Using Mnova to Process and Analyze NMR on Your Desktop

Version 6.1 and 6.2

Sept. 2010

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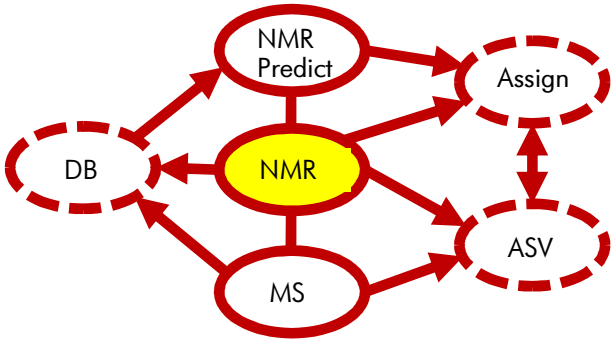
Contents

- Use **Mnova NMR** to
  - Open and transform your NMR data
  - Process, analyze and report a ^{1}H spectrum
- Use **Mnova NMRPredict Desktop** to
  - Predict ^{1}H and ^{13}C and verify your structure
  - Assign peaks



Mnova: An integrated system for analytical chemistry

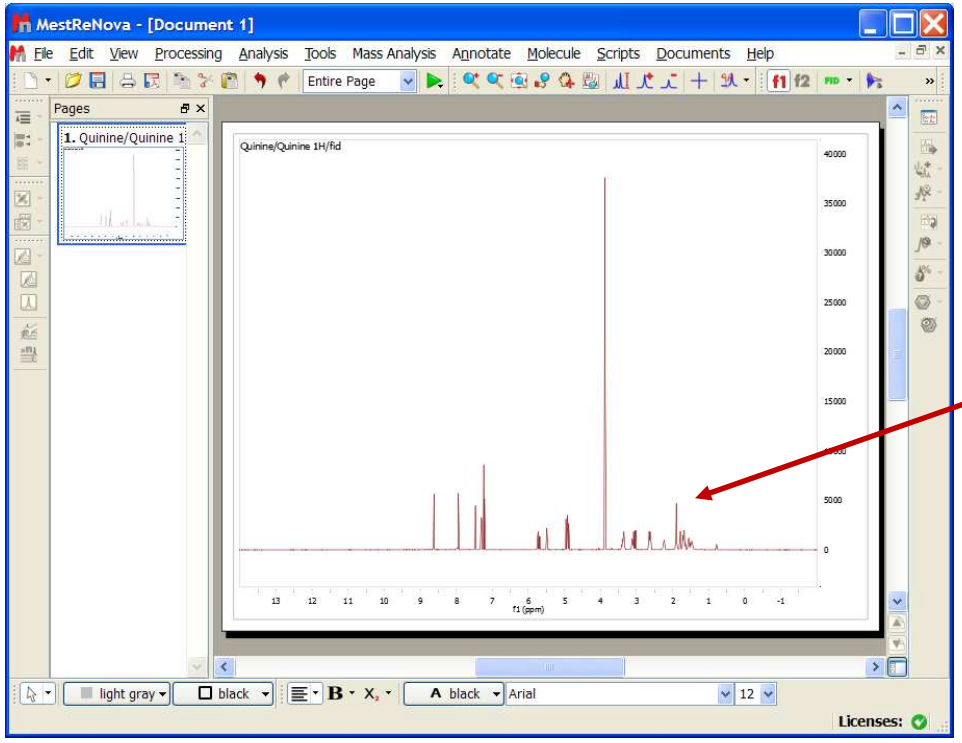
Mnova NMR

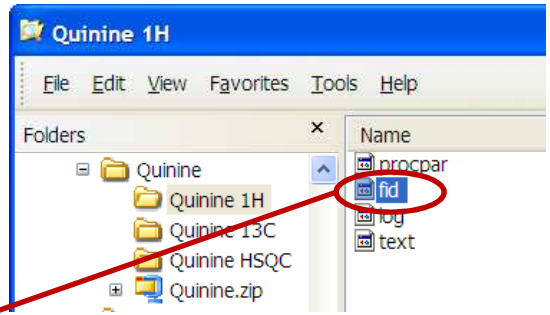
- Quickly process and analyze 1D NMR, and report your chemical shifts and J-couplings in journal format
- Process, analyze and assign multiple 2D spectra together with 1D*
- Advanced tools for automation, quantitation, reaction monitoring, diffusion & relaxation studies*
- Mnova NMR license required

Those features are not illustrated in this tutorial. See Mnova **Help > Contents for more details*

To open and transform your NMR data

- Choose **File | Open** to open the **fid** file
- Or drag an **fid** file from Windows Explorer to Mnova *
- Mnova automatically transforms the raw file into frequency domain (*including Windowing function, Fourier transform, phase correction etc)* **





Drag & drop

You can drag **multiple folders that contain **fid** (or **ser**) to Mnova to open multiple spectra simultaneously.*

***Parameters from the raw data are used for processing. You can view or change the processing parameters by choosing **Processing | Processing Parameters.** See **Help > Contents > Processing Basics** for more details*

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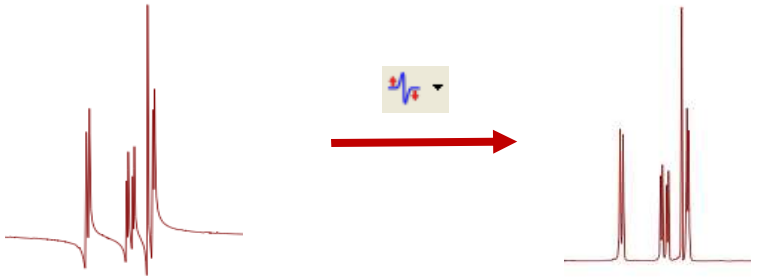
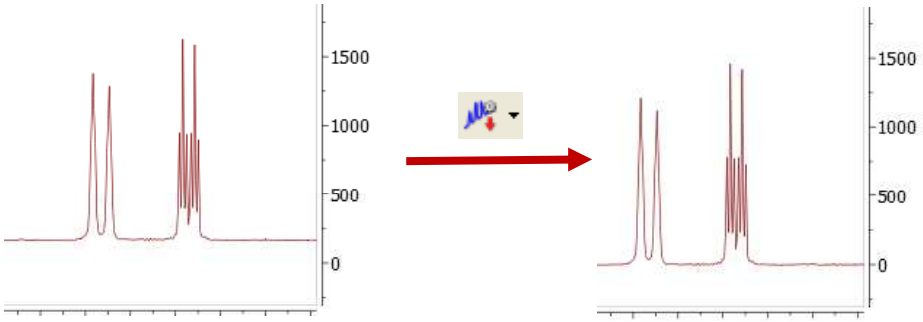
To correct phasing, baseline & reference

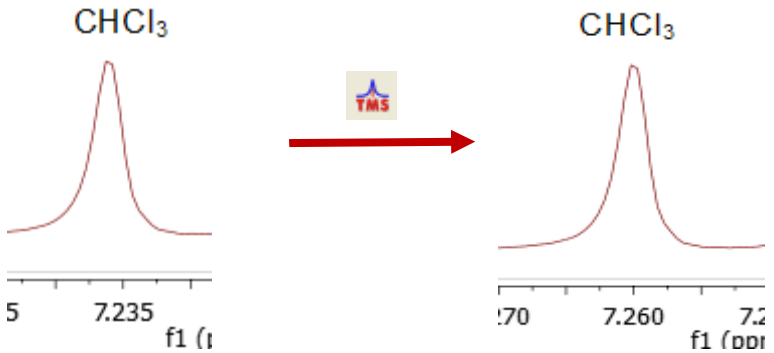
- Click  for **phase correction** if peaks are not symmetric*



- Click  for **baseline correction** if baseline is not zero *



- Click  to calibrate the **chemical shift reference** if the solvent or TMS peak is not at the right ppm



**Click the arrow next to the tool icon for options.*

*See **Help > Contents > Processing Basics** for more details*

To visualize your spectrum

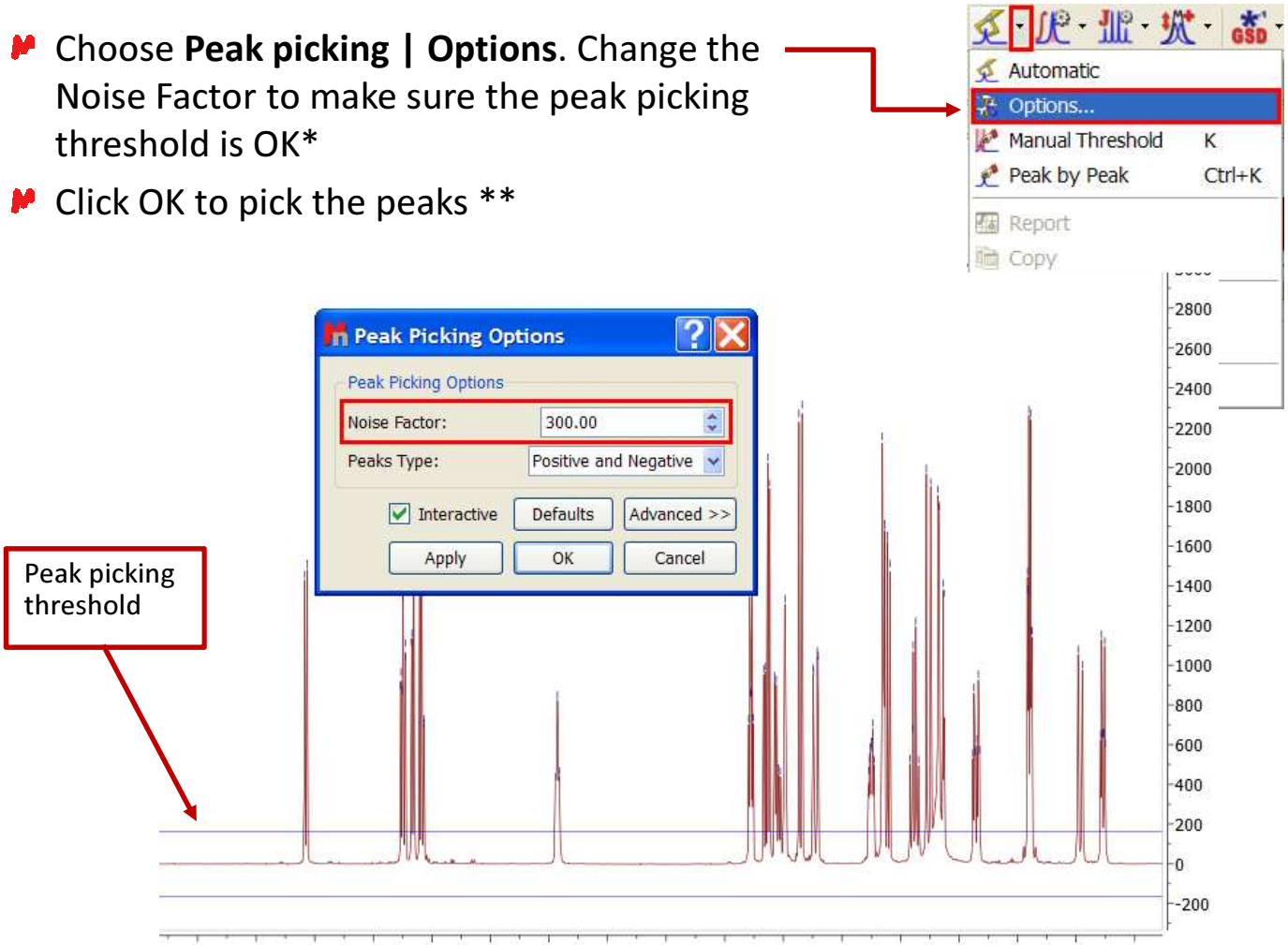
- Zoom in/Zoom out (or press Z) *
- Full spectrum (or press F)
- Manual Zoom in to defined ppm range
- Pan spectrum (or press P)**
- Expansion – click&drag to draw an inlet (or press E)
- Fit to Height (or press H)
- Increase/Decrease Intensity (or move mouse wheel)
- Crosshair Cursor (or press C) for measuring *J*-couplings
- Cut (or press X) to hide parts of the spectrum

**Press Z several times to toggle between horizontal/vertical/box zoom*

*** Press P several times to toggle between free/horizontal/vertical panning*

To analyze multiplets manually (1)

- Choose **Peak picking | Options**. Change the Noise Factor to make sure the peak picking threshold is OK*
- Click OK to pick the peaks **

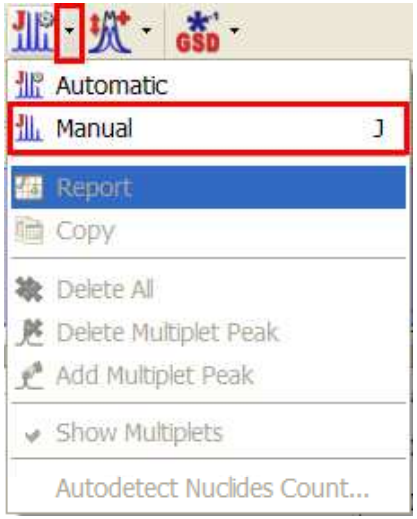


** The threshold is determined by multiplying the automatically calculated Noise Level by the Noise Factor you enter.*

*** It is OK if some unwanted peaks are picked, or some real peaks are missing. In the later steps you can add or delete peaks for multiplets.*

To analyze multiplets manually (2)

- Choose **View | Full View** to show the Full View window.
- Zoom into one or more multiplets
- Press **J** to switch to Manual Multiplet mode
- Click and drag to include peaks for a multiplet
- Double click on the multiplet label to open the **Multiplet Manager Panel** (see next slide)



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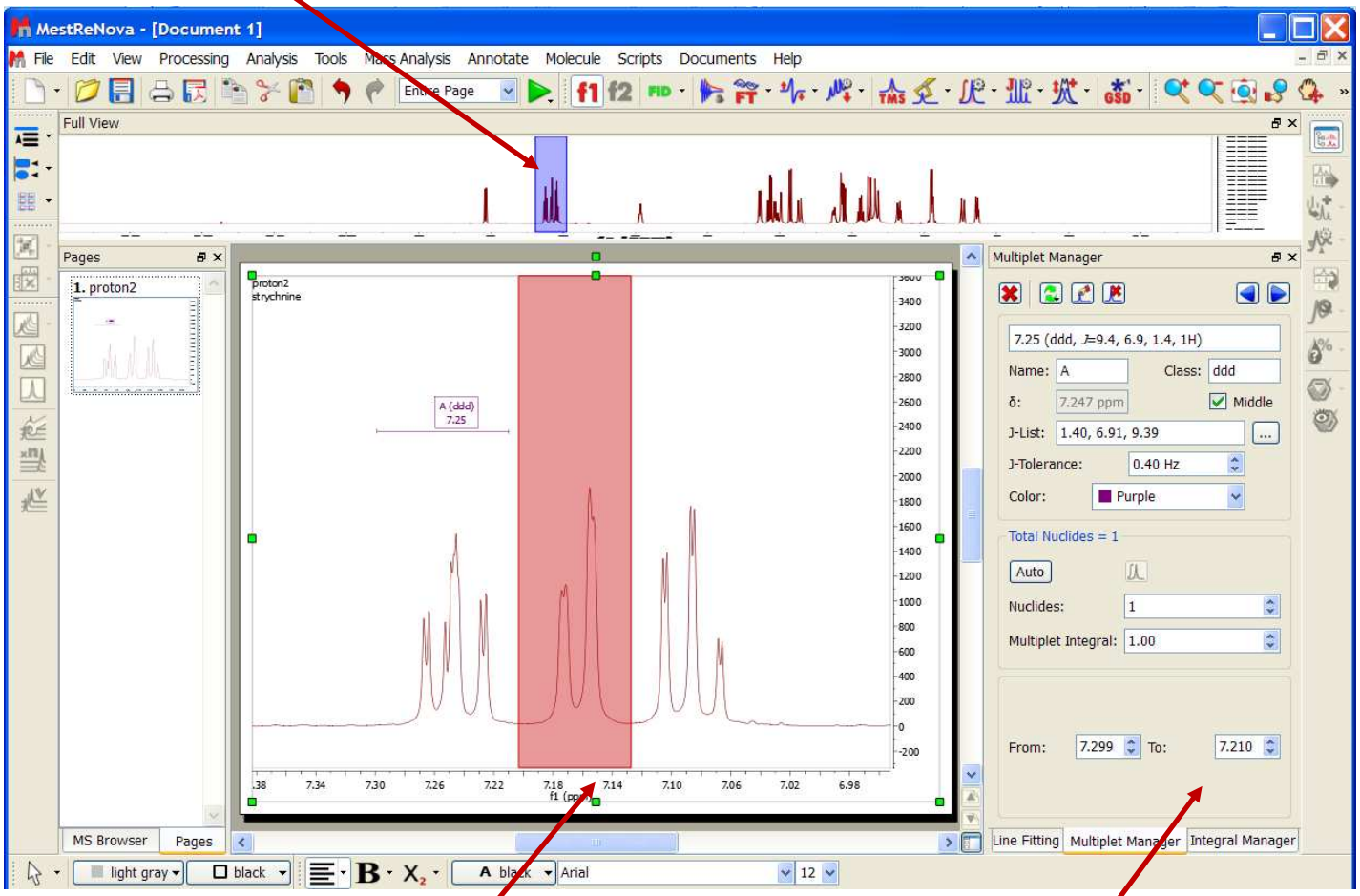
To analyze multiplets manually (3)

Full View: The whole spectrum and zoom-in area.
Drag the blue box to move to other multiplets

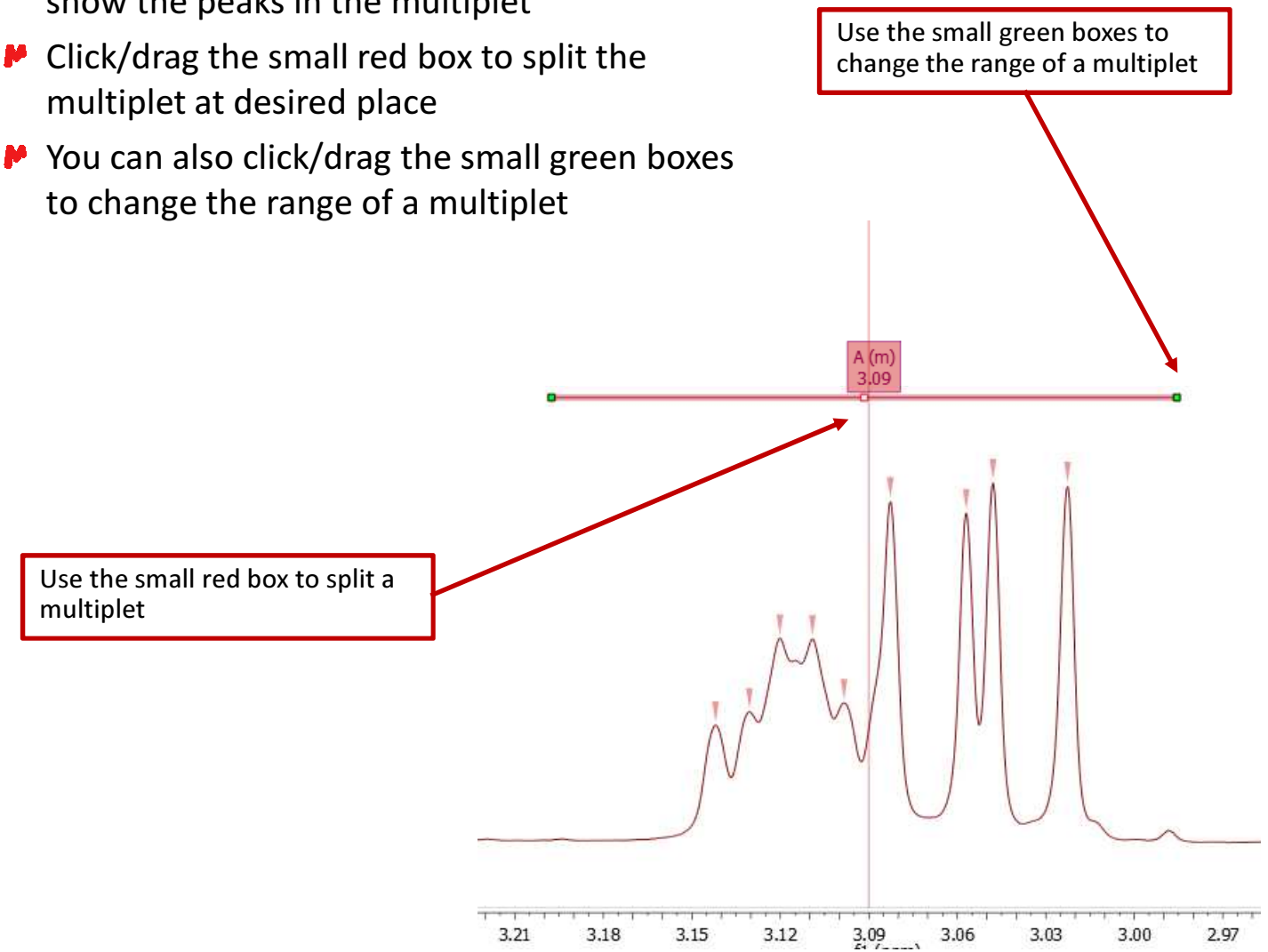


Manual multiplet analysis: Click **J**, then click and drag to define a multiplet

Multiplet Manager shows the properties of the current multiplet

To edit multiplet results (1)

- Hover the cursor on the multiplet label to show the peaks in the multiplet
- Click/drag the small red box to split the multiplet at desired place
- You can also click/drag the small green boxes to change the range of a multiplet



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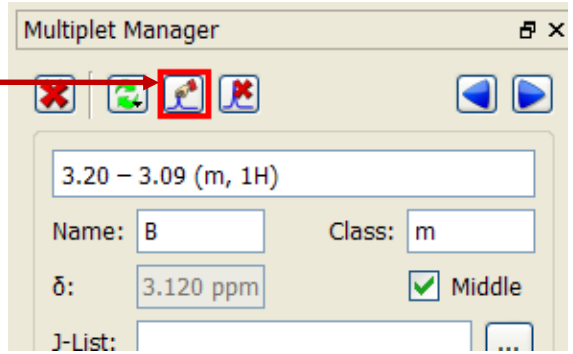
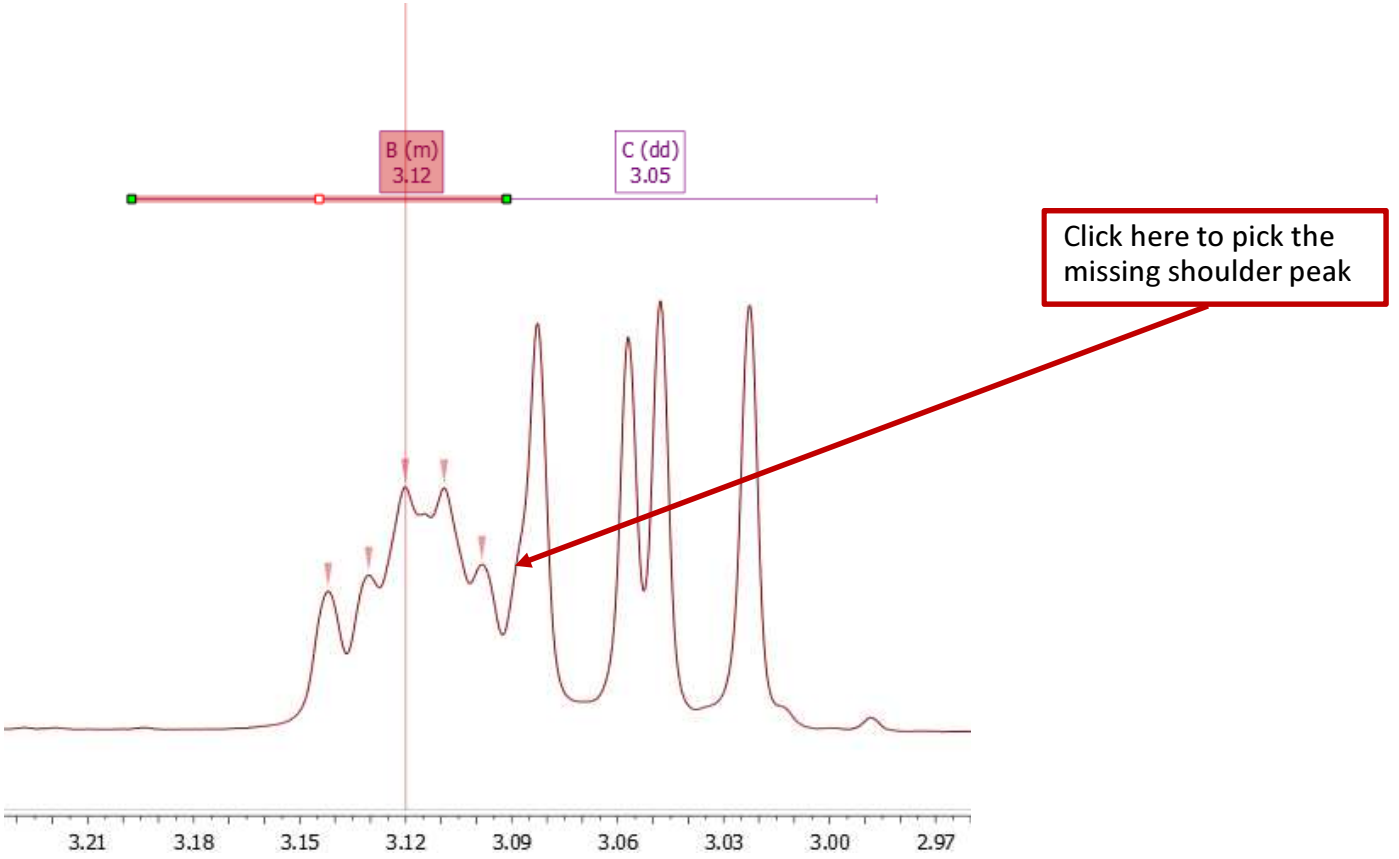
To edit multiplet results (2)

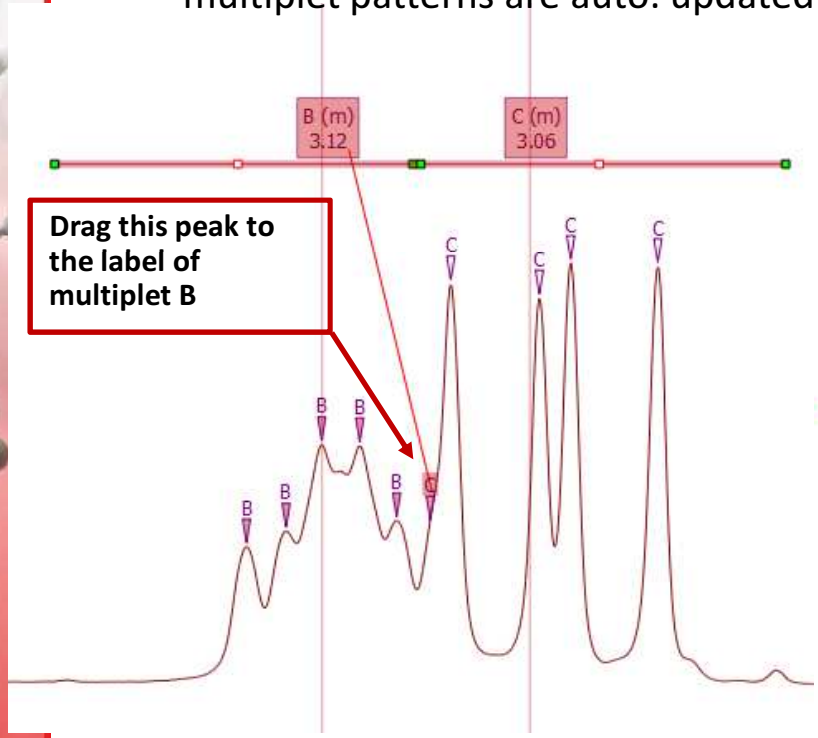
- Select the Add Multiplet Peak tool
- Click SHIFT key once to switch to free peak picking mode
- Click on the shoulder peak at around 3.09 ppm

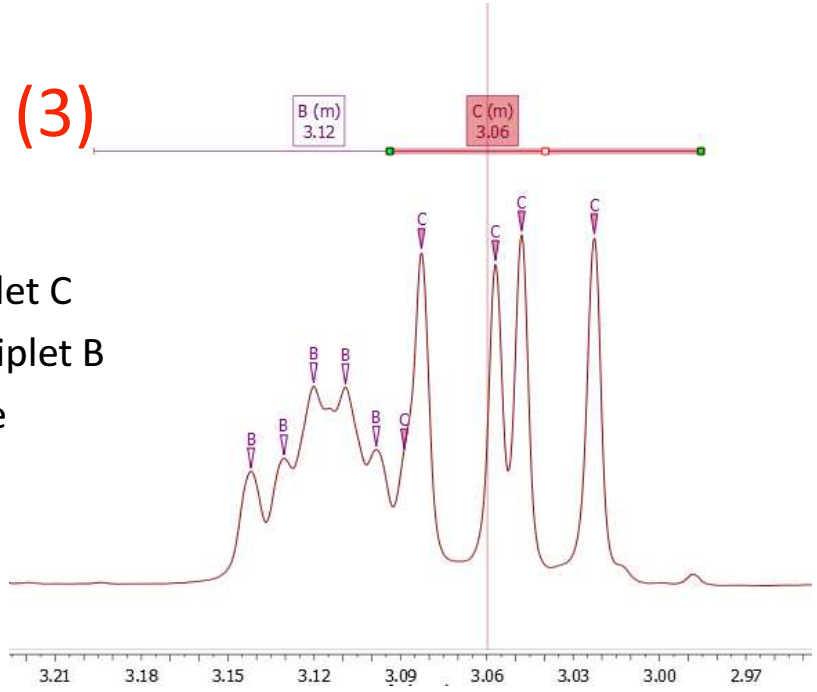


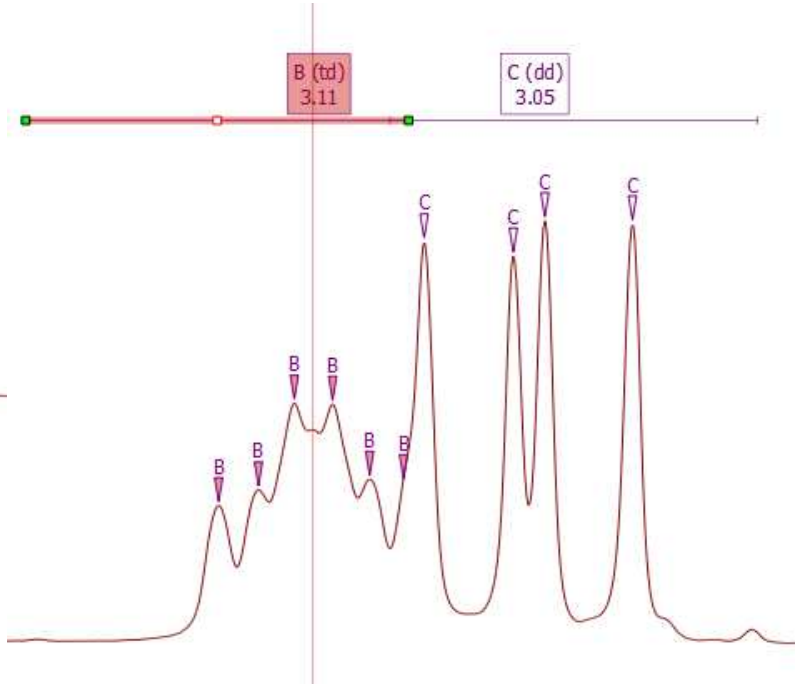


To edit multiplet results (3)

- The new peak is added to multiplet C because it falls in the range of multiplet C
- Click on that peak and drag it to multiplet B
- It belongs to multiplet B now, and the multiplet patterns are auto. updated







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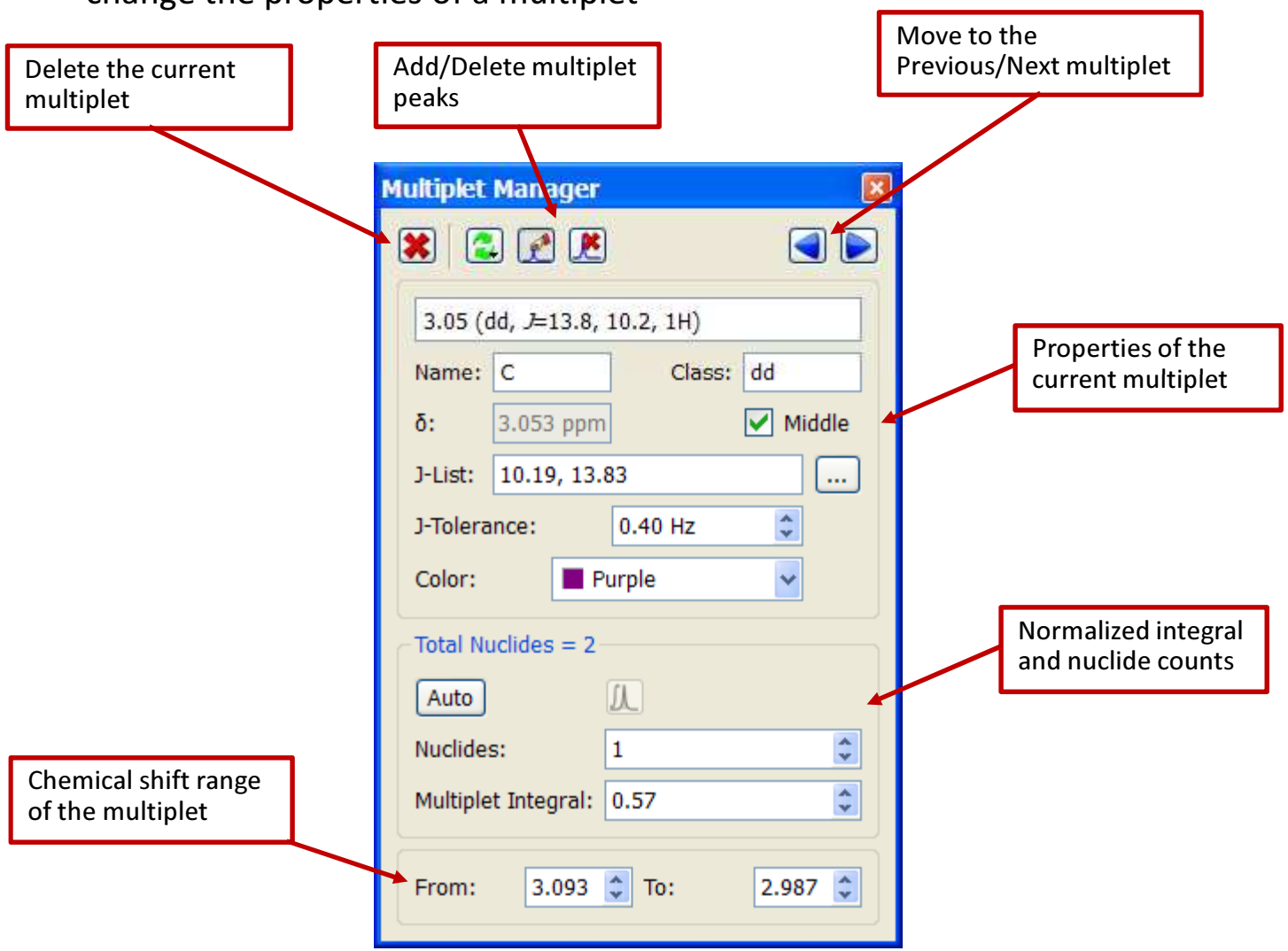
NMR Solutions

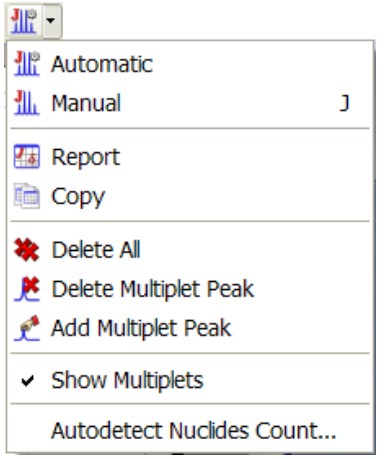
To edit multiplet results (4)

- Use the Multiplet Manager to inspect and change the properties of a multiplet



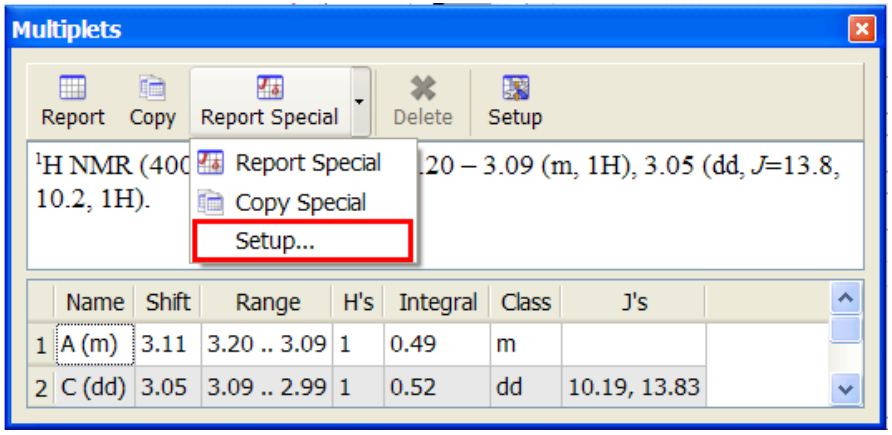
To report multiplets

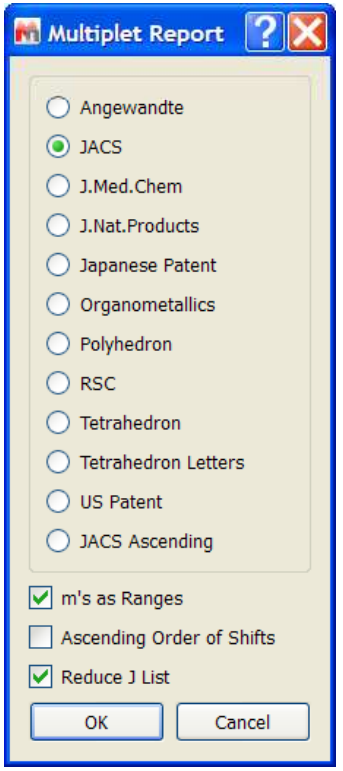
- Click **Multiplet Analysis | Report** to report the results in a journal format:



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.5 Hz, 1H), 7.95 (d, *J* = 9.2 Hz, 1H), 7.46 (d, *J* = 4.5 Hz, 1H), 7.30 (dd, *J* = 9.2, 2.7 Hz, 1H), 7.21 (d, *J* = 2.7 Hz, 1H), 5.80 – 5.66 (m, 1H), 5.48 (d, *J* = 4.1 Hz, 1H), 4.92 (ddt, *J* = 13.3, 10.3, 1.4 Hz, 2H), 3.87 (s, 3H), 3.46 – 3.27 (m, 2H), 3.18 – 3.00 (m, 2H), 2.63 (ddd, *J* = 12.6, 7.1, 3.9 Hz, 2H), 2.32 – 2.08 (m, 1H), 1.90 (s, 2H), 1.83 – 1.63 (m, 3H), 1.51 (dddd, *J* = 12.4, 7.3, 5.7, 2.5 Hz, 2H).

- To change journal format: choose **View | Tables | Multiplets** to display the Multiplets Table. Click **Report Special Options > Setup ***

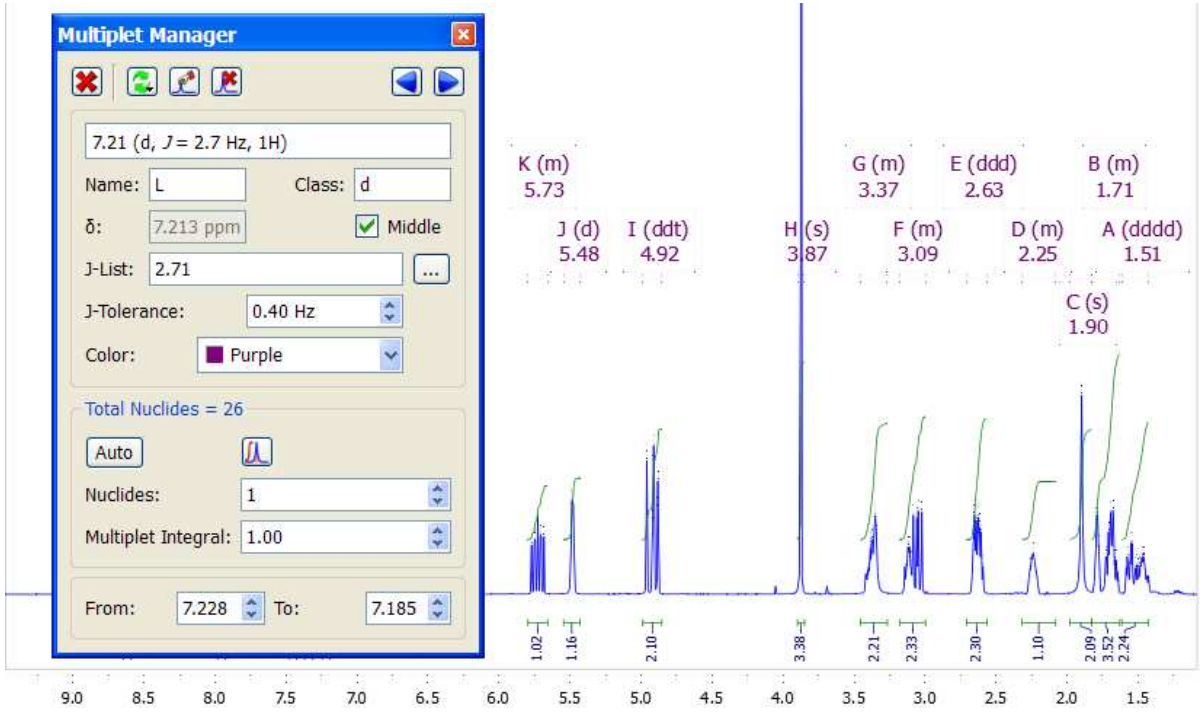




**The Multiplet Report dialog is from Mnova 6.2. Older versions have fewer options*

Other ways of multiplets analysis

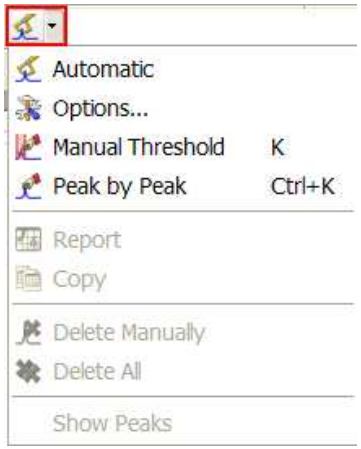
- 1st: Do peak picking. Clean up the peaks
- 2nd: Do integration. Clean up the integrals
- 3rd: Do auto. multiplet analysis for the whole spectrum using the picked peaks and integrals
- Finally edit and report the multiplet results as described in the previous slides



MESTRELAB RESEARCH
NMR Solutions

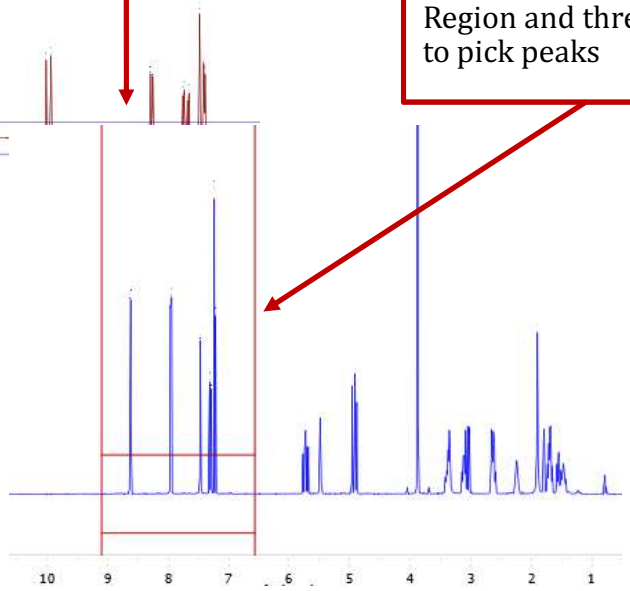
To pick peaks

- Click  to do **auto peak picking**.
  If results are not good, click
  Options to change the threshold:*



Threshold for picking positive and negative peaks

Region and threshold to pick peaks



- Or choose **Manual Threshold** (or press **K**), click&drag to define the region and threshold to pick peaks

- Choose **Peak by Peak** (or press **Ctrl+K**) to pick one peak at a time**

** Threshold is the (auto estimated) noise level multiplied by the Noise Factor (user-defined).*

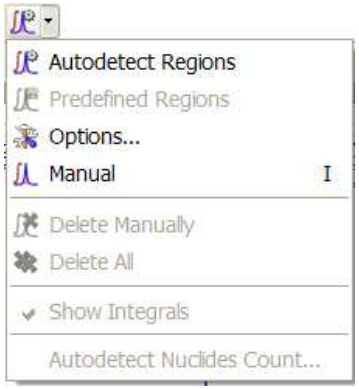
*** By default, Mnova automatically locates the peak tops. Press **Shift** key to turn it off when picking shoulder peaks.*

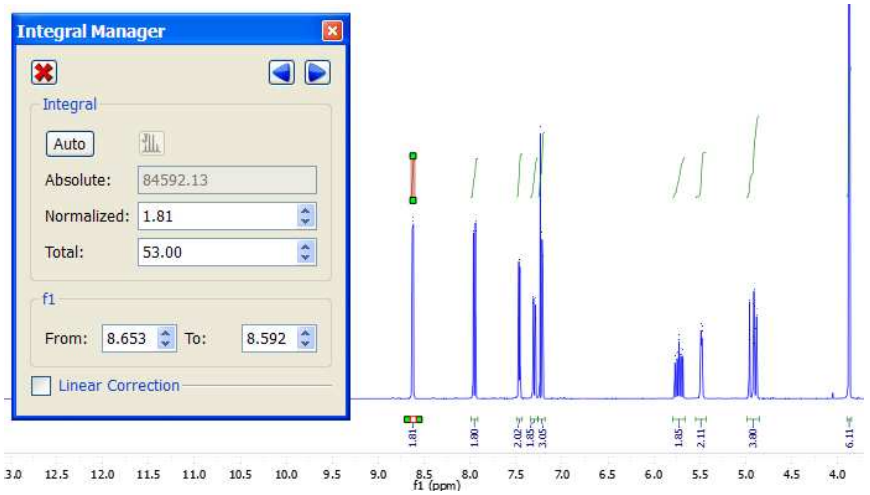
*Tip: Choose **Edit | Properties** to change the way to display peaks*

MESTRELAB RESEARCH
NMR Solutions

To integrate peaks

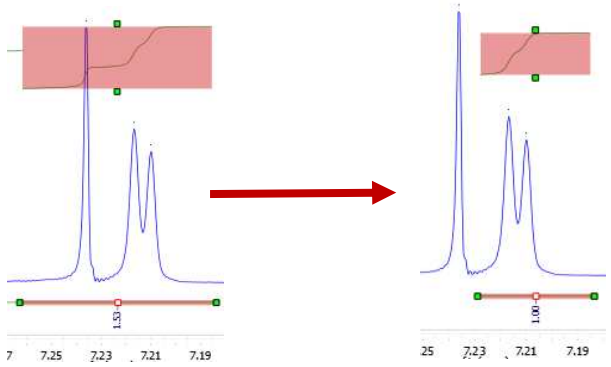
- Click  to do auto integration
- Double click on an integral curve to popup Integral Manager:





- Type a Normalized value to normalize the integrals
- Browse, delete, change, split integrals interactively if needed

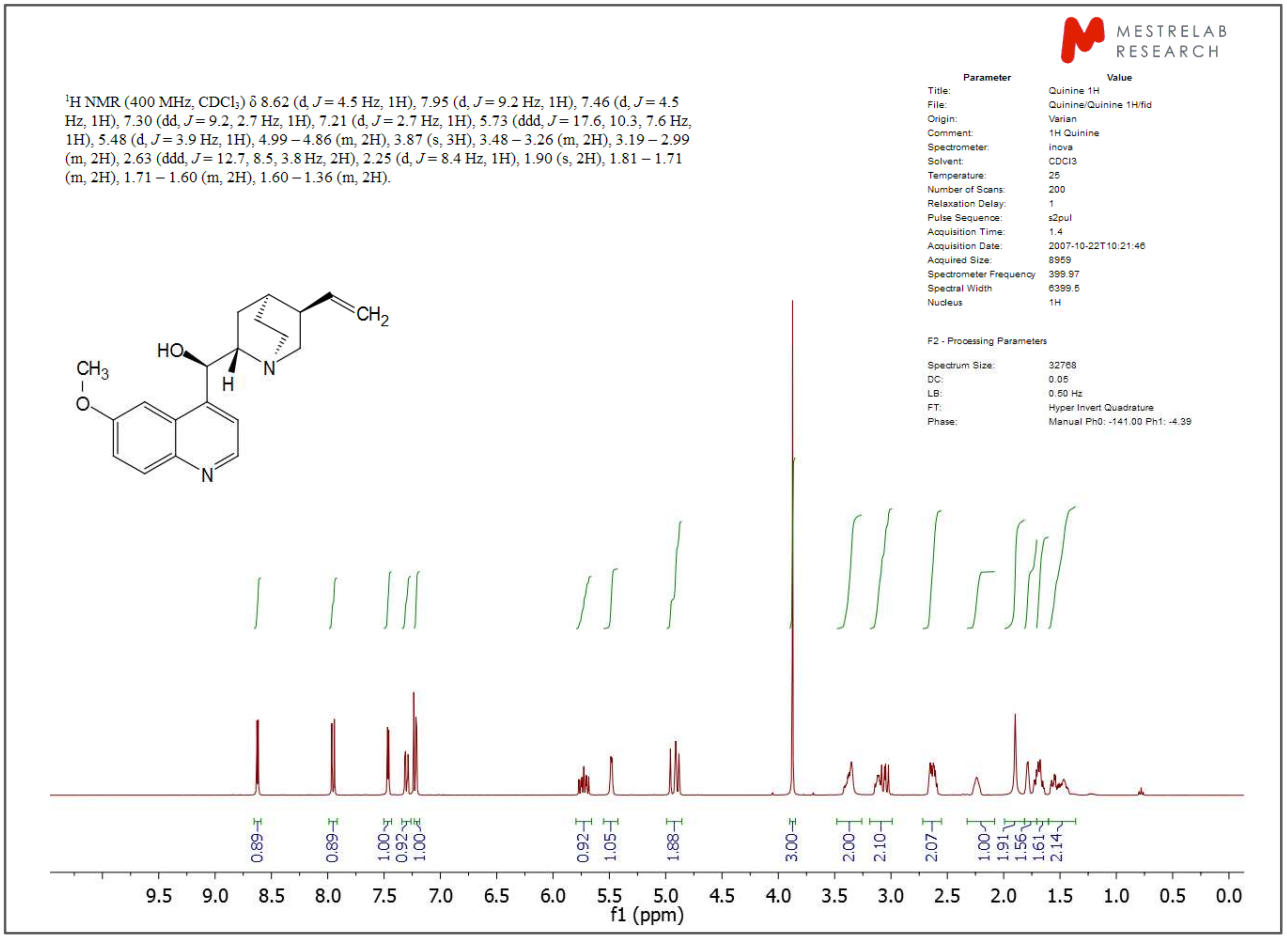
Click and drag the left green box to change the range of the integral



Tip: You can click and drag an integral curve to move them up or down, and change their sizes.
*See **Help > Contents > Analysis tools > Integration** for more details.*

To report using the **R** script*

- Choose **Scripts | R** to report in a predefined format
- Click  to generate PDF, or copy/paste all objects to your documents

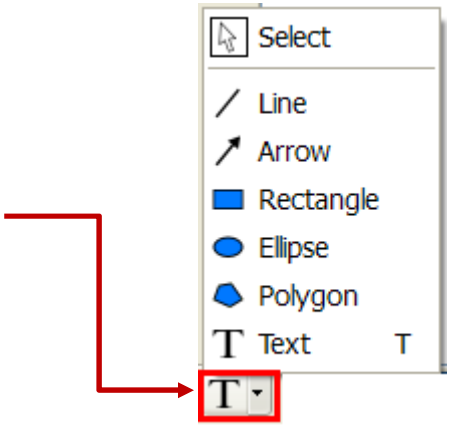


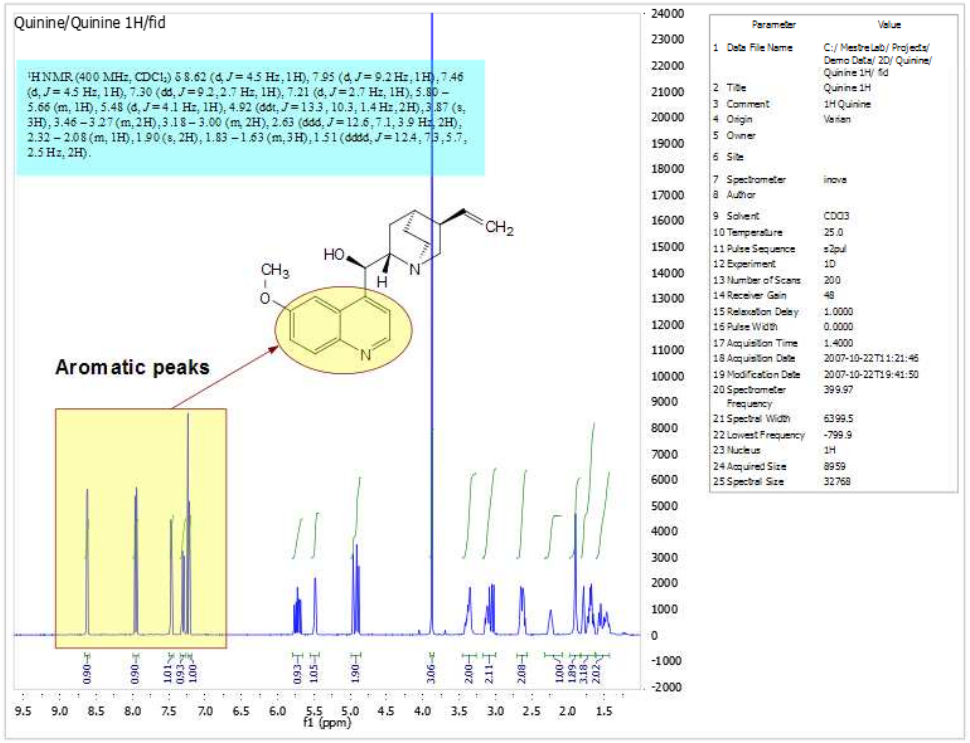
** You need to install R script. Write to sales@mestrelab.com for details.*

*Tip: You can copy a **molecule** from ChemDraw, Isis/Draw or ChemSketch, or open .mol or .sdf files.*

To annotate and report manually

- Click the **Annotation Options** button at the bottom-left corner of Mnova window
- Or press **T** to insert a text box
- All objects can be customized by right clicking on it and then selecting the **Properties** command
- **Tables of Peaks, Integrals, Parameters** etc can be opened by **View | Tables.** Report from there





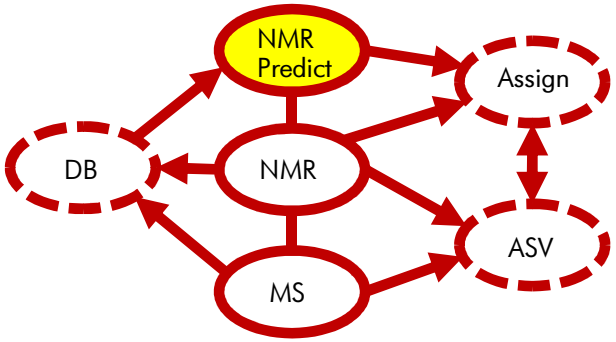
Tips:

Copy a **molecule from ChemDraw or Isis/Draw, or open .mol or .sdf files*

Use **View | Layout Templates menu to generate and apply layout templates, or request an auto **formatting script** from Mestrelab.*

****Copy/paste** any object(s) to your document with high resolution*

Click to export **PDF*



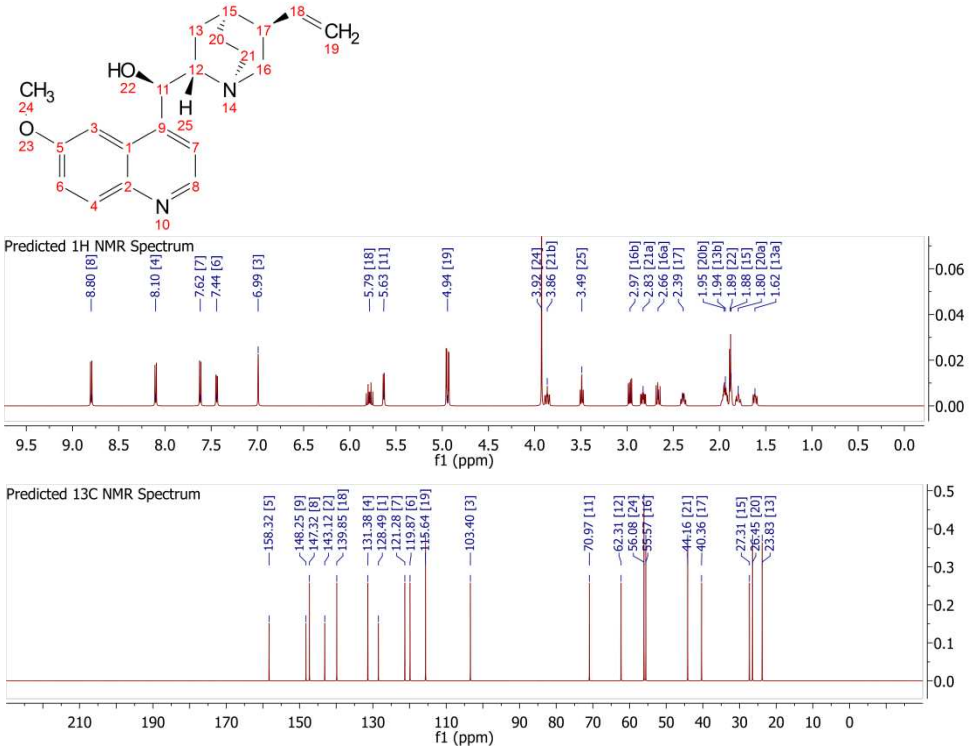
Mnova: An integrated system for analytical chemistry

Mnova NMRPredict Desktop

- Predict ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{29}Si, and ^{31}P spectra
- Predict and verify a structure and do peak assignment interactively
- Mnova NMRPredict Desktop license required

To predict NMR from a structure

- Open a new document (**File | New**) or a new page (**Edit | Create New Page**)
- Copy a structure from ChemDraw, Isis/Draw or ChemSketch, and paste to Mnova, or open a .mol or a .sdf file
- Choose an option from the **Predict** menu



Tips:

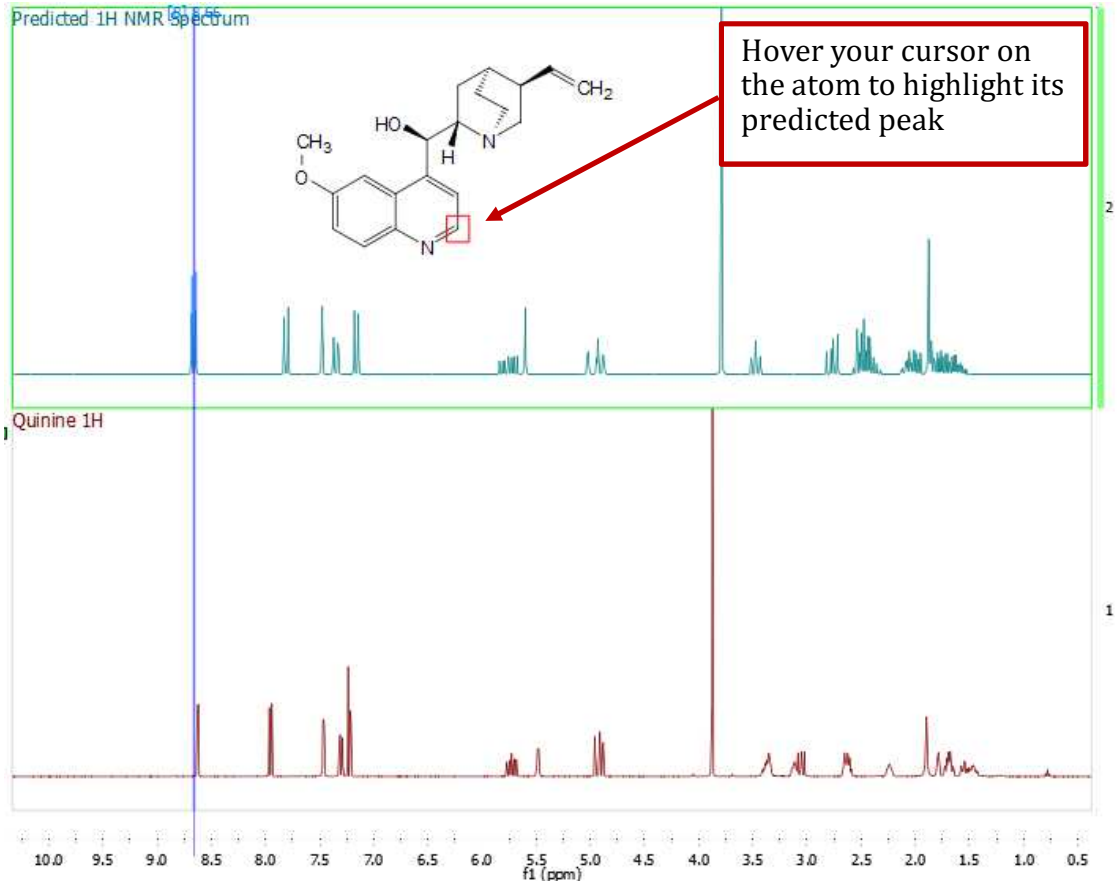
*1. Choose **Molecules | Prediction Options** to change settings*

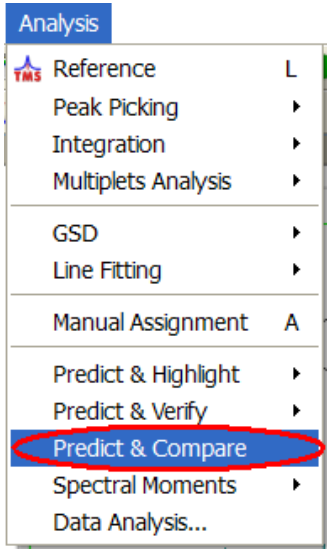
2. You can turn on/off the atom numbers by right-clicking on the structure and choose Properties.

MESTRELAB RESEARCH
NMR Solutions

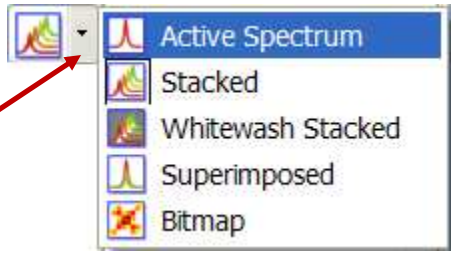
To predict NMR & verify your structure

- Open your ^{1}H (or ^{13}C) **spectrum** in a new page
- Copy your **structure** from ChemDraw or Isis/Draw
- Choose **Analysis | Predict & Compare.** The predicted spectrum is stacked with the experimental one for visual comparison





To assign NMR multiplets to atoms (1)



- Do **Multiplet Analysis** to get the multiplet labels
- Do **Predict and Compare**
- Change the stacking mode to "**Active Spectrum**", press Shift + Up Arrow Key to make sure the experimental spectrum is displayed (so that the multiplet labels are visible)
- Hover the cursor on an atom to see its predicted peak (in blue).
- Press **A**, and click on an atom to assign
- Click on the multiplet label to assign to that atom

Tips:

1. The predicted spectrum helps you assign peaks, but you don't have to have it for assignment.

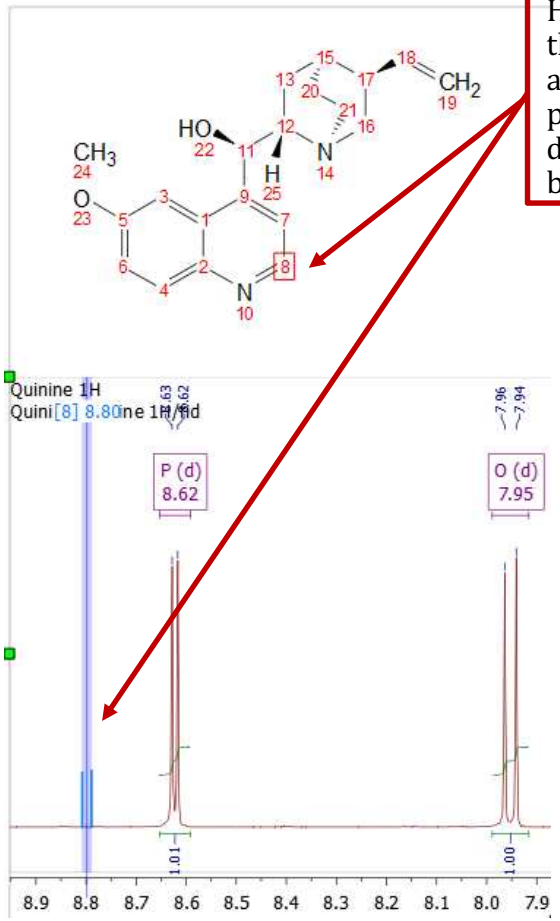
*2. After **Predict and Compare**, the two spectra are stacked. In the Stacked Mode, the multiplet labels are not displayed. You have to change to Active Spectrum mode to see the multiplet labels.*

*2. Press **ESC** to exit assignment mode.*

*3. Choose **View | Tables | Assignment** to report the assignments.*

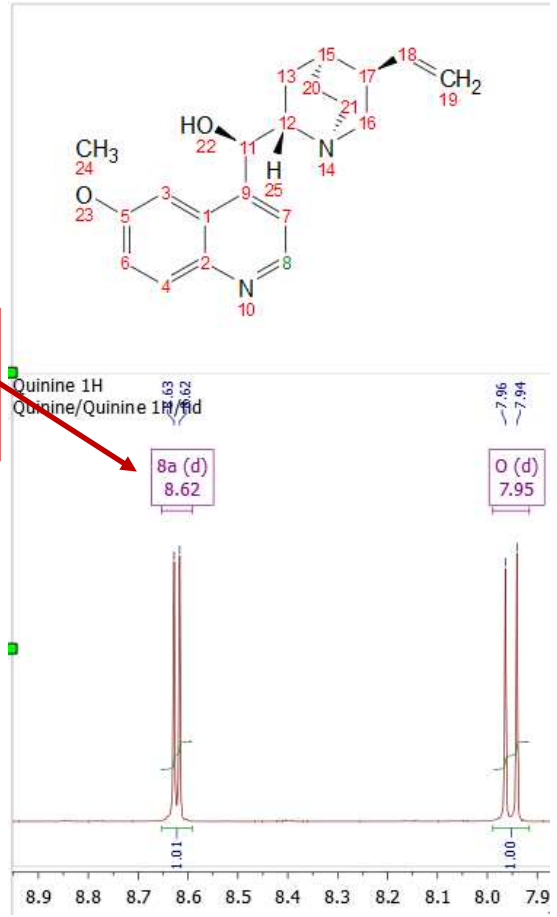
4. Multiple 1D and 2D spectra can be assigned simultaneously in this way.

To assign NMR multiplets to atoms (2)



Hover the cursor on the atom (#8) to assign. The predicted peak is displayed as the blue doublet.

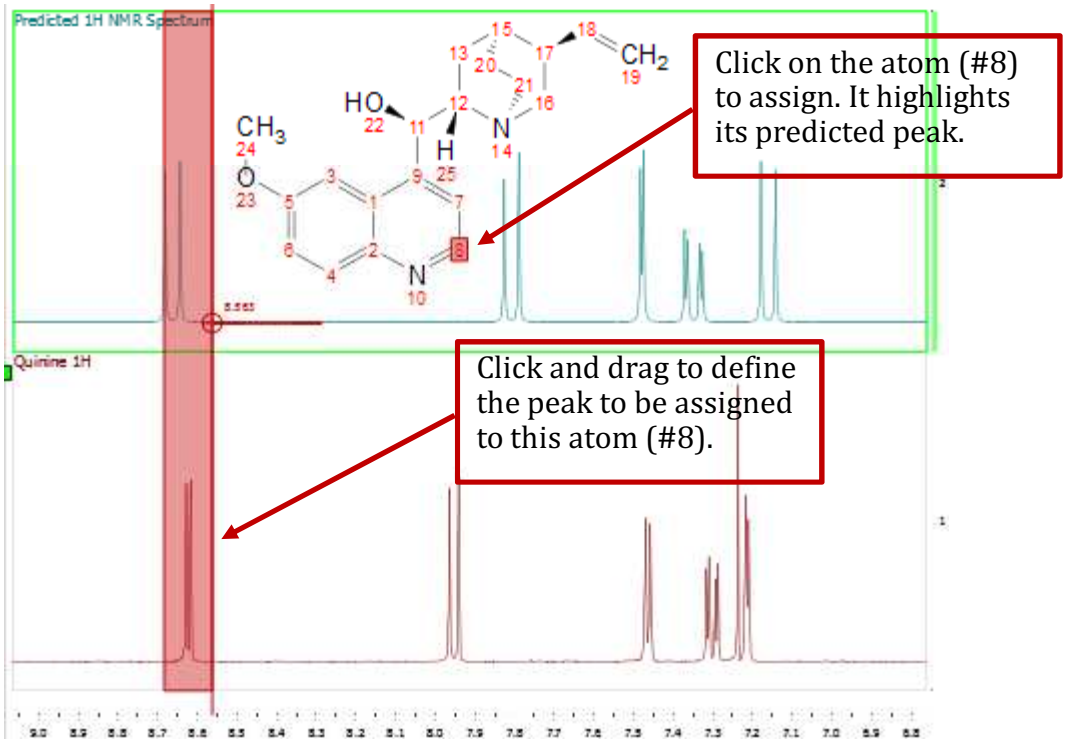
Click on atom #8 and then on this multiplet label to sign it to atom #8.



MESTRELAB RESEARCH
NMR Solutions

To assign NMR peaks to atoms without multiplet analysis

- Do **Predict and Compare** first
- Press **A**, and click on an atom to assign
- Click and drag on the experimental spectrum to include the multiplet to assign
- Or click on a peak top to assign



Tips:

1. The predicted spectrum helps you assign peaks, but you don't have to have it.

*2. Press **ESC** to exit assignment mode.*

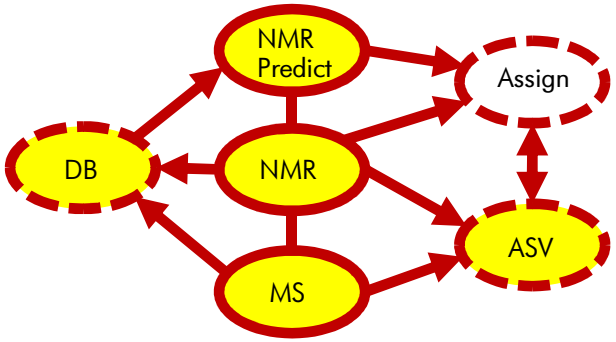
*3. Choose **View | Tables | Assignment** to report the assignments.*

4. Multiple 1D and 2D spectra can be assigned simultaneously in the same document.

*5. Use **Predict | Update 1H (or 13C) User DB** to save your assignment for improving the prediction (Mnova 6.2 only)*

MESTRELAB RESEARCH
NMR Solutions

Starting from here…



Mnova: An integrated system for analytical chemistry

- There are much more Mnova can do, such as
  - Processing and analyzing 2D NMR like a breeze
  - Opening and stacking multiple spectra for comparison
  - Special applications, such as deconvolution, diffusion, relaxation, kinetics studies etc.
  - Scripting for auto batch processing, reporting and structure verification*
  - Processing, analysis and reporting of LC/GC/MS data**
  - Database management of your molecules and analytical data***
- If you have questions,
  - Visit www.mestrelab.com/resources for manuals and tutorials
  - Check **Help > Contents** in Mnova
  - Email to chen.peng@mestrelab.com or support@mestrelab.com

**Automated structure verification needs a separate license of Mnova ASV.*

***Needs a separate license of Mnova MS*

**** Needs a separate license of Mnova DB.*