

Mnova 7.1 NMR Basics

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

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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

Drag & Drop Raw Data Here

Drag & Drop Raw Data Here

- You can drop multiple folders. Each data set shows in a separate “slide”
- Alternatively, open data from **File**→**Open...** or **Open Directoty ...**
- Data are auto- processed after loading.

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: 0.00 +180 PH1: 0.00

Pivot Point

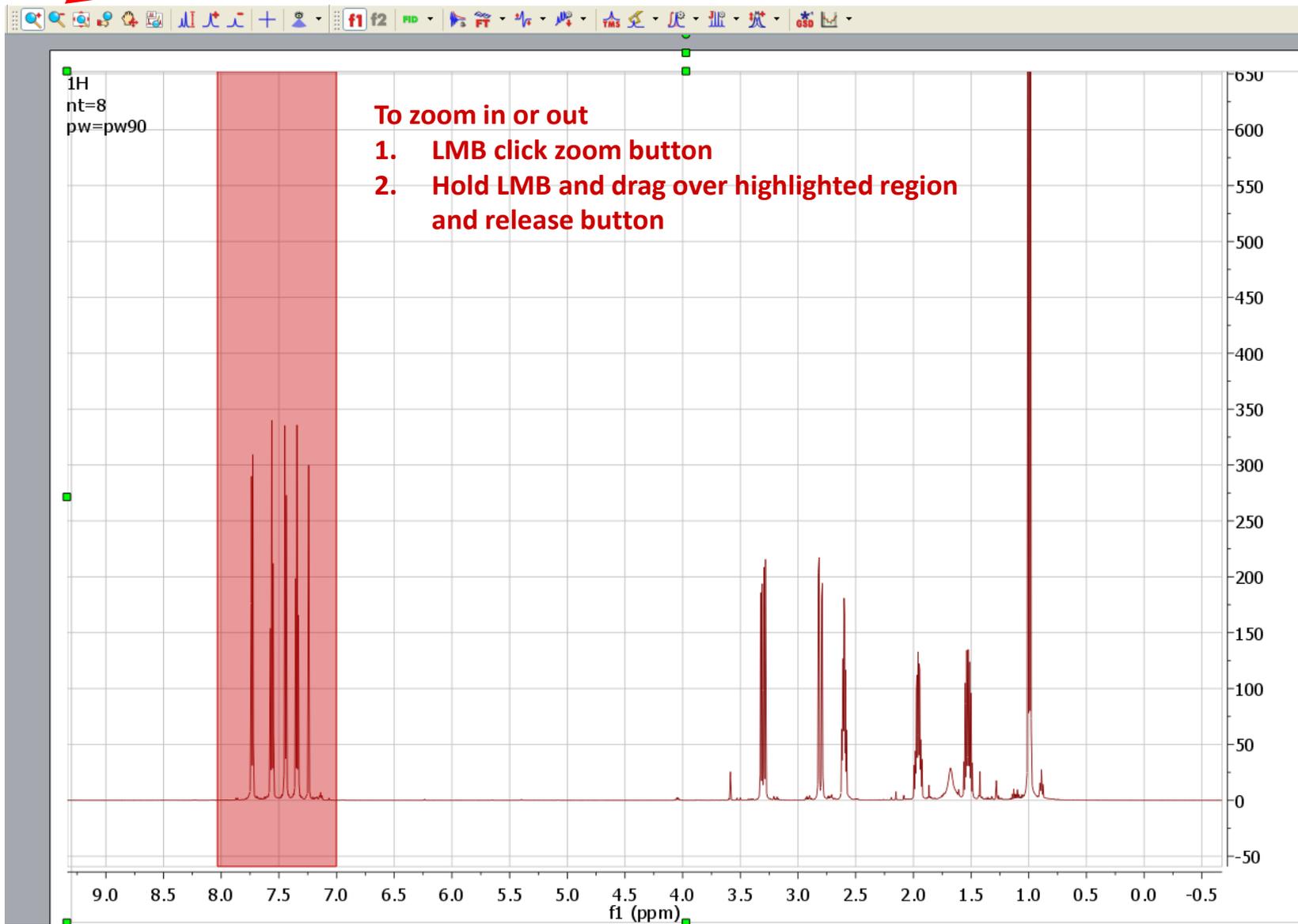
Position: 0.000 Biggest

light gray black

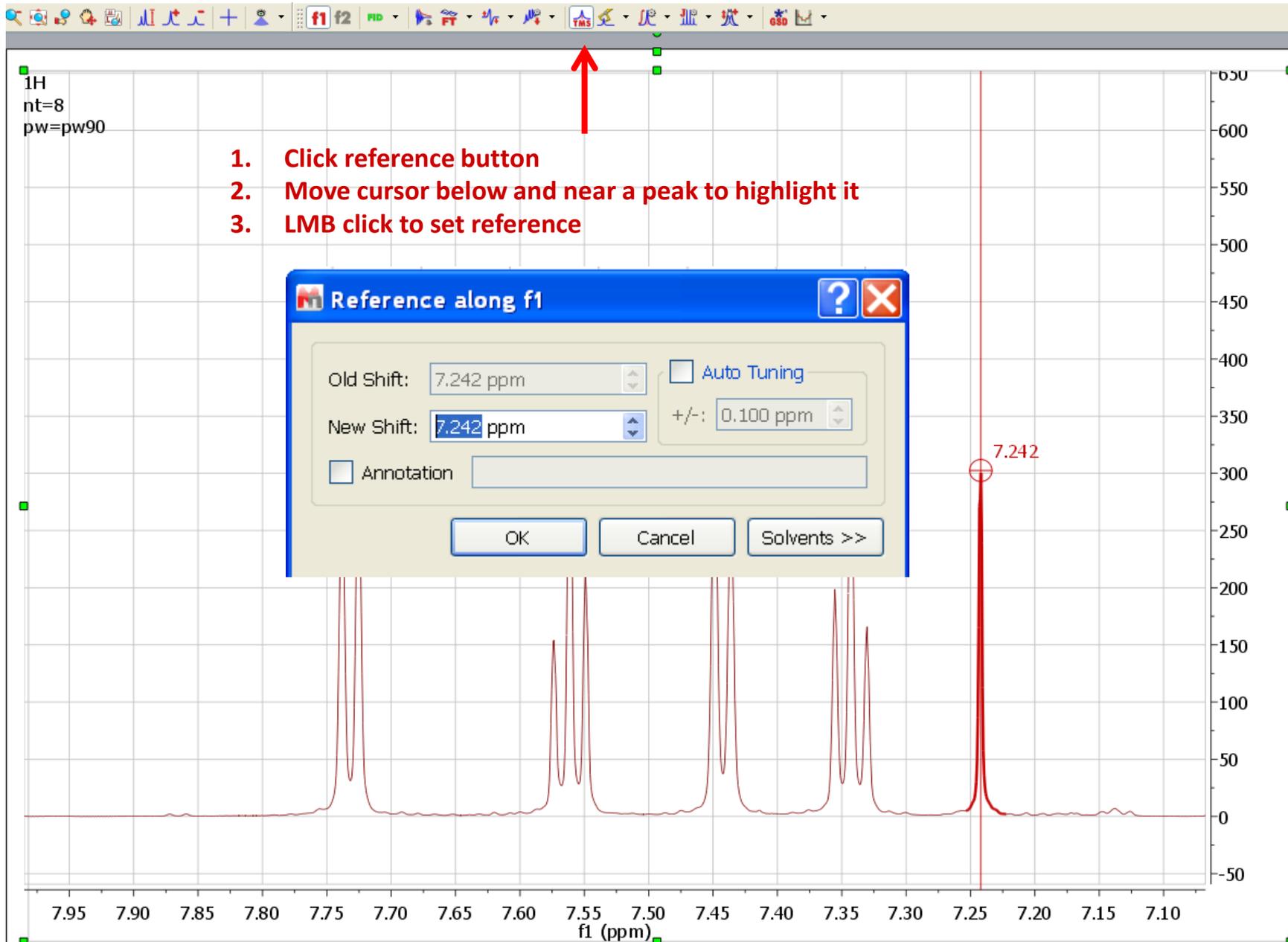
B X₂ A black Arial 12

Licenses: !

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



Reference by Peak



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

Enter phase mode

The screenshot displays the MestReNova software interface. The main window shows a 1D ¹H NMR spectrum with a chemical shift range from 9.0 to -0.5 ppm. The spectrum features several peaks, with a prominent one at approximately 1.0 ppm. The software's menu bar includes File, Edit, View, Processing, Analysis, Advanced, Stack, Predict, Annotate, Scripts, Documents, and Help. The toolbar contains various icons for file operations and processing. A context menu is open over the spectrum, listing options such as Phase Correction, Baseline, Peak Picking, Integration, Reference, Cut, Copy, Paste, Delete, Select All, Alignment, Properties, and Customize Context Menus. The 'Phase Correction' sub-menu is expanded, showing 'Automatic Options...', 'Manual Correction', 'Magnitude', and 'Power'. A red arrow points to the 'Phase mode' icon in the toolbar, which is highlighted in the 'Phase Correction' sub-menu. A red arrow also points to the 'Manual Correction' option in the sub-menu. A red text annotation 'OR: RMB click inside to open menu' is placed near the spectrum. The status bar at the bottom shows 'light gray', 'black', 'A black', 'Arial', and '12'.

Phase mode

OR: RMB click inside to open menu

1H
F1=8
pw=pw90

Phase Correction

- Automatic Options...
- Manual Correction
- Magnitude
- Power

Automatic Options...

Manual Correction

Magnitude

Power

light gray black

A black Arial 12

Licenses: ⚠

Phase Panel Opened

The screenshot displays the MestReNova software interface. The main window shows an NMR spectrum with a prominent peak at approximately 1.0 ppm. A 'Phase Correction' dialog box is open, centered over the spectrum. The dialog box contains the following text and controls:

Phase Correction

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: -120.98 +180 PH1: 0.00

Pivot Point

Position: 0.995 Biggest

The background spectrum shows a peak at 1.0 ppm with a height of approximately 1500. The x-axis ranges from 2.5 to -0.5 ppm, and the y-axis ranges from -100 to 1600. A red arrow points from the text 'Drag & drop phase panel here' to the 'Phase Correction' dialog box.

Drag & drop phase panel here

Phasing steps:

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

The screenshot displays the MestReNova software interface. The main window shows an NMR spectrum with a vertical blue line at 0.995 ppm, labeled as the pivot point for 1st order phasing. A red arrow points to this line. The text "MMB scroll to change vertical scaling" is overlaid on the spectrum. The left sidebar contains a "Phase Correction" panel with the following settings:

- PH0: -120.98
- PH1: 0.00
- Pivot Point Position: 0.995
- Buttons: +180, Biggest

Red arrows point to the "0.995" input field and the "Biggest" button, with the text "Adjust pivot point" below them. The top menu bar includes File, Edit, View, Processing, Analysis, Advanced, Stack, Predict, Annotate, Scripts, Documents, and Help. The bottom status bar shows font settings: Arial, size 12, and a license notice.

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

Toggle Zoom mode on/off
Hold LMB to select region

Set fixed range

The screenshot shows the MestReNova software interface with the following components and annotations:

- Top Menu Bar:** File, Edit, View, Processing, Analysis, Advanced, Stack, Predict, Annotate, Scripts, Documents, Help.
- Toolbar:** Contains icons for zooming, selection, and analysis. Annotations include:
 - Red arrow pointing to the zoom icon: "Toggle Zoom mode on/off"
 - Red arrow pointing to the selection icon: "Hold LMB to select region"
 - Red arrow pointing to the zoom icon: "Set fixed range"
 - Red arrow pointing to the zoom icon: "Click to return to full spectrum"
- Pages Panel (Left):** Shows a thumbnail of the full spectrum labeled "1. 1H".
- Phase Correction Panel (Bottom Left):**
 - Buttons for "f2" and "f1".
 - Text: "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)".
 - Input fields: PH0: -121.88, PH1: 5.00.
 - Pivot Point section: Position: 7.731, Biggest.
 - Annotation: "Adjust pivot point" with red arrows pointing to the position input field.
- Main Spectrum Plot (Right):**
 - Y-axis: Intensity (0 to 500).
 - X-axis: Chemical shift (ppm) from 8.4 to 6.7.
 - Annotation: "Set pivot to left side peak Adjust zero-order phase so that this peak to pure absorptive" with a red arrow pointing to a peak at approximately 7.73 ppm.
- Bottom Panel:** Includes a color palette (light gray, black), font settings (Arial, size 12), and a license notice.

1st order Phasing

The screenshot displays the MestReNova software interface for NMR data analysis. The main window shows a 1H NMR spectrum with a vertical scale from -1 to 11. A zoomed-in view of a peak at approximately 7.7 ppm is shown in the center, with a vertical blue line indicating the pivot point. The software interface includes a menu bar (File, Edit, View, Processing, Analysis, Advanced, Stack, Predict, Annotate, Scripts, Documents, Help), a toolbar, and a sidebar with various tool icons. The 'Phase Correction' panel on the left contains the following controls:

- Buttons for **f2** and **f1**.
- Instructional text: "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: -121.88 (with a +180 button)
- PH1: 5.00
- Pivot Point section with "Position: 7.731" and a "Biggest" button.

The zoomed-in plot includes the text: "Scroll MMB to increase vertical scale to observe phase distortion". The x-axis is labeled "f1 (ppm)" and ranges from 9.0 to -0.5. The y-axis ranges from -1 to 11. The plot shows a complex multiplet with a phase correction line at 7.731 ppm.

At the bottom of the interface, there are controls for background color (light gray, black), font style (B, X), font color (A black), font family (Arial), and font size (12). A "Licenses: !" icon is visible in the bottom right corner.

1st order Phasing

The screenshot displays the MestReNova software interface for 1st order phasing. The main window shows a 1H NMR spectrum with a red trace and a blue vertical line at 7.731 ppm. The x-axis is labeled 'f1 (ppm)' and ranges from 9.0 to -0.5. The y-axis ranges from -1 to 11. The spectrum shows several peaks, with the most prominent one at approximately 7.7 ppm. A blue vertical line is positioned at 7.731 ppm, and a red square is at the top of this line. A red arrow points to the 'PH1: 1.00' field in the Phase Correction panel.

Pages
1. 1H

Phase Correction

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)

Hold/drag RMB to adjust 1st order phase

Watch right side spectrum for good phase while adjusting 1st order phase

Click up/down to fine adjust values

PH0: -121.24 +180 PH1: 1.00

Pivot Point
Position: 7.731 Biggest

light gray black B X₂ A black Arial 12

Licenses: !

Full Auto Polynomial Baseline Correction for Simple Baseline Defects

The screenshot displays the MestReNova software interface. The main window shows a 1H NMR spectrum with a red baseline. A context menu is open over the spectrum, with the 'Baseline' option selected. A red arrow points to the 'Full Auto (Bernstein Polynomials)' option within the 'Baseline' submenu. The 'Phase Correction' panel is visible in the bottom left, with a red arrow pointing to its close button and the text 'Close phase panel if needed'. The software's menu bar and toolbar are visible at the top, and the status bar at the bottom shows the font and license information.

RMB click and select "Full Auto"

Close phase panel if needed

Phase Correction

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: -121.24 +180 PH1: 1.00

Pivot Point
Position: 7.731 Biggest

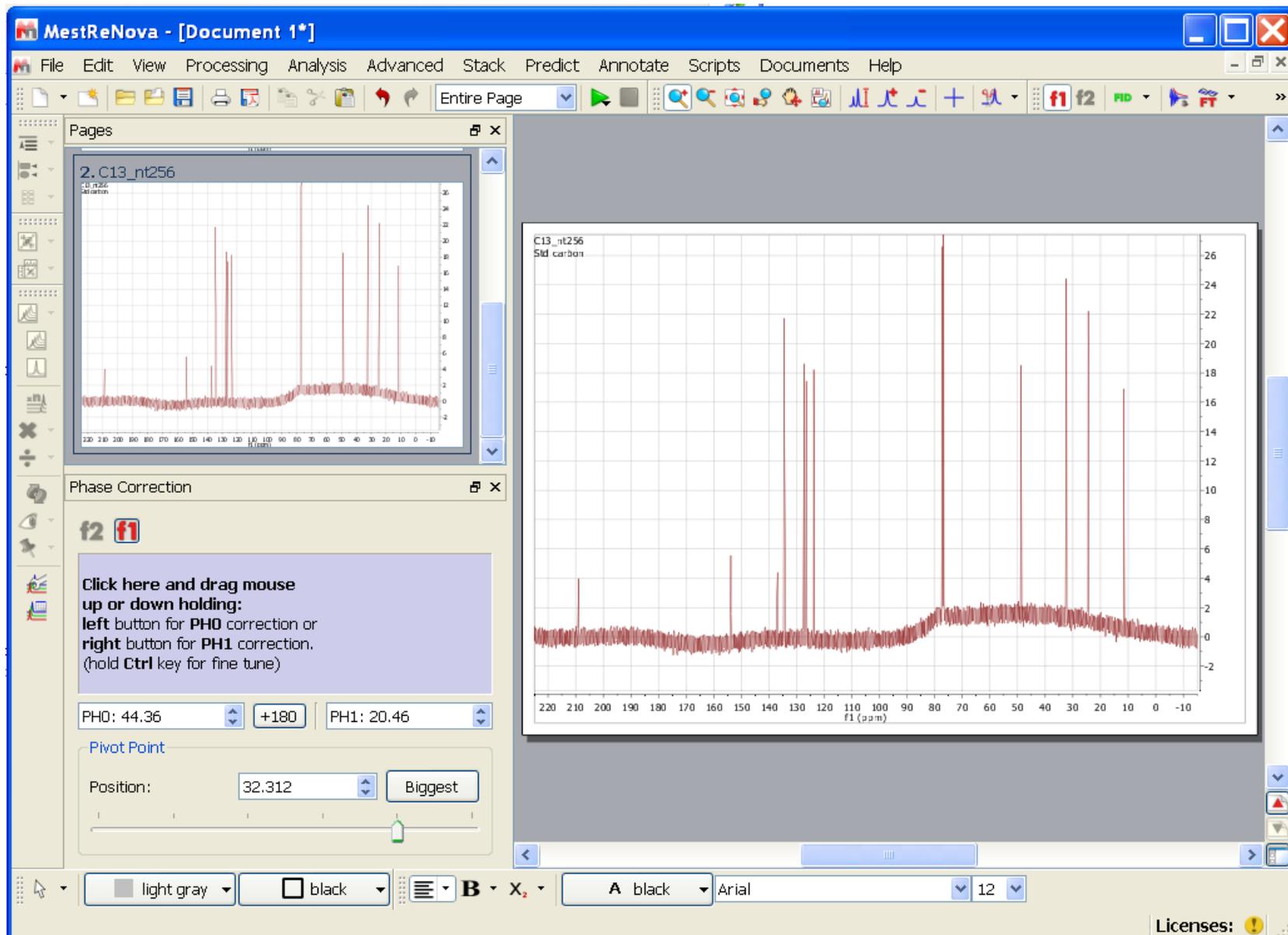
Phase Correction

- Phase Correction
- Baseline
 - Baseline Correction...
 - Full Auto (Bernstein Polynomials)
 - Multipoint Baseline Correction
- Peak Picking
- Integration
- Reference L
- Cut Ctrl+X
- Copy Ctrl+C
- Paste Ctrl+V
- Delete Del
- Select All Ctrl+A
- Alignment
- Properties...
- Customize Context Menus...

light gray black B X₂ A black Arial 12 Licenses: !

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

MestReNova - [Document 1*]

File Edit View Processing Analysis Advanced Stack Predict Annotate Scripts Documents Help

Pages

2. C13_nt256

Phase Correction

f2 f1

Click here and drag mouse up or down holding:
left button for PHD correction or
right button for PH1 correction.
(hold Ctrl key for fine tune)

PHD: 44.36 +180 PH1: 20.46

Pivot Point

Position: 32.312 Biggest

light gray black

B X₂ A black Arial 12

Baseline Correction also...

Method: Bernstein Polynomial Fit

Parameters: Polynomial Order: 3

Ok Cancel Extract

Adjust order and watch blue line match

Watch to get best blue fit line match with actual baseline

13_nt256 Std. carbon

f1 (ppm)

Licenses: !

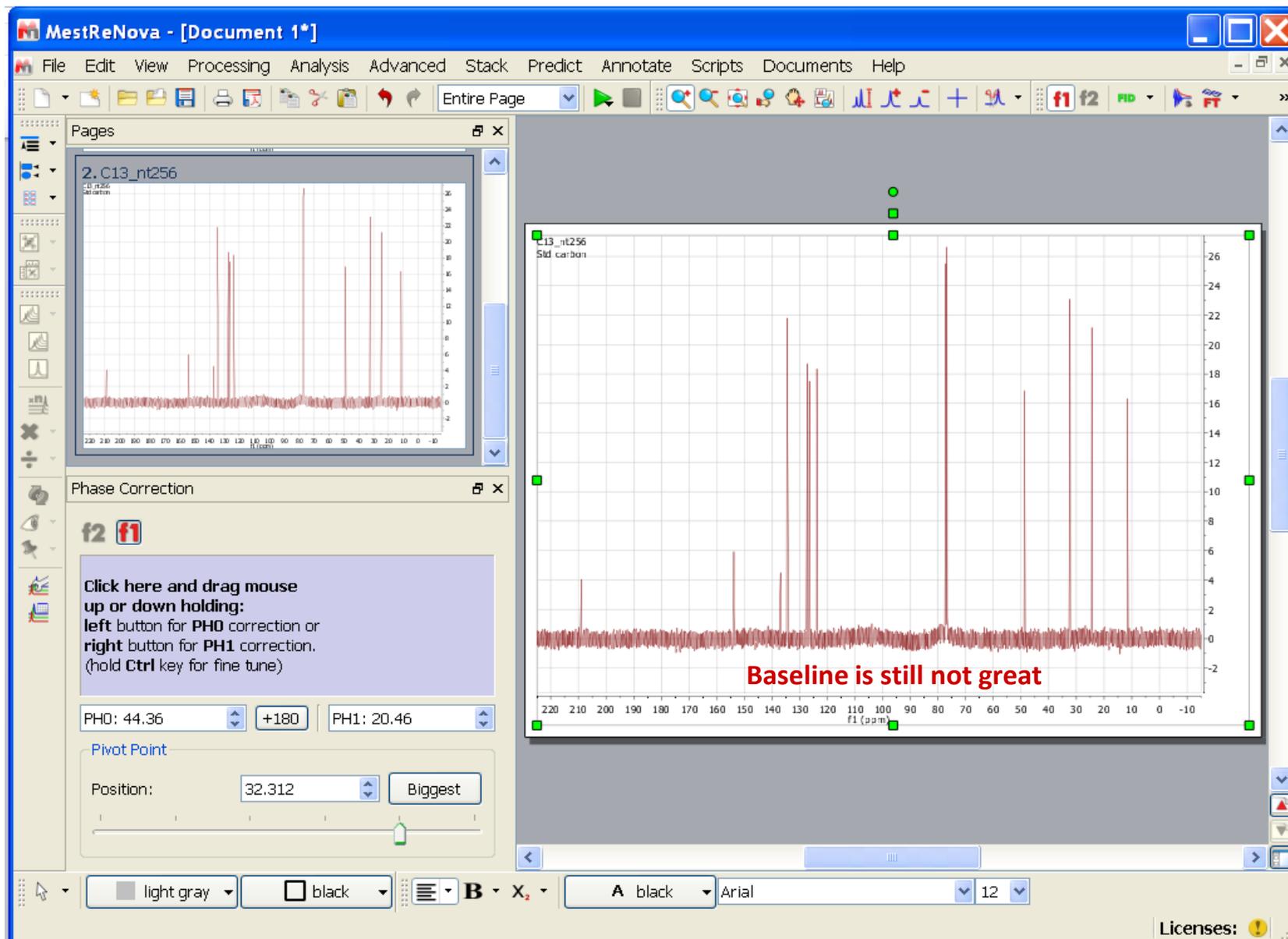
Default Full Auto Baseline Correction with Bernstein Polynomial Fit Order 20

The screenshot displays the MestReNova software interface. The main window shows a chromatogram titled 'C13_nt256 Std carbon' with a baseline correction applied. A dialog box titled 'Baseline Correction' is open, showing the following settings:

- Method: Bernstein Polynomial Fit
- Parameters: Polynomial Order: 20

A red arrow points to the '20' in the Polynomial Order field, with the text 'Order 20 (max) works best' written in red. The software interface includes a menu bar (File, Edit, View, Processing, Analysis, Advanced, Stack, Predict, Annotate, Scripts, Documents, Help), a toolbar, and a sidebar with various tool icons. The bottom status bar shows 'light gray', 'black', 'B', 'X', 'A black', 'Arial', and '12'.

Result from Baseline Correction with Bernstein Polynomial Fit Order 20



Best Result Comes with Whittaker Smoother

The screenshot displays the MestReNova software interface. The main window shows a 13C NMR spectrum of a standard carbon sample. The x-axis is labeled 'f1 (ppm)' and ranges from 220 to -10. The y-axis represents intensity. A blue fit line is overlaid on the spectrum, following the baseline. A red arrow points to this fit line, and text below it reads 'blue fit line matches actual baseline well'. A dialog box titled 'Baseline Correction along f1' is open, showing the 'Whittaker Smoother' method selected. The parameters are: Filter (4.42 Hz) set to 8, Smooth Factor set to 20000, and both 'Autodetect' checkboxes are checked. The software interface includes a menu bar (File, Edit, View, Processing, Analysis, Advanced, Stack, Predict, Annotate, Scripts, Documents, Help), a toolbar, and a sidebar with various tools and panels like 'Pages', 'Phase Correction', and 'f2 f1'.

Baseline Correction along f1

Method: Whittaker Smoother

Parameters:

- Filter (4.42 Hz): 8 Autodetect
- Smooth Factor: 20000 Autodetect

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: 44.36 +180 PH1: 20.46

Pivot Point

Position: 32.312 Biggest

light gray black

A black Arial 12

Licenses: !

Perfect Baseline Correction with Whittaker Smoother

The screenshot displays the MestReNova software interface. The main window shows a ¹³C NMR spectrum for 'C13_nt256' (Std carbon) with a flat baseline. The x-axis is labeled 'f1 (ppm)' and ranges from 220 to -10. The y-axis ranges from -2 to 26. The spectrum shows several sharp peaks, with the most prominent one at approximately 77 ppm. The baseline is very flat, indicating successful correction.

The 'Phase Correction' panel on the left contains the following information:

- Buttons for **f2** and **f1**.
- Instruction: "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: 44.36 [+180] PH1: 20.46
- Pivot Point: Position: 32.312 [Biggest]

The bottom status bar shows the following settings:

- Background: light gray
- Color: black
- Font: Arial, size 12
- License status: Licenses: !

Peak Integration

The screenshot displays the MestReNova software interface for peak integration. The main window shows a 1H NMR spectrum with several peaks. A context menu is open over the spectrum, listing various integration options. A red arrow points to the 'Integration' icon in the top toolbar.

MestReNova - [Document 1*]

File Edit View Processing Analysis Advanced Stack Predict Annotate Scripts Documents Help

Pages: 1. 1H

Integration

- Autodetect Regions
- Predefined Regions
- Options...
- Manual
- Delete Manually
- Delete All
- Show Integrals
- Autodetect Nuclides Count...

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: -121.24 +180 PH1: 1.00

Pivot Point

Position: 7.731 Biggest

light gray black B X A black Arial 12

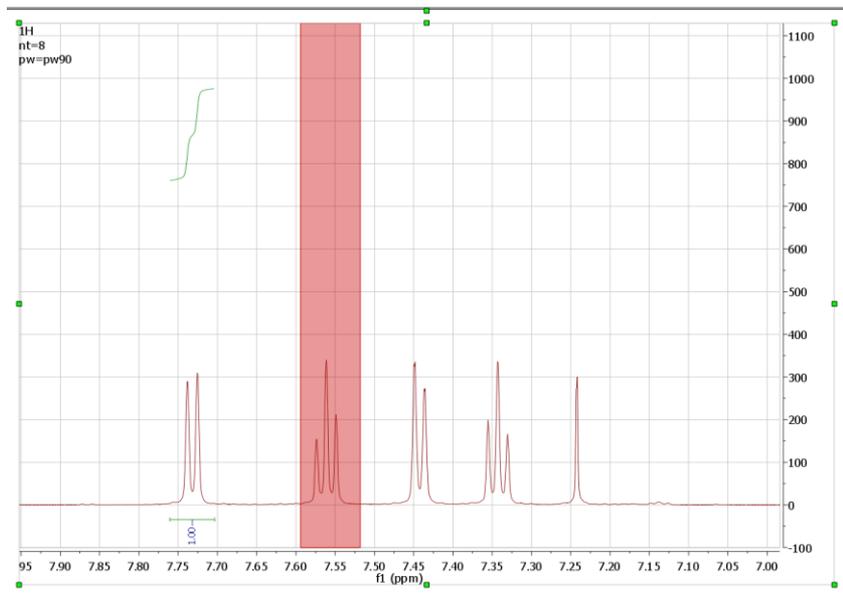
Licenses: !

Methods:

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

For full manual integration:

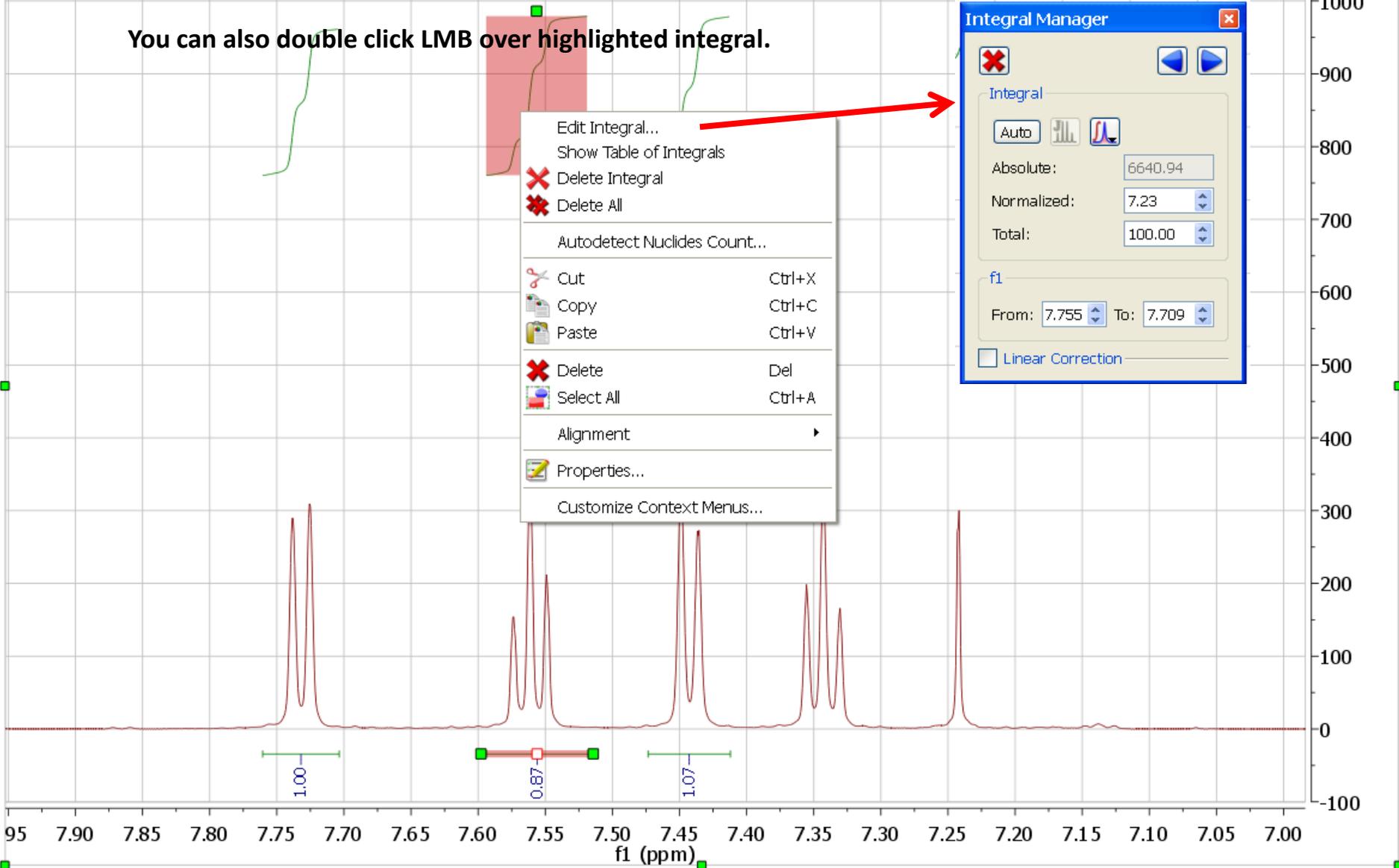
1. If integrals exist, select **Analysis**→**Integration** →**Delete all**
2. If an integration symbol appears, hold and drag LMB over peak region to define integral region as the highlighted area.
3. To delete an integral, LMB click over green integral line to select integral and RMB to select **Delete 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 [Bar Chart Icon] [Line Graph Icon]

Absolute: 6640.94

Normalized: 7.23

Total: 100.00

f1

From: 7.755 To: 7.709

Linear Correction

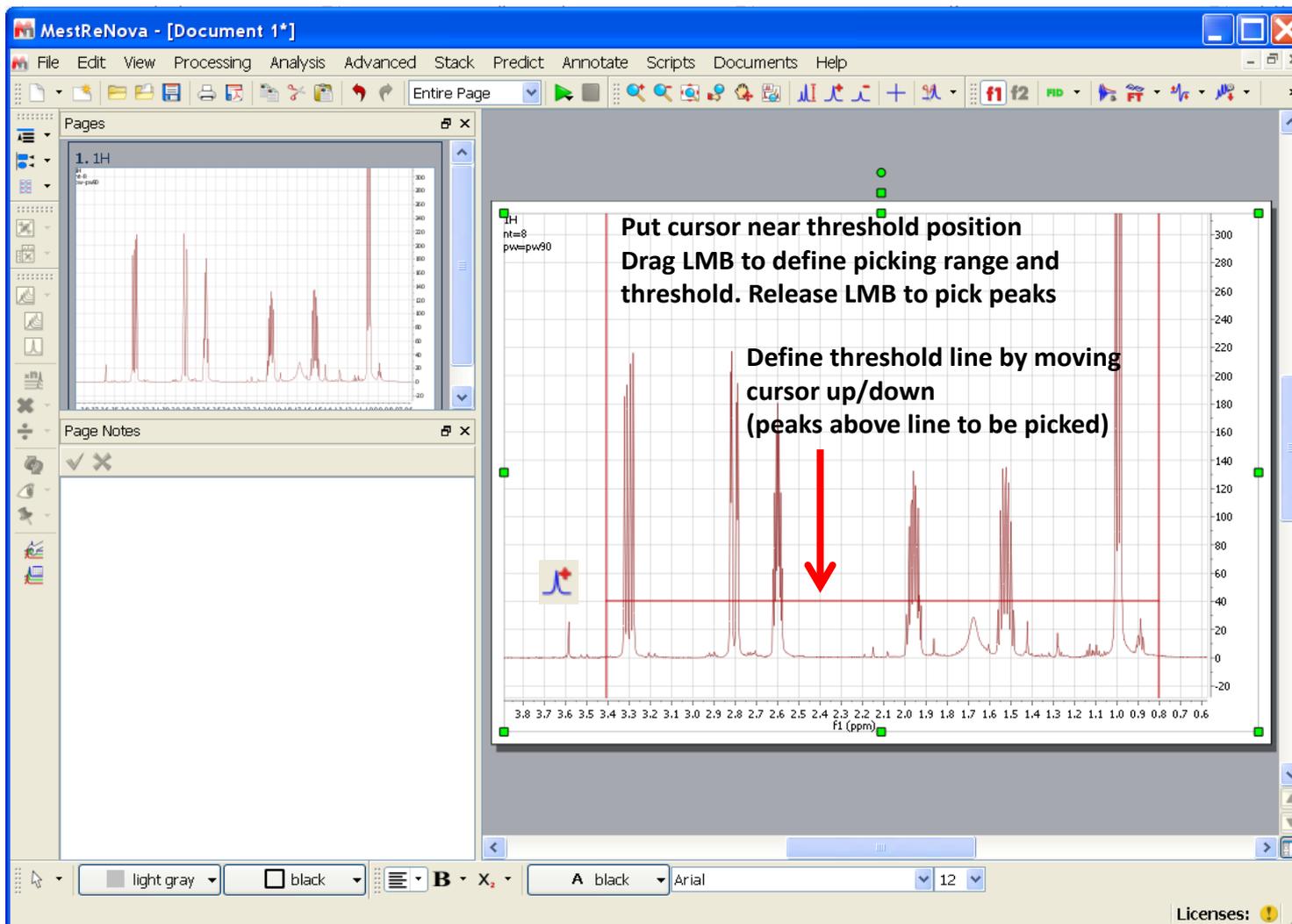
Analysis → Peak Picking

Enter Peak Picking Mode

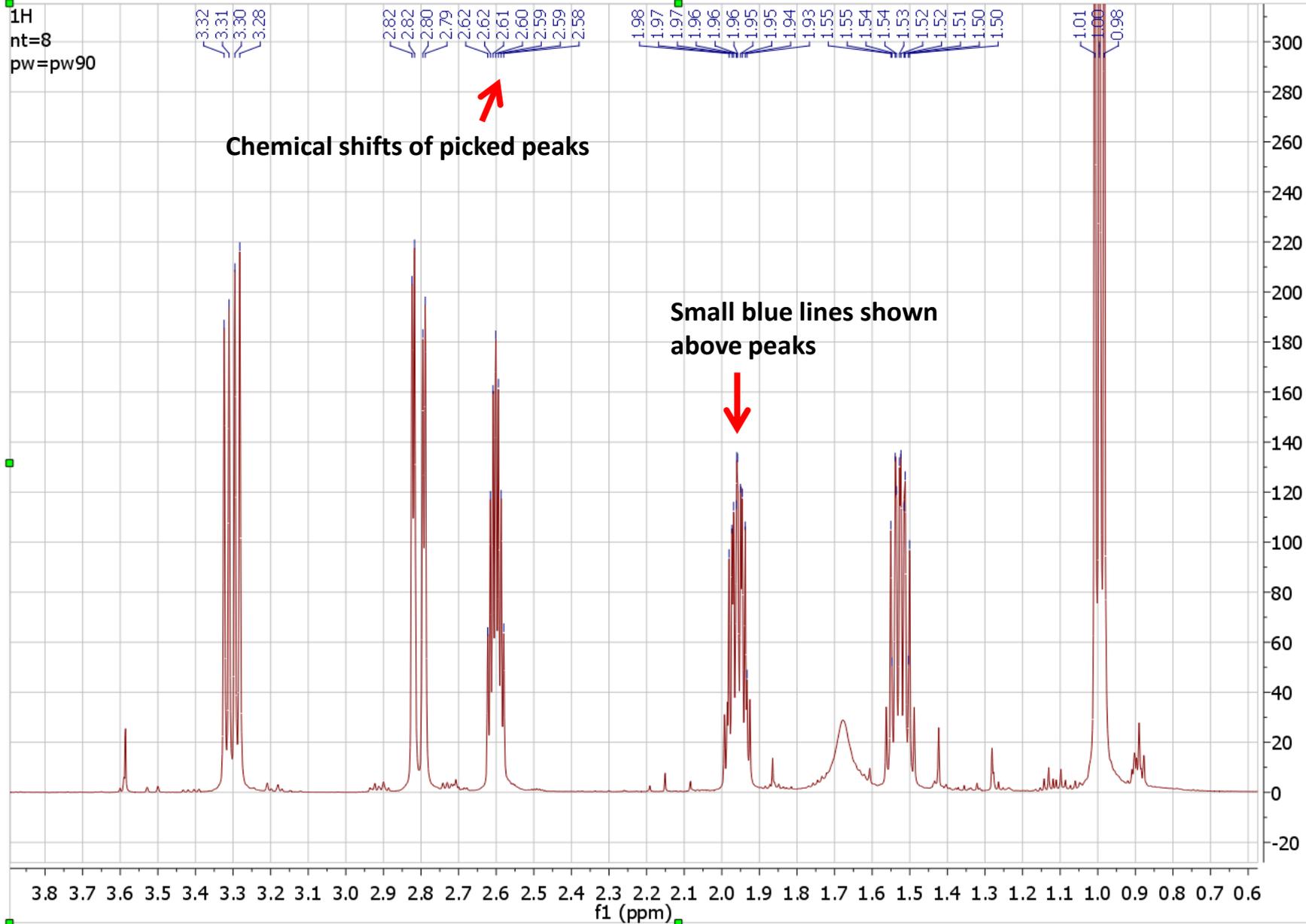
The screenshot displays the MestReNova software interface. The 'Analysis' menu is open, and 'Peak Picking' is selected. The context menu for 'Peak Picking' is also open, showing options like 'Automatic', 'Options...', 'Manual Threshold', 'Peak by Peak', 'Delete Manually', and 'Delete All'. The 'Manual Threshold' option is highlighted, and a red arrow points to its icon, labeled 'Shown in manual picking mode'. The main plot shows an NMR spectrum with several peaks. A red arrow points to the 'Peak Picking' icon in the toolbar, labeled 'Peak picking'. The x-axis is labeled 'F1 (ppm)' and ranges from 3.60 to 2.35. The y-axis ranges from -100 to 1600. The software title bar shows 'MestReNova - [Document 1]'. The status bar at the bottom shows 'light gray', 'black', 'B', 'X', 'A black', 'Arial', and '12'. The license information is visible in the bottom right corner.

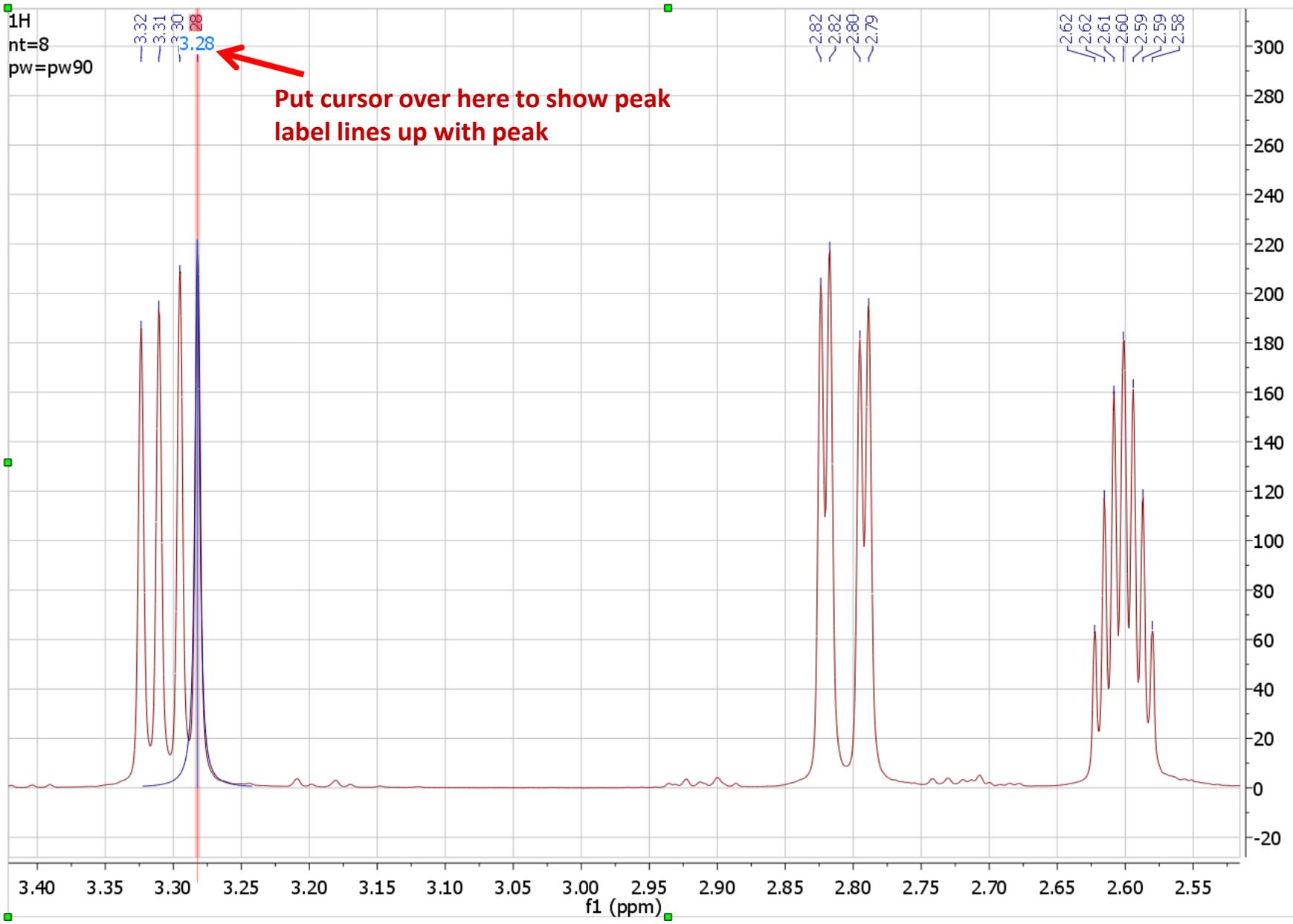
Peak Picking: Manual Threshold Mode

Positive and negative peaks carry same threshold magnitude by default

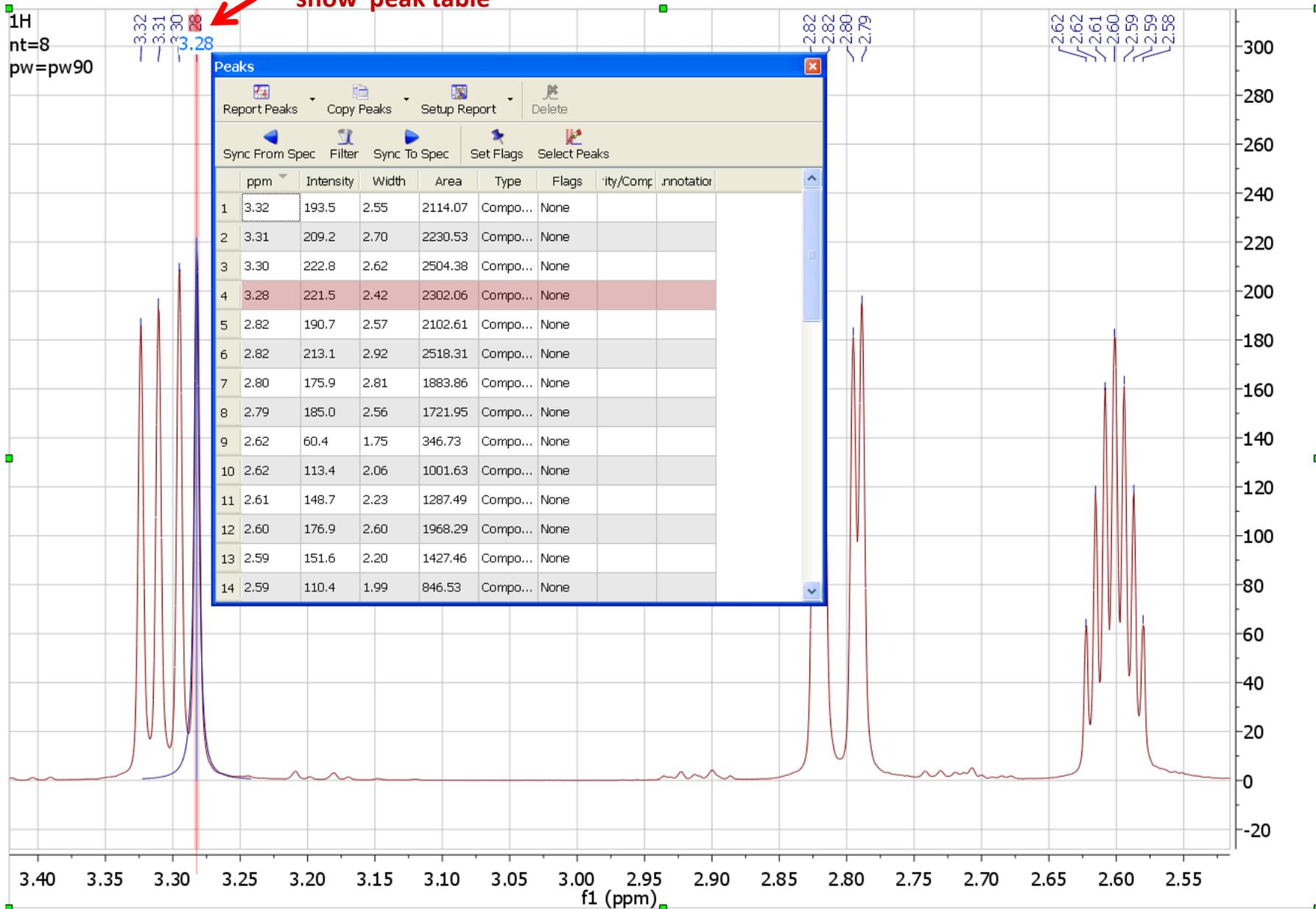


Peak Picking





LMB click in highlighted peak label to show peak table



¹H
nt=8
pw=pw90

3.32
3.31
3.30
3.28

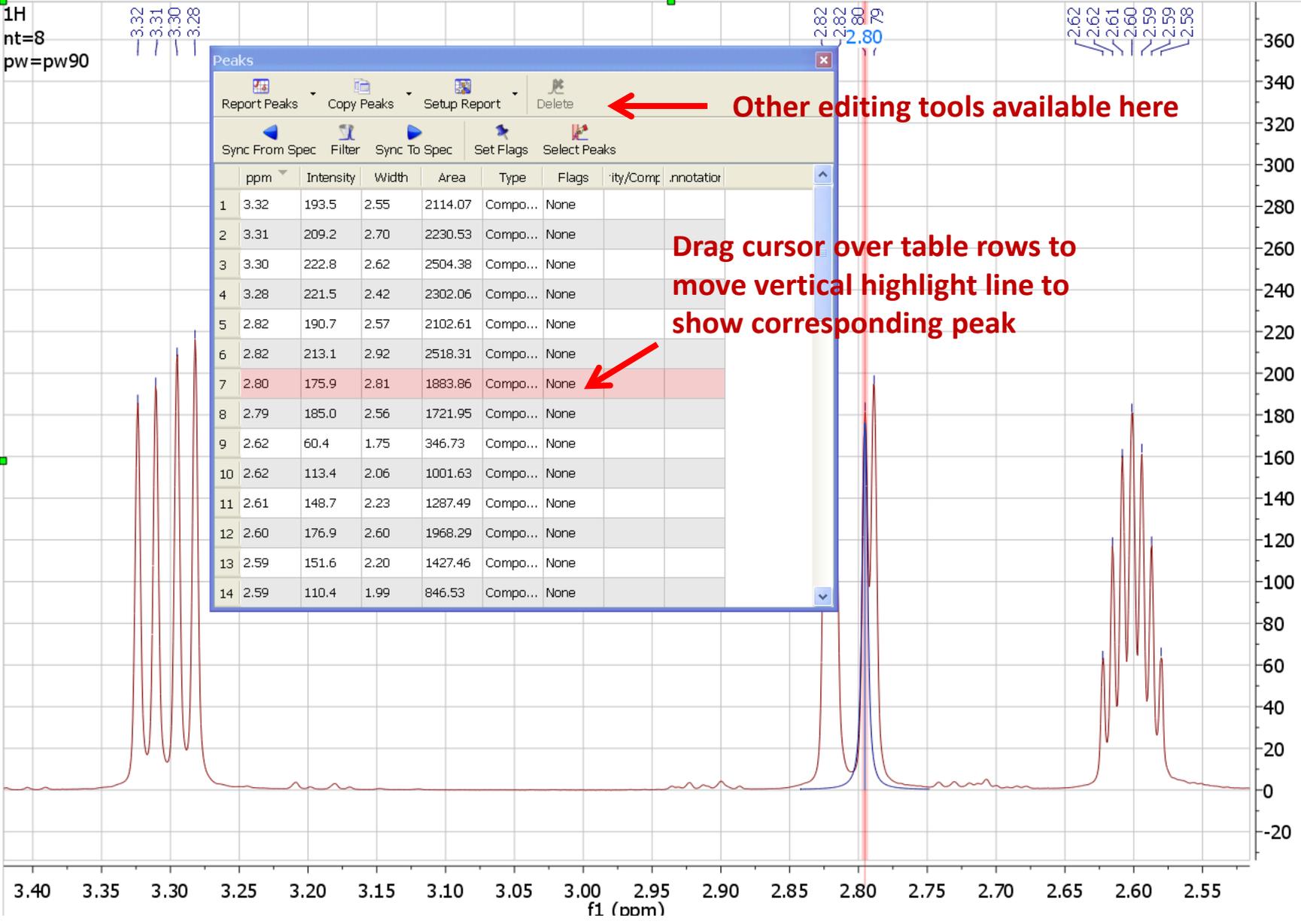
2.82
2.80
2.79

2.62
2.61
2.60
2.59
2.58

	ppm	Intensity	Width	Area	Type	Flags	ity/Comp	.nnotation
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		

Other editing tools available here

Drag cursor over table rows to move vertical highlight line to show corresponding peak



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

The screenshot displays the MestReNova software interface. The main window shows a 2D NMR spectrum (likely a 2D COSY or HSQC) with the following axes:

- Vertical axis (f1): ppm, ranging from 0 to 150.
- Horizontal axis (f2): ppm, ranging from 0.5 to 8.5.

The spectrum shows several cross-peaks, indicating correlations between protons. A 1D 1H NMR spectrum is visible in the top-left corner of the main window, showing peaks at approximately 7.5, 7.2, 6.8, 6.5, 3.5, 3.2, 2.8, 2.5, 2.0, 1.5, and 1.0 ppm.

The software interface includes a menu bar (File, Edit, View, Processing, Analysis, Advanced, Stack, Predict, Annotate, Scripts, Documents, Help) and a toolbar. The File menu is open, showing options such as New Document, Open..., Open Directory..., Close, Save, Save As..., Page Setup..., Print..., Export to PDF..., Recent Documents, Recent Files, and Exit.

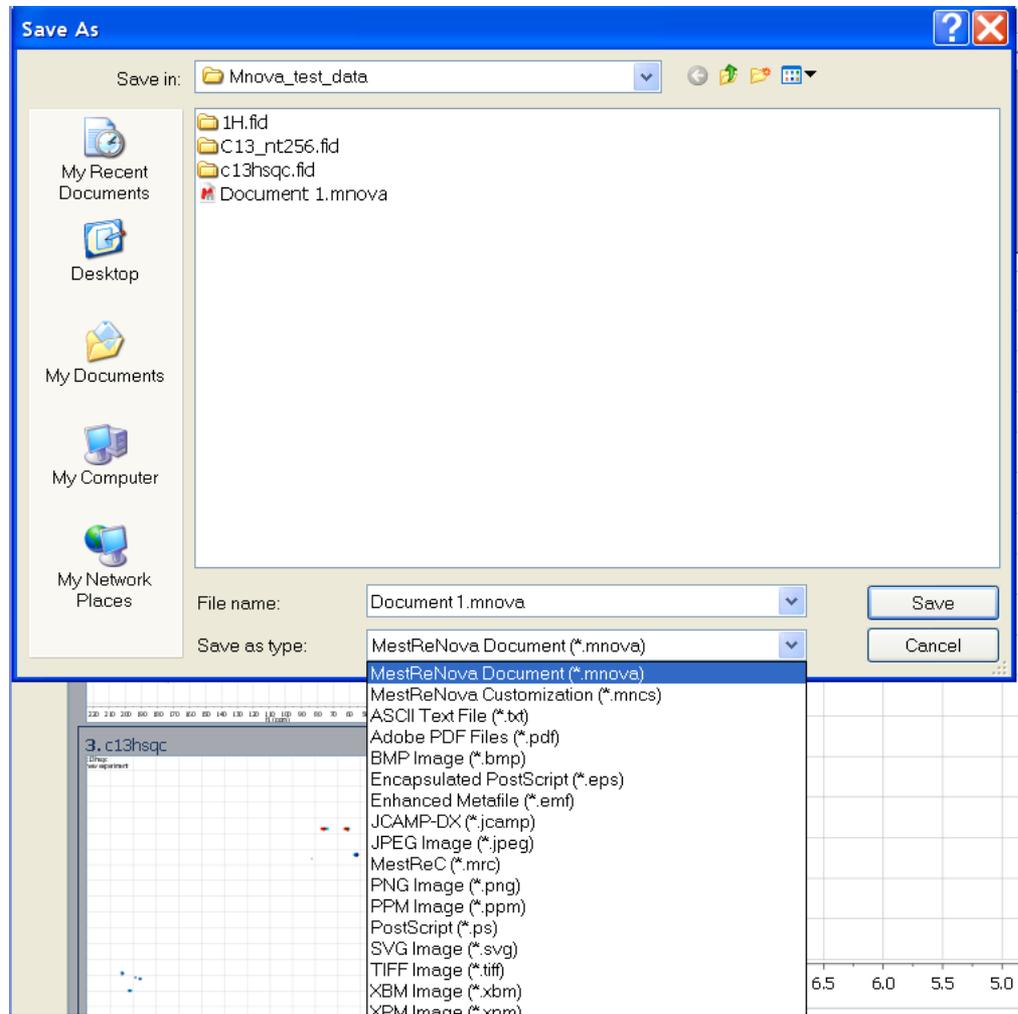
Overlaid on the main window is a red text box with the following text:

**Saved .mnova file retains all data and information.
It can be opened later for further processing.**

At the bottom of the interface, there is a status bar with a color selection dropdown (light gray, black), a font size dropdown (12), and a license indicator.

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

The screenshot displays the MestReNova software interface. The main window shows three NMR spectra panels on the left: 1. ¹H, 2. C13_nt256, and 3. c13hsqc. The central panel displays a 2D c13hsqc spectrum with the title 'c13hsqc new experiment'. An 'Export to PDF' dialog box is open, showing the 'Range' options: 'Current Page', 'Selected Pages', and 'Whole Document' (which is selected). The dialog box has 'OK' and 'Cancel' buttons. The software interface includes a menu bar (File, Edit, View, Processing, Analysis, Advanced, Stack, Predict, Annotate, Scripts, Documents, Help), a toolbar, and a status bar at the bottom with font settings (Arial, size 12) and a license indicator.

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

¹H
nt=8
pw=pw90

RMB click

- Phase Correction >
- Baseline >
- Peak Picking >
- Integration >
- Reference L
- Cut Ctrl+X
- Copy Ctrl+C
- Paste Ctrl+V
- Delete Del
- Select All Ctrl+A
- Alignment >
- Properties...**
- Customize Context Menus...

Properties

Geometry NMR Spectrum

General

- Title
- Grid
- 1D
- Scales
 - Horizontal
 - Vertical
- Peaks
- Integrals
 - Multiplets
 - Integrals
- Fitting
- Assignments

Background

Color:

Opacity: 0 %

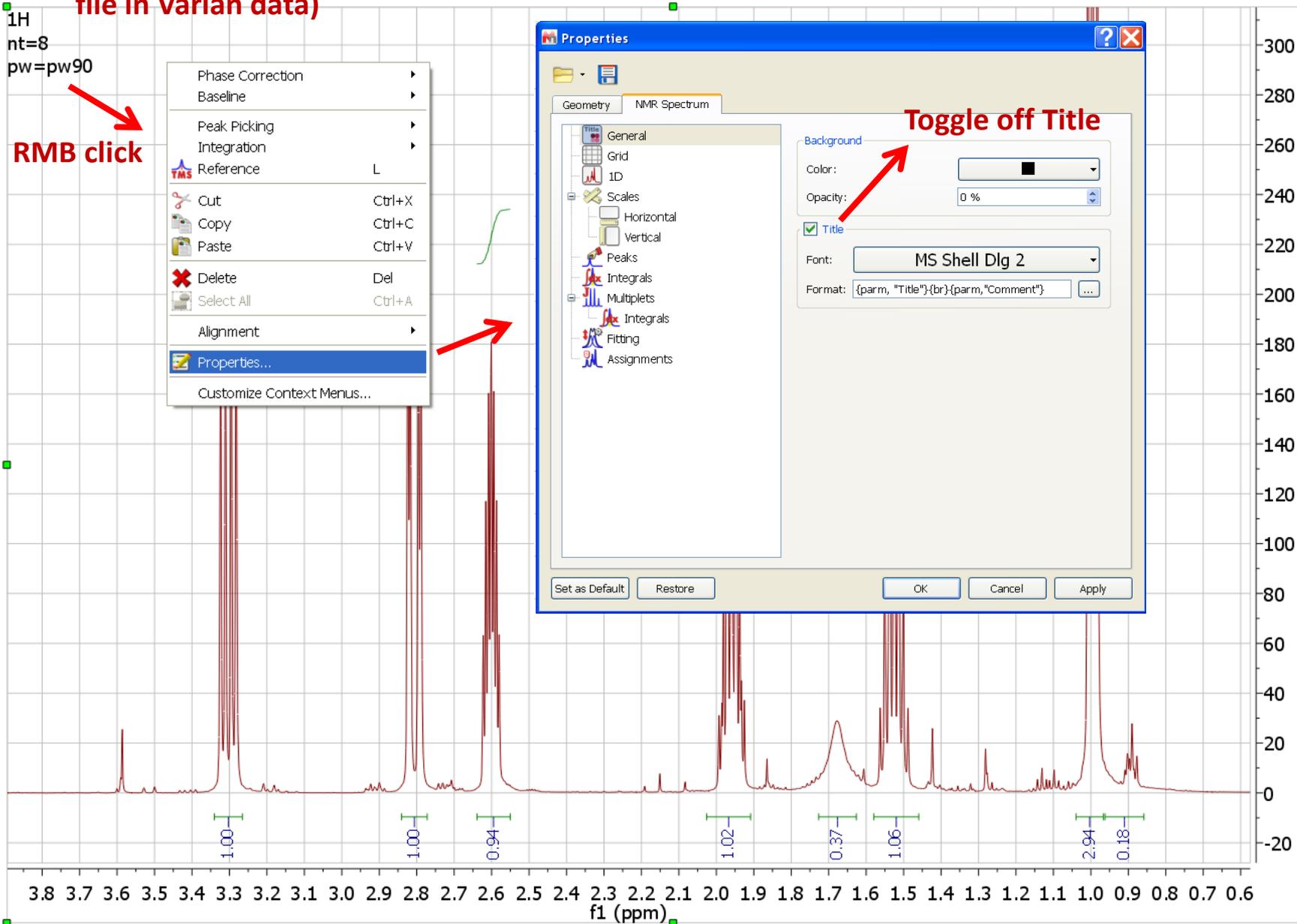
Title

Font: MS Shell Dlg 2

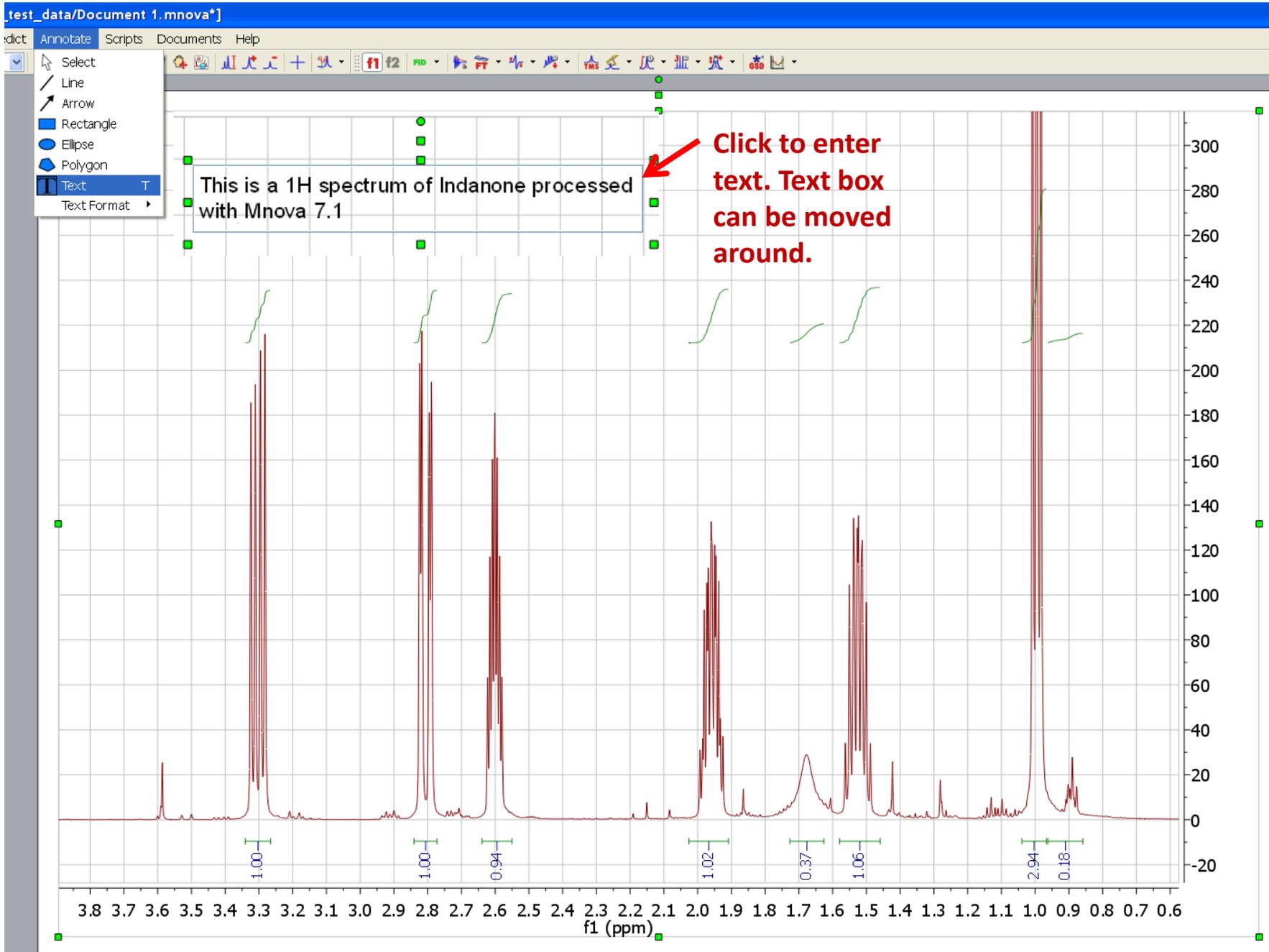
Format: {parm, "Title"}{br/>{parm, "Comment"} ...

Set as Default Restore OK Cancel Apply

Toggle off Title



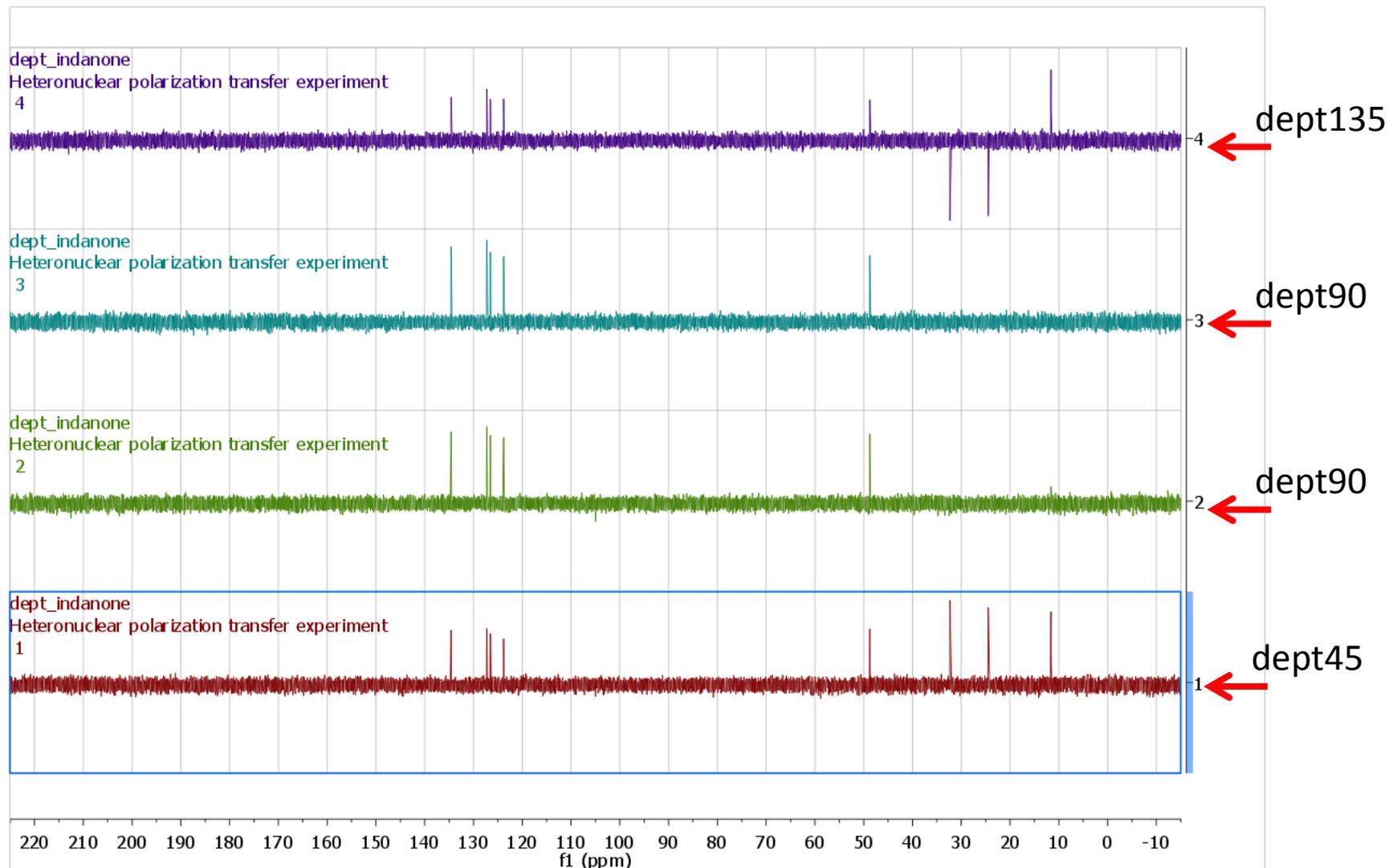
To annotate spectrum



Process Arrayed Experiment: DEPT

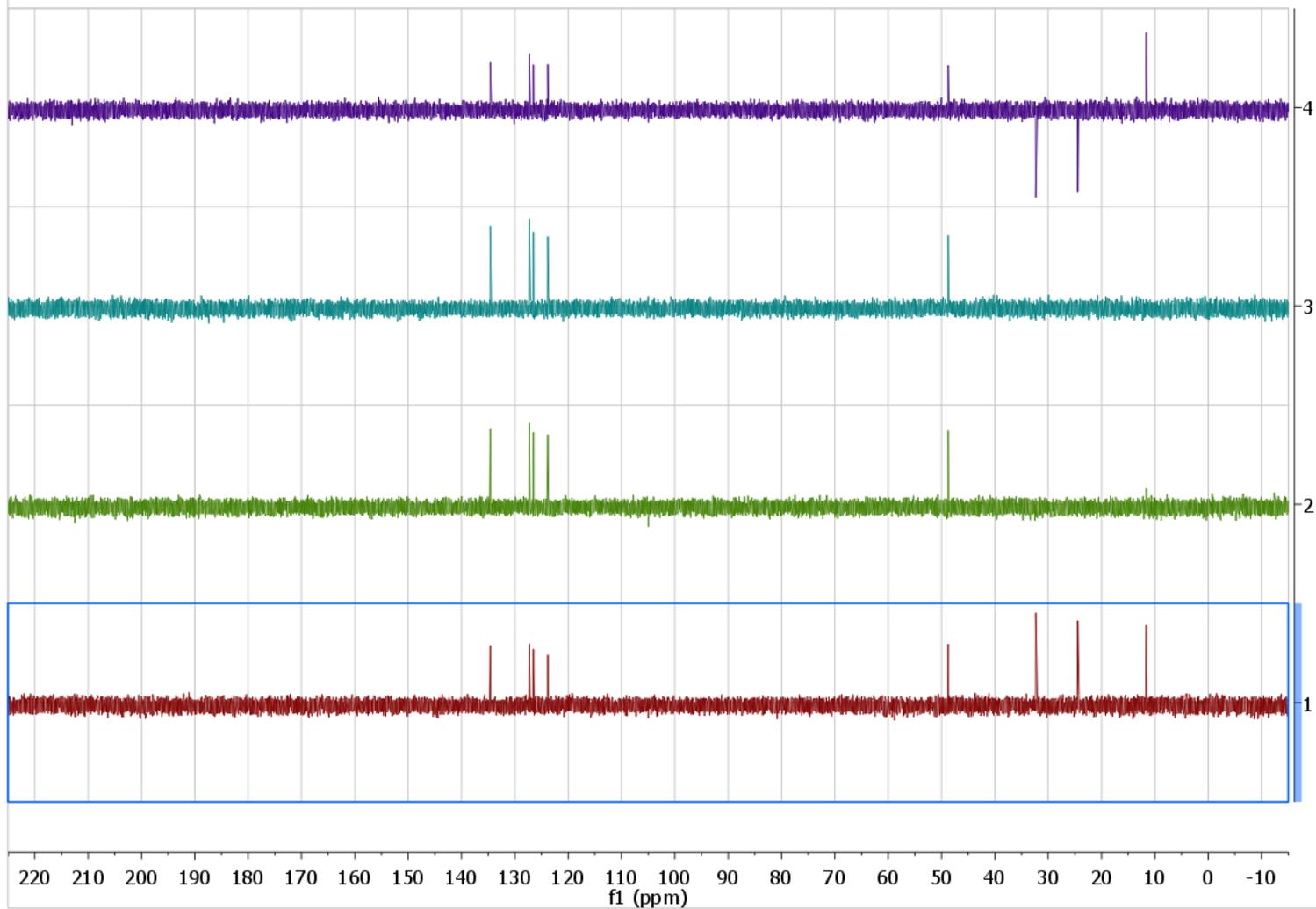
Drag & drop to load/autoprocess data

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

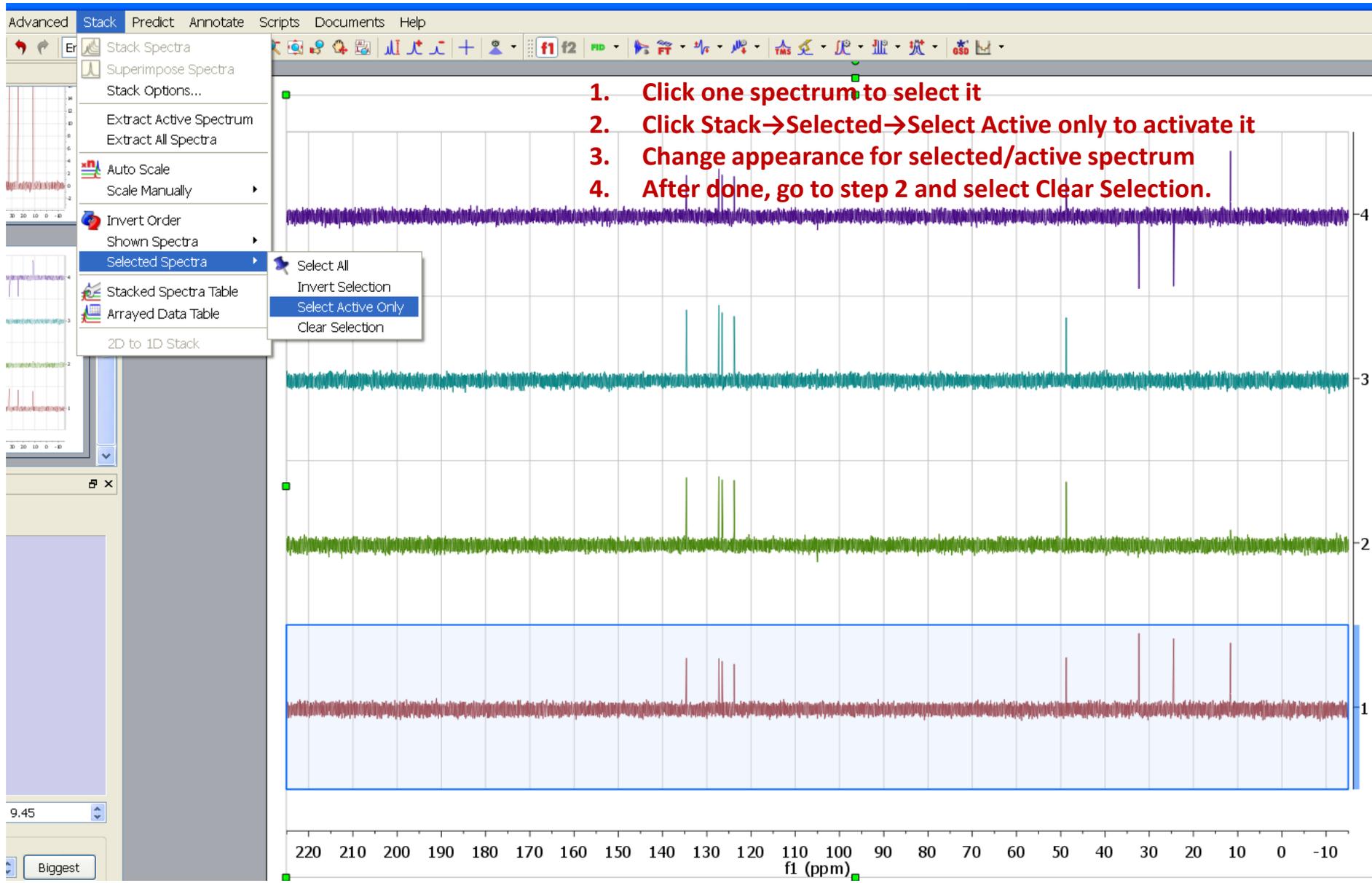


See Facility website: <http://nmr.chem.ucsb.edu/protocols/DEPT.html> for more details

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

Pages

5. dept

- Select active spectrum to display single spectrum (boxed with blue line)
- Select stacked to display stacked spectra array

Active Spectrum

Stacked

Whitewash Stacked

Superimposed

Bitmap

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

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

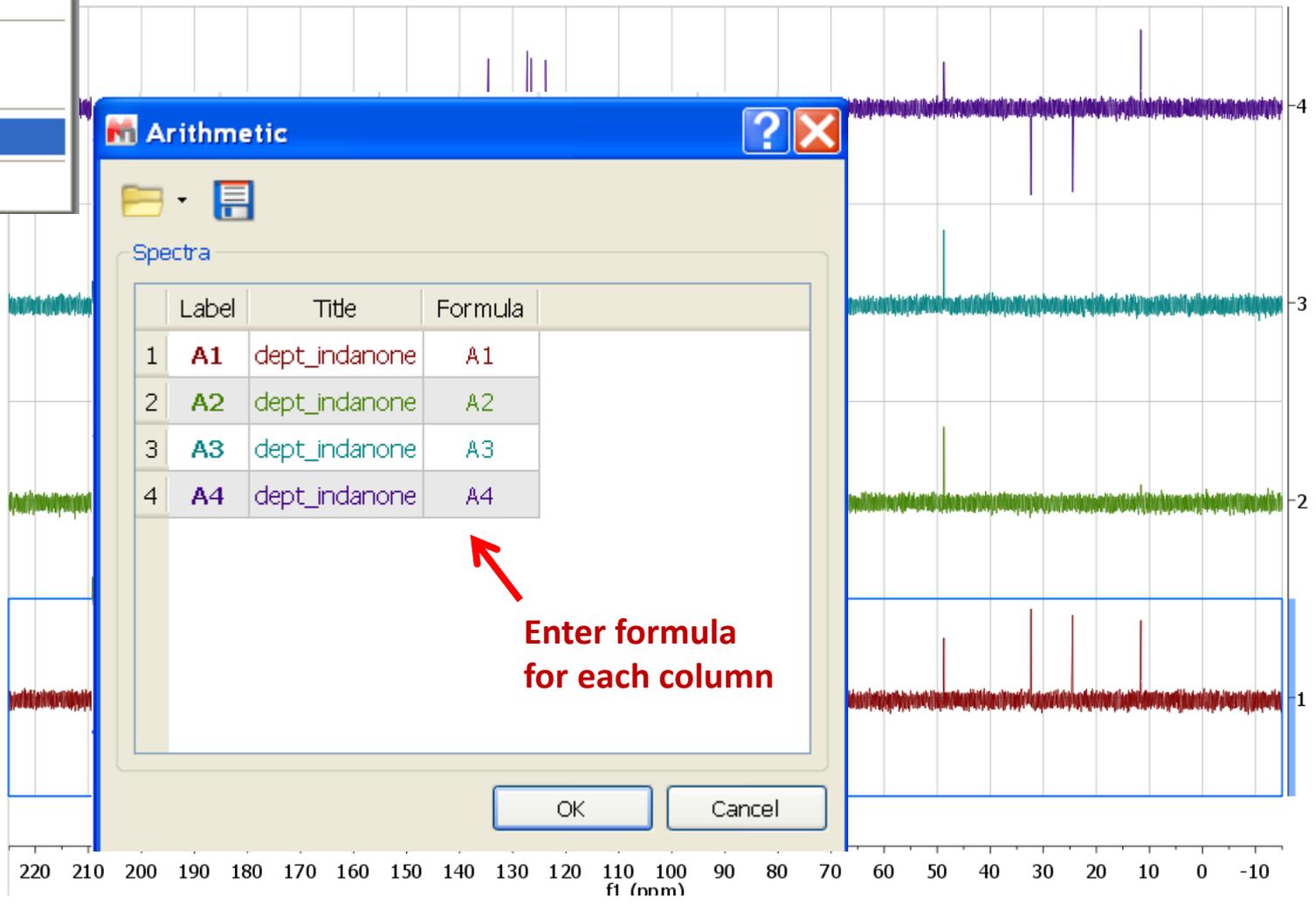
light gray black

A black Arial 12

Licenses: !

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

- Advanced
- Stack
- Predict
- Anr
- Line Fitting
- Bayesian DOSY Transform...
- Data Analysis...
- Align Spectra
- Reference Alignment
- J-Correlator...
- Filter False Positives
- Arithmetic...
- Spin Simulation...



Arithmetic

Spectra

	Label	Title	Formula
1	A1	dept_indanone	A1
2	A2	dept_indanone	A2
3	A3	dept_indanone	A3
4	A4	dept_indanone	A4

OK Cancel

Enter formula
for each column

Re-processed Varian DEPT Data

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

Save formula for future use

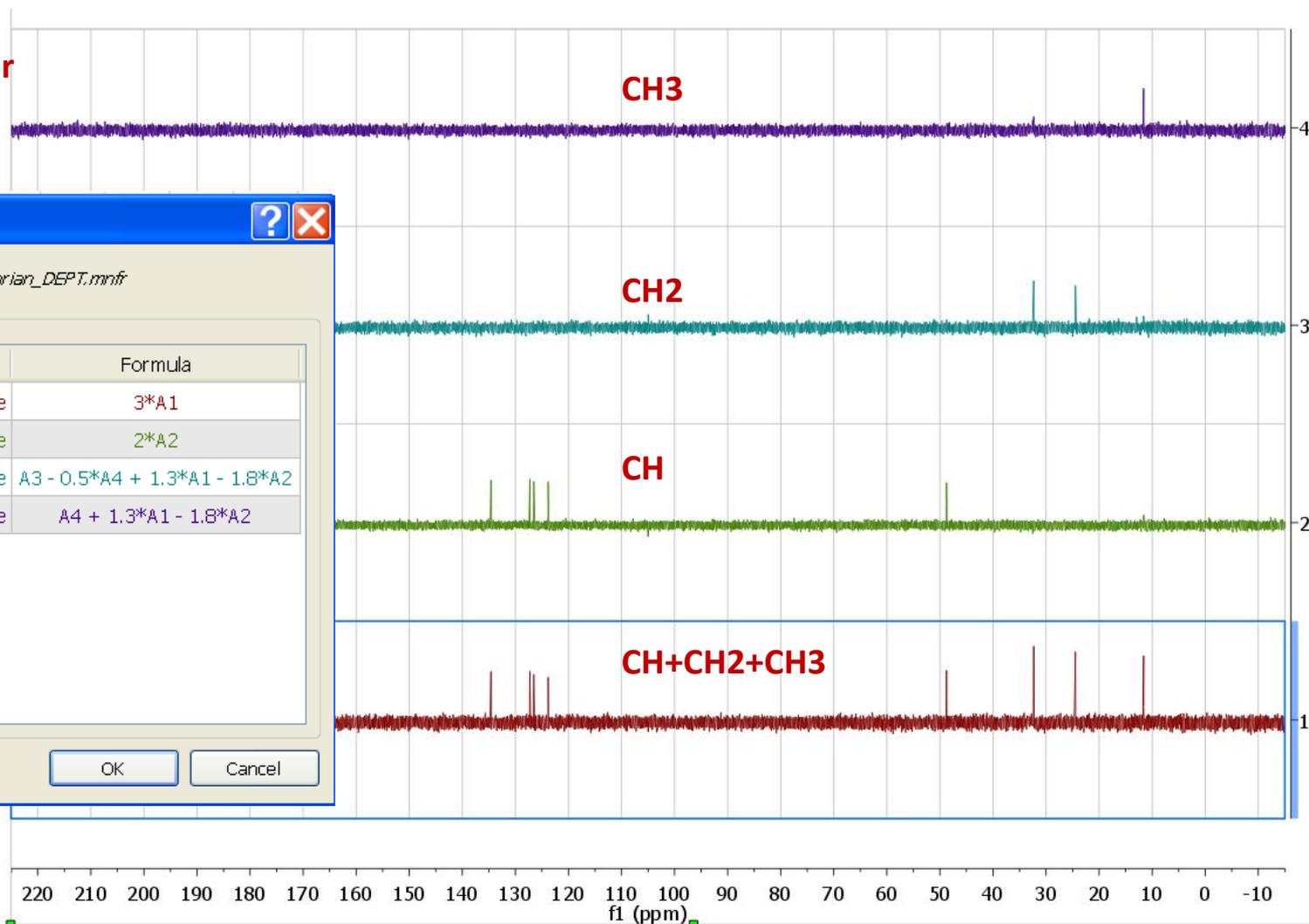
Arithmetic

Filename: *Varian_DEPT.mnfr*

Spectra

	Label	Title	Formula
1	A1	dept_indanone	3*A1
2	A2	dept_indanone	2*A2
3	A3	dept_indanone	A3 - 0.5*A4 + 1.3*A1 - 1.8*A2
4	A4	dept_indanone	A4 + 1.3*A1 - 1.8*A2

OK Cancel



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

Superimposition of Several Spectra

The screenshot displays the MestReNova software interface. The 'Stack Spectra' menu is open, showing options such as 'Superimpose Spectra', 'Stack Options...', 'Extract Active Spectrum', 'Extract All Spectra', 'Auto Scale', 'Scale Manually', 'Invert Order', 'Shown Spectra', 'Selected Spectra', 'Stacked Spectra Table', 'Arrayed Data Table', and '2D to 1D Stack'. A red arrow points to the 'Superimpose Spectra' option. The main plot area shows a 1D NMR spectrum with a large peak at approximately 125 ppm. The x-axis is labeled 'f1 (ppm)' and ranges from 230 to -50. The y-axis ranges from -5000 to 55000. A red text overlay reads 'Click Superimpose Spectra'. In the background, two other spectra are visible, labeled '7. Mnova_Test_data/CHO_C13.fid' and '8. Mnova_Test_data/C13_C13.fid'. A red text overlay reads 'Hold Shift Key and select multiple spectra' with a red arrow pointing to the '8. Mnova_Test_data/C13_C13.fid' file name. The software title bar reads 'MestReNova - [Document 1*]'. The bottom status bar shows 'Superimpose Selected Spectra' and 'Licenses: !'.

Hold Shift Key and select multiple spectra

Click Superimpose Spectra

7. Mnova_Test_data/CHO_C13.fid

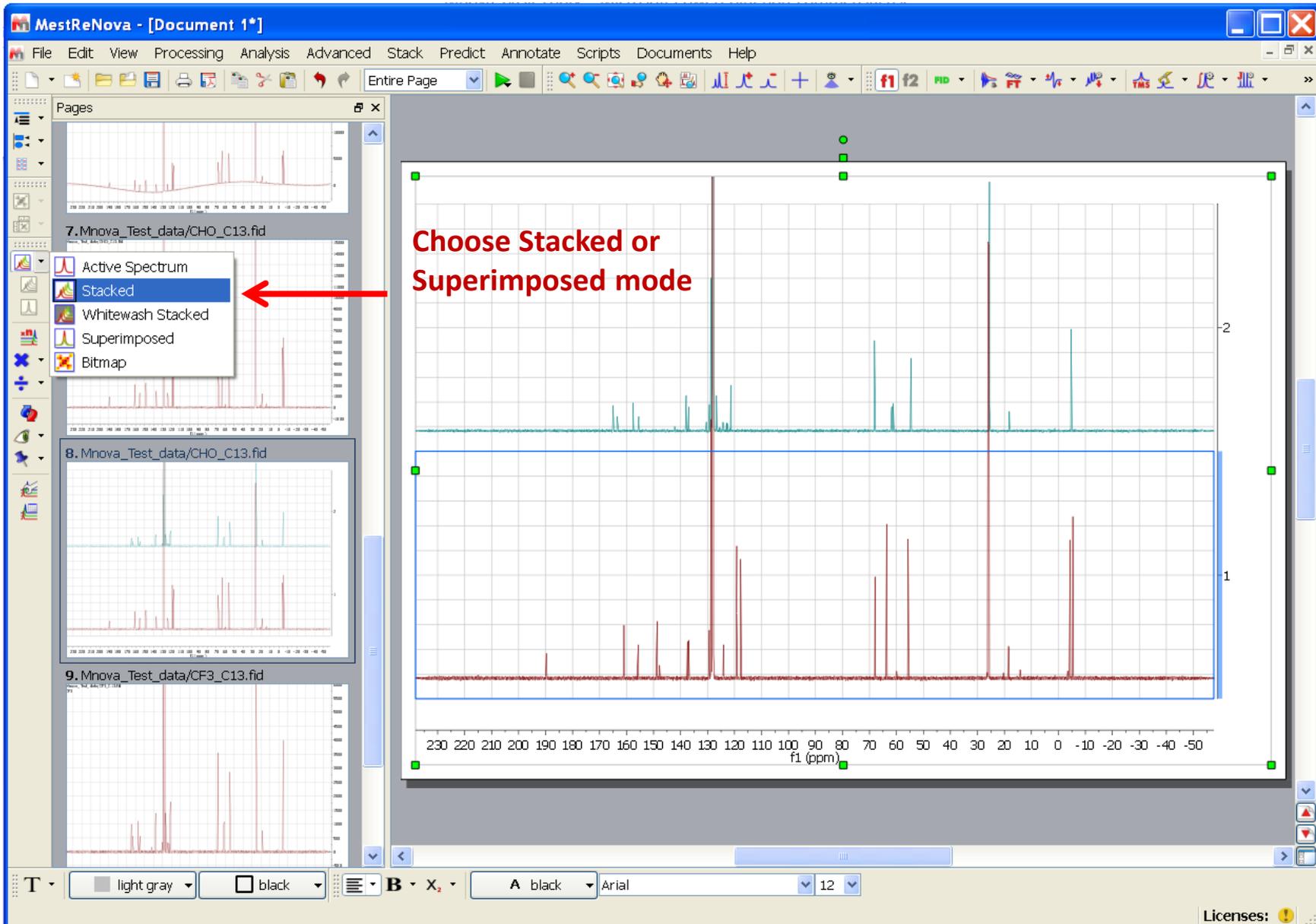
8. Mnova_Test_data/C13_C13.fid

9.

light gray black

B X₂ A black Arial 12

Superimpose Selected Spectra Licenses: !



Choose Stacked or Superimposed mode

