Mnova 7.1 NMR Basics

Hongjun Zhou
Department of Chemistry and Biochemistry
University of California Santa Barbara

Last Updated on October 26, 2011

All data were collected at UCSB Chem NMR Facility.

Mnova 7.1 NMR Basics

- Interface and operation resemble MS Powerpoint
- Nearly all onscreen items editable
- Both auto- and manual- processing possible

NOTE:
- Multiple ways (e.g., menu buttons or RMB click) to access the same function are available

Typical three mouse button control
- Left mouse button (**LMB**): selection
- Middle mouse (scroll) button (**MMB**): change vertical scaling
- Right mouse button (**RMB**): show menu

Typical 1D Processing in sequential order
- Load data (and auto-process)
- Adjust processing parameters if necessary (line broadening, number of points, referencing, etc.)
- Adjust phases (zero and 1st order)
- Baseline correction
- Peak integration
- Peak picking
- Save, print, report, etc.

Hot Keys
- Press **Esc** to exit interactive mode
- Press **i** to enter integration mode
- Press **k** to enter peak picking/manual threshold mode
- Press **p** to enter panning mode
- Press **z** to zoom in
- Press **t** to enter text annotation

Hot Keys
- Press **f** to display full spectrum
- Press **h** to fit tallest peak to window height
- Press **m** to set manual zoom range
- Press **c** to show cross hair mark as cursor moves
- Press **x** (then hold left cursor and drag) to cut/delete region of spectrum
- Press **+**/**-** to increase/decrease vertical scale
- Press **→ ← ↑ ↓** to move spectrum right/left/up/down

Overview

- **1D data processing (H1 and C13)**
  - Referencing
  - Phasing
  - Baseline correction
  - Integration
  - Peak picking

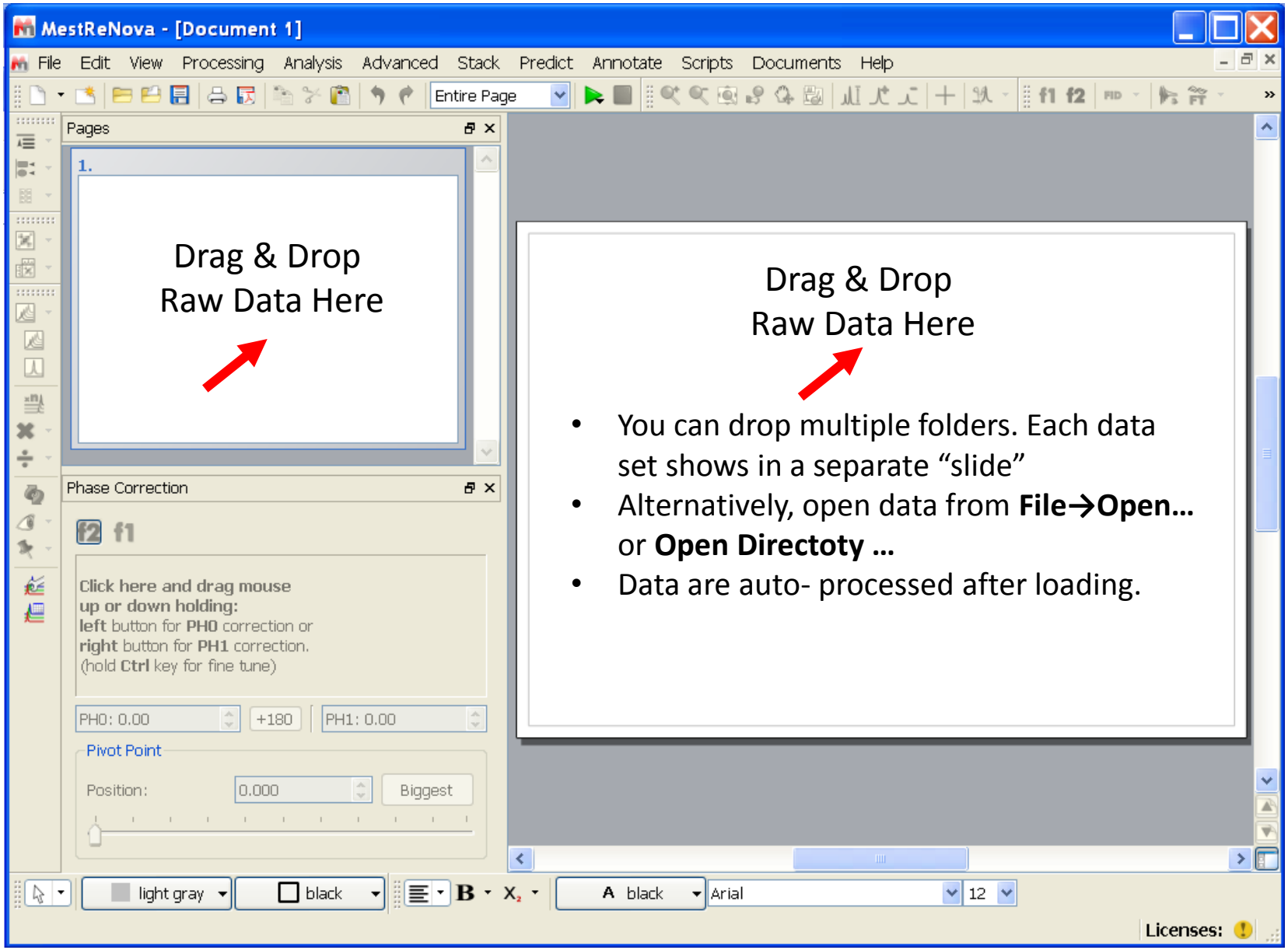
- **1D arrayed data processing: DEPT**
  - Straight processing of Varian DEPT data
  - Separation of CH, CH2, CH3 groups with formula

- **Superimpose multiple spectra**

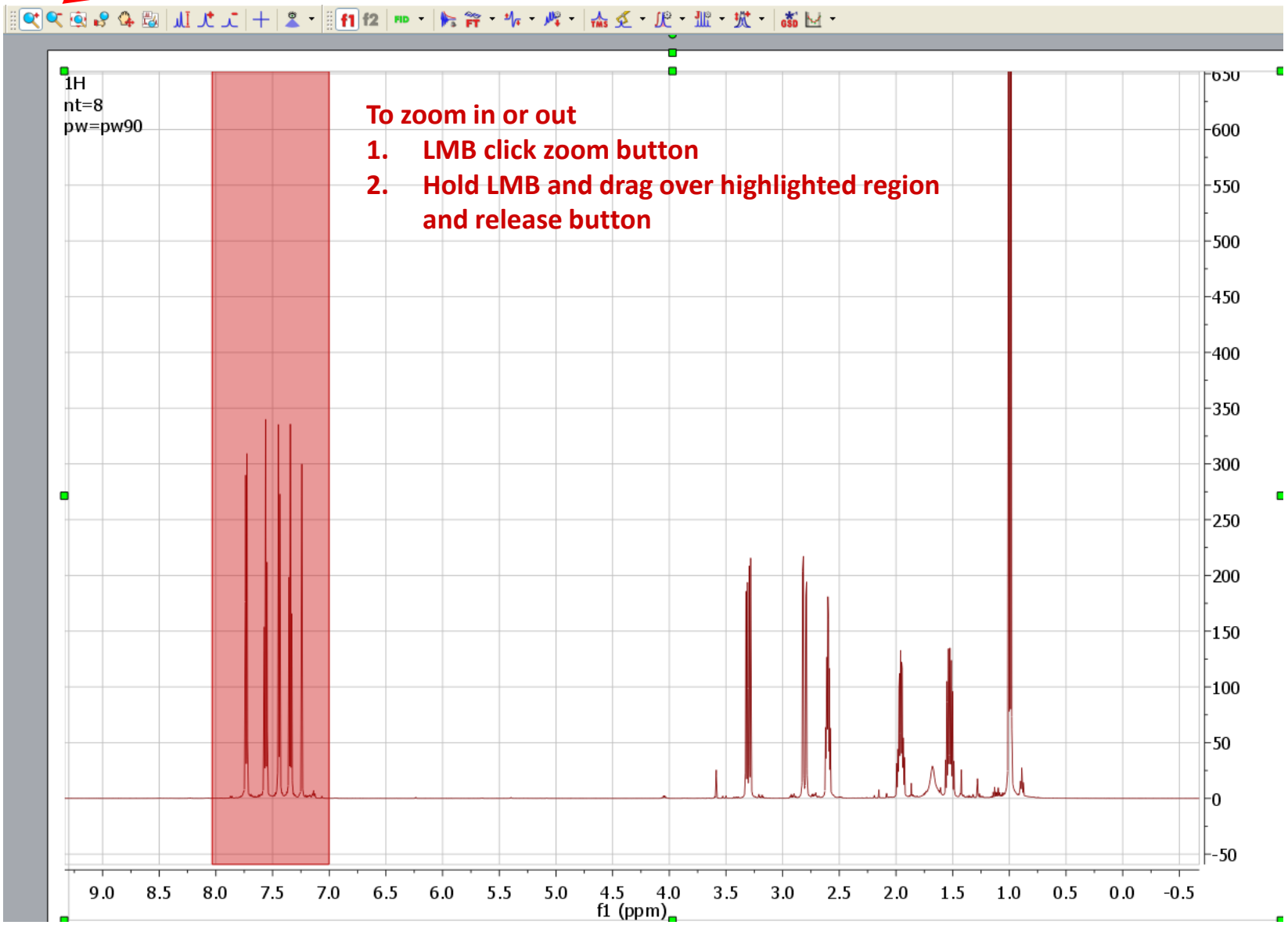
- **Test data available**
  - H1.fid
  - C13.fid
  - dept.fid

Load Raw NMR Data Folder

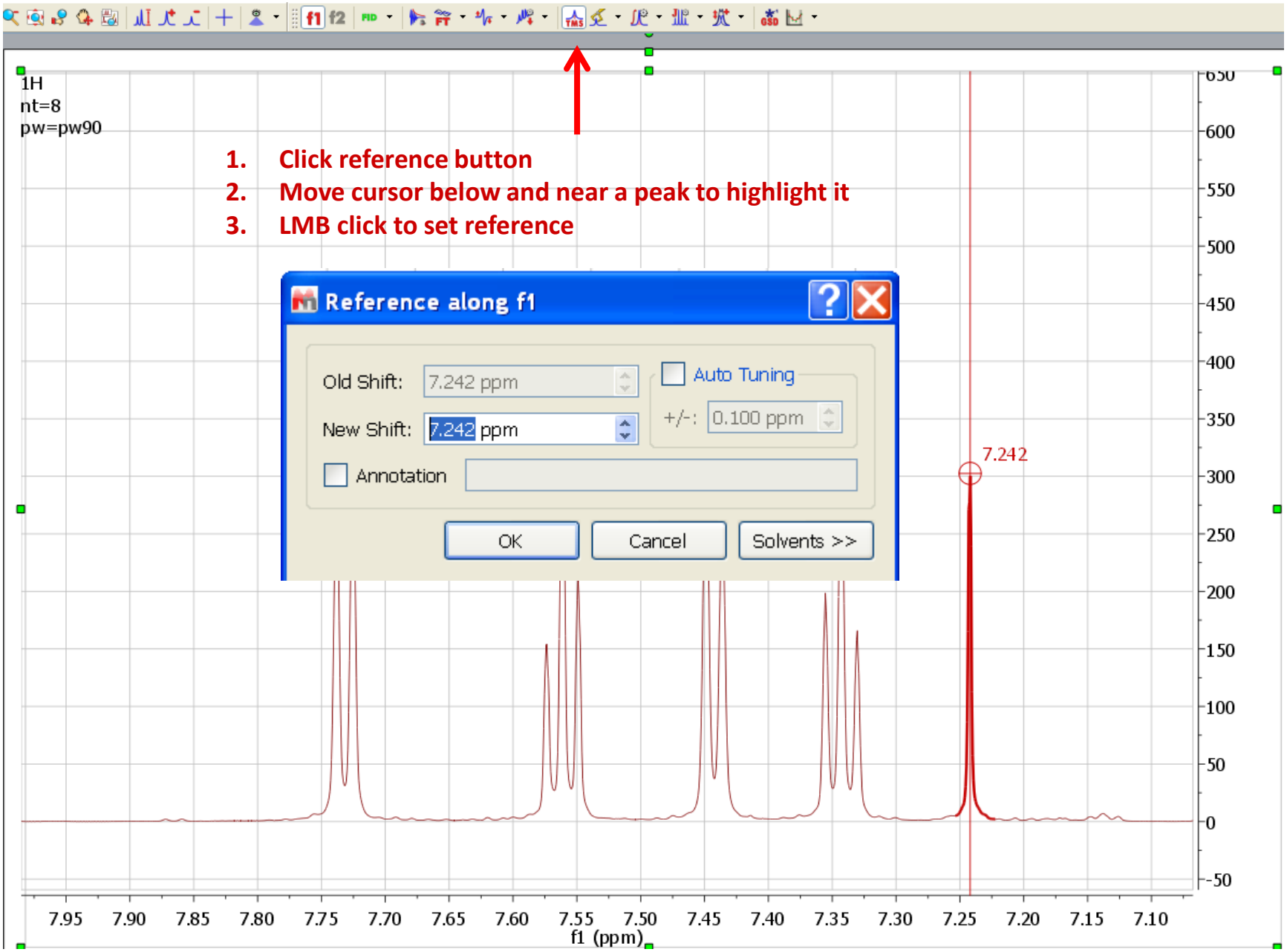
Drag and drop Varian .fid folder or Bruker data folder



Zoom in/out/full range/manual range/pan

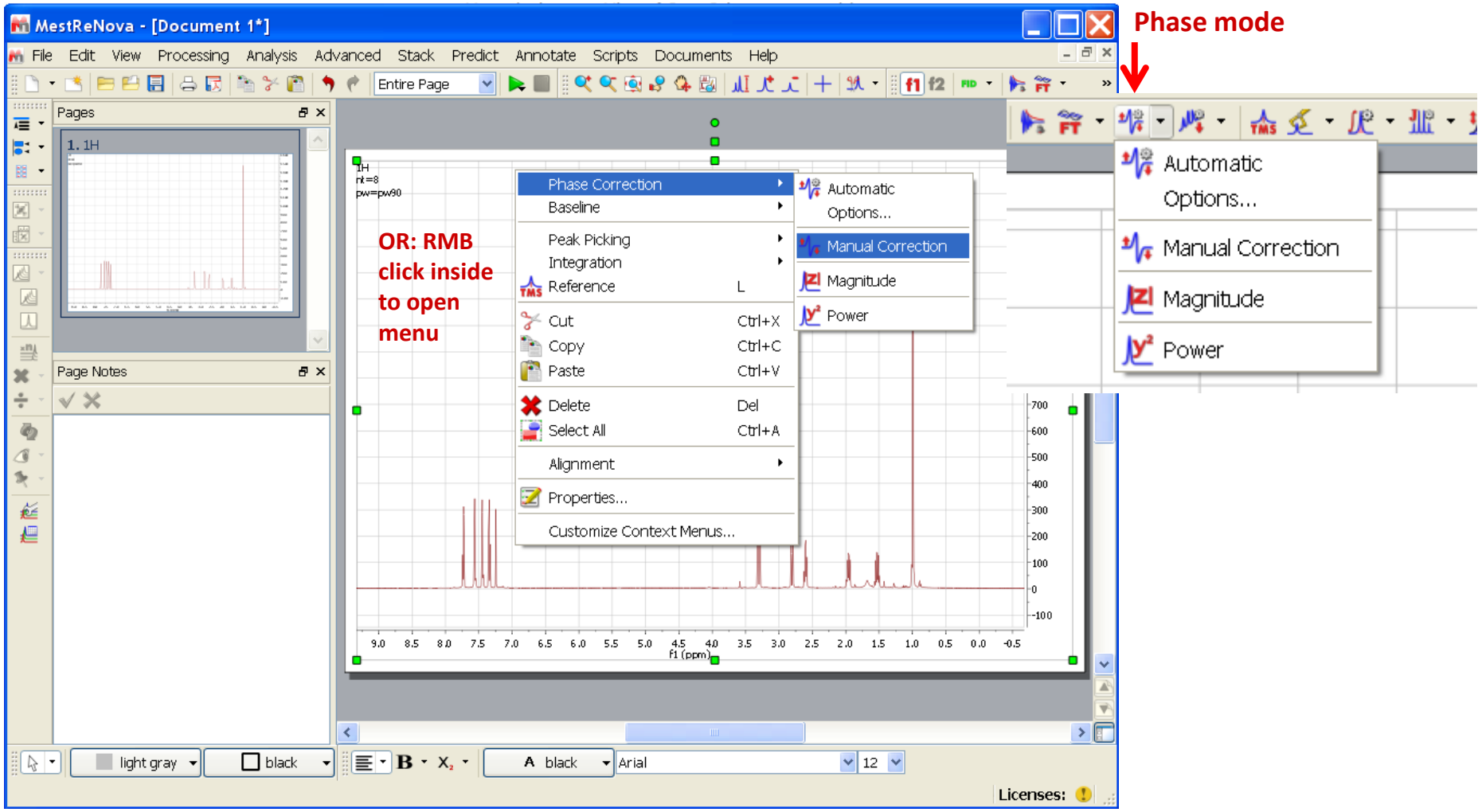


Reference by Peak

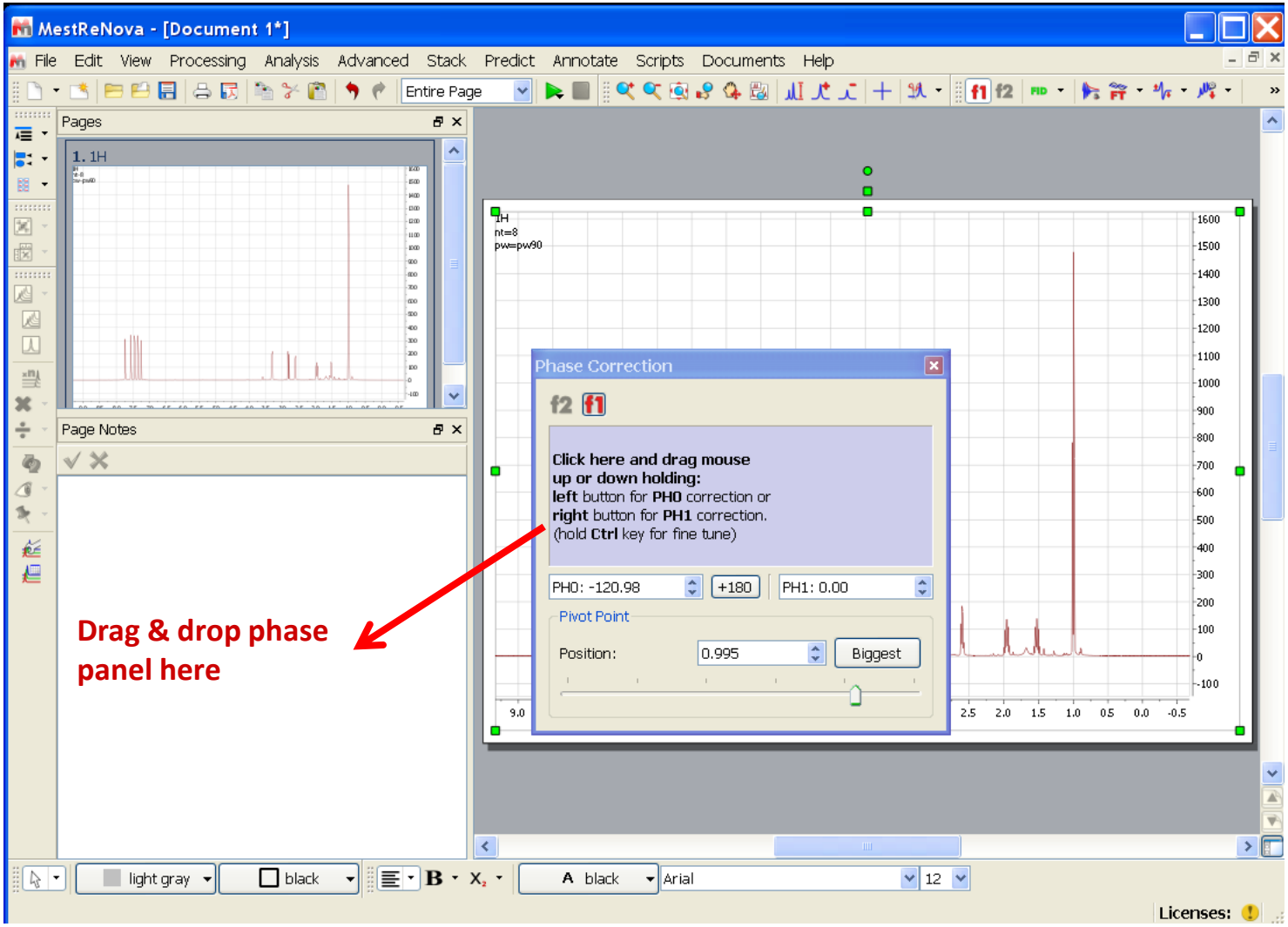


1D 1H Spectrum after Data Loading and Auto-processing

Enter phase mode

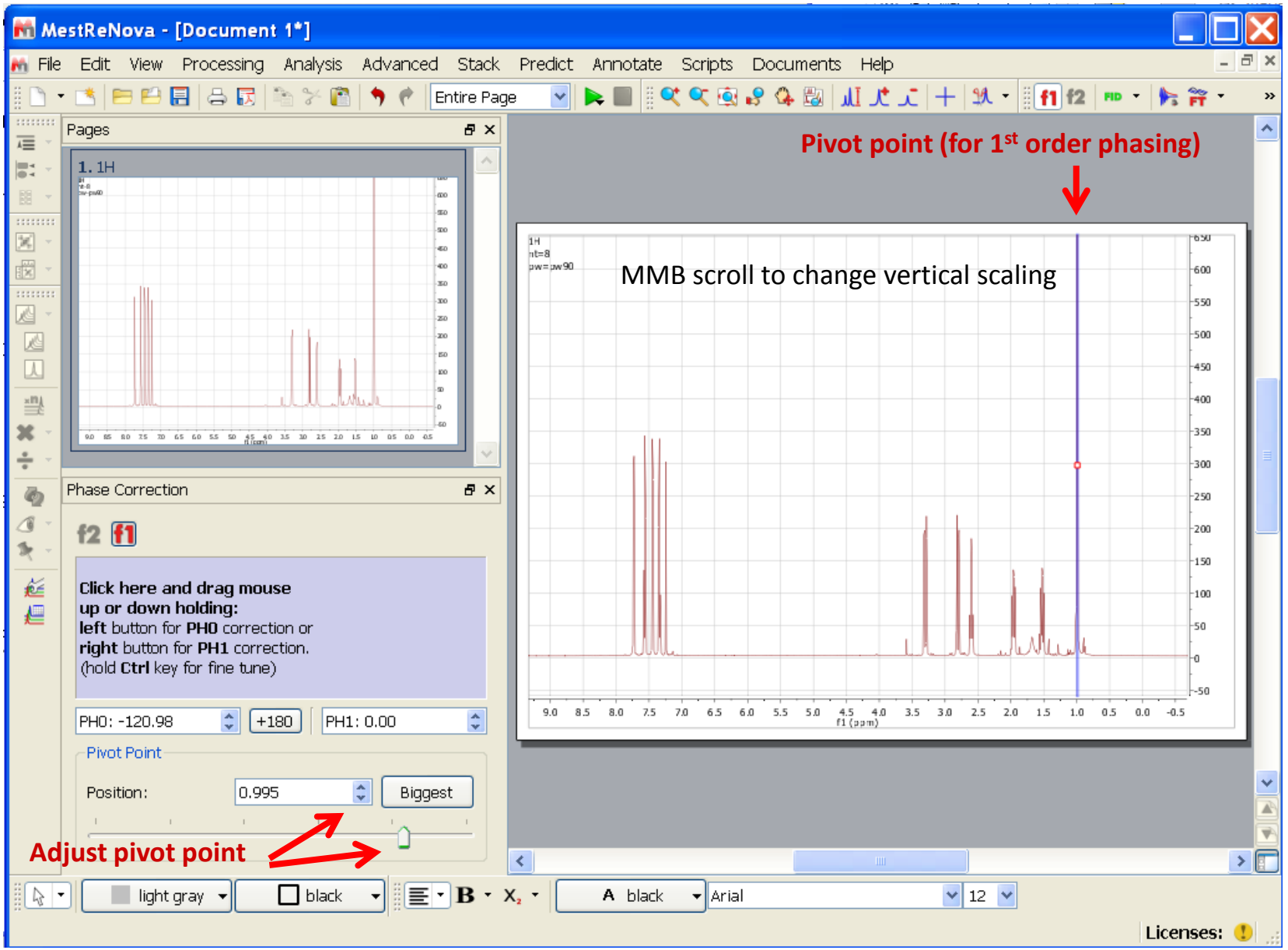


Phase Panel Opened



Phasing steps:

1. **Adjust zero-order phase**
2. **Select pivot and adjust 1st-order phase**



Phasing

Spectra in **phase-sensitive mode** (such as HSQC and NOESY) need to be phased to absorptive mode where peaks are symmetric around the baseline and are either up or down.

Spectra in **absolute-value or magnitude mode** (such as common COSY and HMBC) have no phase information and do not need to be phased.

Phasing involves:

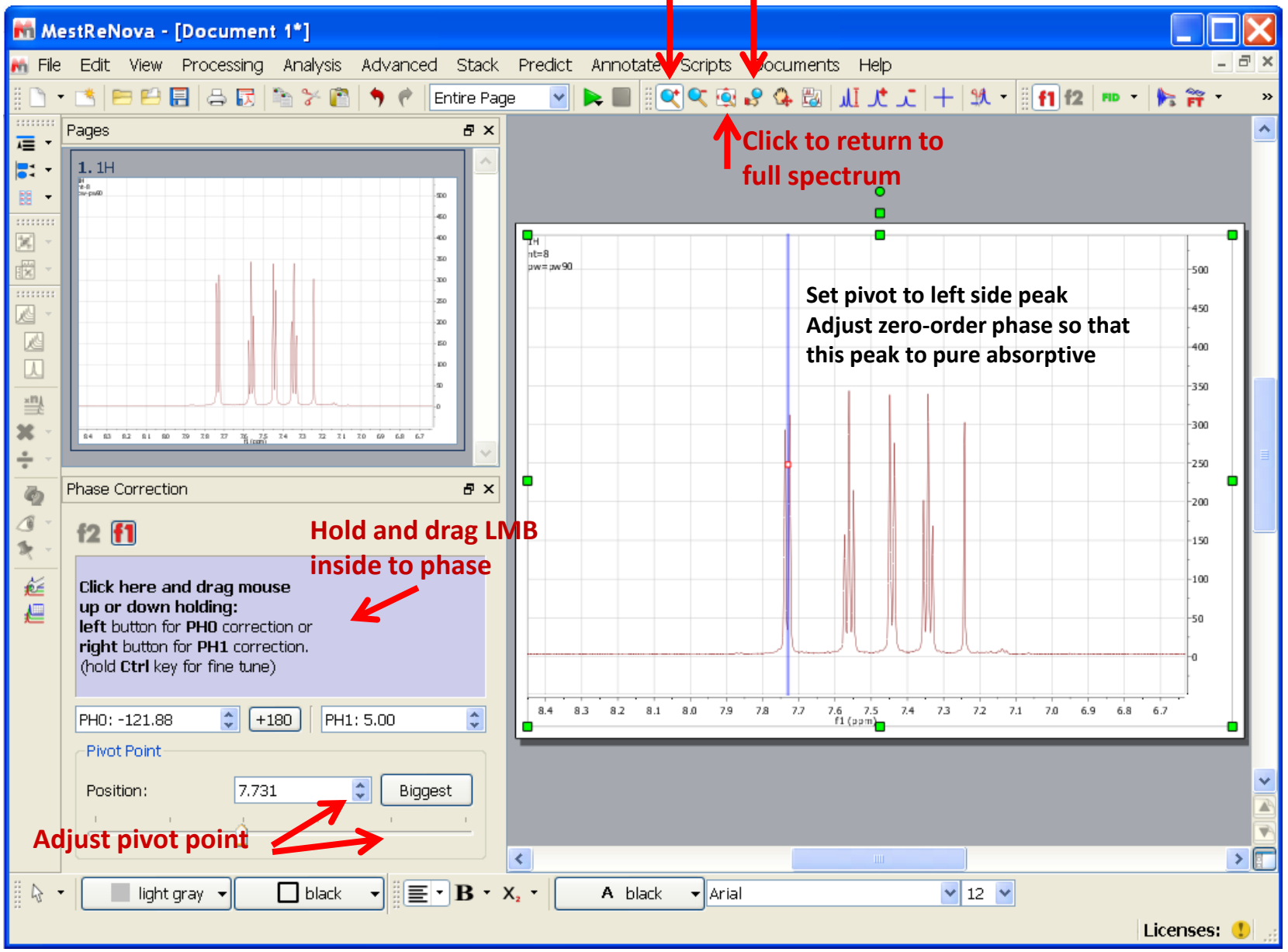
1. Adjust **zero-order phase** (constant across the spectrum)
2. Adjust **1st-order phase** (linear change away from pivot point)

Before 1st-order phase adjustment, pick a peak on the left or right side of the spectrum as the **pivot**.

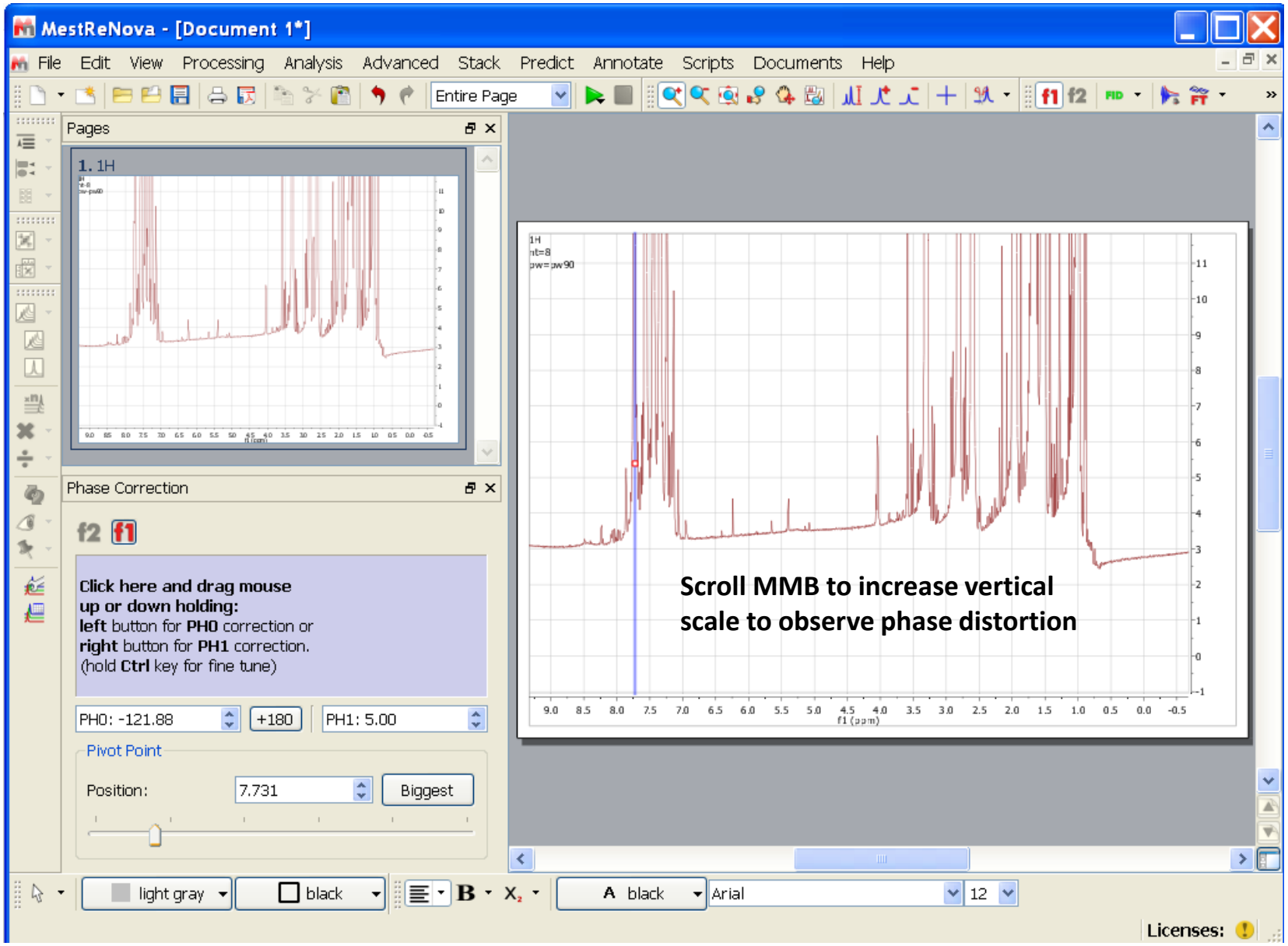
The pivot is where the 1st order phase is always zero and more linear phase is applied away from this point. Adjust 1st order phase so that the peaks away from the pivot become in-phase absorptive.

The phasing concept here applies to all NMR data along all dimensions.

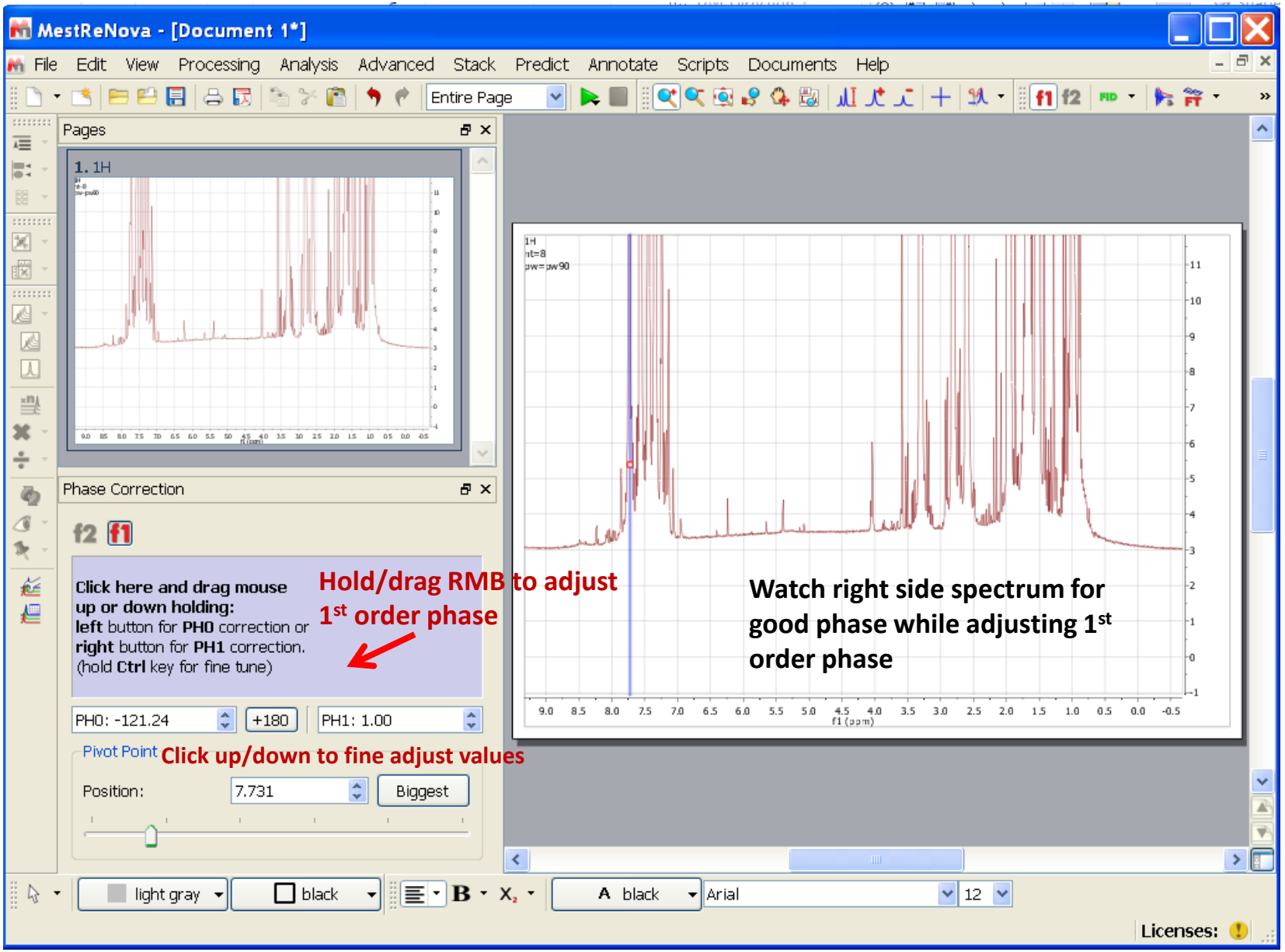
- **Zero order Phasing**
- **Select pivot**



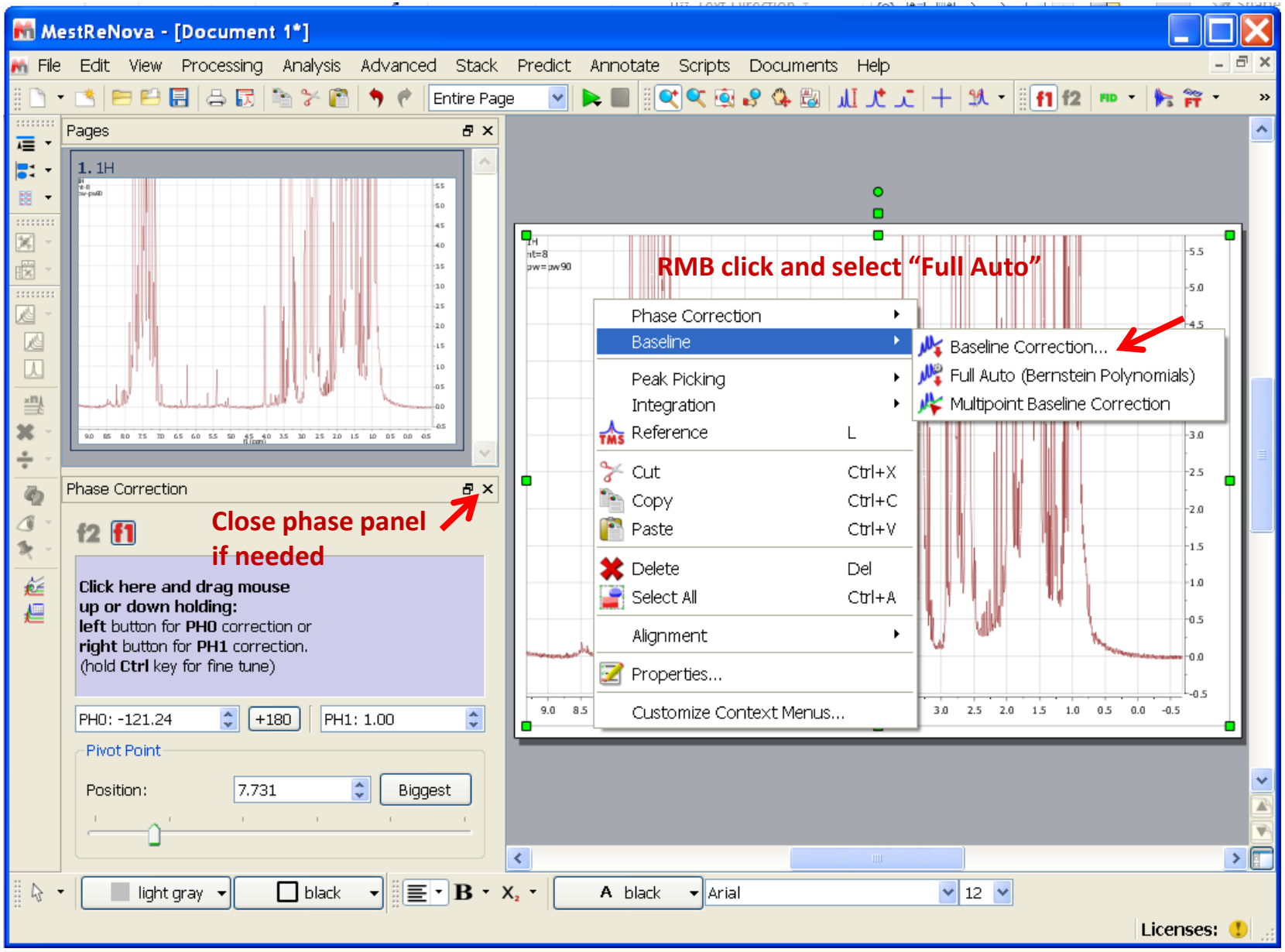
1st order Phasing



1st order Phasing

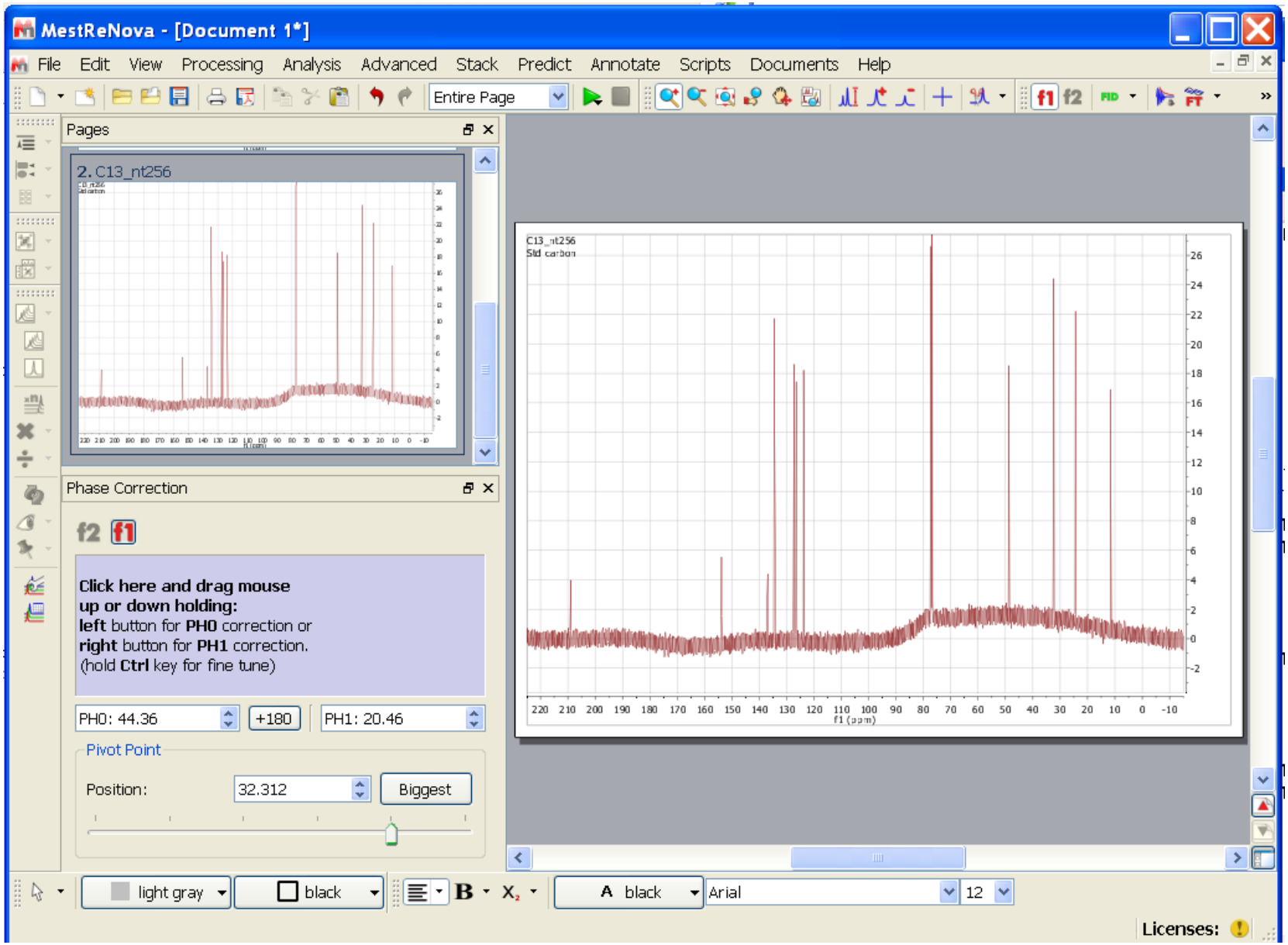


Full Auto Polynomial Baseline Correction for Simple Baseline Defects

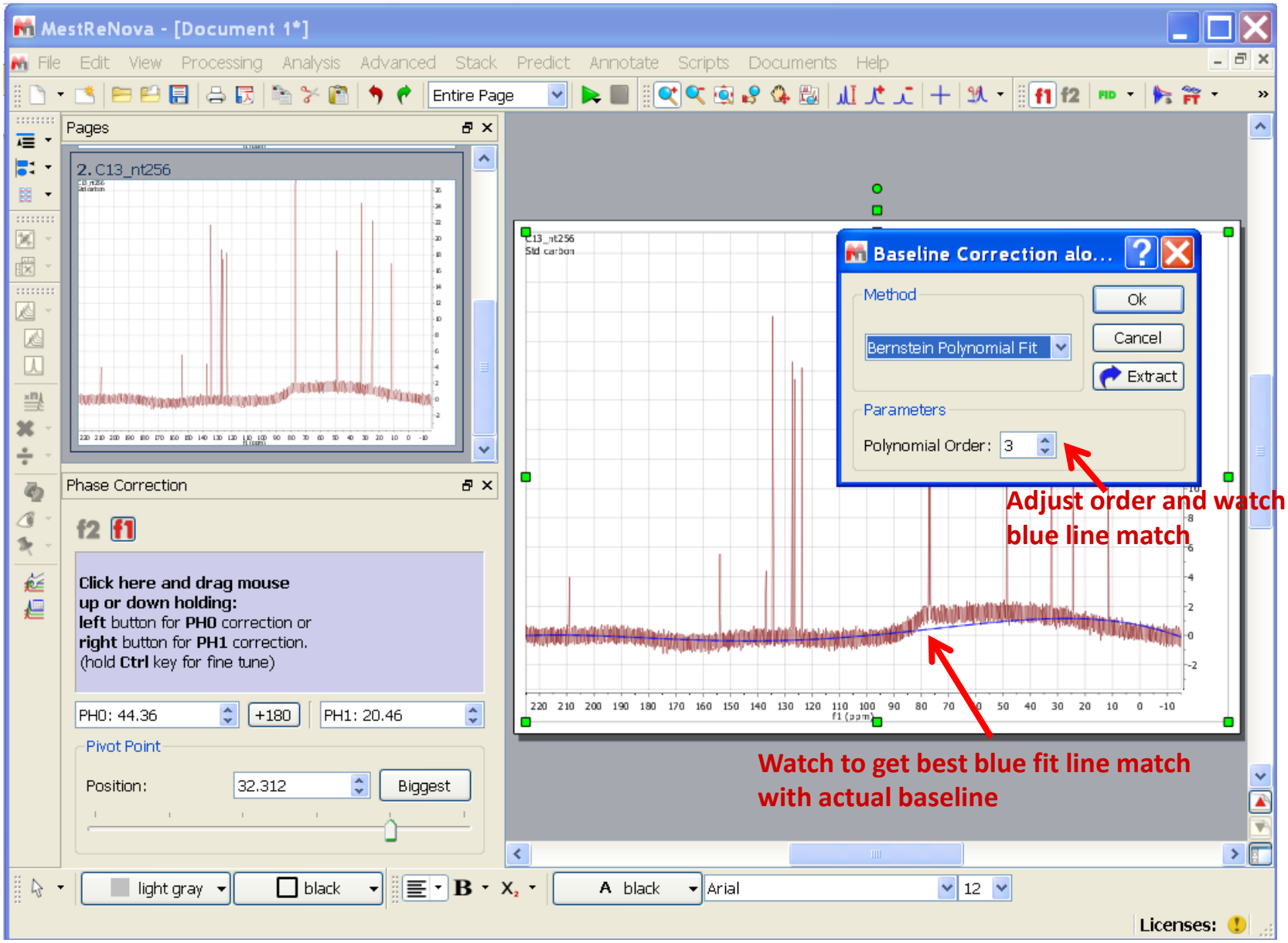


Baseline Correction for Complex Baseline Roll

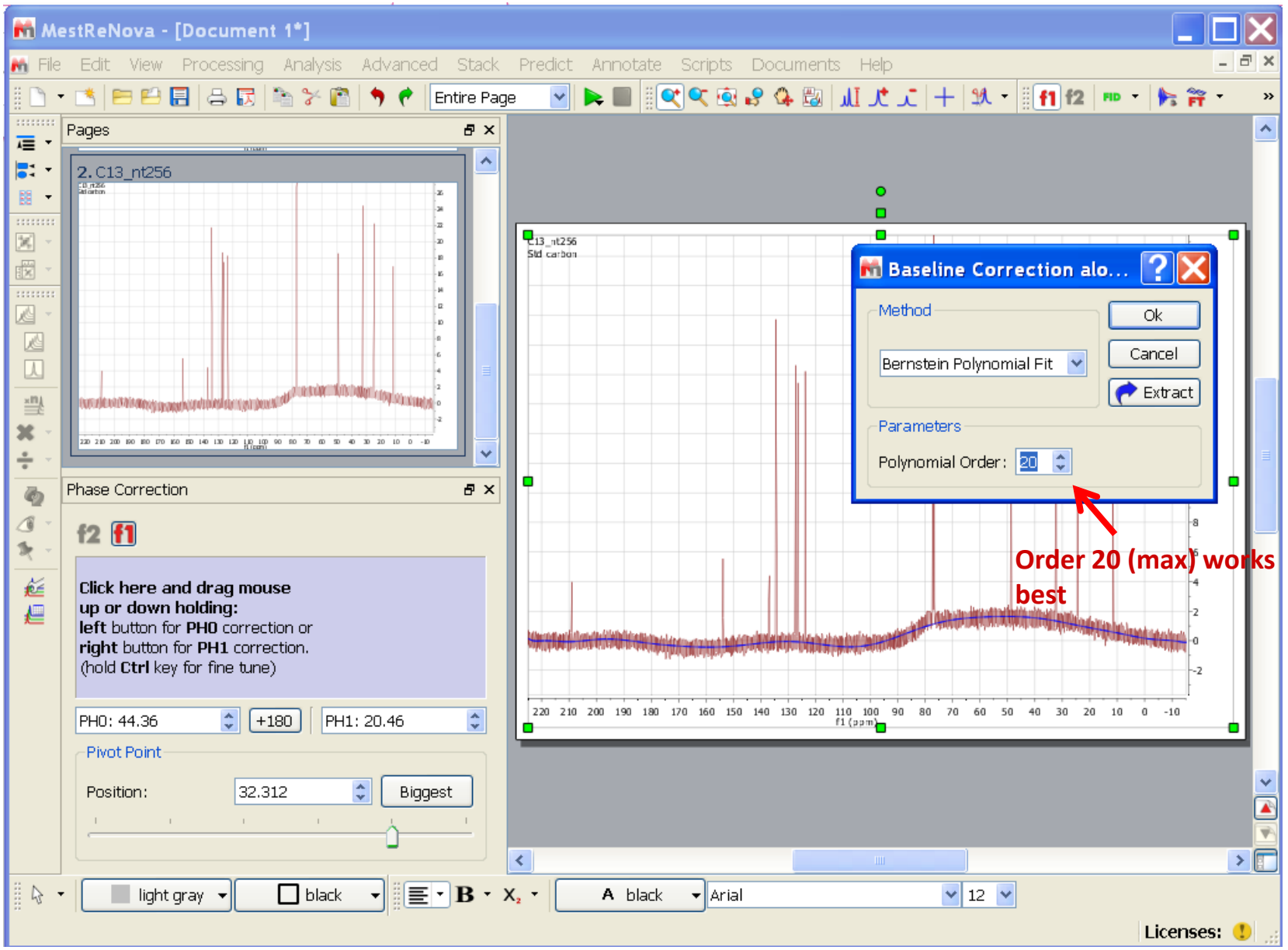
(Seen in some C13 spectra and on certain probes)



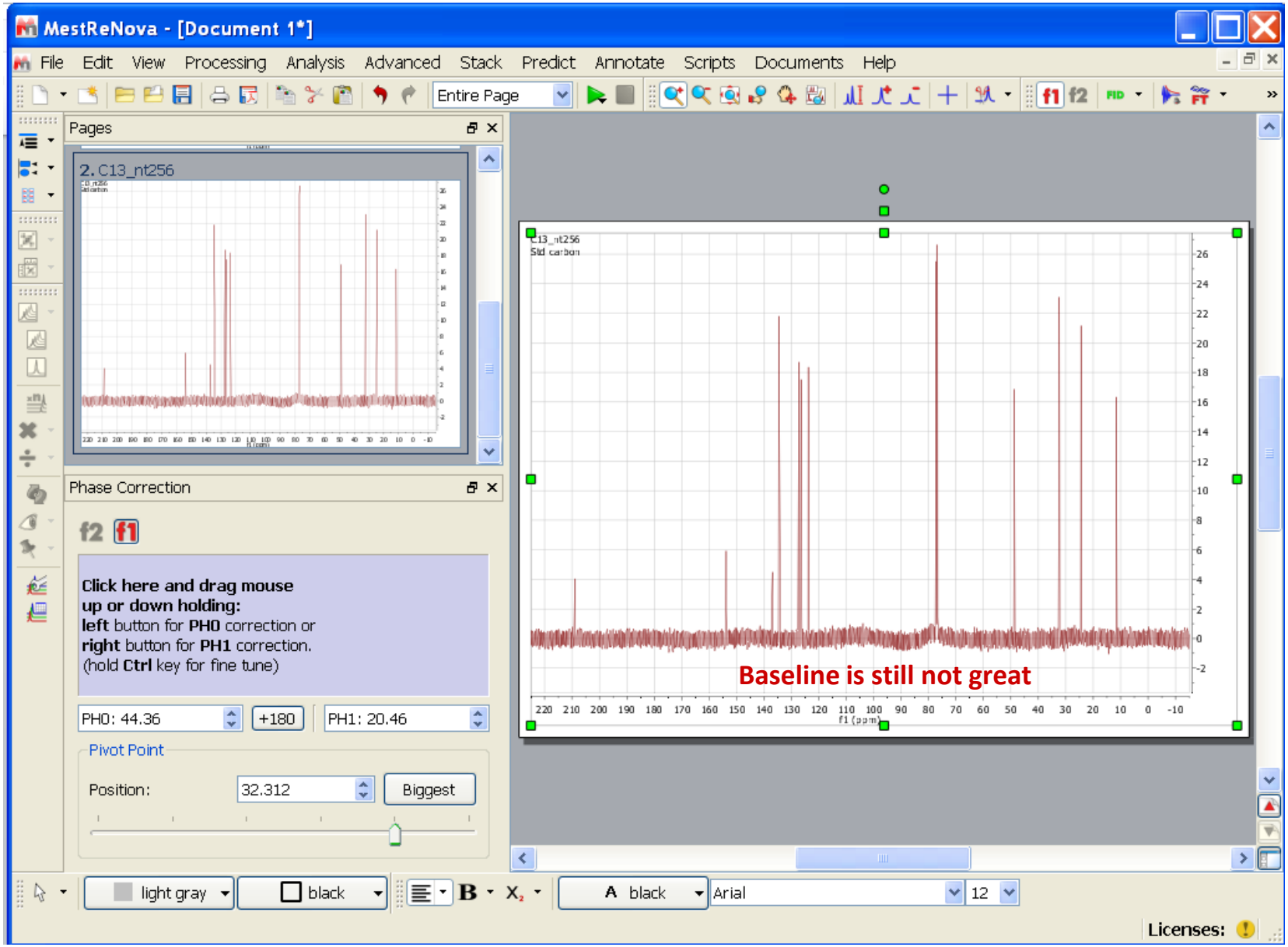
Default Full Auto Baseline Correction with Bernstein Polynomial Fit Order 3



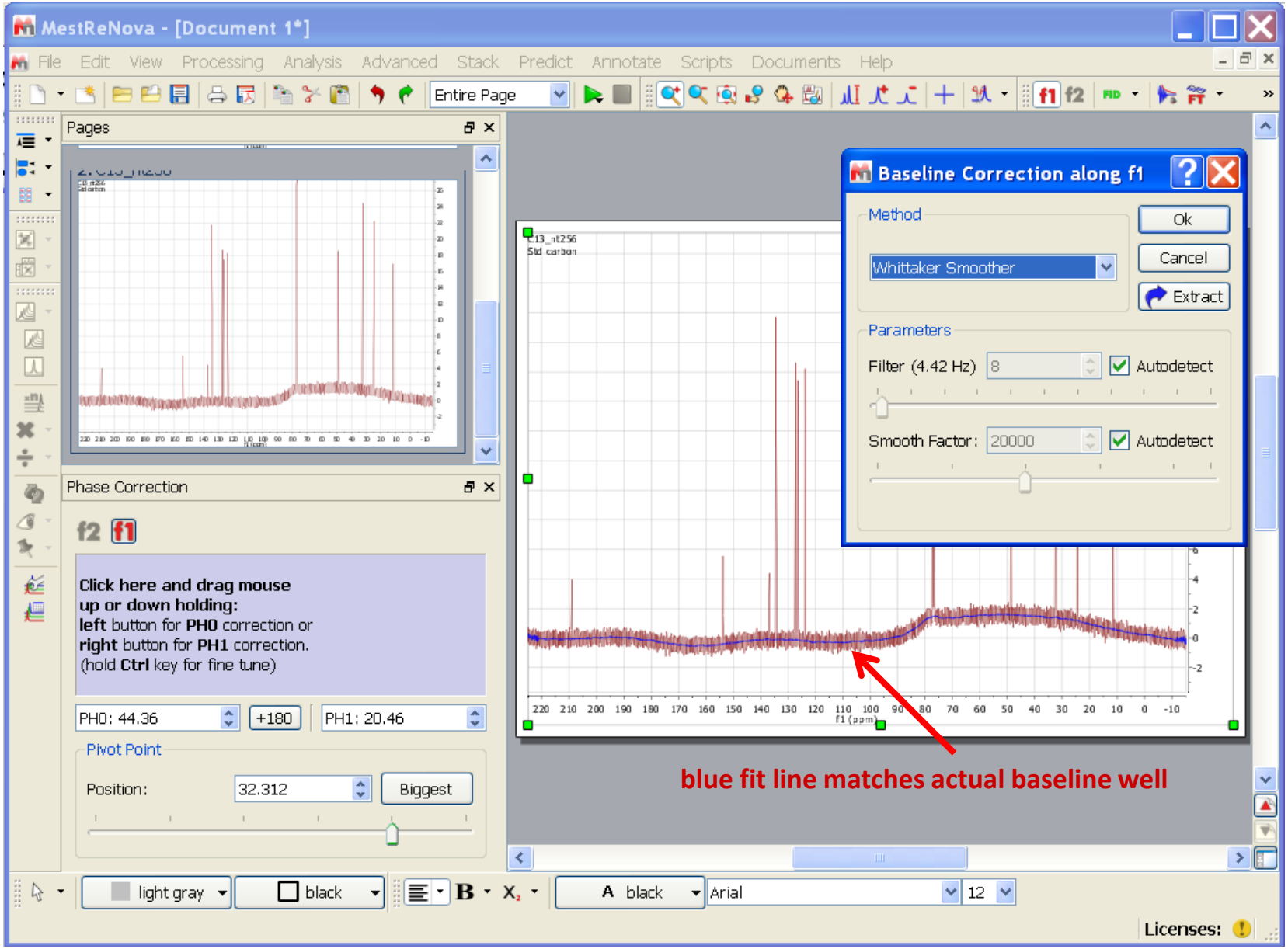
Default Full Auto Baseline Correction with Bernstein Polynomial Fit Order 20



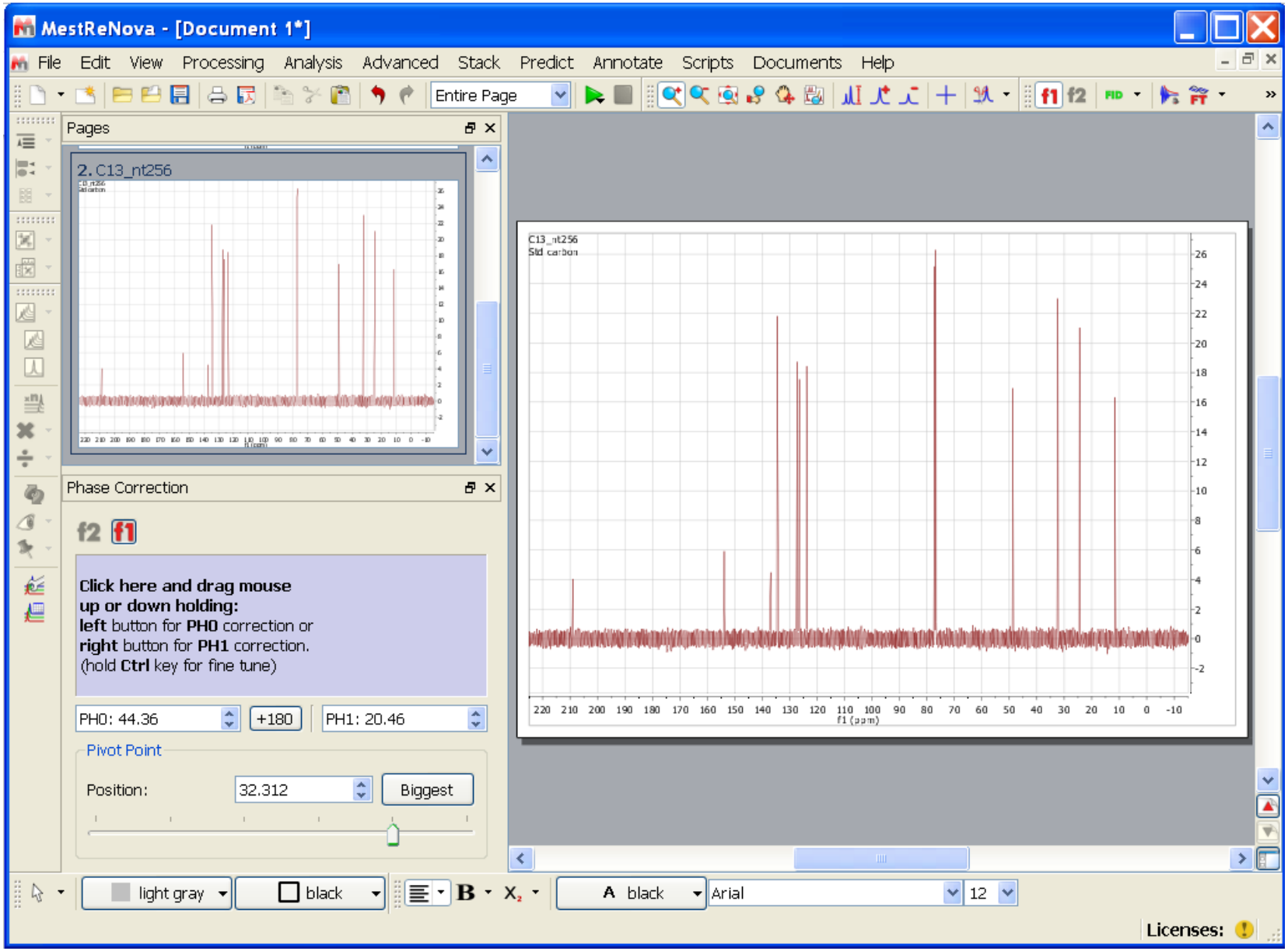
Result from Baseline Correction with Bernstein Polynomial Fit Order 20



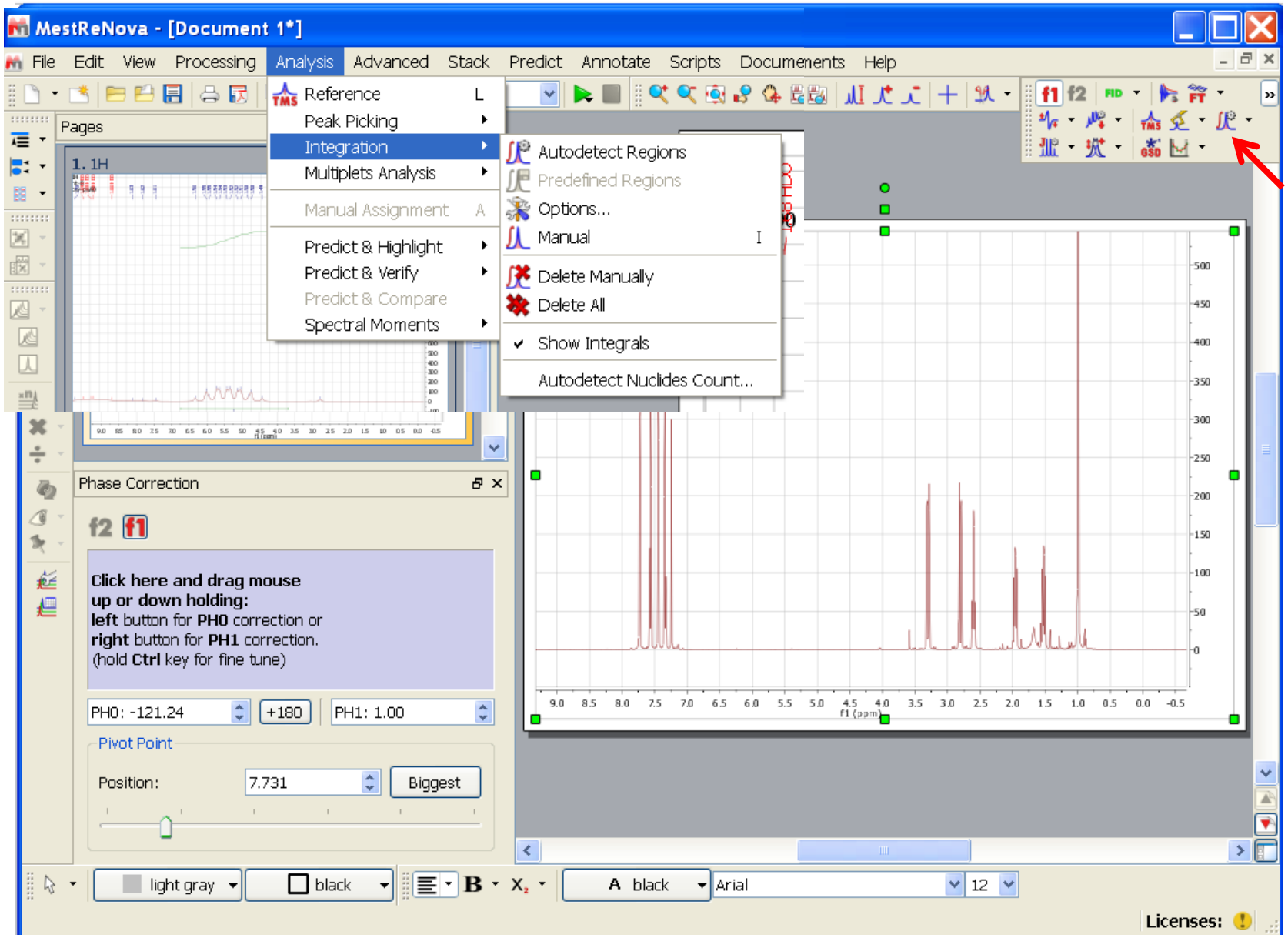
Best Result Comes with Whittaker Smoother



Perfect Baseline Correction with Whittaker Smoother



Peak Integration

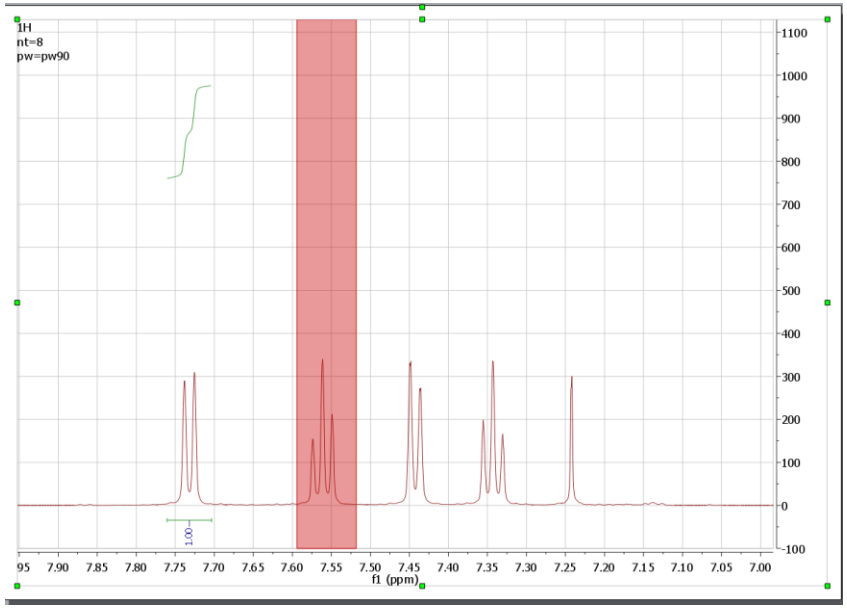


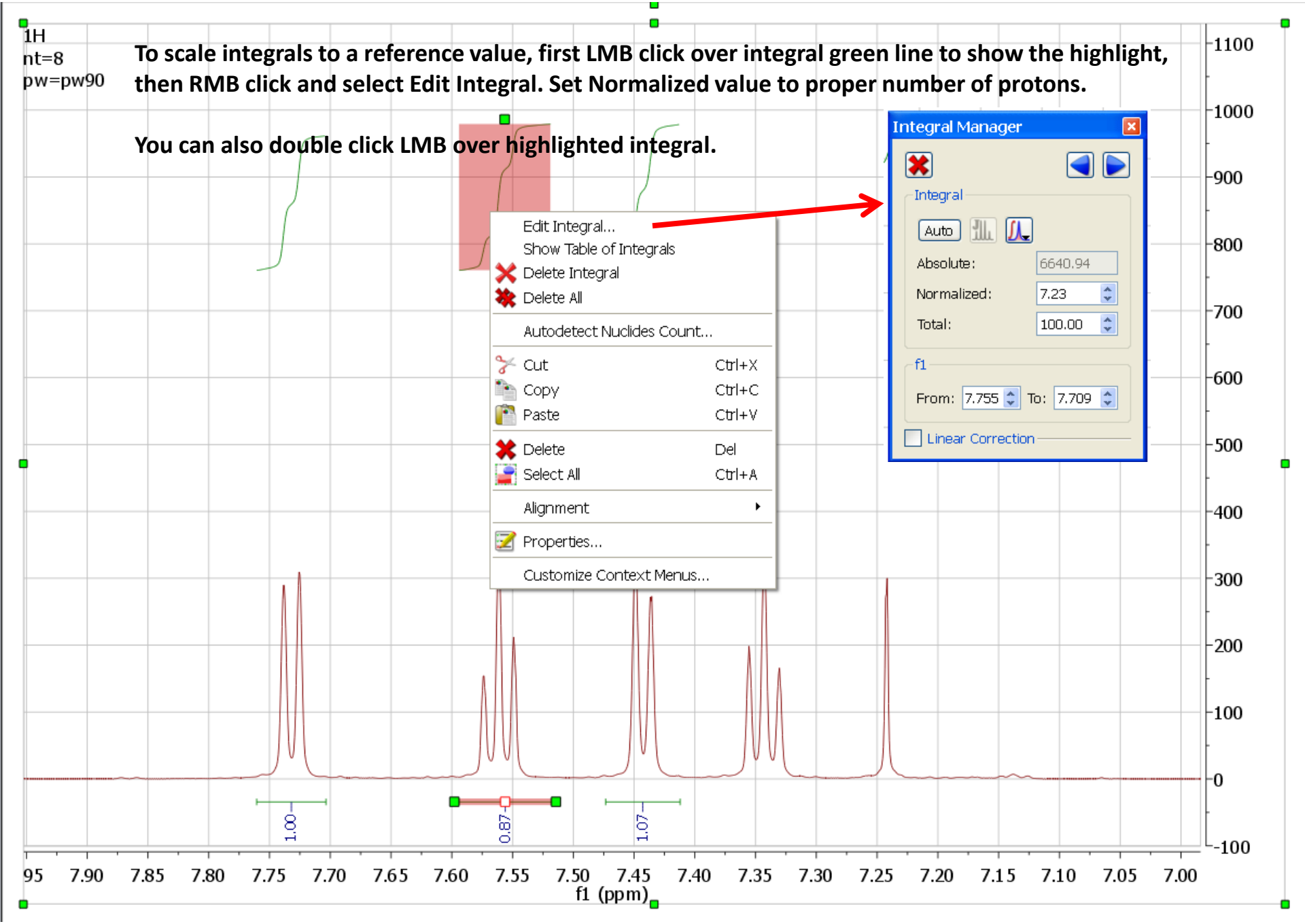
Methods:

1. Try auto-detect regions then manual adjustment (click **Autodetect Regions**)
2. OR: Full manual integral region picking

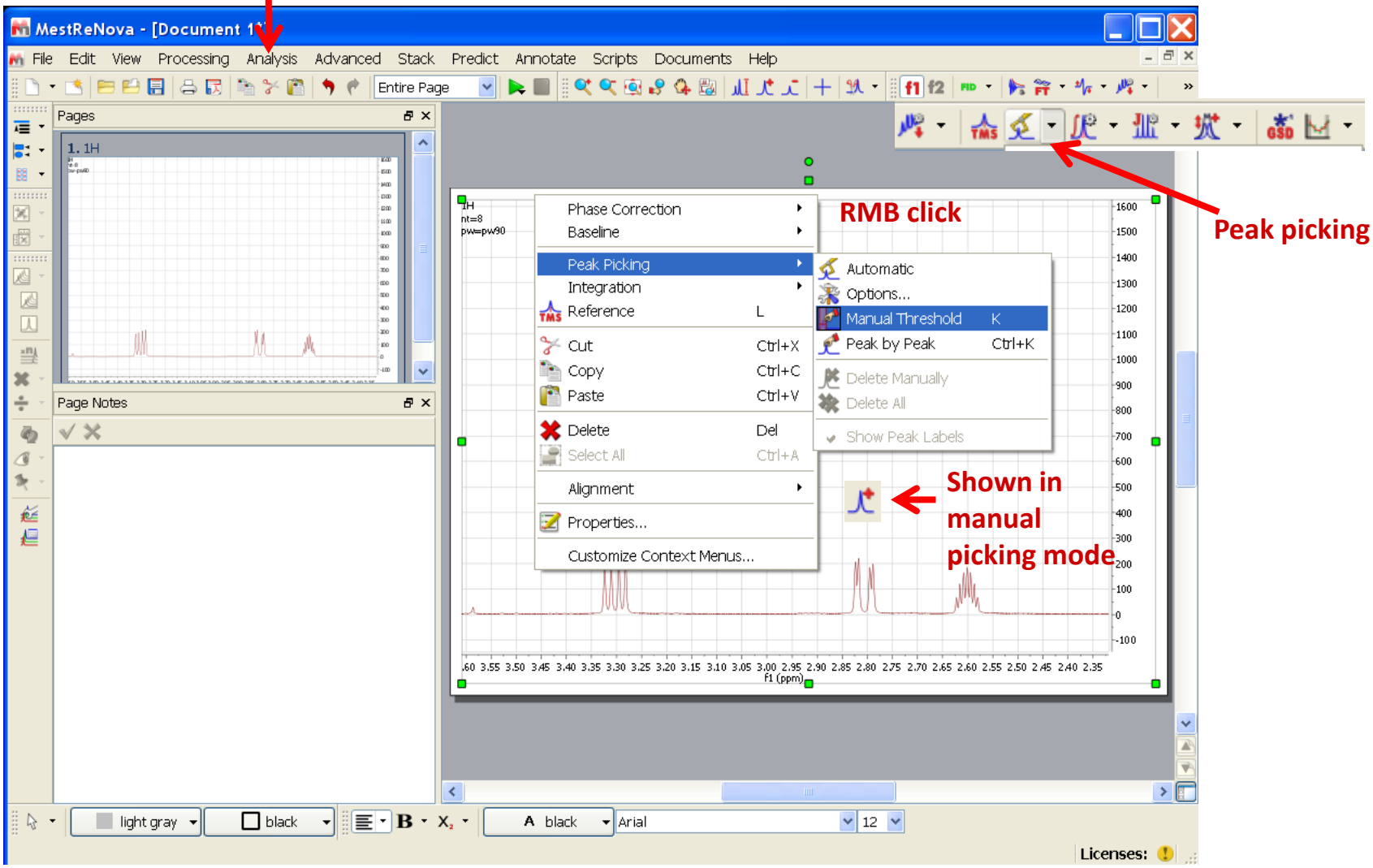
For full manual integration:

1. If integrals exist, select **Analysis→Integration →Delete all**
2. If an integration symbol appears, hold and drag LMB over peak region to define integral region as the highlighted area.
3. To delete an integral, LMB click over green integral line to select integral and RMB to select **Delete Integral** (DO NOT select **Delete** which deletes current spectrum).
4. To exit integration mode, press **Esc** key.



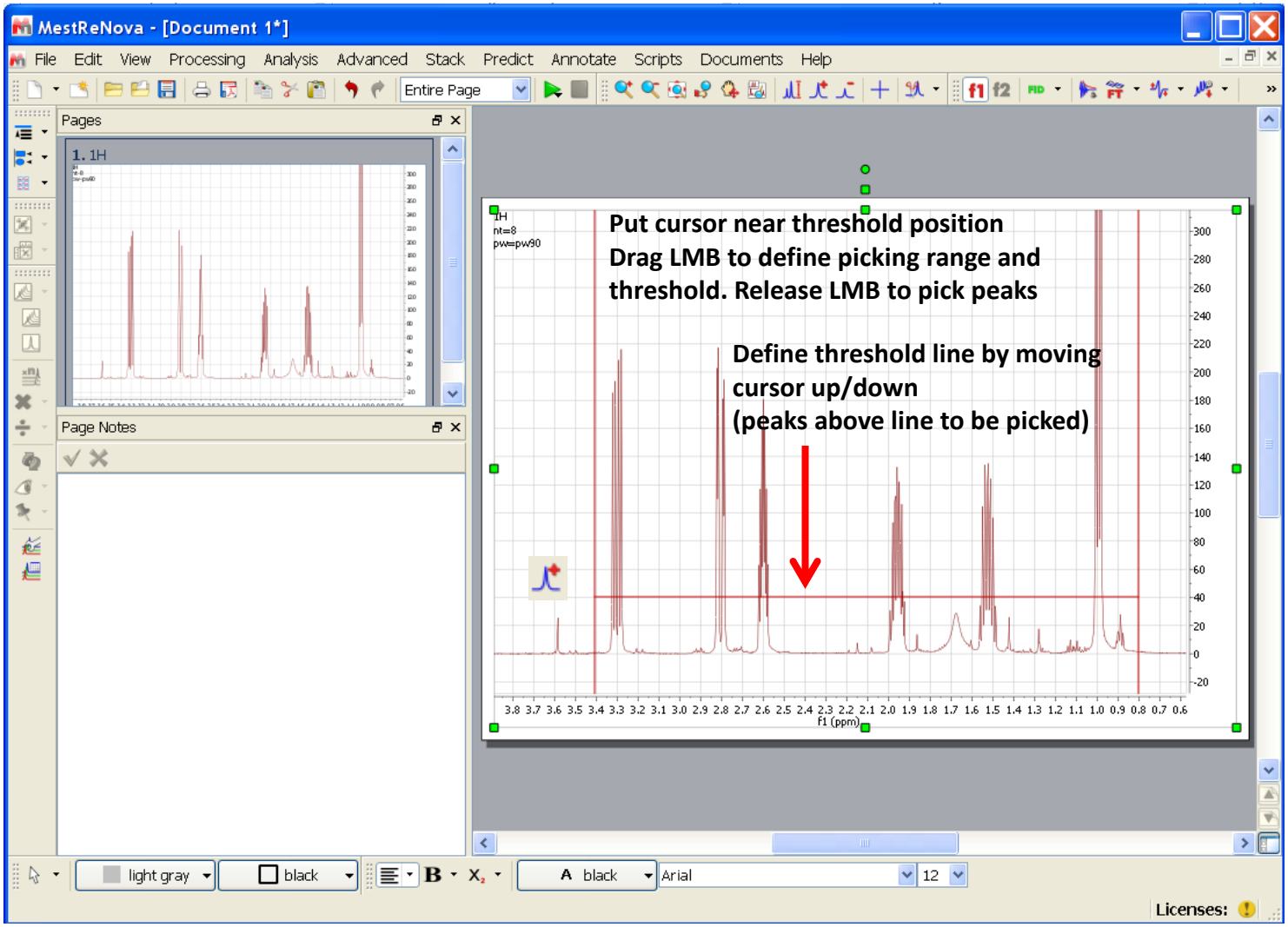

1H
nt=8
pw=pw90
To scale integrals to a reference value, first LMB click over integral green line to show the highlight, then RMB click and select Edit Integral. Set Normalized value to proper number of protons.
You can also double click LMB over highlighted integral.
Edit Integral...
Show Table of Integrals
Delete Integral
Delete All
Autodetect Nuclides Count...
Cut Ctrl+X
Copy Ctrl+C
Paste Ctrl+V
Delete Del
Select All Ctrl+A
Alignment
Properties...
Customize Context Menus...
Integral Manager
Integral
Auto
Absolute: 6640.94
Normalized: 7.23
Total: 100.00
f1
From: 7.755 To: 7.709
Linear Correction
1.00
0.87
1.07
f1 (ppm)

Enter Peak Picking Mode

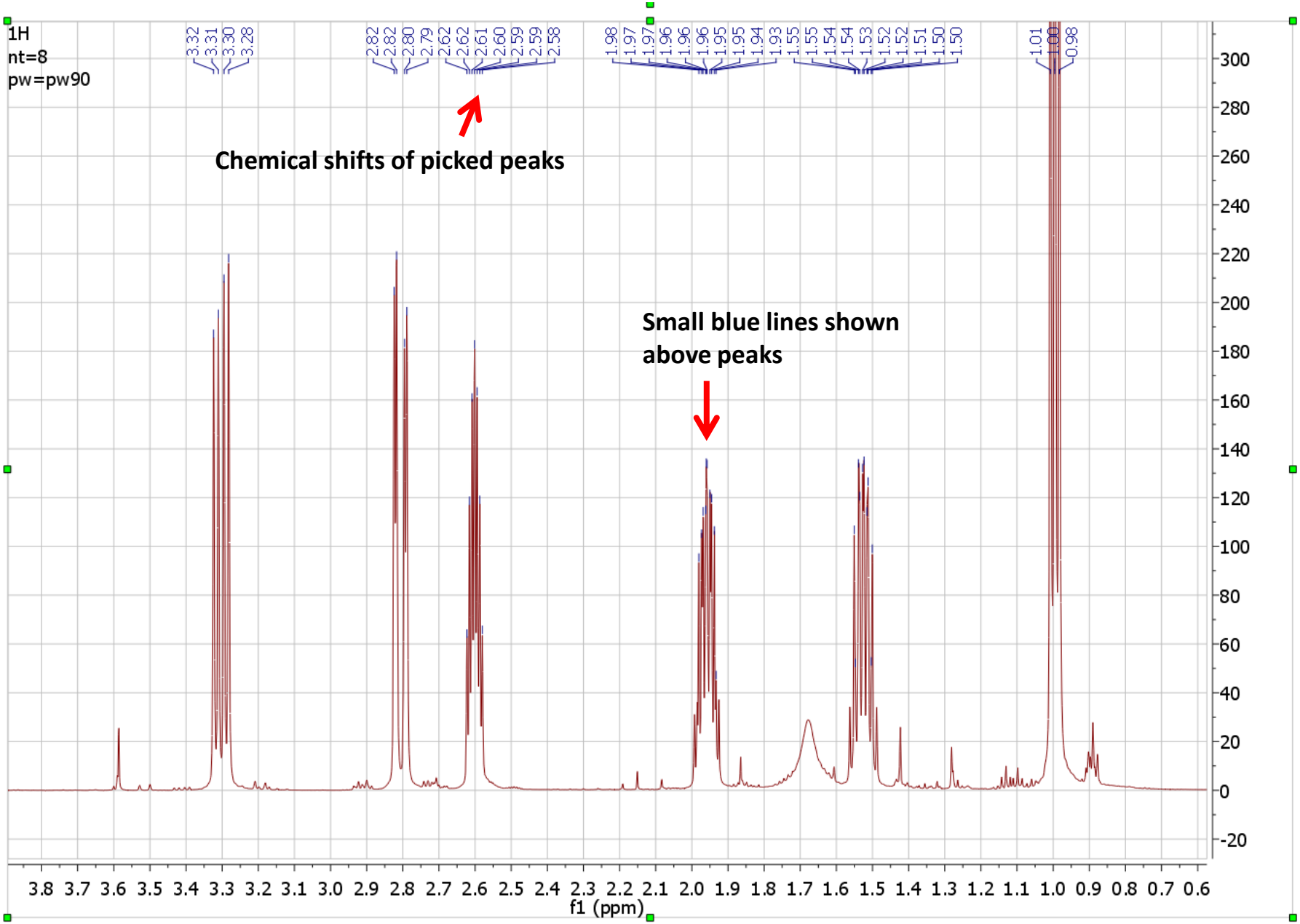


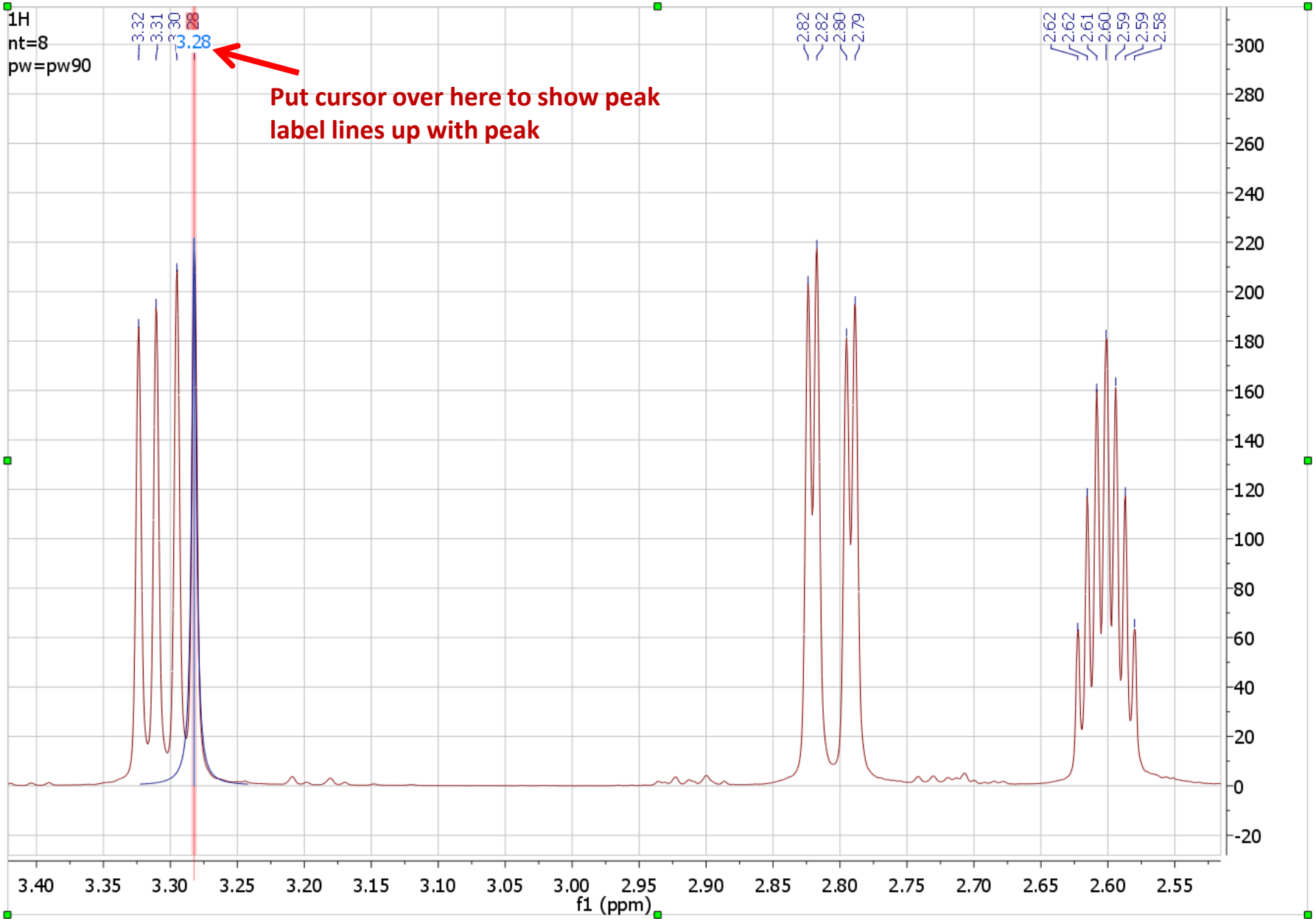
Peak Picking: Manual Threshold Mode

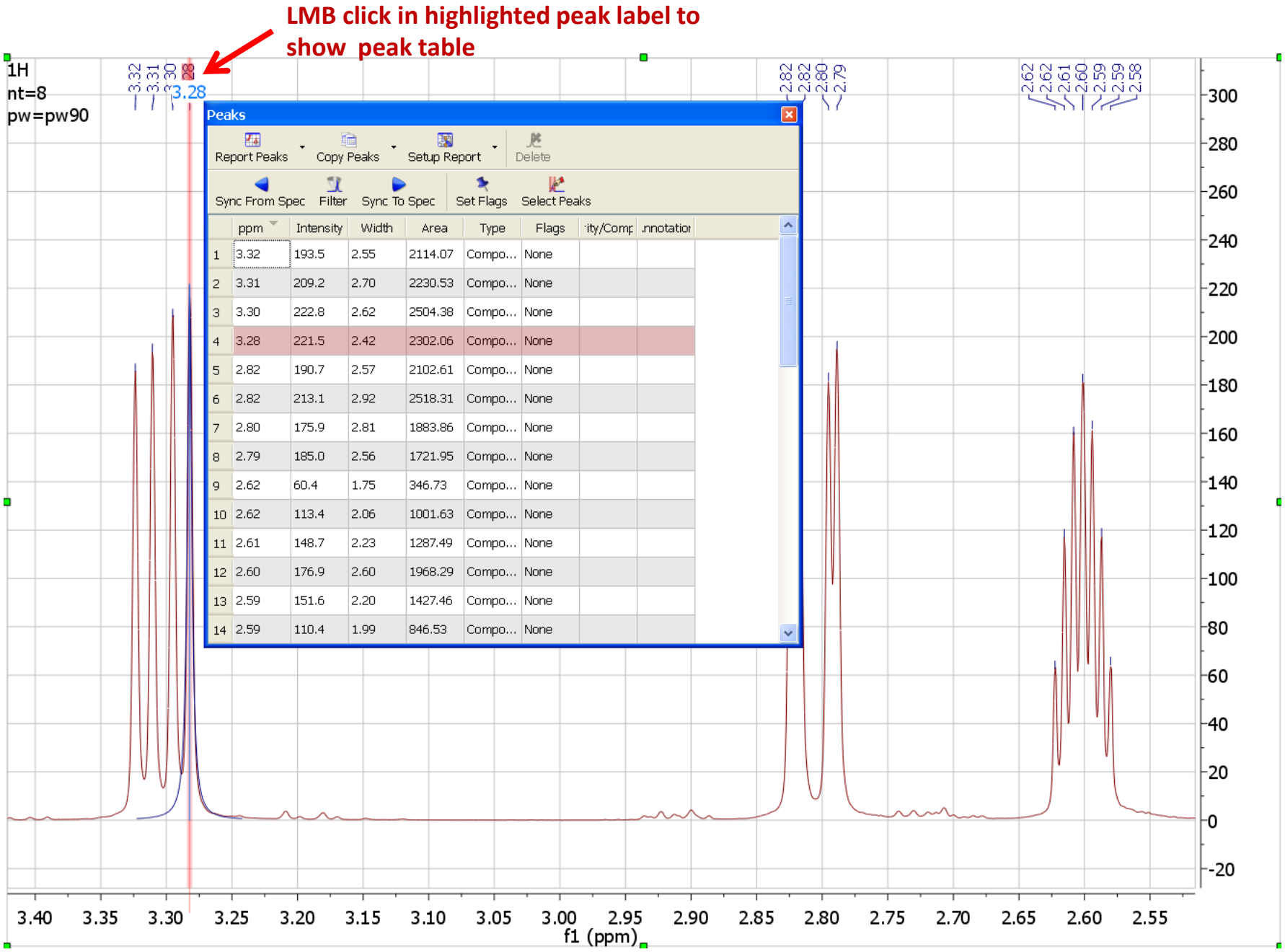
Positive and negative peaks carry same threshold magnitude by default

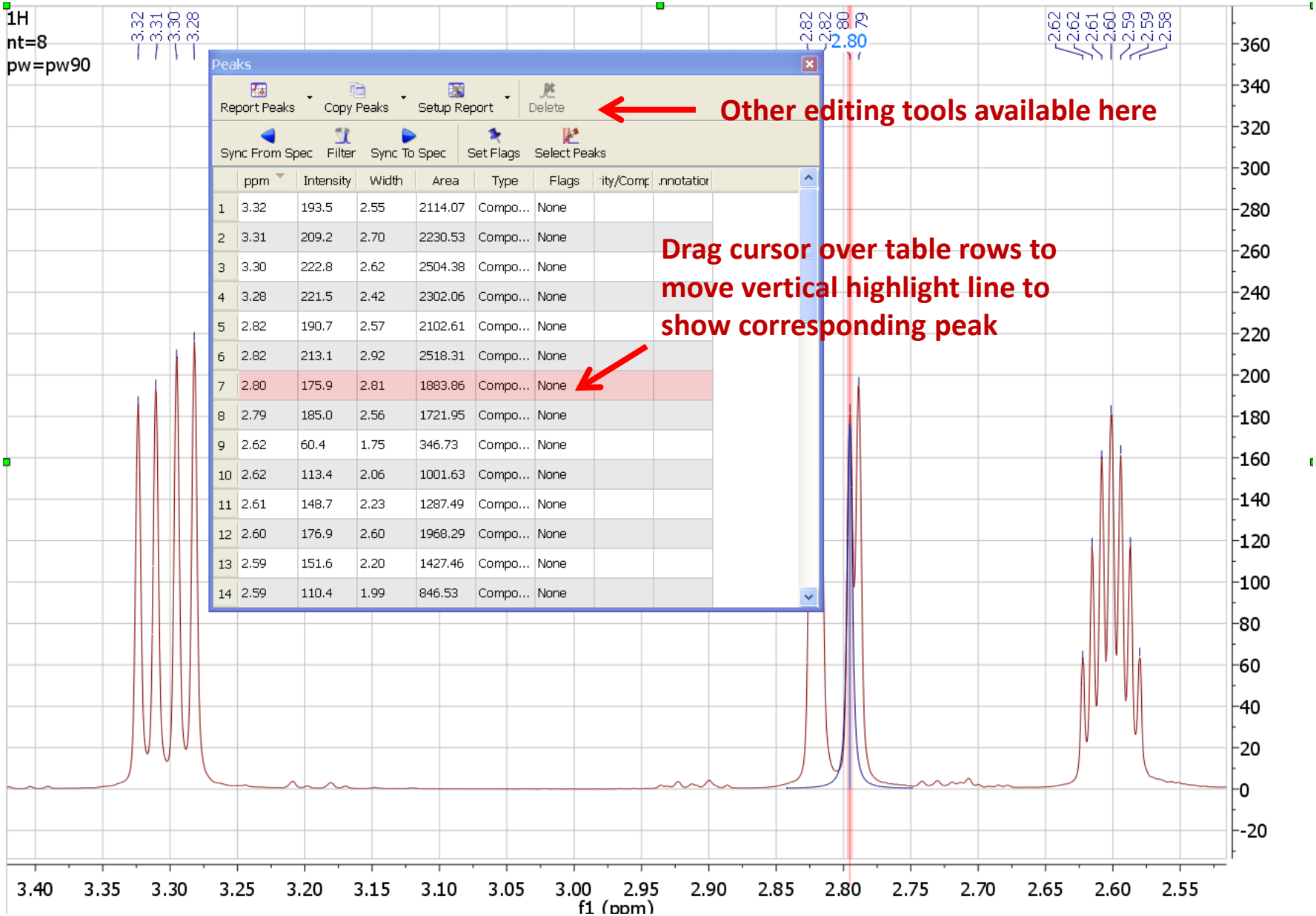


Peak Picking

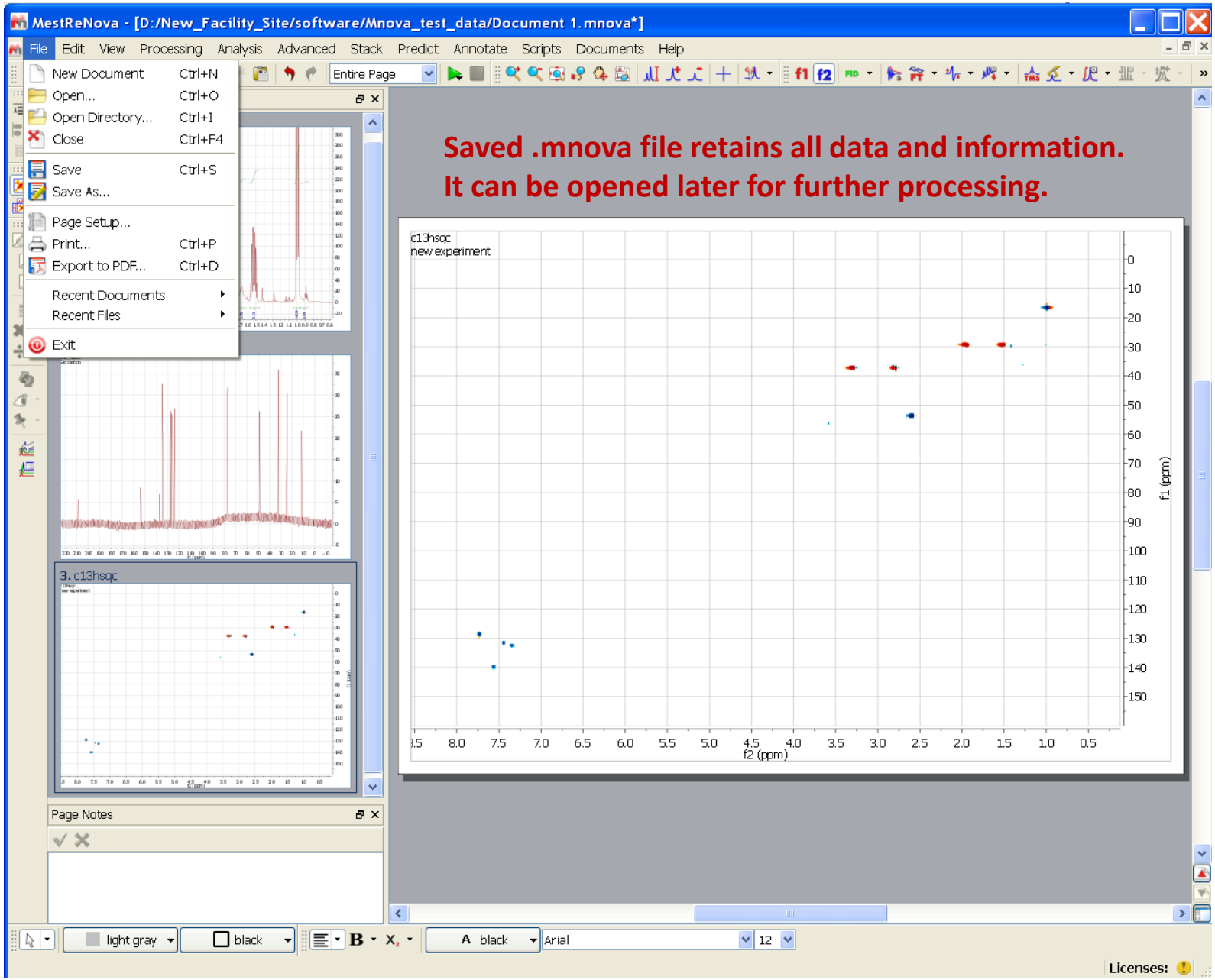



1H
nt=8
pw=pw90
3.32
3.31
3.30
3.28
3.28
Put cursor over here to show peak label lines up with peak
2.82
2.82
2.80
2.79
2.62
2.62
2.61
2.60
2.59
2.59
2.58
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
3.40
3.35
3.30
3.25
3.20
3.15
3.10
3.05
3.00
2.95
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
f1 (ppm)


LMB click in highlighted peak label to show peak table
1H
nt=8
pw=pw90
3.32
3.31
3.30
3.28
2.82
2.82
2.80
2.79
2.62
2.62
2.61
2.60
2.59
2.59
2.58
Peaks
Report Peaks
Copy Peaks
Setup Report
Delete
Sync From Spec
Filter
Sync To Spec
Set Flags
Select Peaks
ppm
Intensity
Width
Area
Type
Flags
1 3.32 193.5 2.55 2114.07 Compo... None
2 3.31 209.2 2.70 2230.53 Compo... None
3 3.30 222.8 2.62 2504.38 Compo... None
4 3.28 221.5 2.42 2302.06 Compo... None
5 2.82 190.7 2.57 2102.61 Compo... None
6 2.82 213.1 2.92 2518.31 Compo... None
7 2.80 175.9 2.81 1883.86 Compo... None
8 2.79 185.0 2.56 1721.95 Compo... None
9 2.62 60.4 1.75 346.73 Compo... None
10 2.62 113.4 2.06 1001.63 Compo... None
11 2.61 148.7 2.23 1287.49 Compo... None
12 2.60 176.9 2.60 1968.29 Compo... None
13 2.59 151.6 2.20 1427.46 Compo... None
14 2.59 110.4 1.99 846.53 Compo... None
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
3.40
3.35
3.30
3.25
3.20
3.15
3.10
3.05
3.00
2.95
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
f1 (ppm)

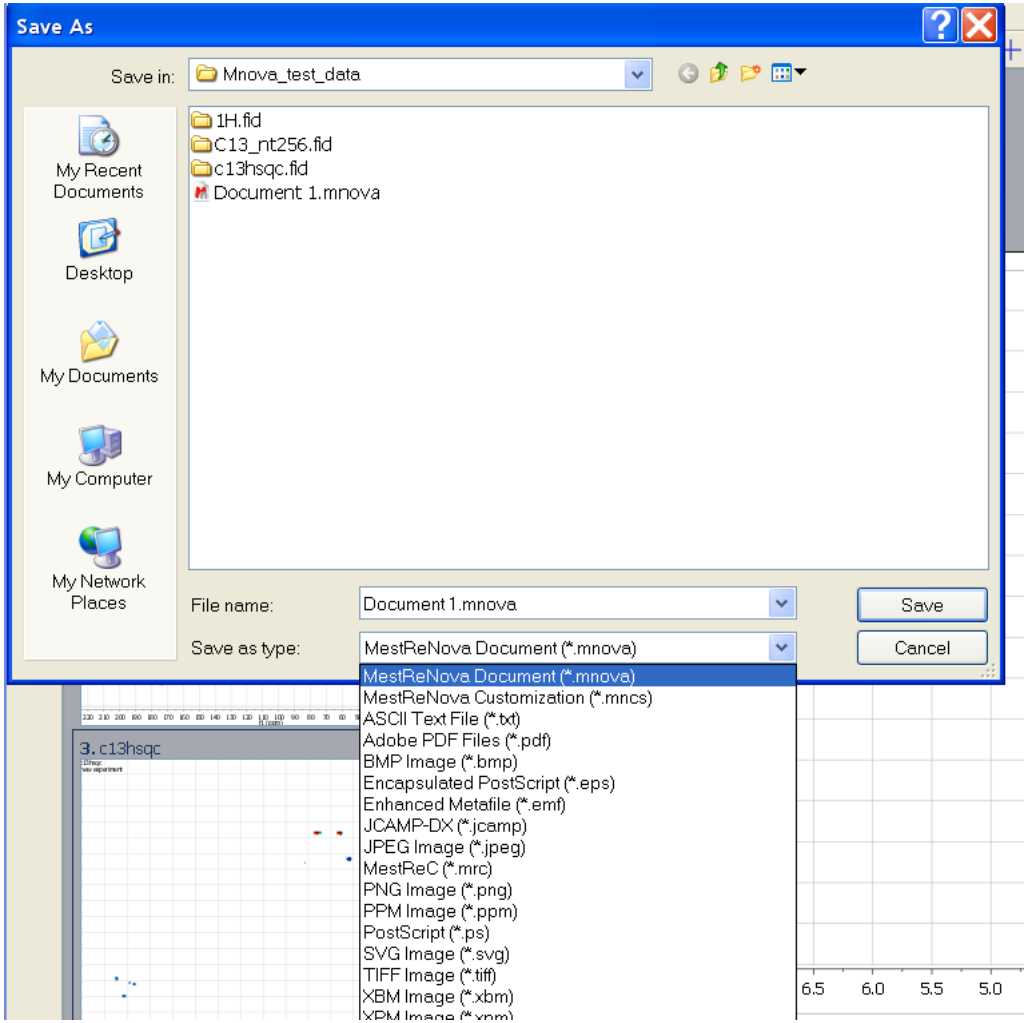

1H
nt=8
pw=pw90
3.32
3.31
3.30
3.28
2.82
2.82
2.80
2.79
2.62
2.62
2.61
2.60
2.59
2.59
2.58
Peaks
Report Peaks
Copy Peaks
Setup Report
Delete
Sync From Spec
Filter
Sync To Spec
Set Flags
Select Peaks
Other editing tools available here
Drag cursor over table rows to move vertical highlight line to show corresponding peak
ppm | Intensity | Width | Area | Type | Flags | ity/Comp | nnotatior
1 | 3.32 | 193.5 | 2.55 | 2114.07 | Compo... | None
2 | 3.31 | 209.2 | 2.70 | 2230.53 | Compo... | None
3 | 3.30 | 222.8 | 2.62 | 2504.38 | Compo... | None
4 | 3.28 | 221.5 | 2.42 | 2302.06 | Compo... | None
5 | 2.82 | 190.7 | 2.57 | 2102.61 | Compo... | None
6 | 2.82 | 213.1 | 2.92 | 2518.31 | Compo... | None
7 | 2.80 | 175.9 | 2.81 | 1883.86 | Compo... | None
8 | 2.79 | 185.0 | 2.56 | 1721.95 | Compo... | None
9 | 2.62 | 60.4 | 1.75 | 346.73 | Compo... | None
10 | 2.62 | 113.4 | 2.06 | 1001.63 | Compo... | None
11 | 2.61 | 148.7 | 2.23 | 1287.49 | Compo... | None
12 | 2.60 | 176.9 | 2.60 | 1968.29 | Compo... | None
13 | 2.59 | 151.6 | 2.20 | 1427.46 | Compo... | None
14 | 2.59 | 110.4 | 1.99 | 846.53 | Compo... | None
360
340
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
3.40
3.35
3.30
3.25
3.20
3.15
3.10
3.05
3.00
2.95
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
f1 (ppm)

To save current data sets and processing results, go to File→Save as … or Save to .mnova format



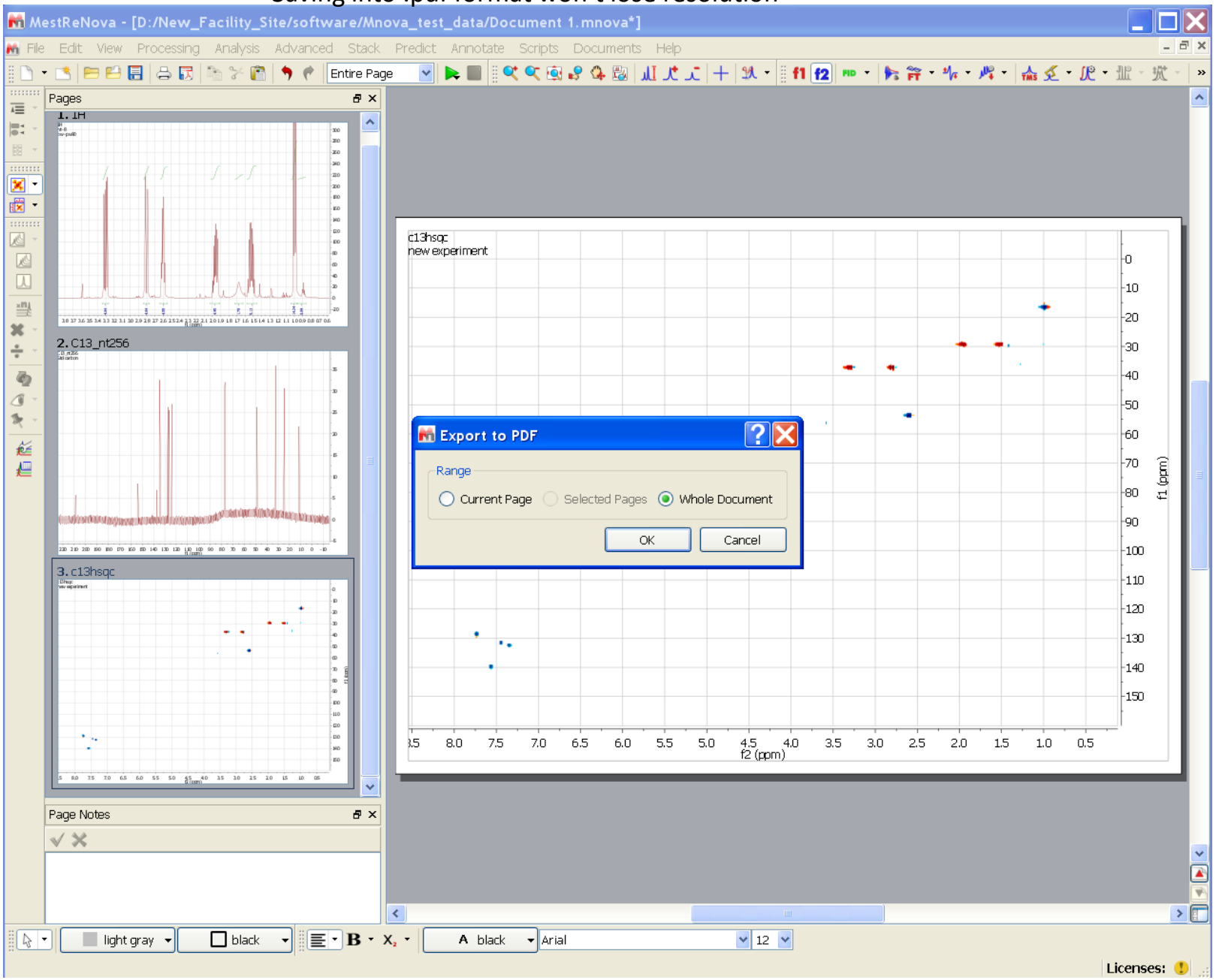
Export Data: many image formats available

.pdf and .eps are vector based and retain native resolution

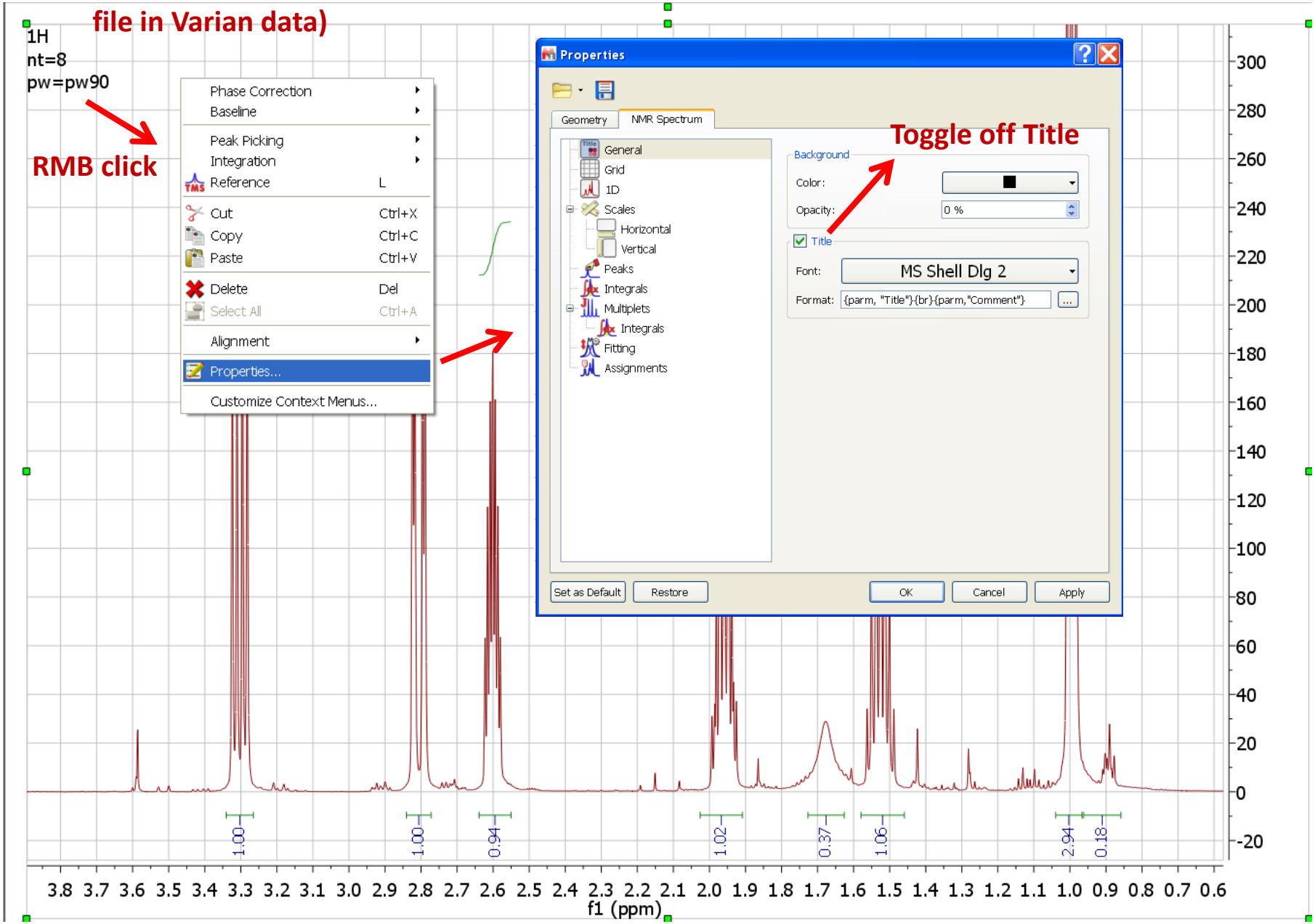


Saving Data: other formats available

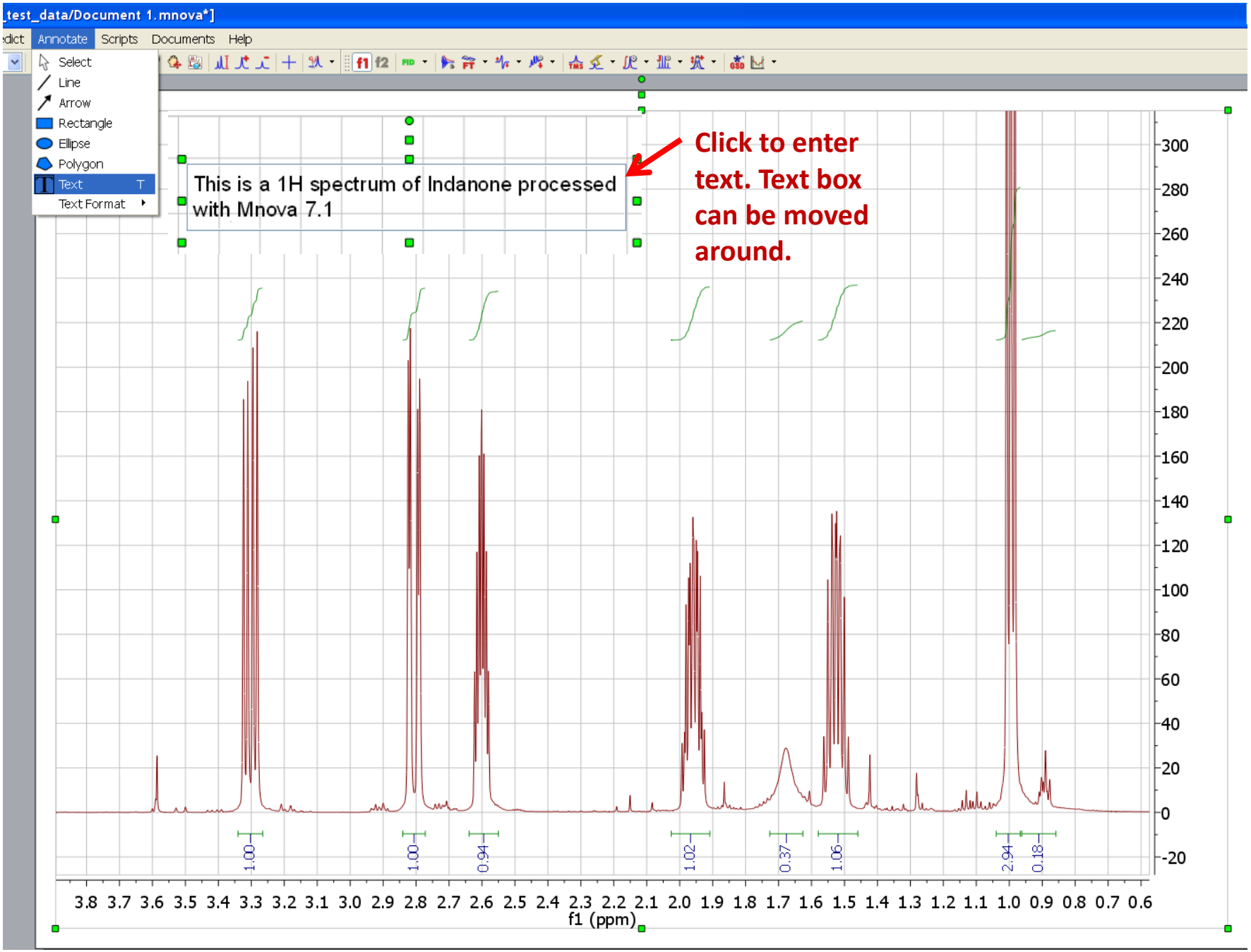
Saving into .pdf format won't lose resolution



To remove experiment title (from comment text file in Varian data)



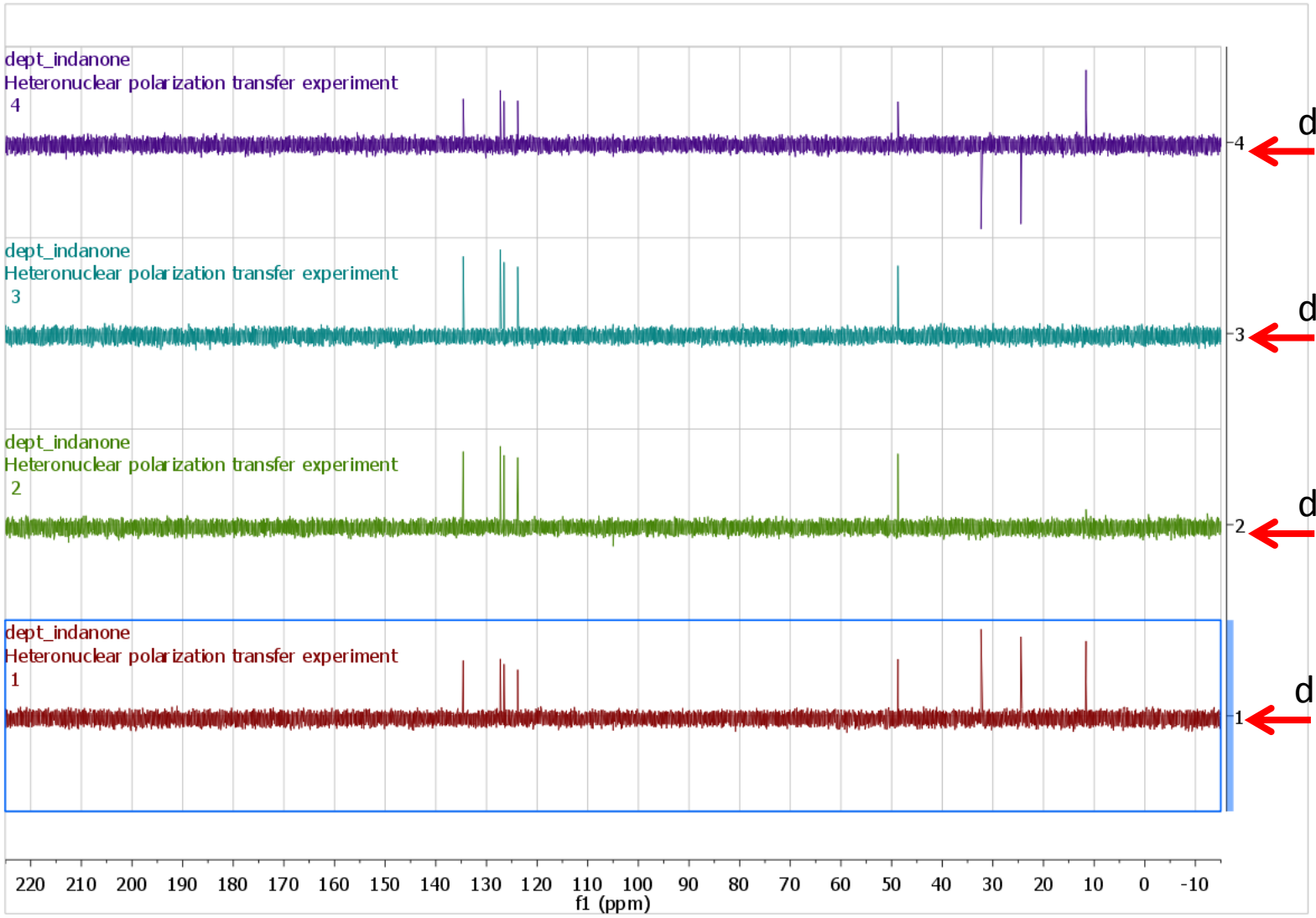
To annotate spectrum



Process Arrayed Experiment: DEPT

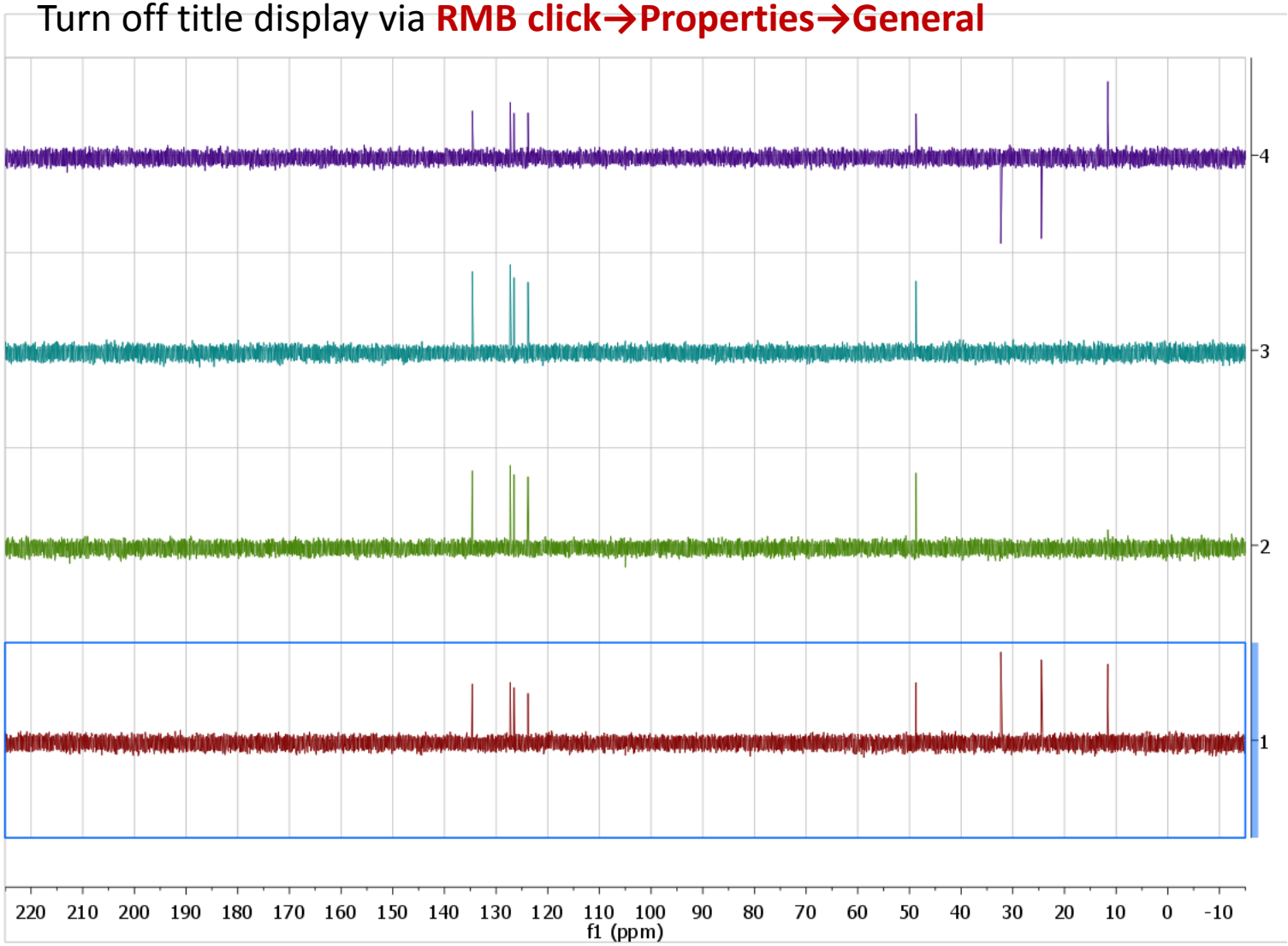
Drag & drop to load/autoprocess data

The following is directly processed Varian DEPT without further separation of CH/CH2/CH3 groups

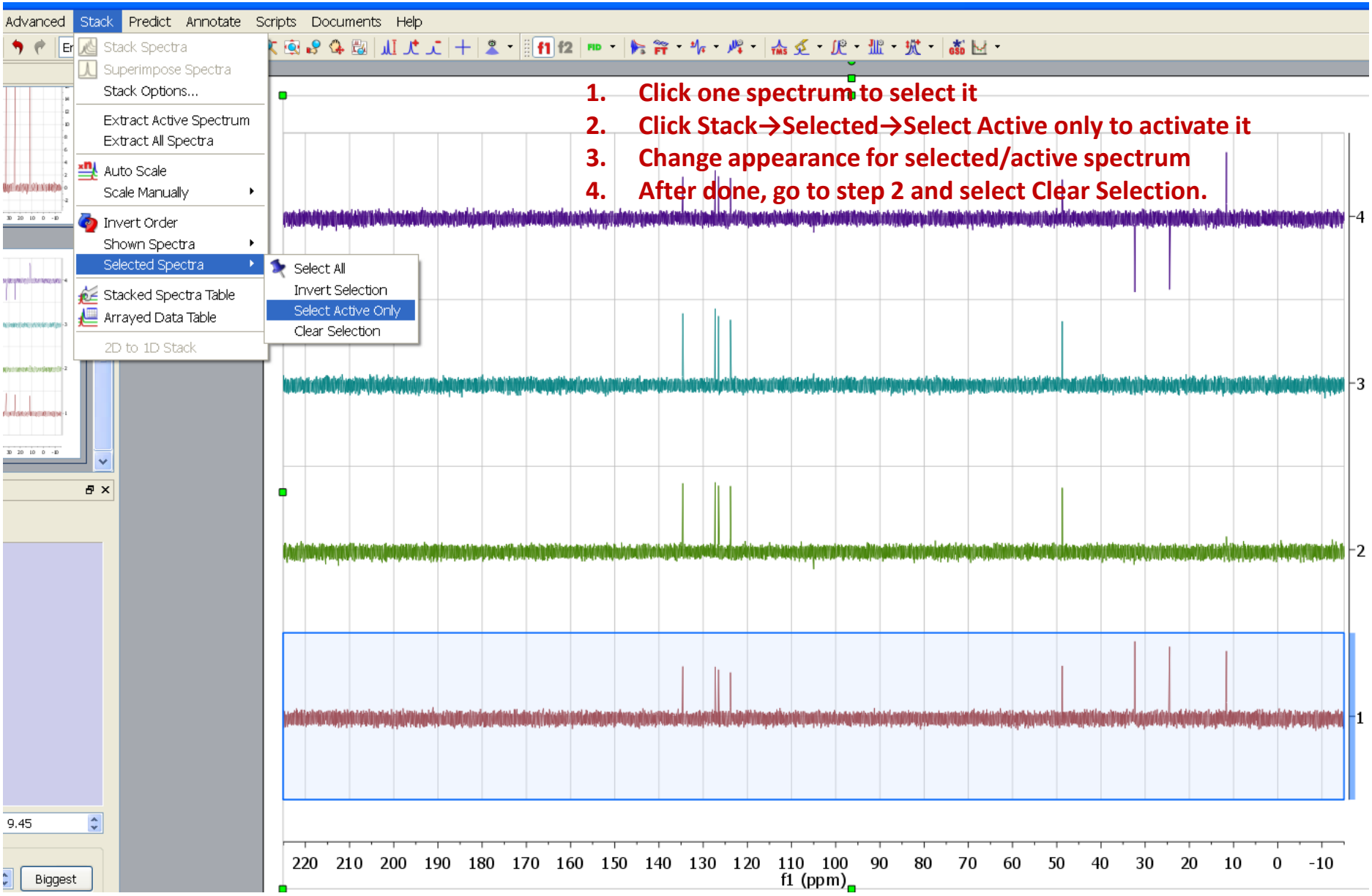


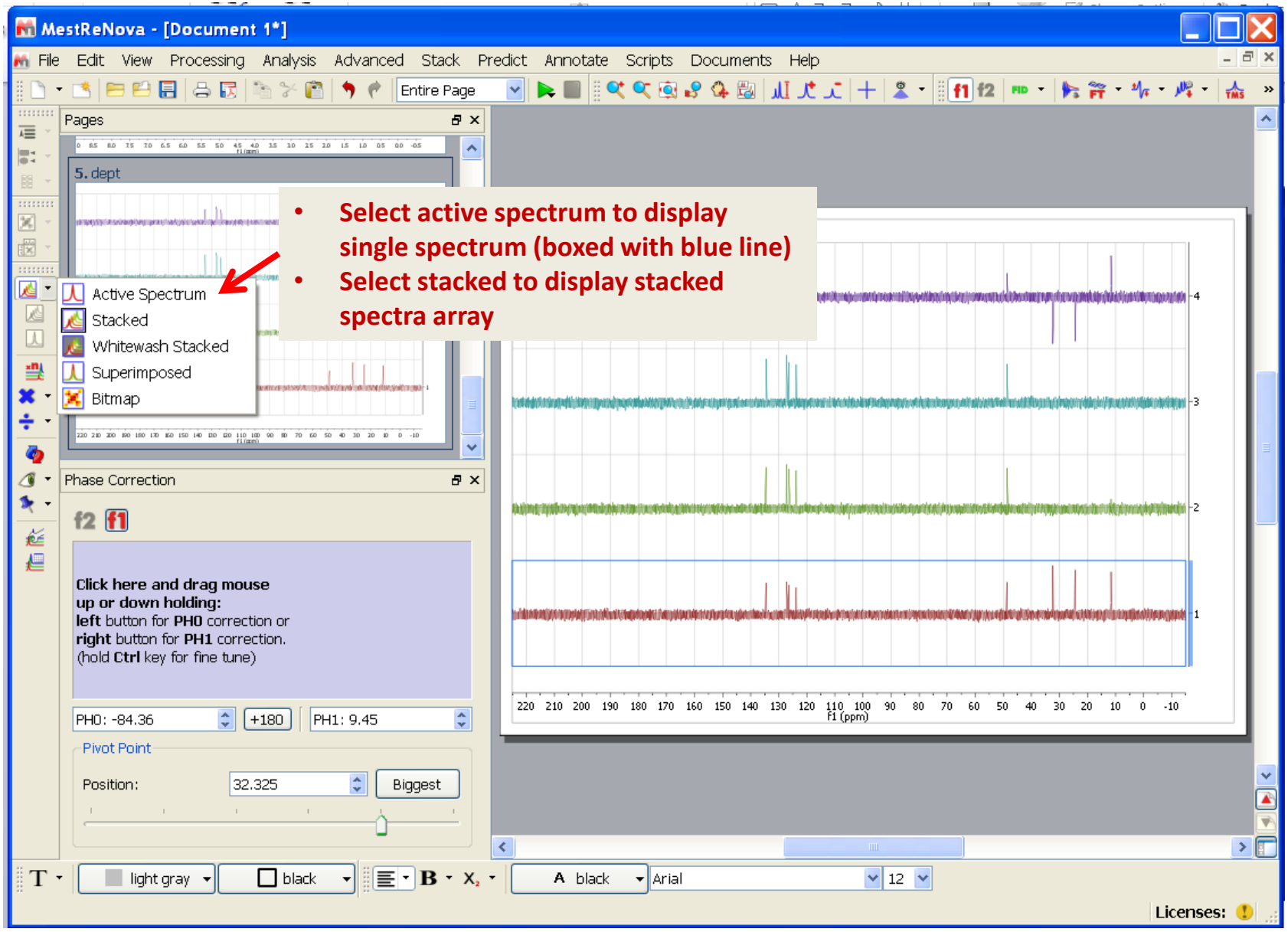
See Facility website: http://nmr.chem.ucsb.edu/protocols/DEPT.html for more details

Turn off title display via **RMB click→Properties→General**

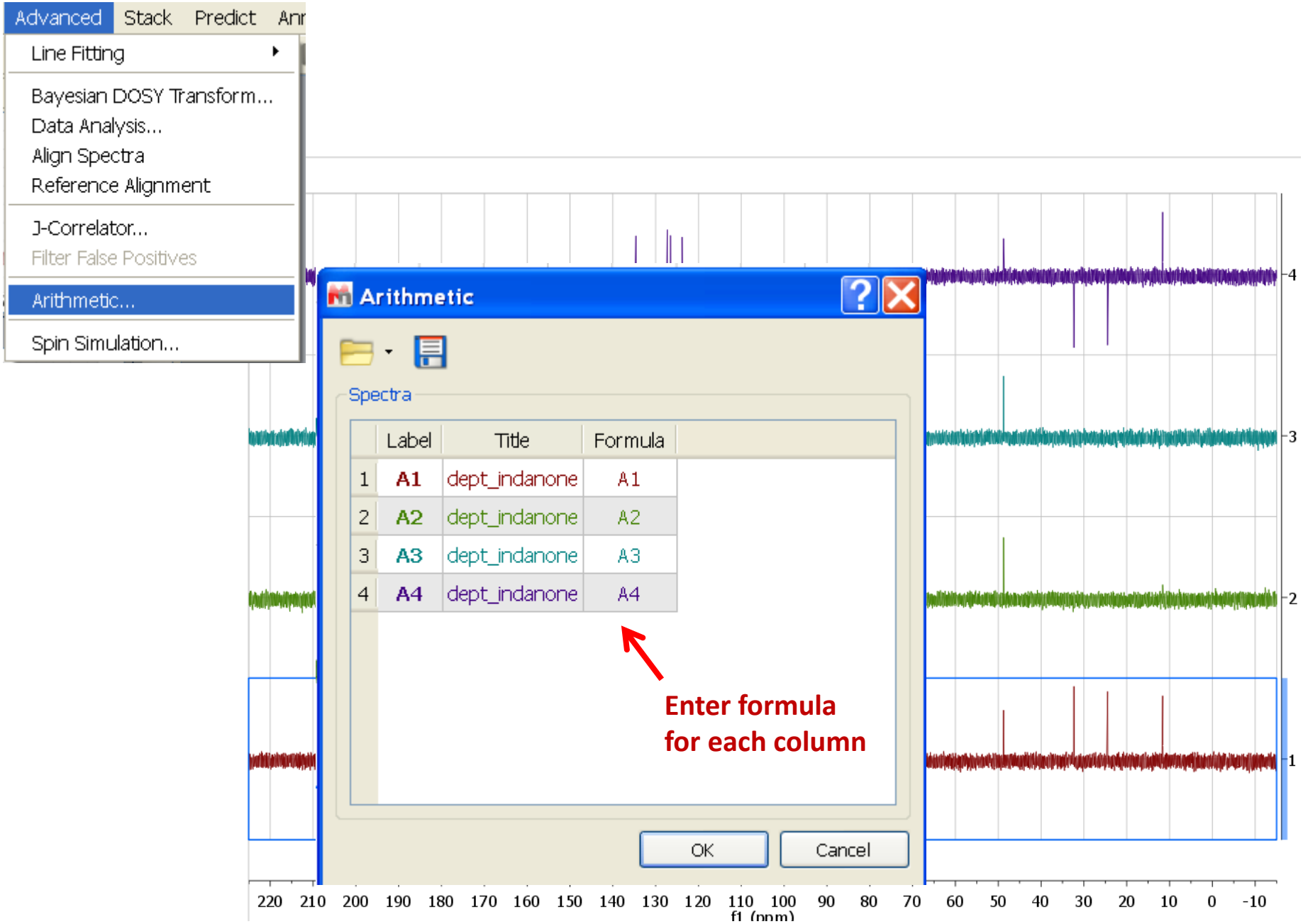


Although it is undesirable for DEPT, phase and appearance of each spectrum can be changed.



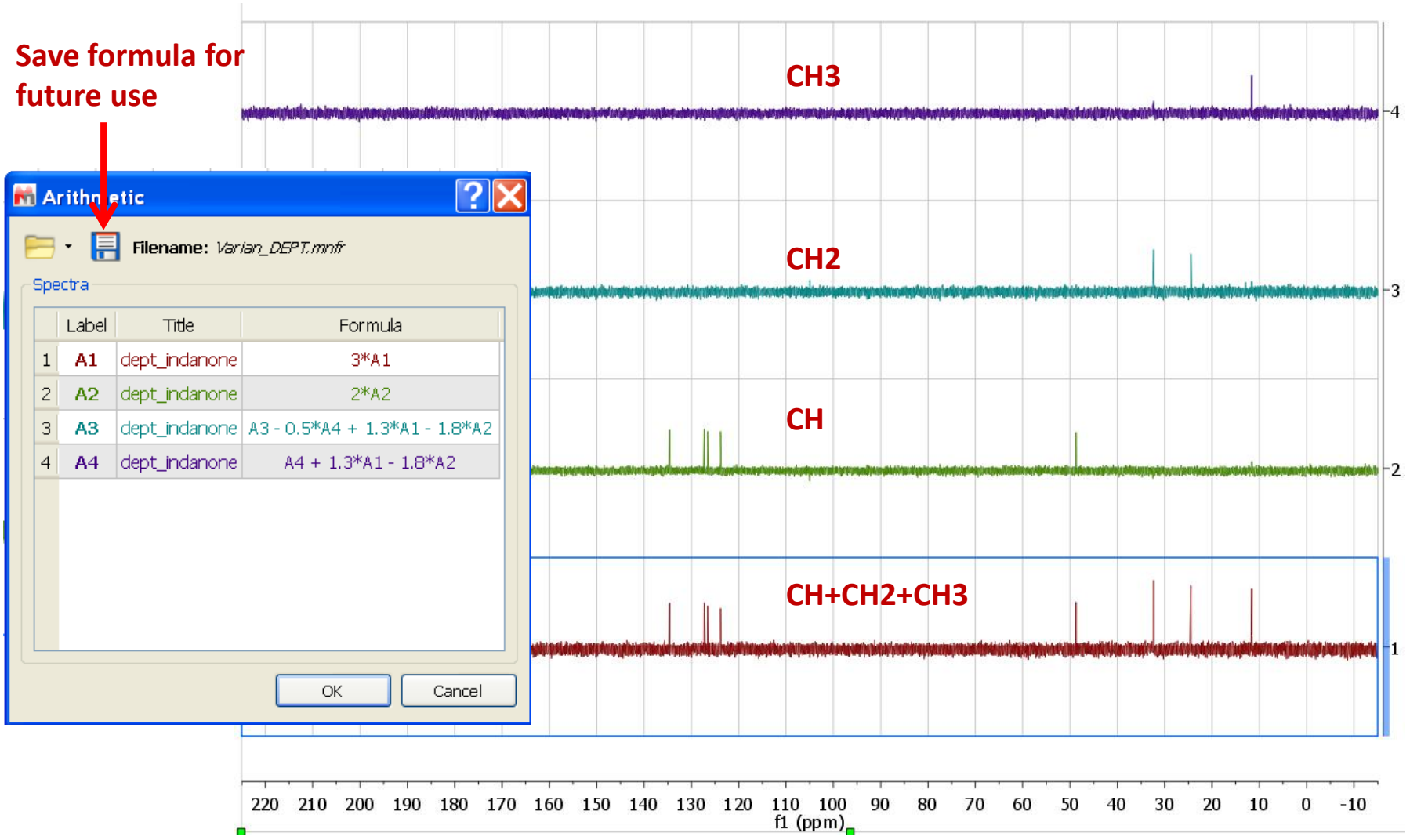

MestReNova - [Document 1*]
File Edit View Processing Analysis Advanced Stack Predict Annotate Scripts Documents Help
Entire Page
Pages
5. dept
Active Spectrum
Stacked
Whitewash Stacked
Superimposed
Bitmap
• Select active spectrum to display single spectrum (boxed with blue line)
• Select stacked to display stacked spectra array
Phase Correction
f2 f1
Click here and drag mouse up or down holding:
left button for PH0 correction or
right button for PH1 correction.
(hold Ctrl key for fine tune)
PH0: -84.36
+180
PH1: 9.45
Pivot Point
Position:
32.325
Biggest
f1 (ppm)
light gray
black
black
Arial
12
Licenses:

Separation of CH/CH2/CH3 peaks with Varian DEPT Data



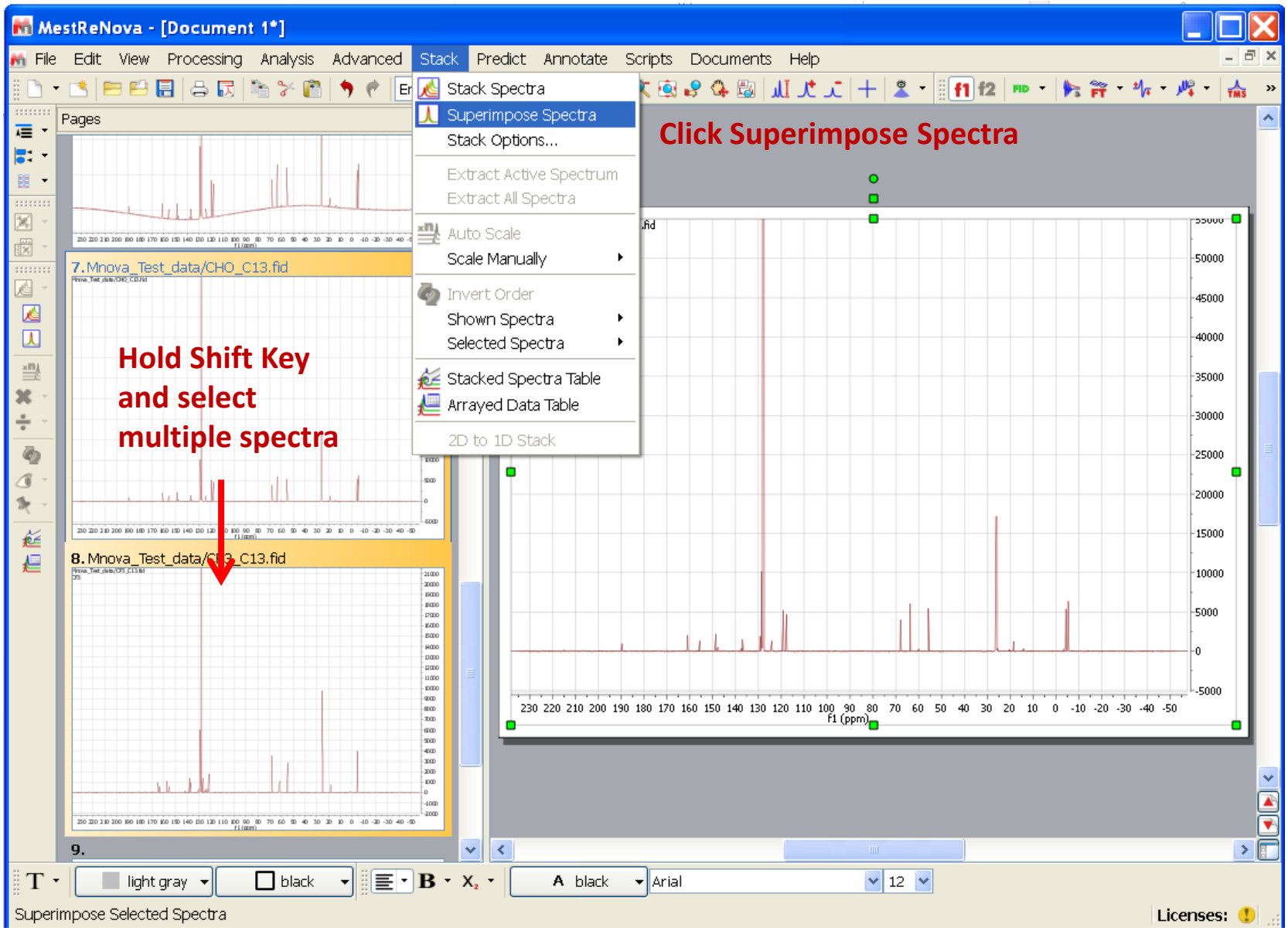
Re-processed Varian DEPT Data

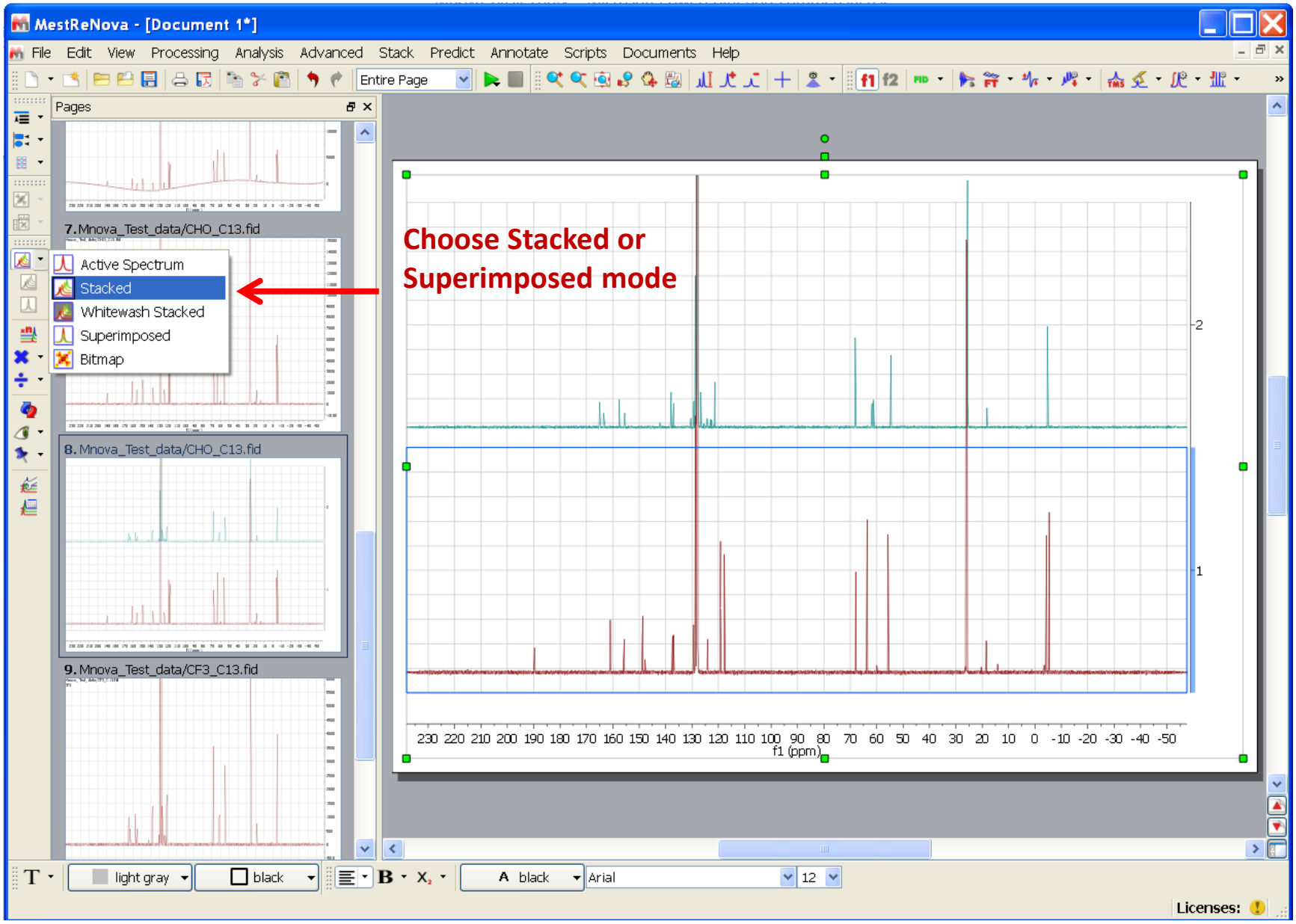
Processing similar to Varian's **adept** macro

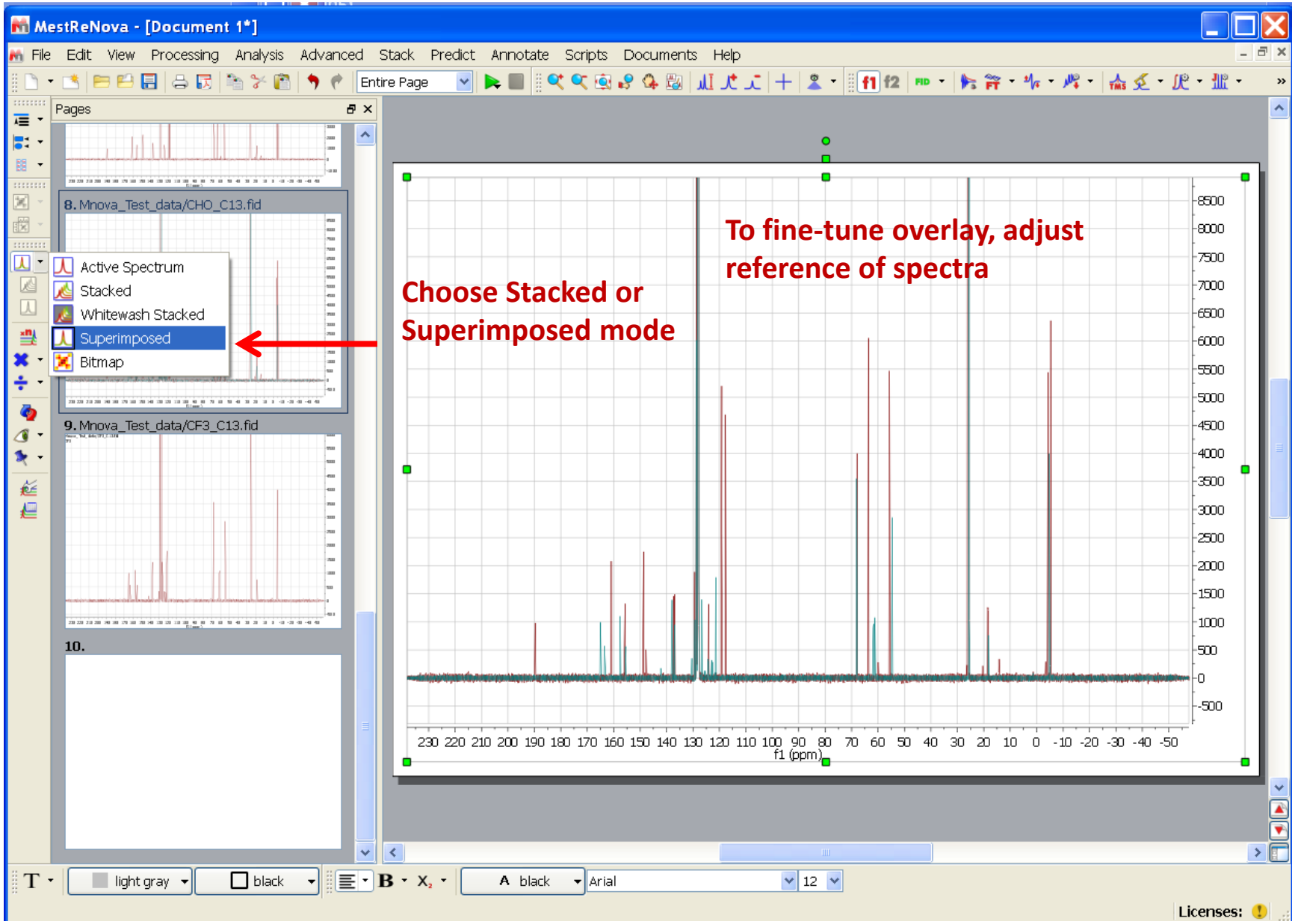


See Facility website: http://nmr.chem.ucsb.edu/protocols/DEPT.html for more details

Superimposition of Several Spectra




MestReNova - [Document 1*]
File Edit View Processing Analysis Advanced Stack Predict Annotate Scripts Documents Help
Entire Page
Pages
7. Mnova_Test_data/CHO_C13.fid
8. Mnova_Test_data/CHO_C13.fid
9. Mnova_Test_data/CF3_C13.fid
Active Spectrum
Stacked
Whitewash Stacked
Superimposed
Bitmap
Choose Stacked or
Superimposed mode
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50
f1 (ppm)
light gray
black
A black
Arial
12
Licenses:


MestReNova - [Document 1*]
File Edit View Processing Analysis Advanced Stack Predict Annotate Scripts Documents Help
Entire Page
Pages
8. Mnova_Test_data/CHO_C13.fid
9. Mnova_Test_data/CF3_C13.fid
10.
Active Spectrum
Stacked
Whitewash Stacked
Superimposed
Bitmap
Choose Stacked or Superimposed mode
To fine-tune overlay, adjust reference of spectra
f1 (ppm)
light gray
black
black
Arial
12
Licenses: