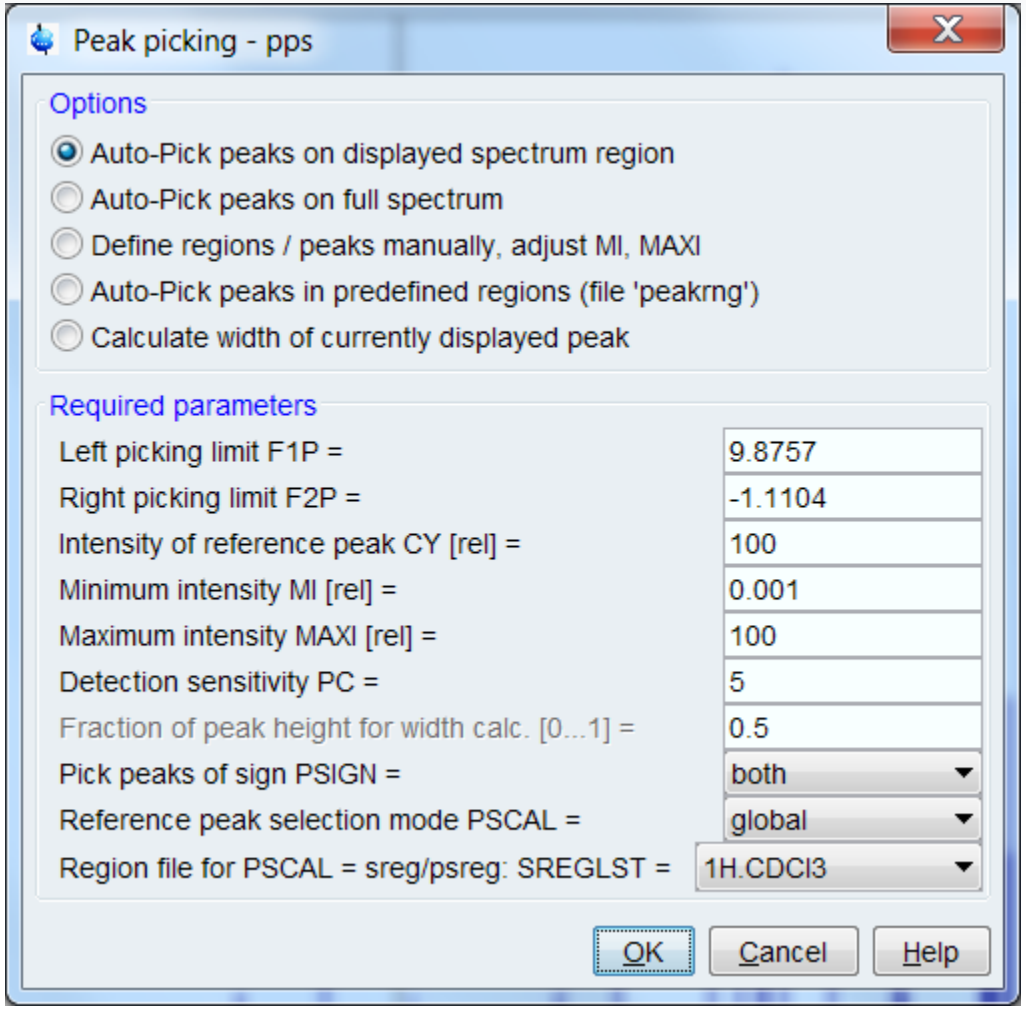
Pick Peaks


File
Start
Process
Analyse
Publish
View
Manage
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata
Spectrum
ProcPars
AcquPars
Title
PulseProg
Peaks
Integrals
Sample
Structure
Plot
Fid
Peak 1
Peak 2
Peak 3
Peak 4
7.6314
7.6159
7.4701
7.4528
[rel]
0
20
40
60
80
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
[ppm]
1 rows selected.

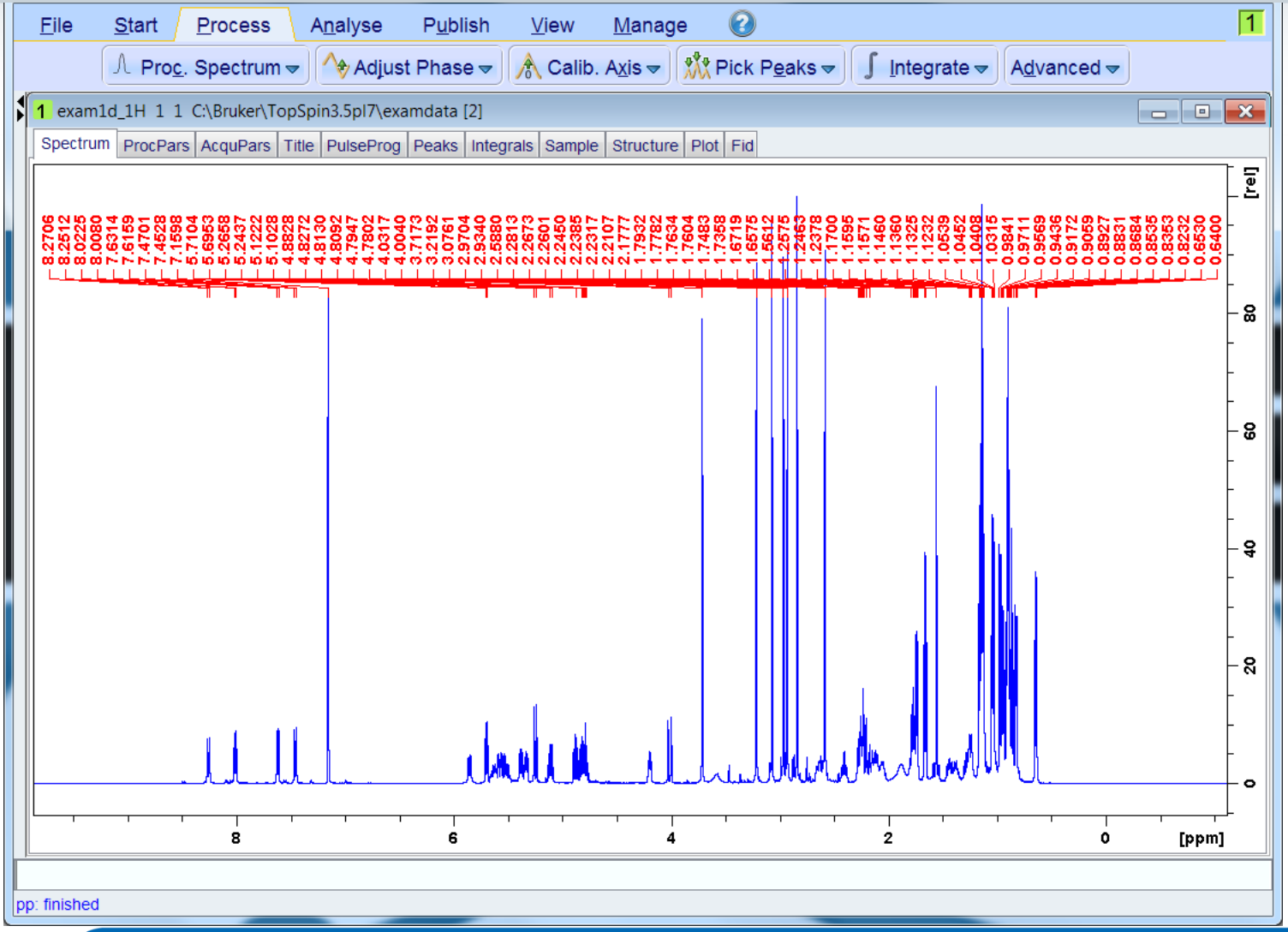
Parameters

- 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 × PC are picked.
- PSIGN defines if only positive or negative peaks or both are picked

Automatic Peak Picking Options [pp]

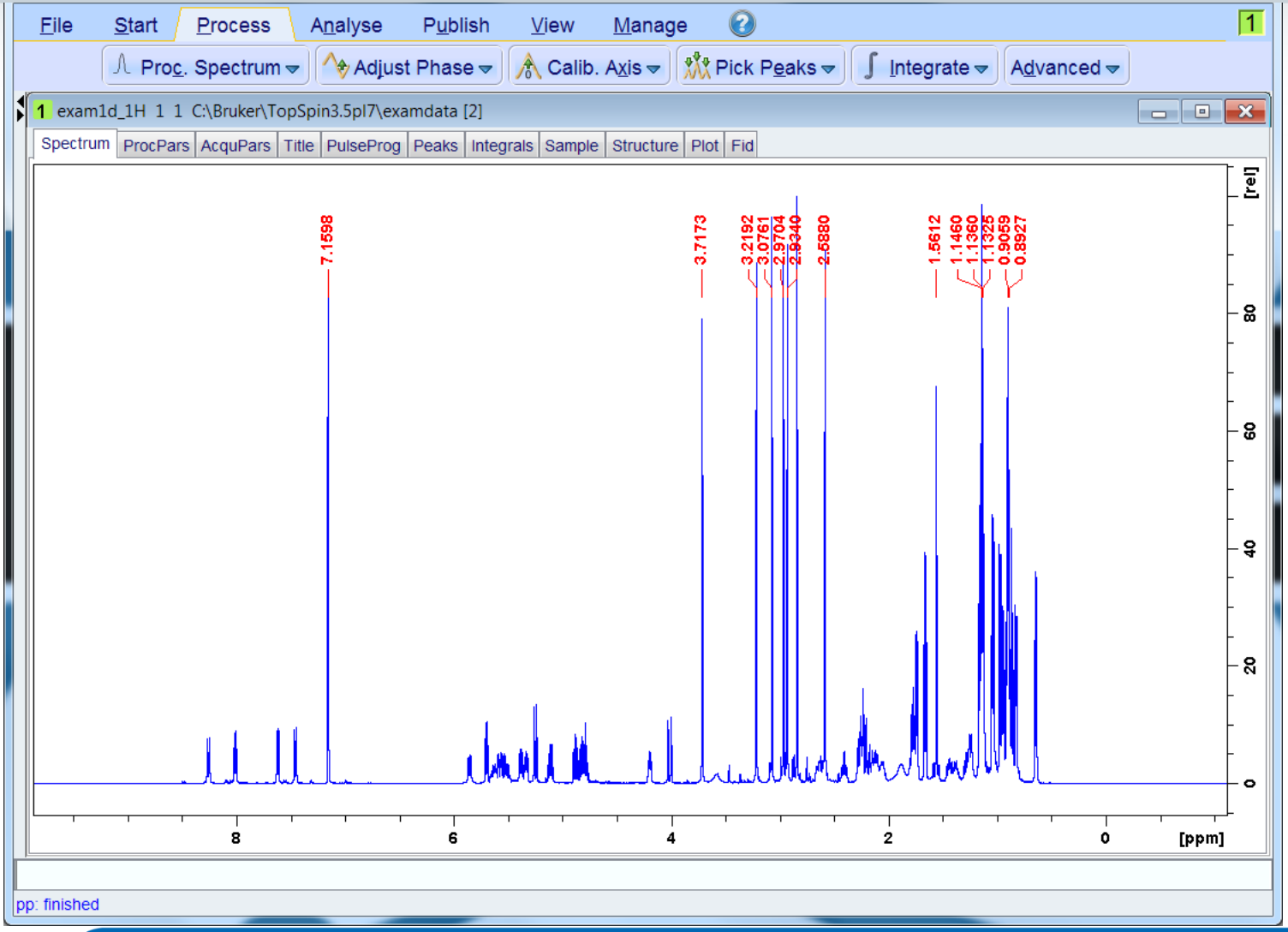


Automatic Peak Picking



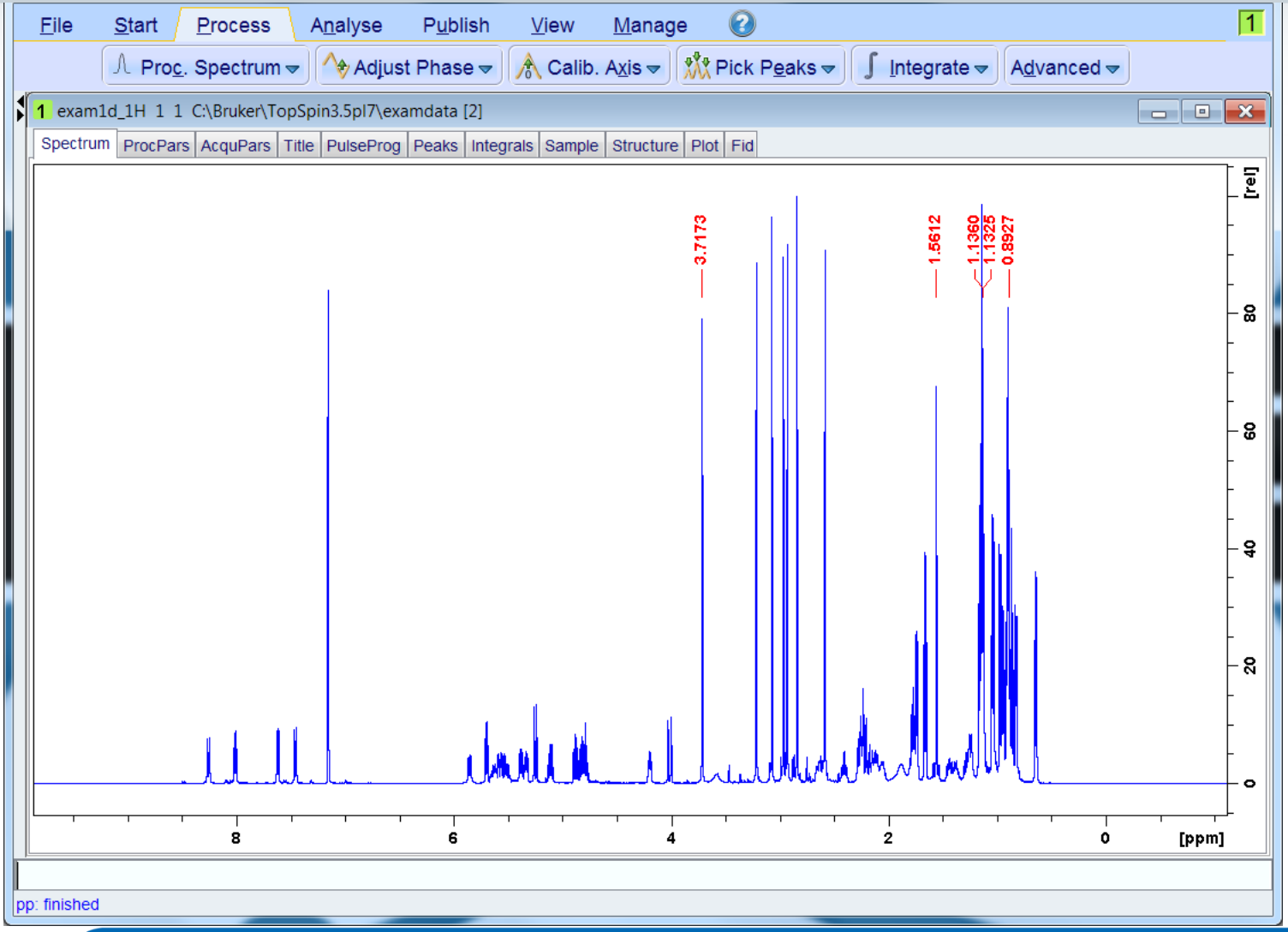
MI: 0.001
MAXI: 100
CY: 100
PC: 1

Automatic Peak Picking



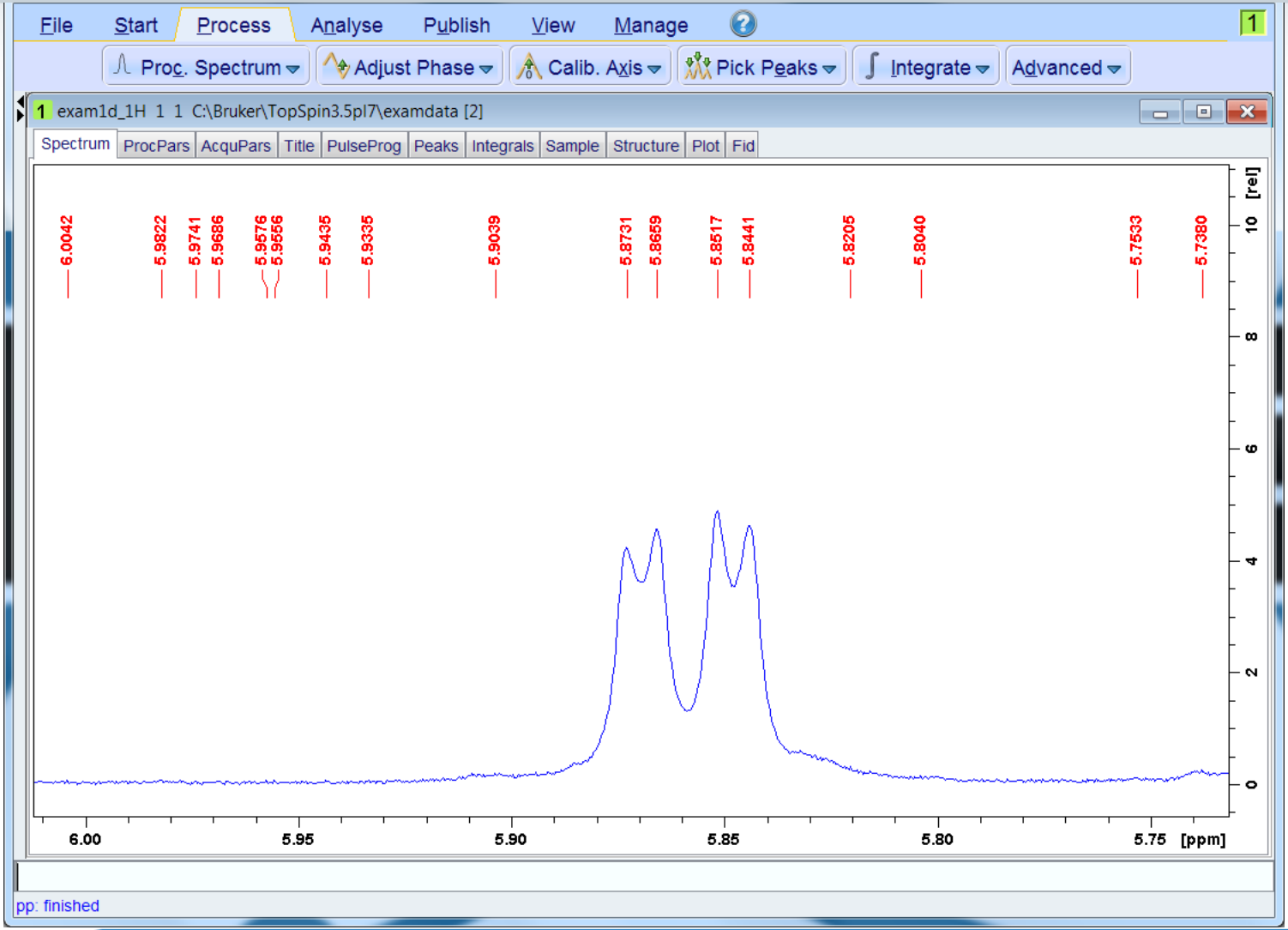
MI: 50
MAXI: 100
CY: 100
PC: 1

Automatic Peak Picking



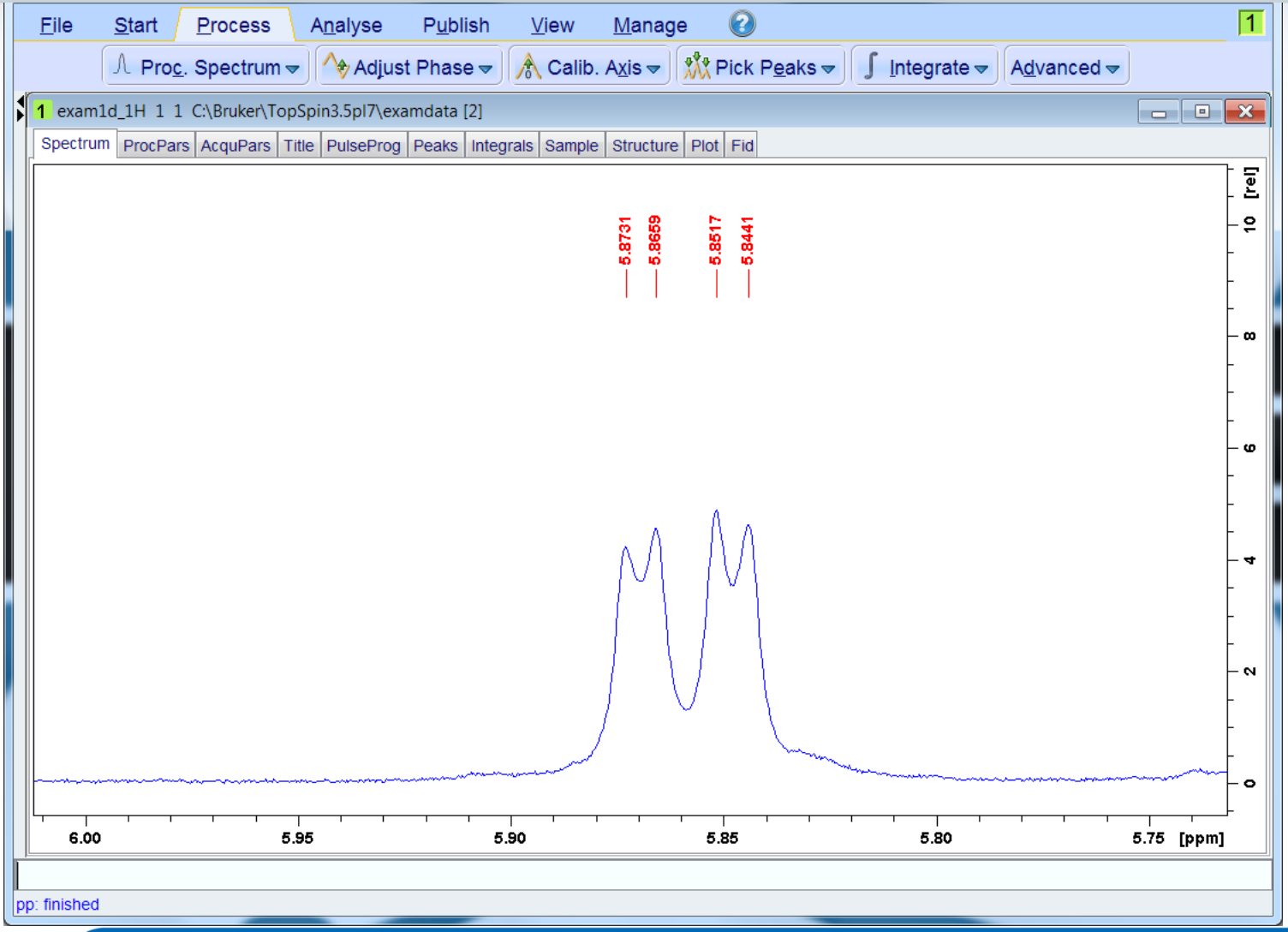
MI: 50
MAXI: 80
CY: 100
PC: 1

Automatic Peak Picking



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

Automatic Peak Picking

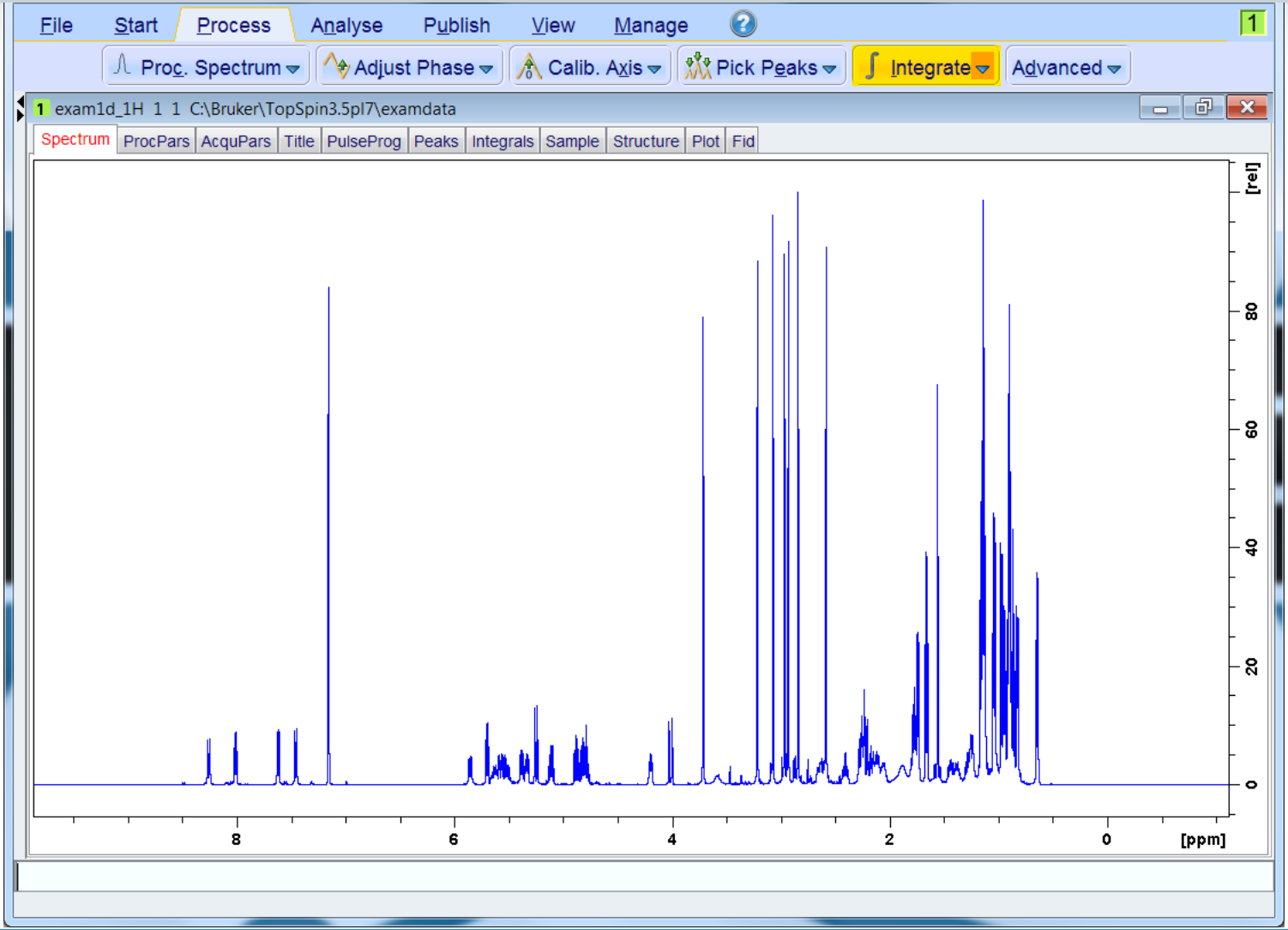


MI: 0.001
MAXI: 100
CY: 100
PC: 5

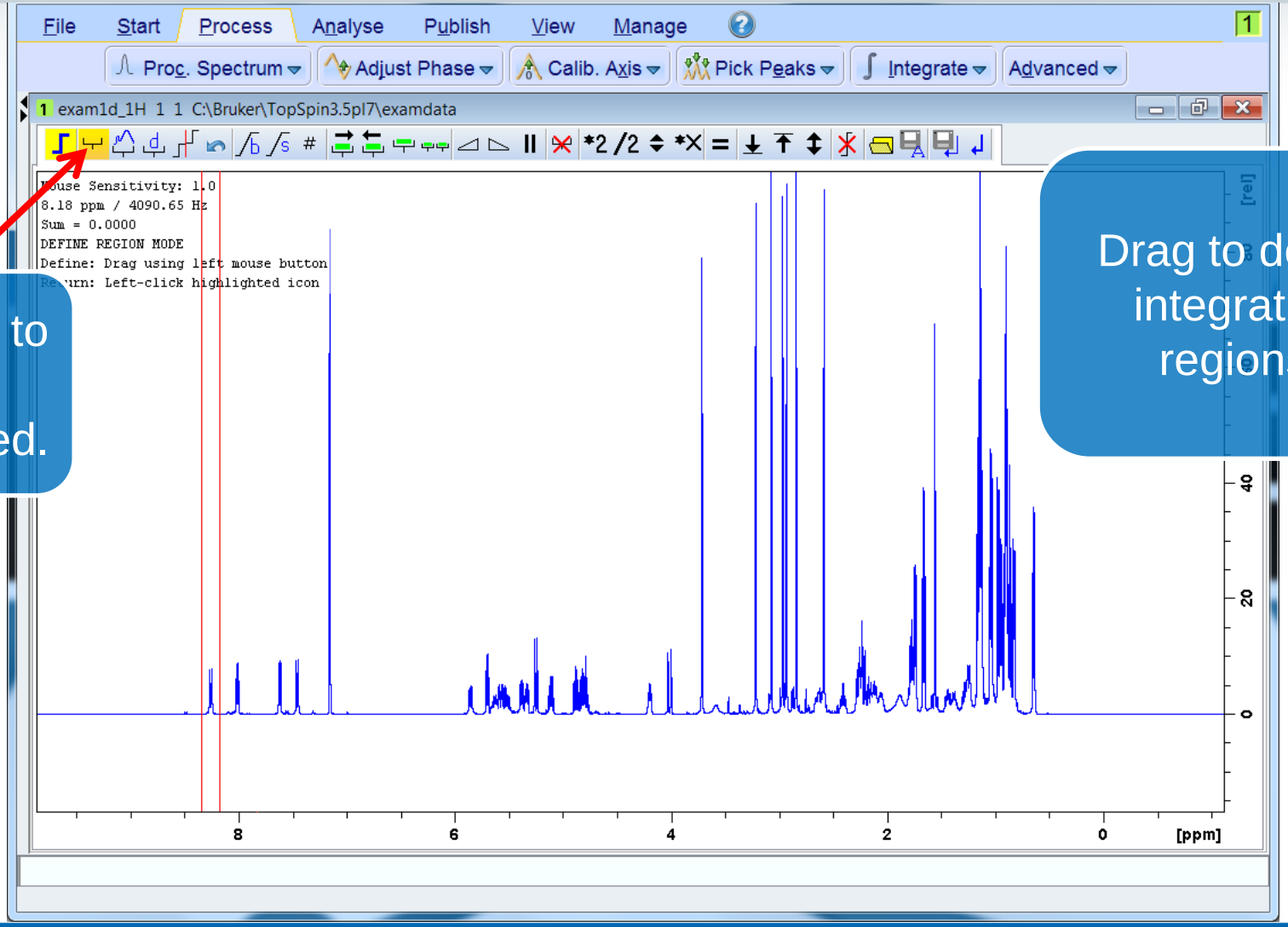
Integrate

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

Manual Integration



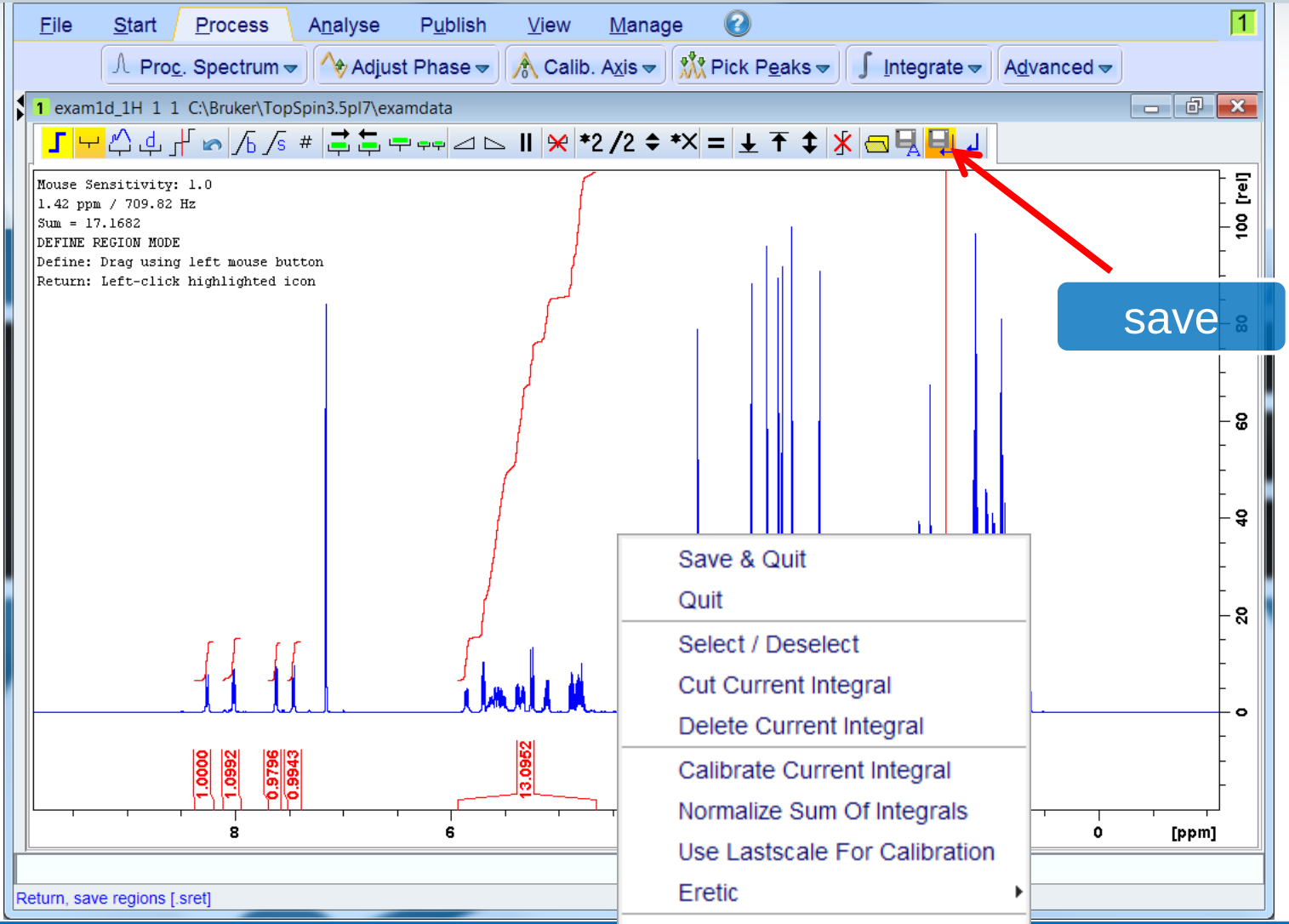
Manual Integration



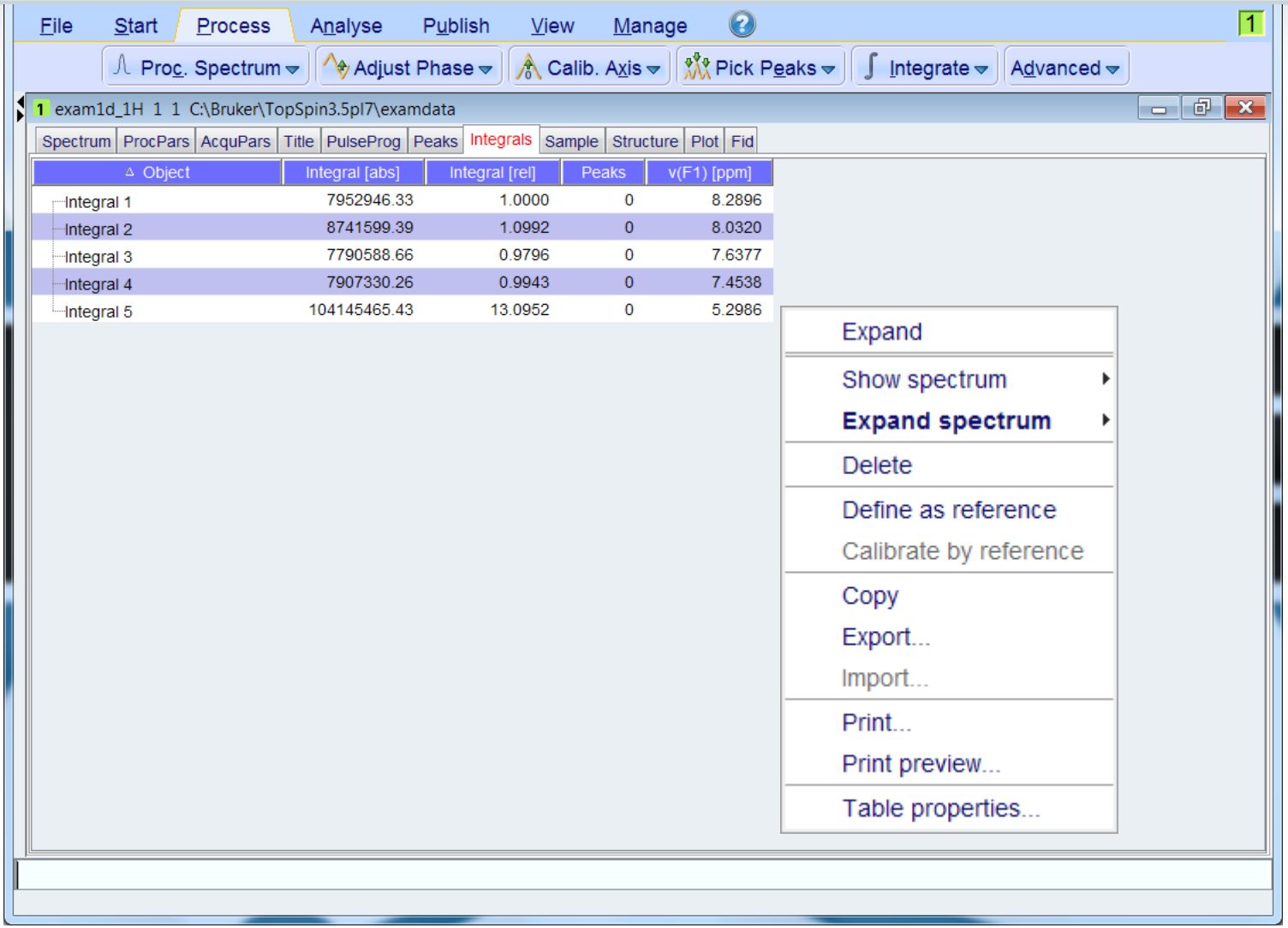
Needs to be selected.

Drag to define integration regions.

Manual Integration



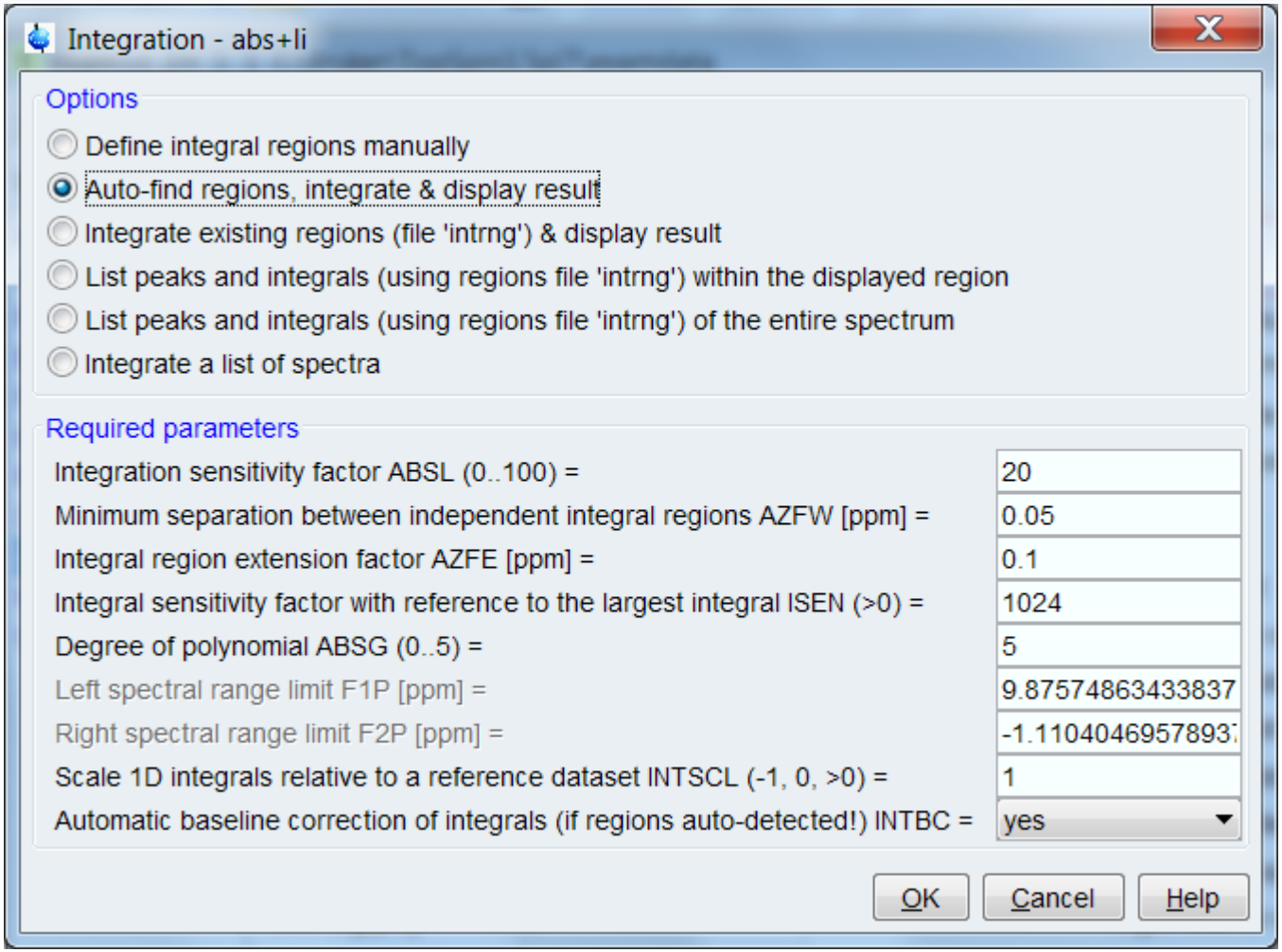
Integrals


File
Start
Process
Analyse
Publish
View
Manage
Proc. Spectrum
Adjust Phase
Calib. Axis
Pick Peaks
Integrate
Advanced
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata
Spectrum
ProcPars
AcquPars
Title
PulseProg
Peaks
Integrals
Sample
Structure
Plot
Fid
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...

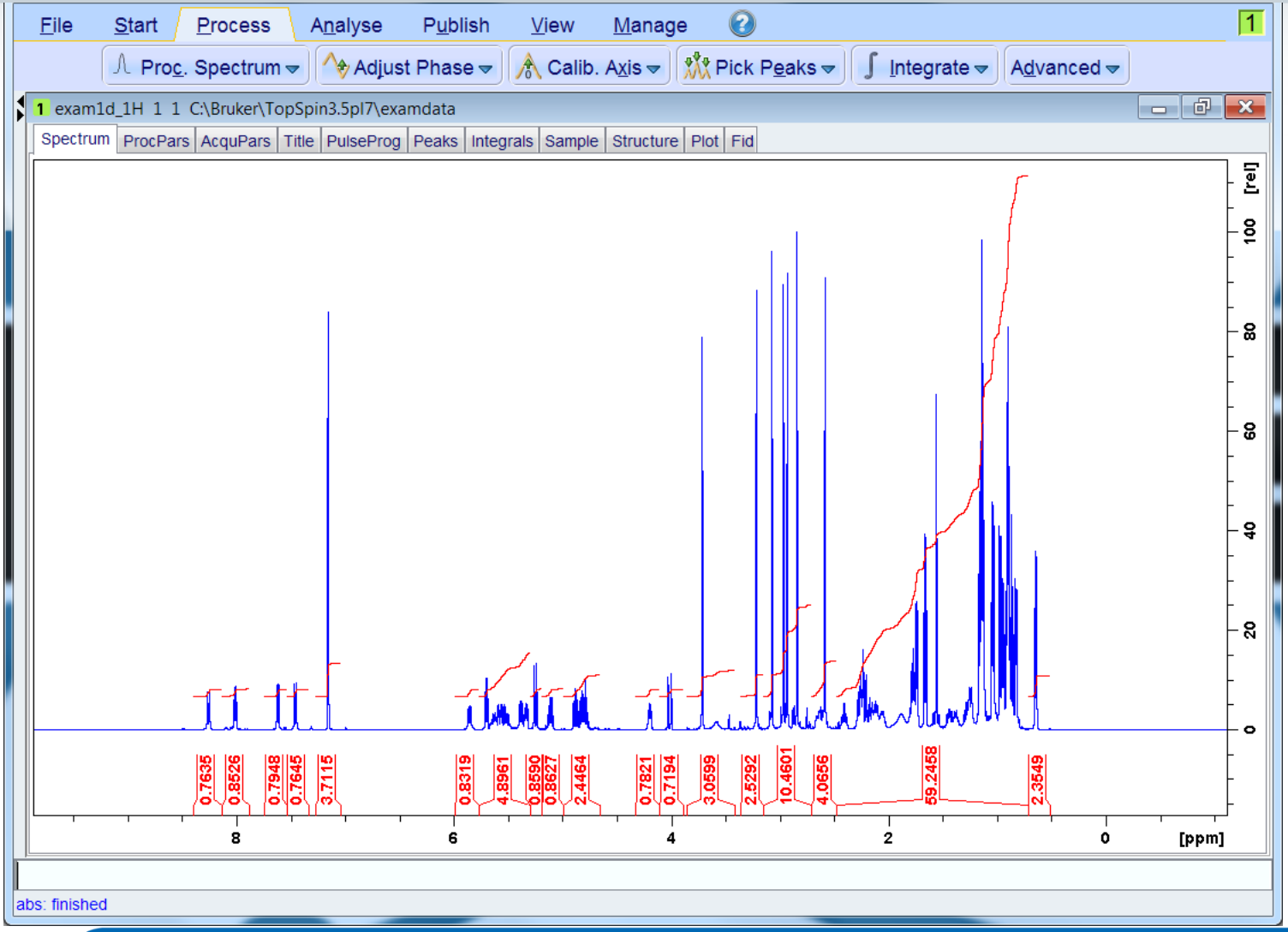
Parameters

- 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]

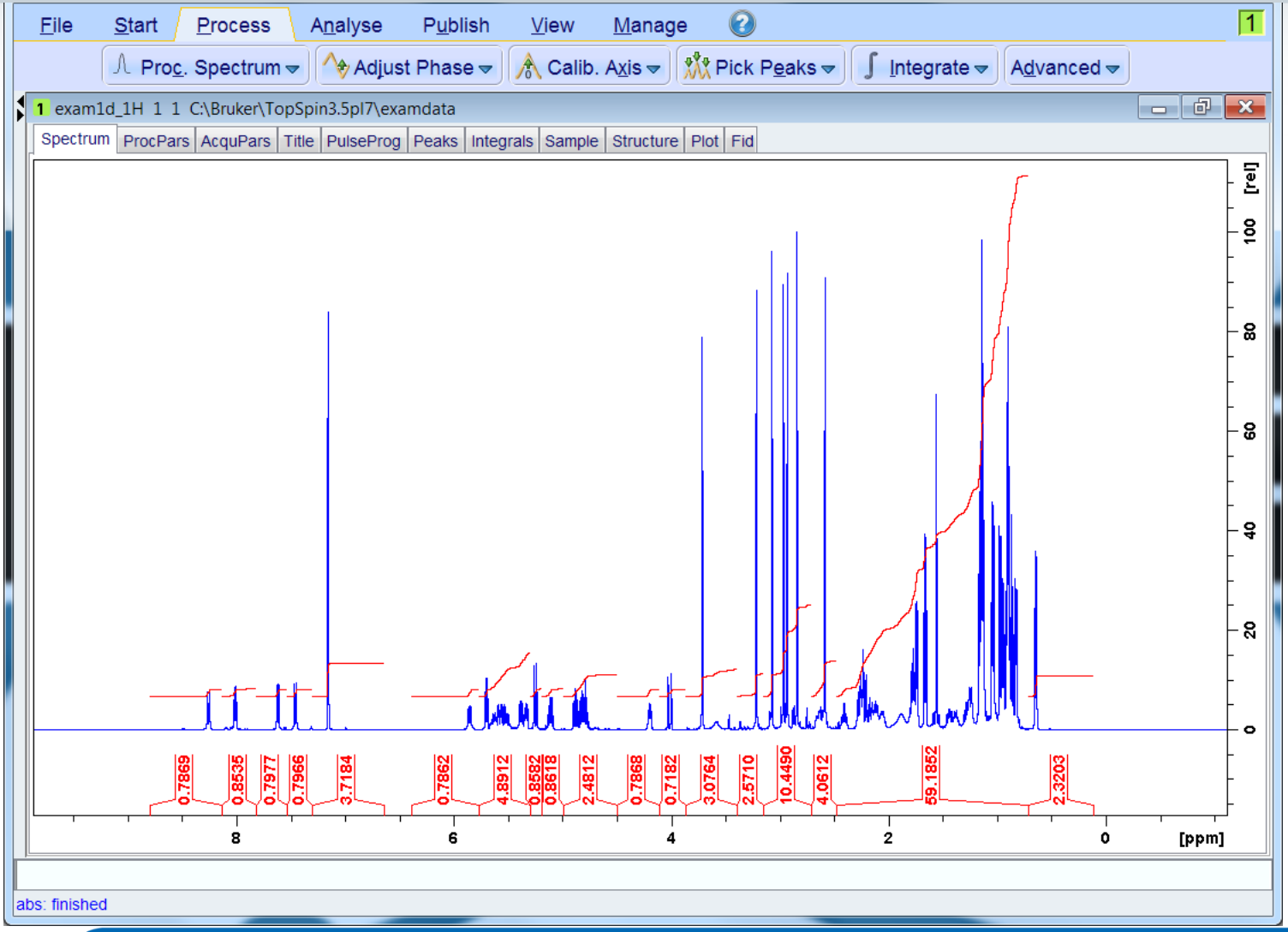


Automatic Integration



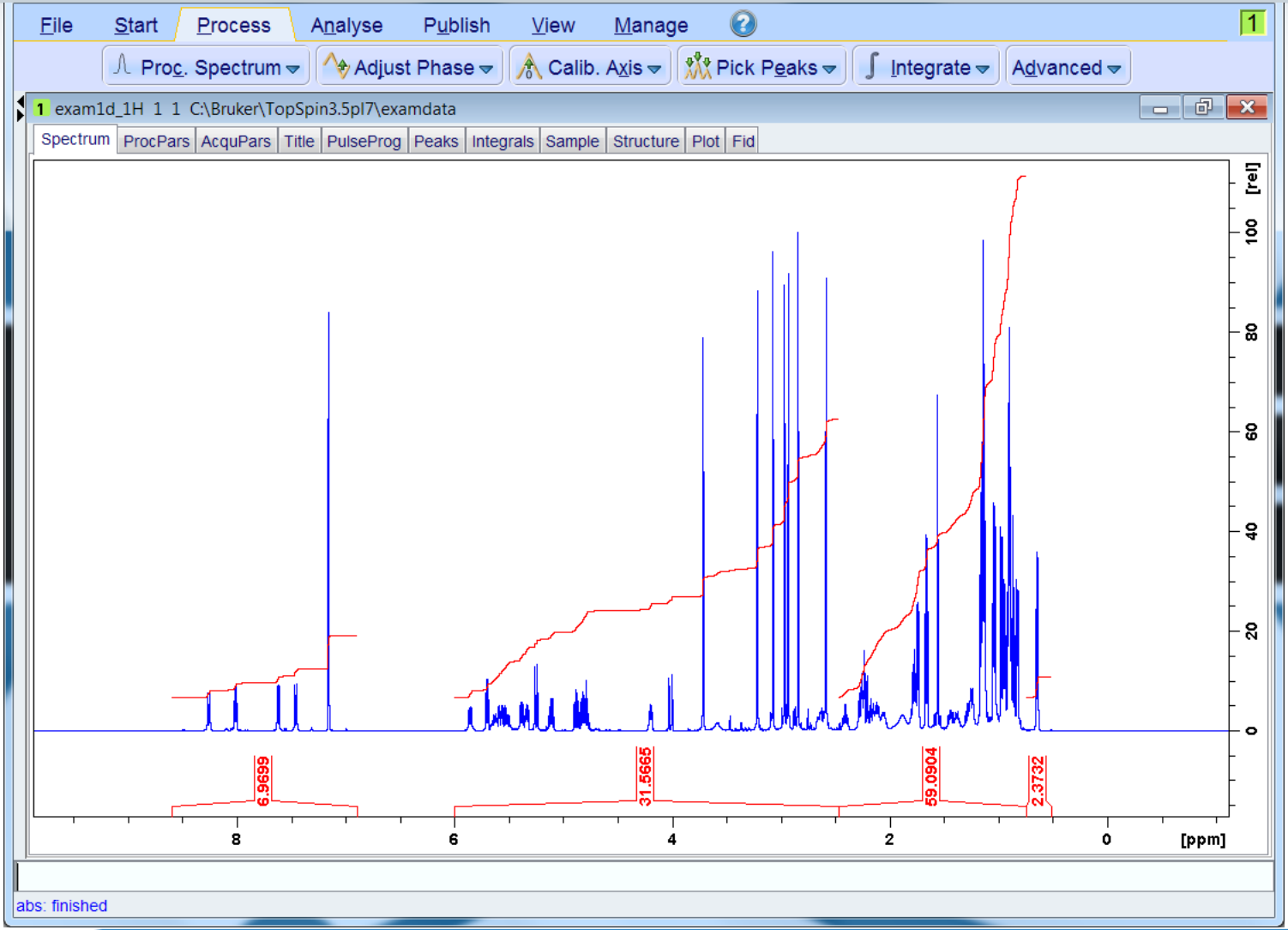
ISEN: 128
AZFE: 0.1
AZFW: 0.05
ABSL: 20

Automatic Integration



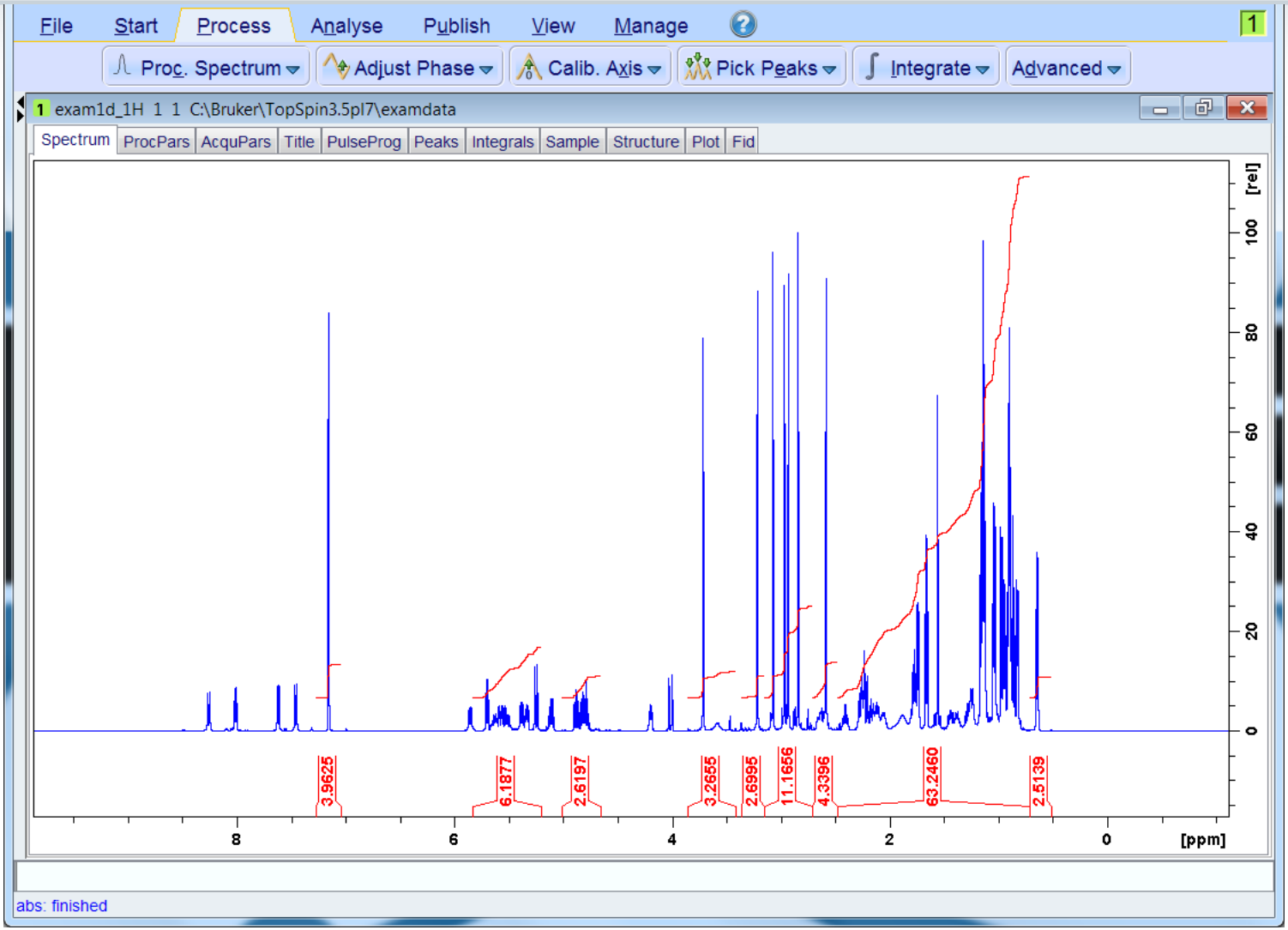
ISEN: 128
AZFE: 0.5
AZFW: 0.05
ABSL: 20

Automatic Integration



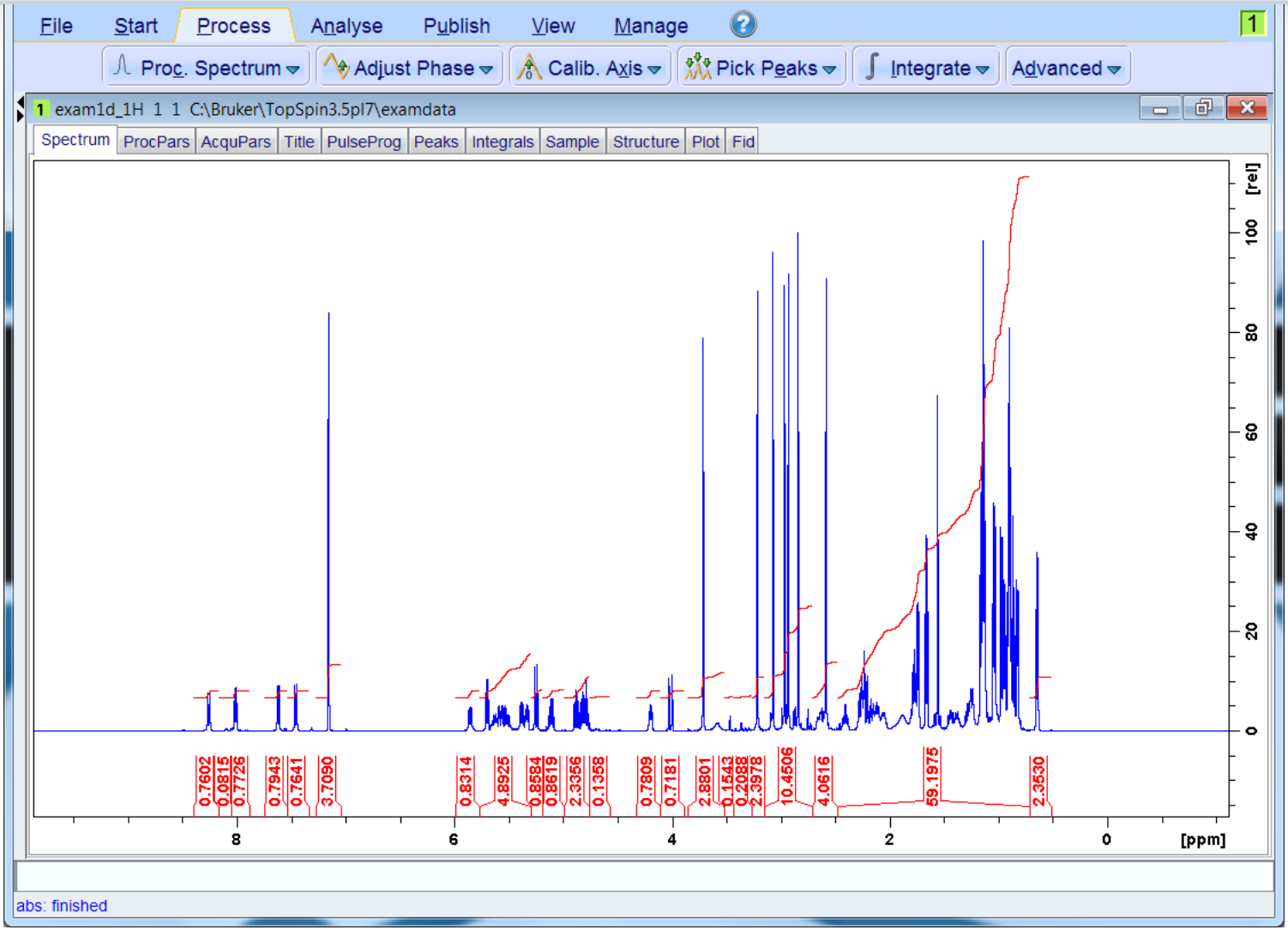
ISEN: 128
AZFE: 0.1
AZFW: 0.5
ABSL: 20

Automatic Integration



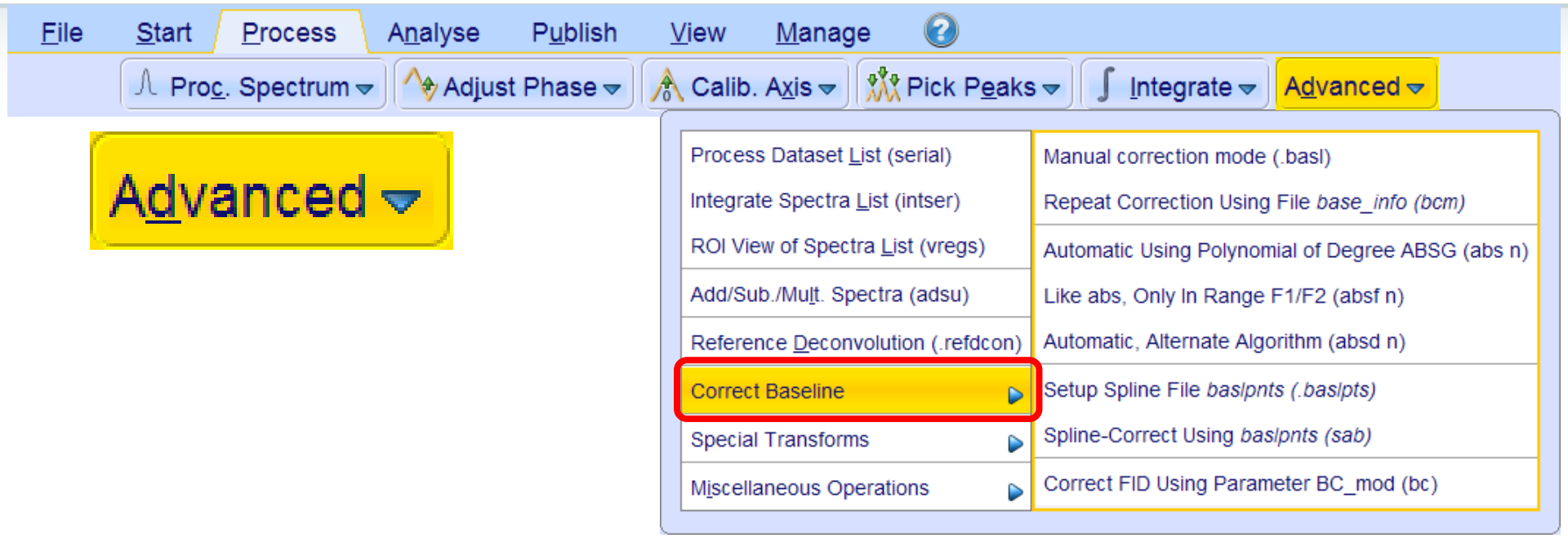
ISEN: 64
AZFE: 0.1
AZFW: 0.05
ABSL: 20

Automatic Integration



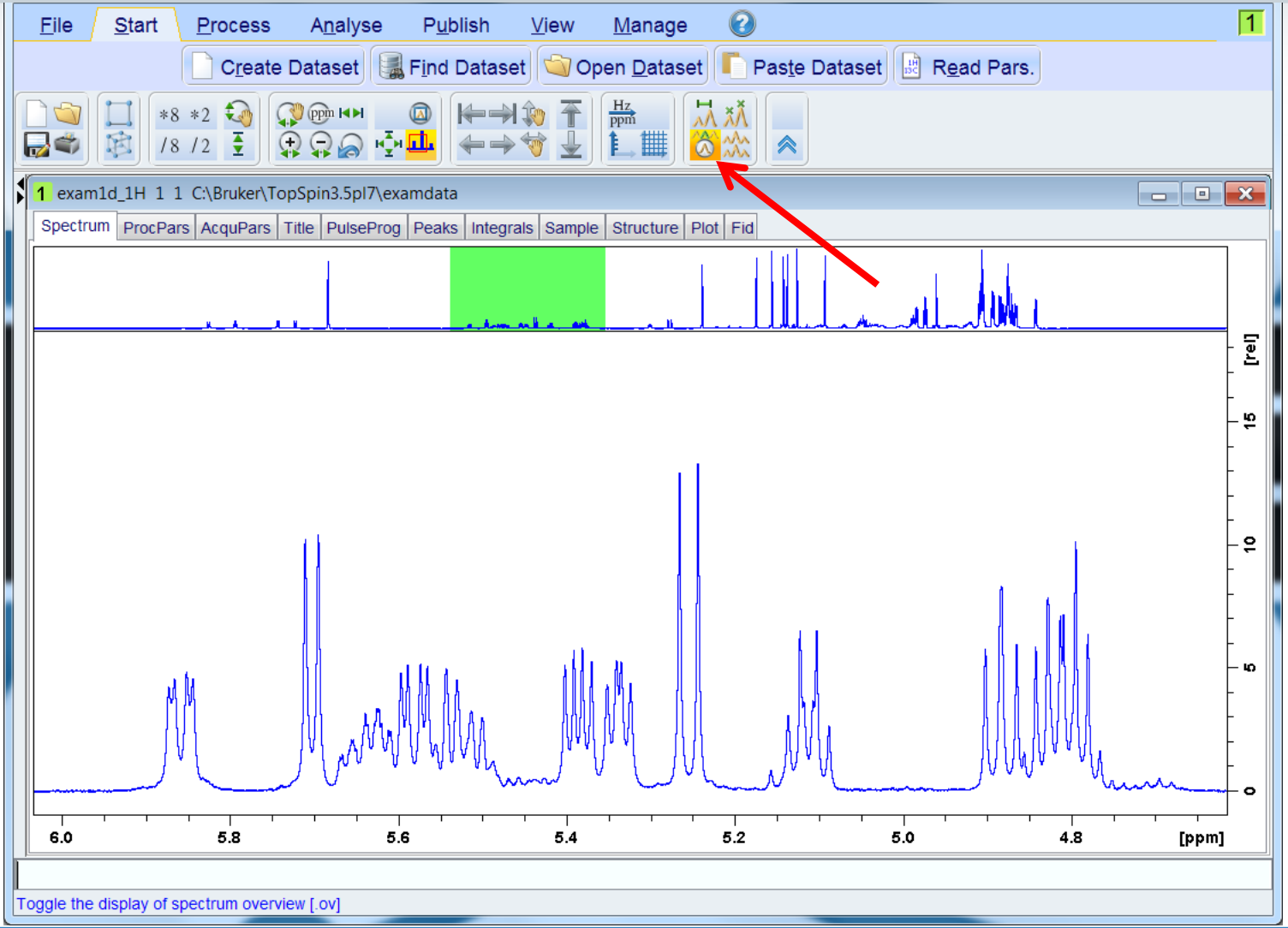
ISEN: 1k
AZFE: 0.1
AZFW: 0.05
ABSL: 20

Advanced

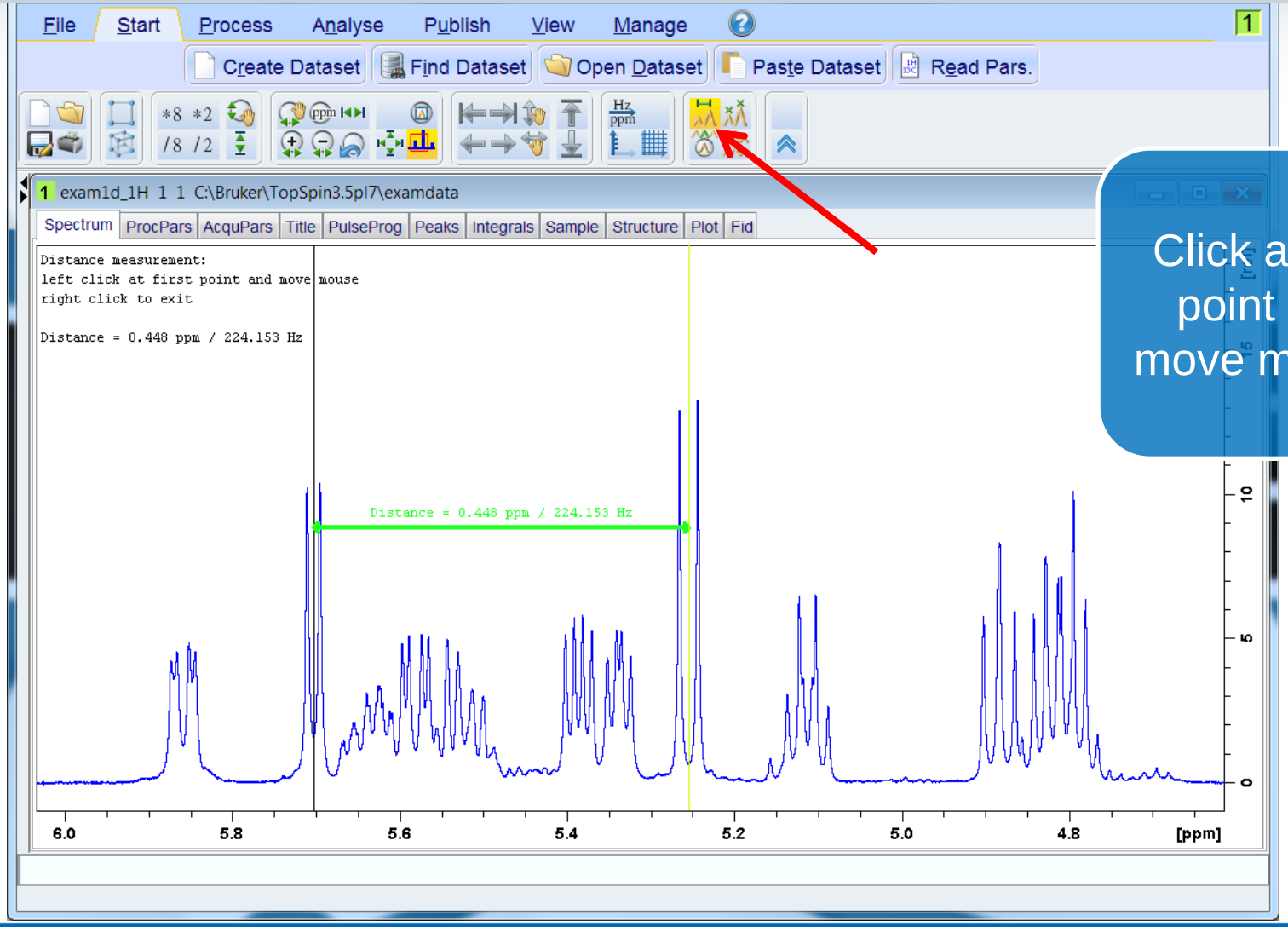


- [**abs**] performs automatic baseline correction and integration
- [**abs n**] performs automatic baseline correction (no integration)
- [**.basl**] manual baseline correction mode
- [**bas**] opens dialog for baseline correction

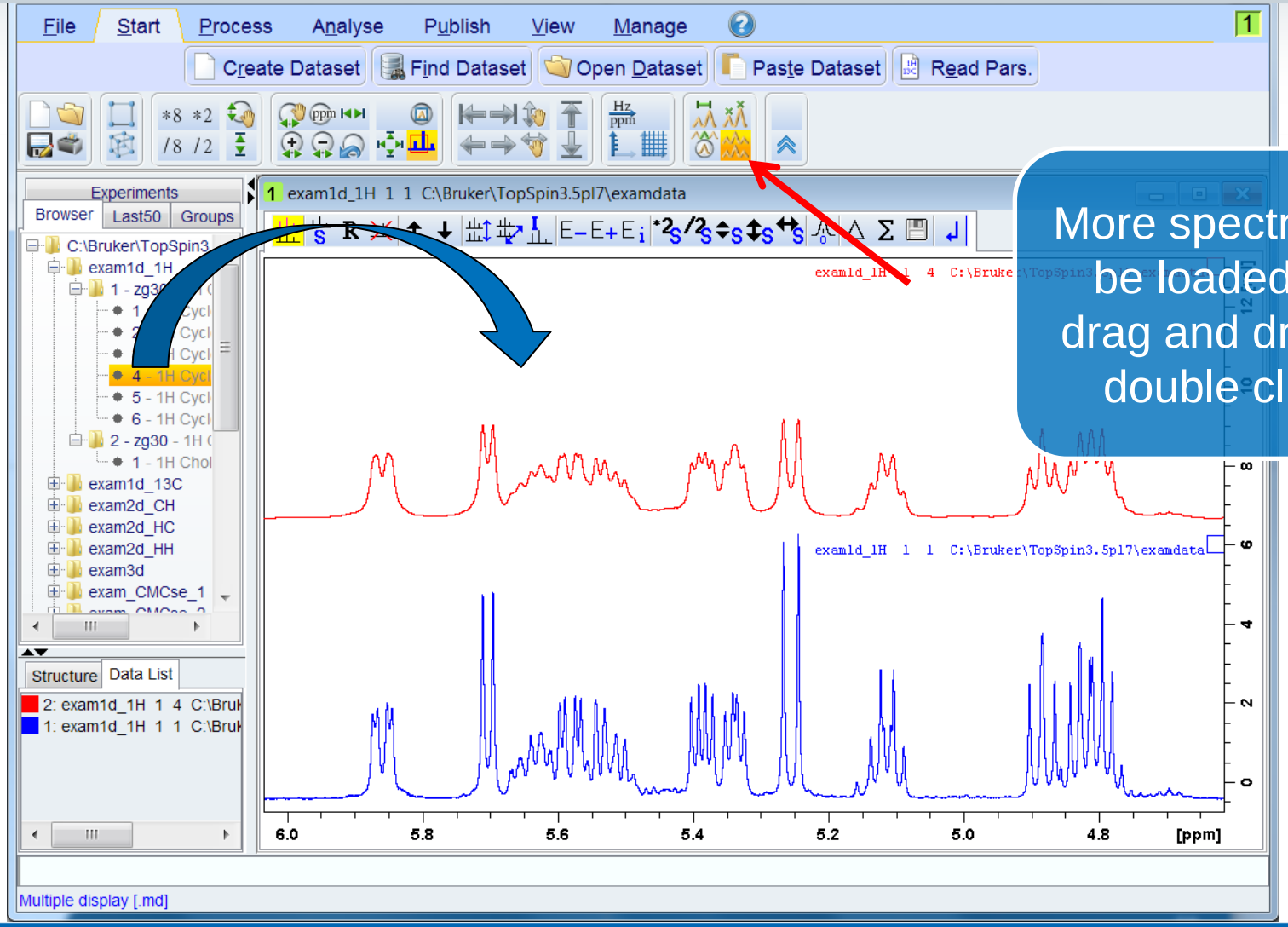
Toggle spectrum overlay



Measure distances

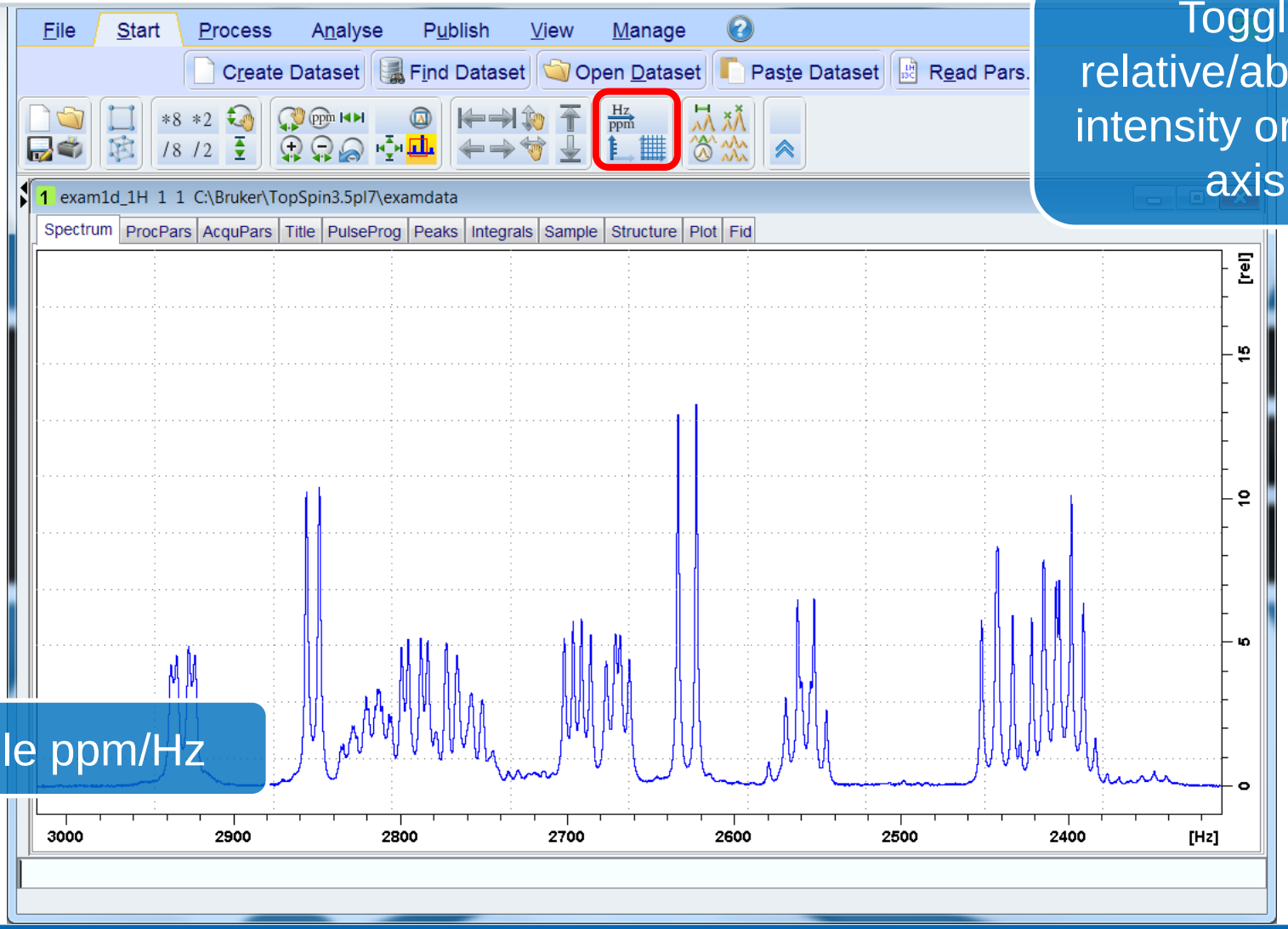


Dual display



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

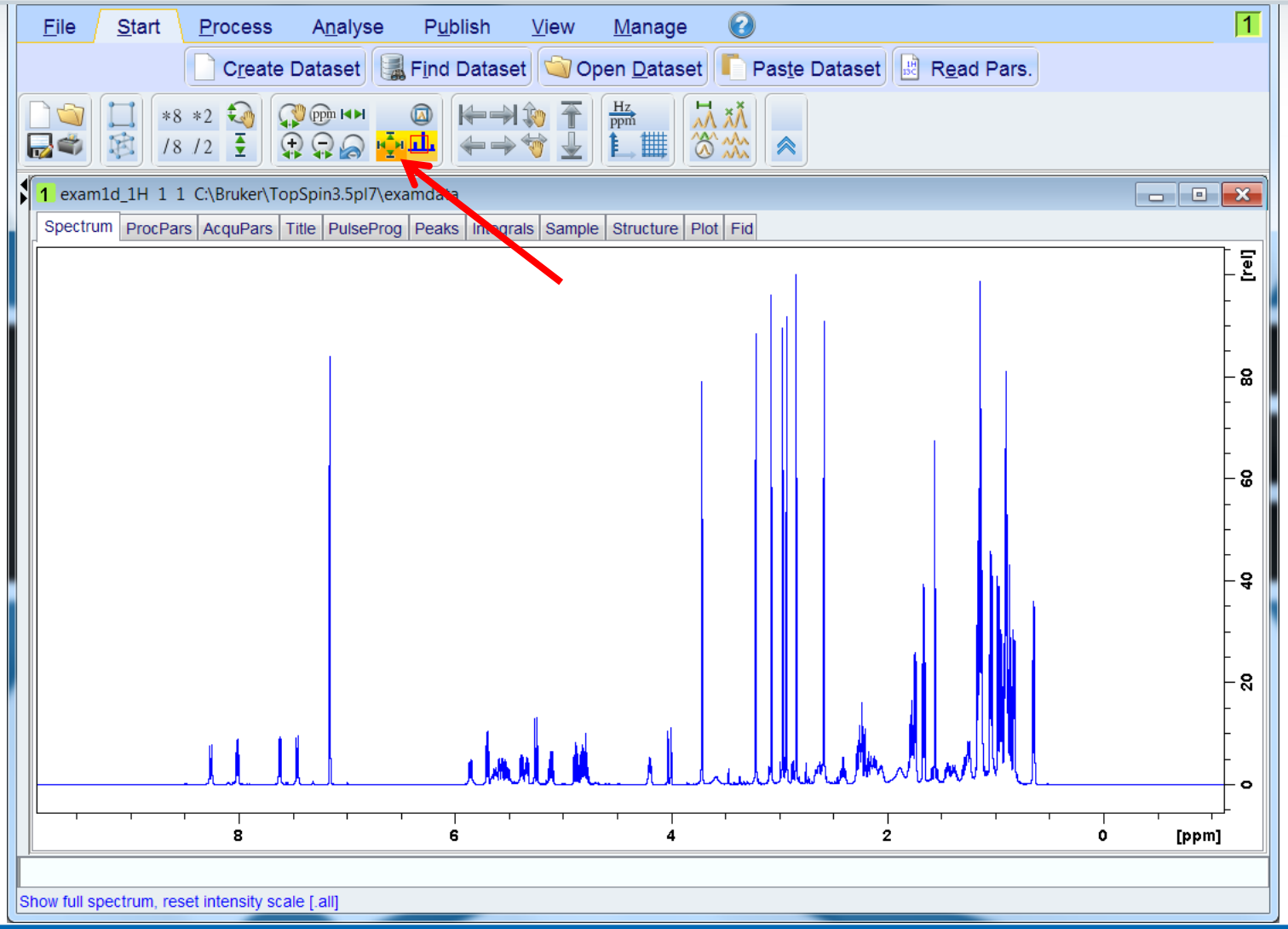
Toggle axis units and grid



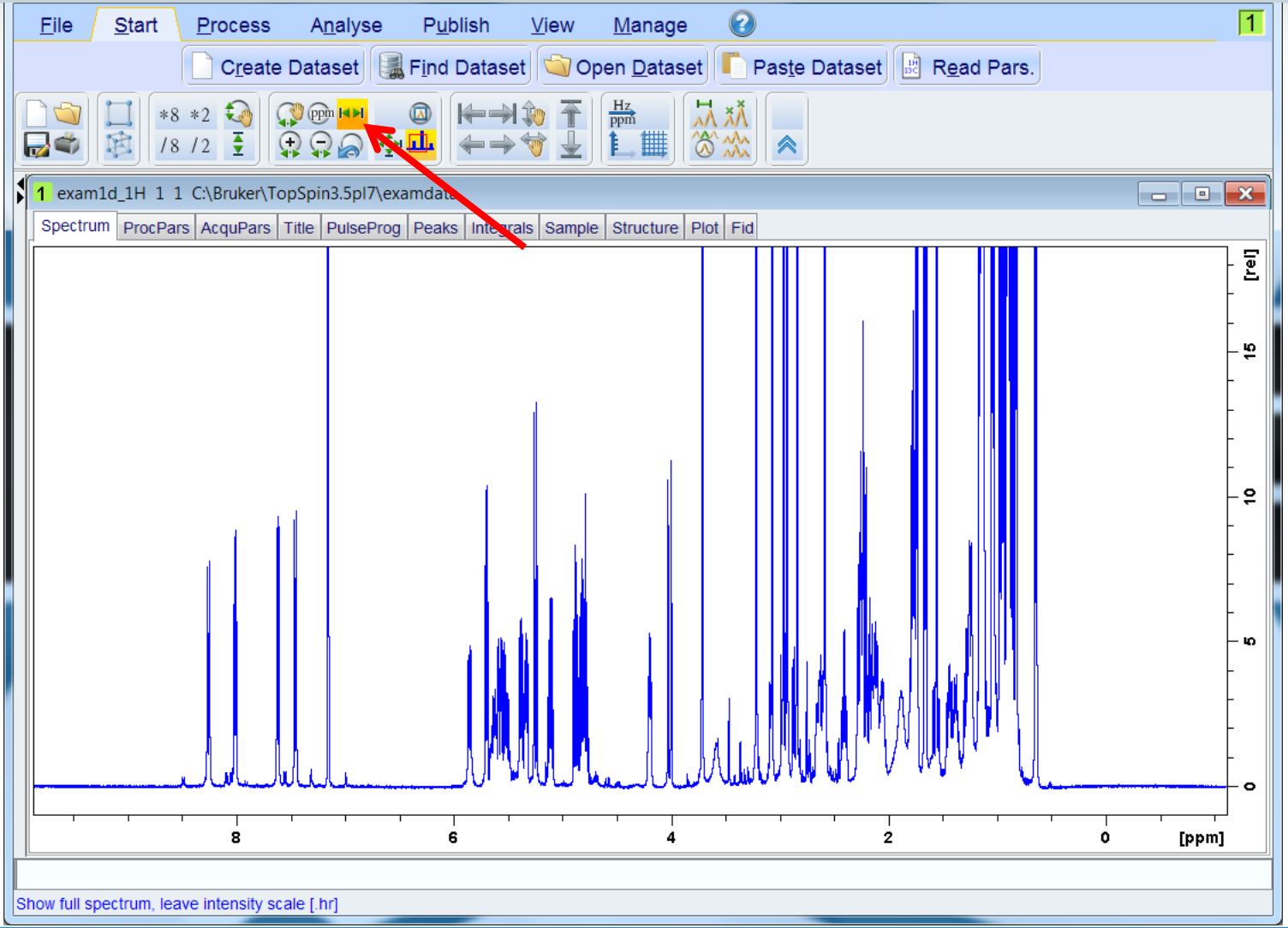
Toggle relative/absolute intensity or hides axis

Toggle ppm/Hz

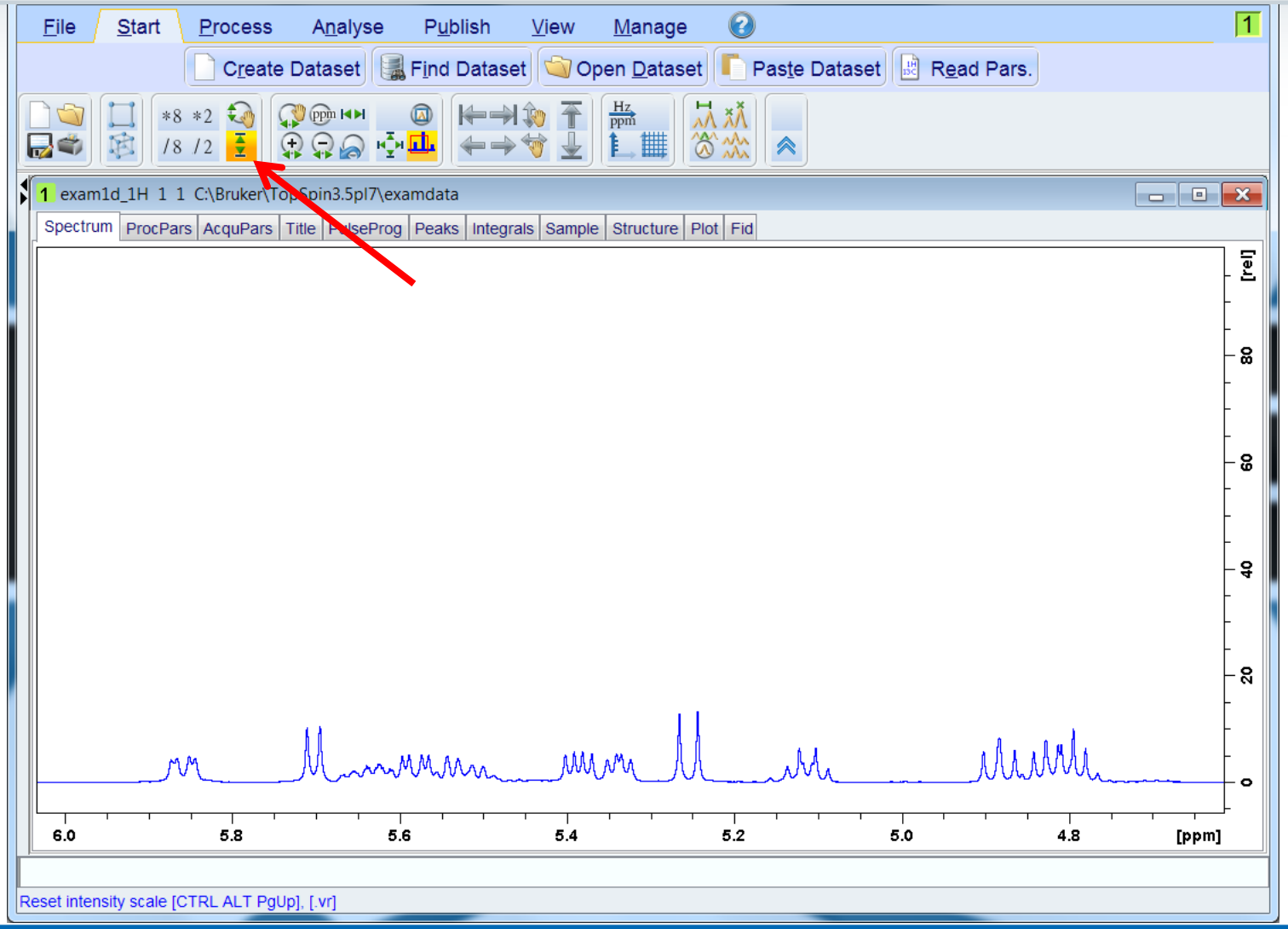
Show full spectrum, reset intensity



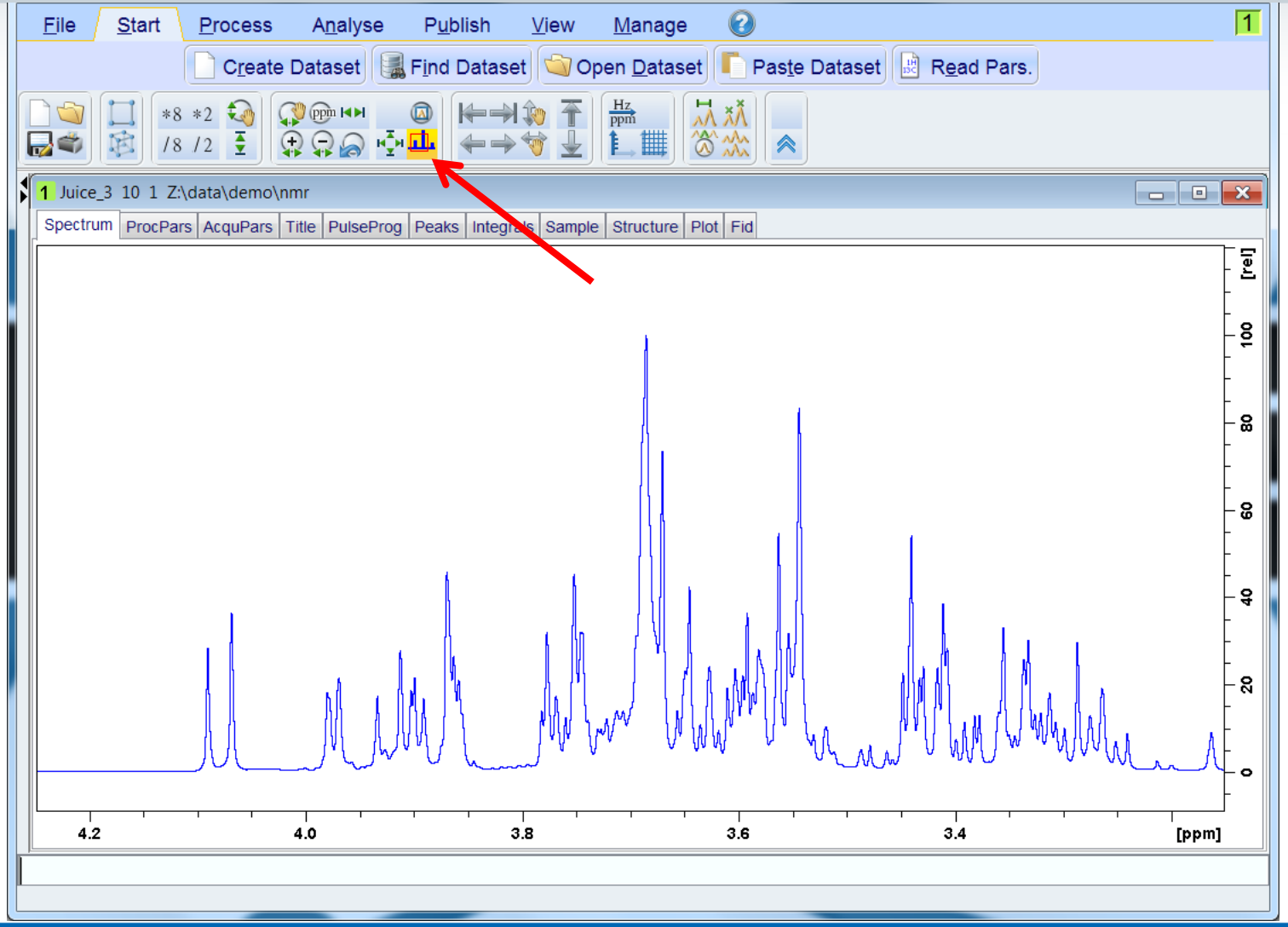
Show full spectrum, do not reset intensity



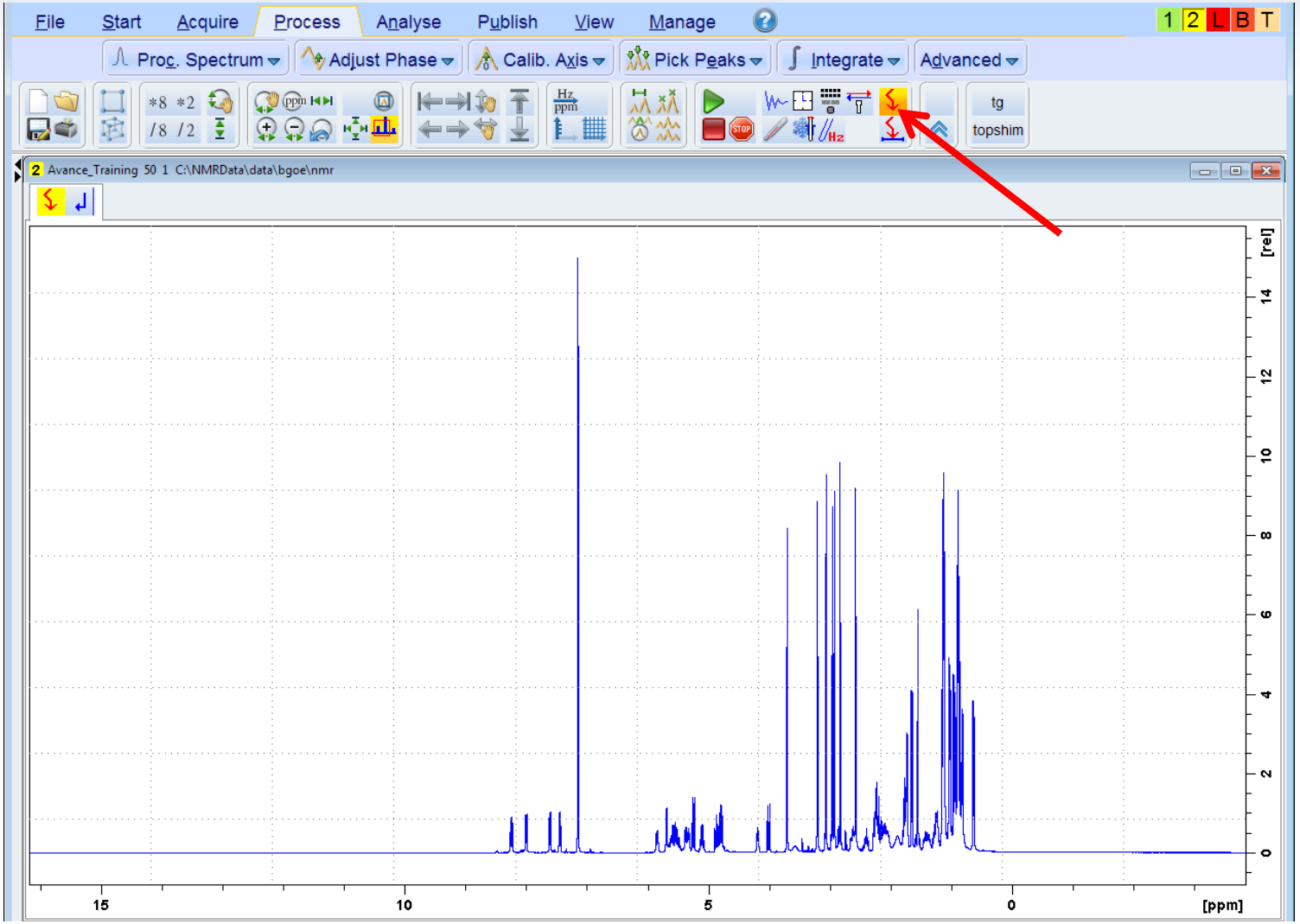
Reset intensity



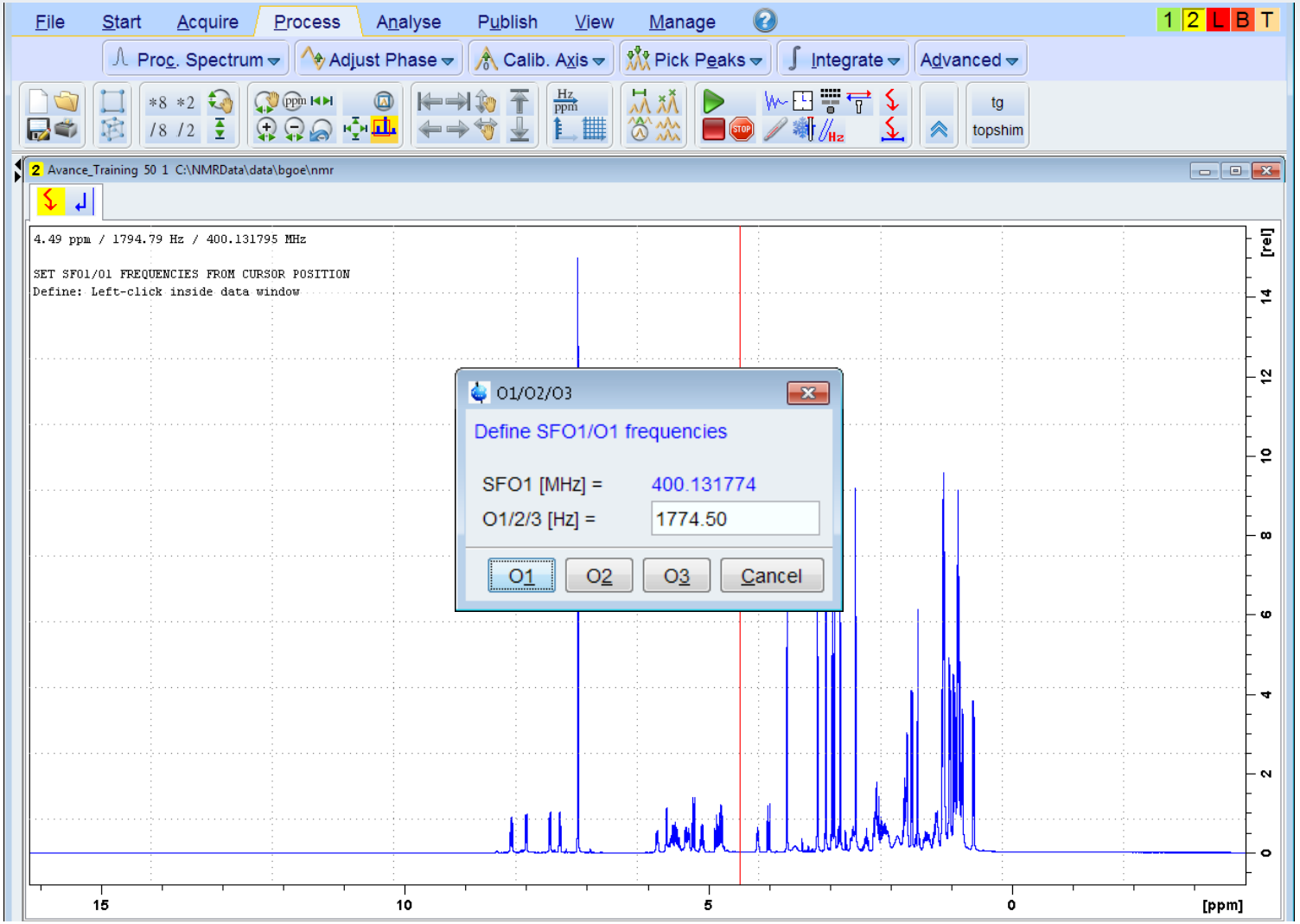
Retain scale and intensity



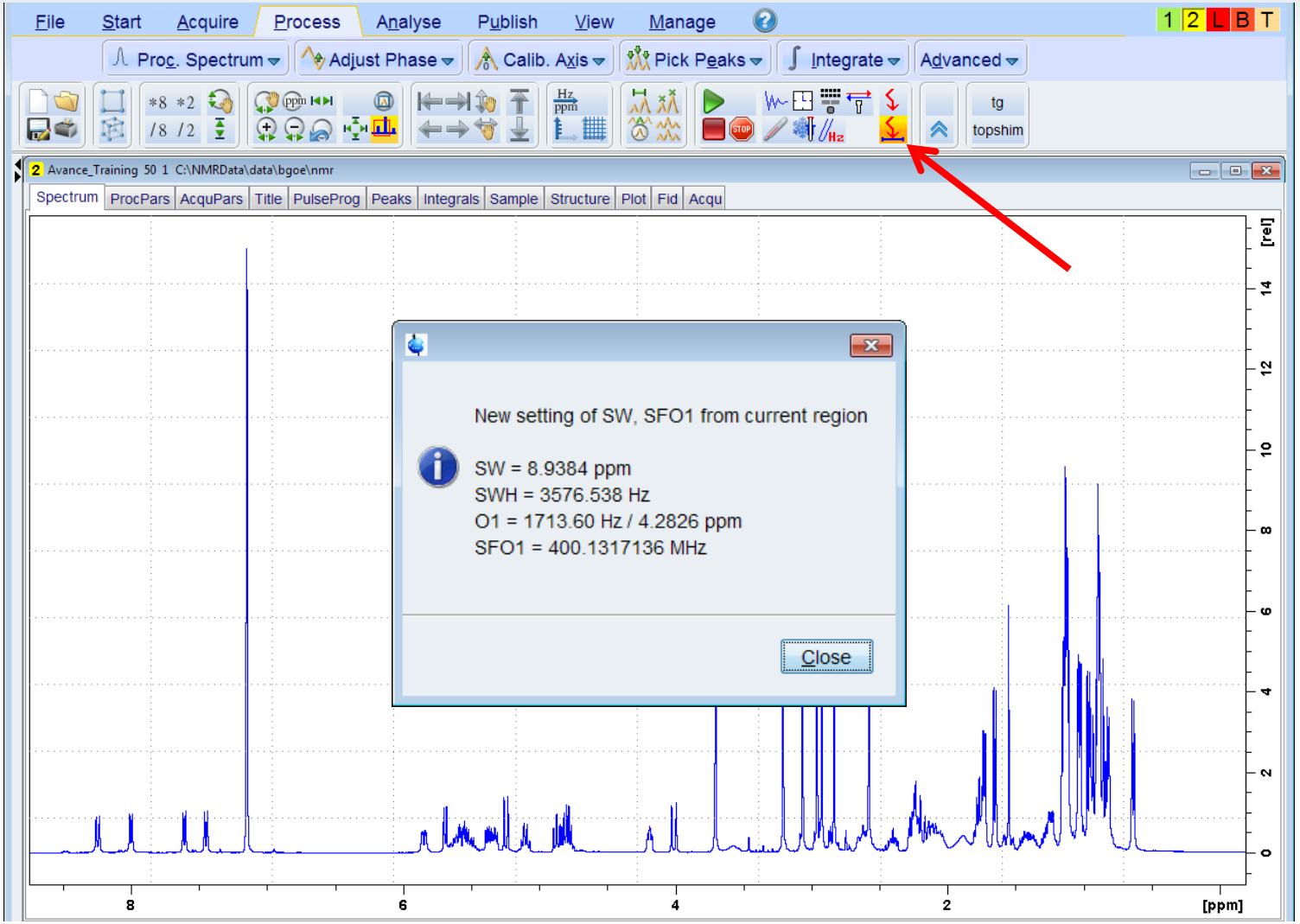
Set transmitter frequency by cursor

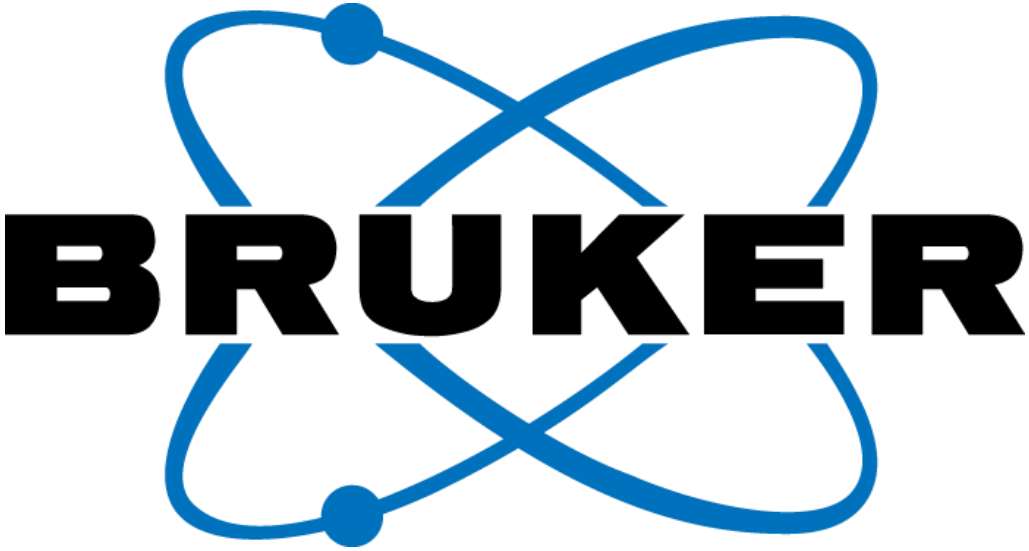


Set transmitter frequency by cursor



Set SW to current region and O1 in center





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