Mestrelab Research

chemistry software solutions

Mnova 11 – Starting guide

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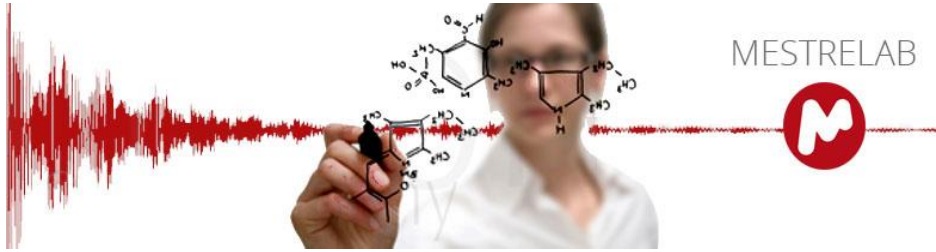
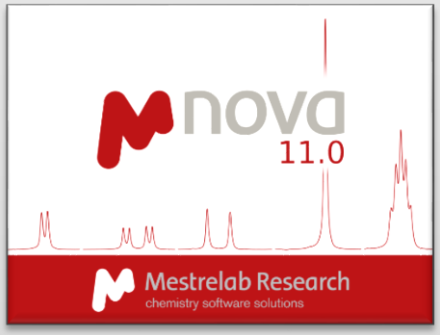
Outline – Starting guide

- Overview of Mestrelab and Mnova
- Open and process 1D and 2D NMR data
- Multiplet Analysis for 1D ^{1}H NMR
- Assign 1D peaks to a structure
- Assign 1D and 2D spectra
- Report analysis results
- Basic handling of multiple spectra
- Predict, assign and verify
- LC/GC/MS data processing



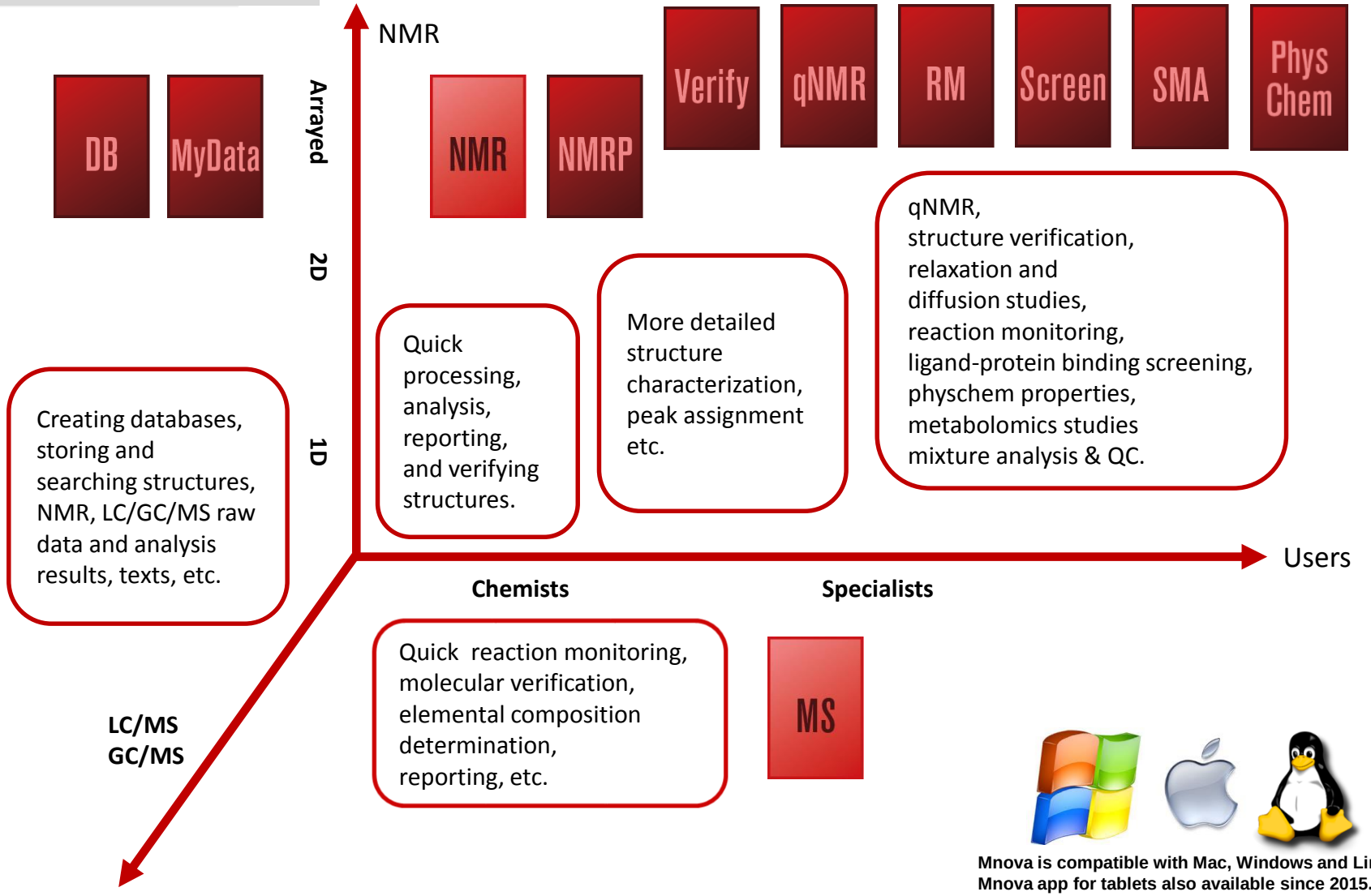
A Fast Growing Company

- 1996: A research project in University of Santiago de Compostela, Spain, developed a free Software, **MestReC**, for NMR processing.
- 2004: **Mestrelab Research** incorporated in Santiago de Compostela.
- 2004: New **MestReNova (Mnova)** platform and **NMR** plugin released.
- 2006: **NMRPredict Desktop** for NMR prediction.
- 2009: **MS** plugin for LC/GC/MS data analysis.
- 2009: **Global Spectral Deconvolution (GSD)** algorithm released for NMR.
- 2011: **DB** plugin for Database Management of NMR and MS.
- 2012: **Verify** plugin for auto structure verification.
- 2012: **qNMR** plugin for quantitative NMR analysis.
- 2013: **Reaction Monitoring** plugin for NMR-based reaction kinetics studies.
- 2014: **Screen** plugin for high-throughput ligand-protein binding analysis.
- 2015: **SMA** (plugin for simple mixture analysis) **Mbook ELN**, **Mnova app for tablets.**
- 2016: **Mnova 11** and many more!



An R&D company with 30 people and >80,000 registered users.

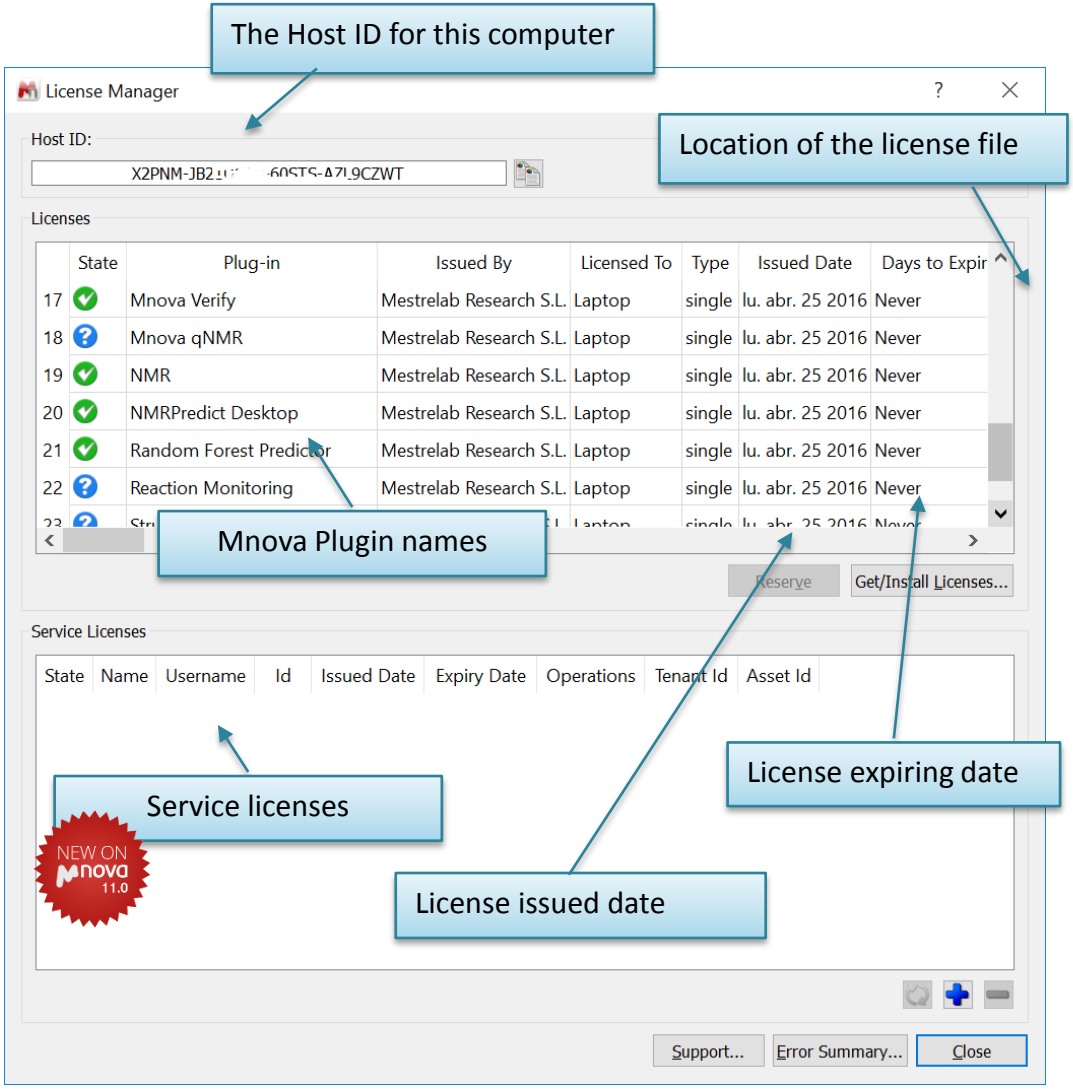
Mnova products and applications



Mnova is compatible with Mac, Windows and Linux.
Mnova app for tablets also available since 2015.

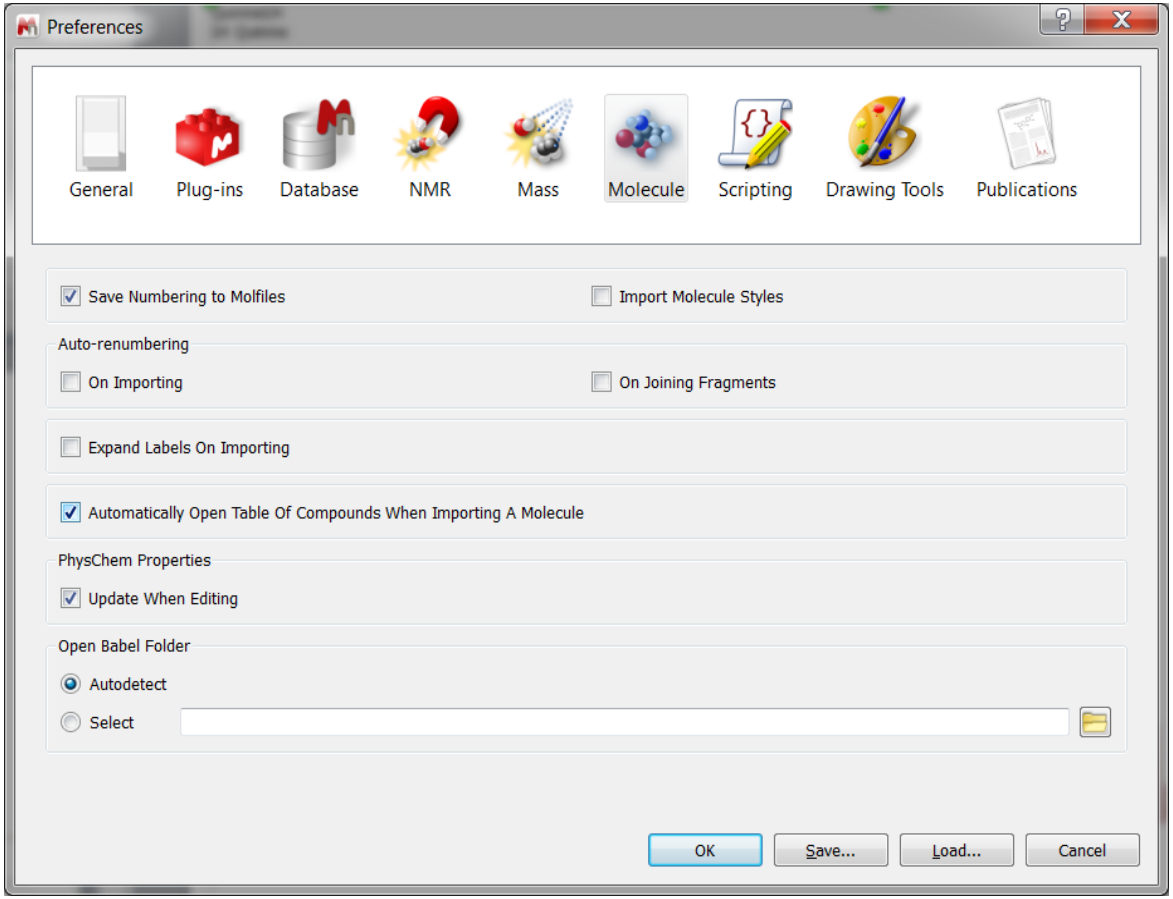
Download and activate your Mnova license

- Download and install Mnova www.mestrelab.com. Choose ***Help > License Manager*** to open the License Manager dialog.
- Activate Mnova using your purchased license files, or apply for 45 day free trial licenses (Click ***Get/Install Licenses***)
- Make sure that you see green checks for NMR and other plugins that you have chosen to activate.
- For managing campus/site/ concurrent licenses, see http://www.mestrelab.com/mlicserver



Mnova preferences

Mnova allows you to change Mnova's interface options for Plugins, Database, NMR, MS, Molecule, Scripting and Publications. You can edit them on **"Mnova/Edit/Preferences".**



Mnova 11 allows you to pop-up the table when opening a new molecule. You can edit this on **"Mnova/Edit/Preferences/ Molecule".**

NEW ON Mnova 11.0

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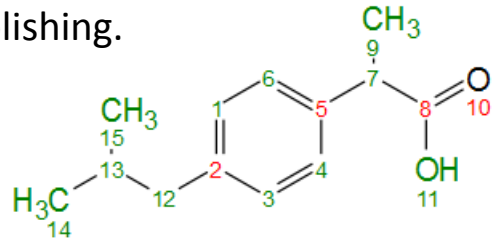
PROCEDURE

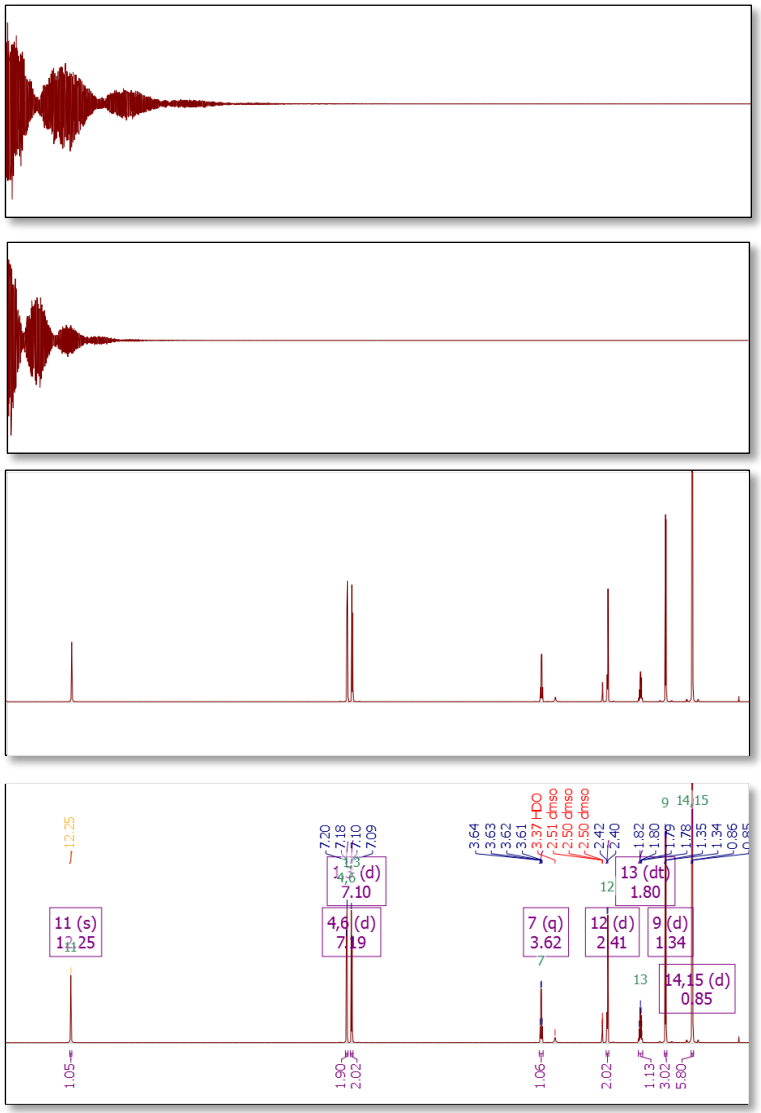
^{1}H processing and analysis: General procedure

- Opening the raw data.
- Preprocessing of FID: drift correction, apodization, zero filling, linear prediction, etc.
- Fourier transform.
- Phase correction and baseline correction.
- Chemical shift referencing.
- Peak picking, integration, multiplet analysis.
- Structure verification and peak assignment.
- Reporting and publishing.



^{1}H NMR (600 MHz, DMSO-d_6) δ 12.25 (s, 1H), 7.19 (d, J = 7.8 Hz, 2H), 7.10 (d, J = 7.9 Hz, 2H), 3.62 (q, J = 7.1 Hz, 1H), 2.41 (d, J = 7.2 Hz, 2H), 1.80 (dt, J = 13.5, 6.8 Hz, 1H), 1.34 (d, J = 7.1 Hz, 3H), 0.85 (d, J = 6.7 Hz, 6H).

Note: Most of these steps are done automatically by Mnova but you have full control.

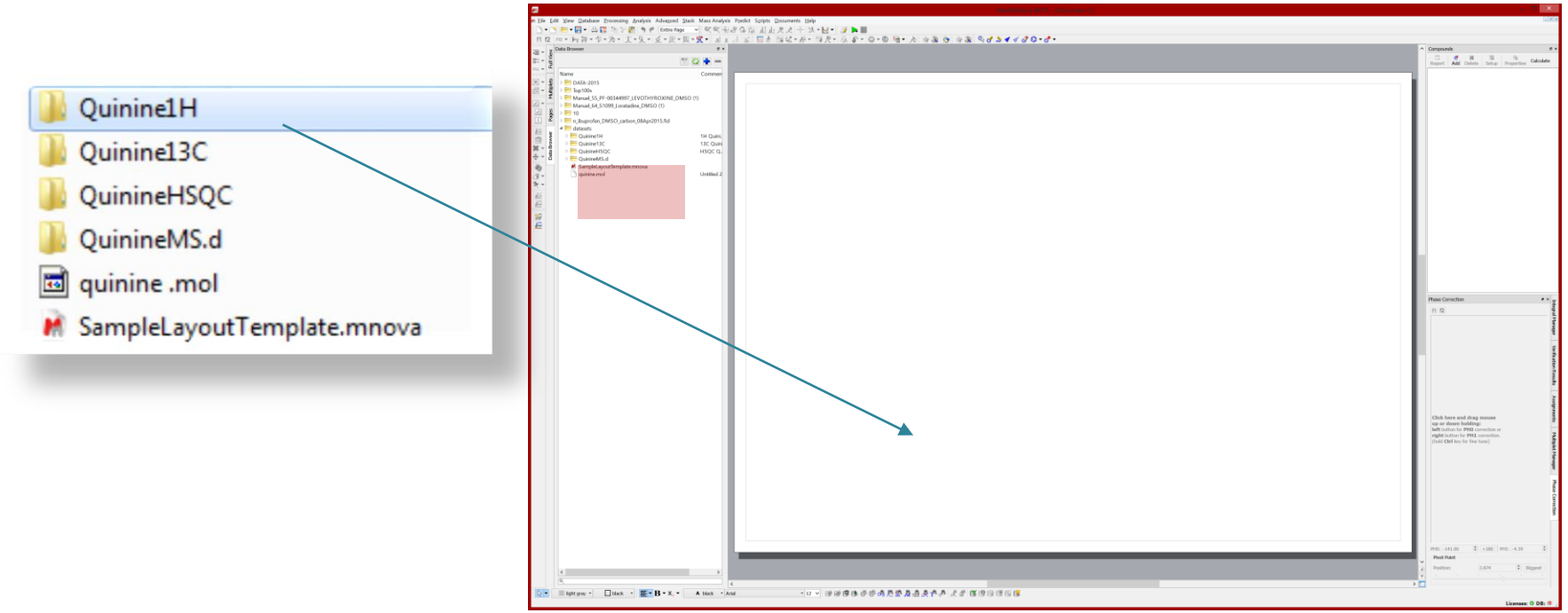


DATA FILE EXAMPLES

Mnova comes with a set of data file examples

- The installation of Mnova comes with a set of 1D and 2D NMR, LC/MS data, and the structure of quinine for your practice. On Windows, they are typically located at: **C:\Program Files (x86)\Mestrelab Research S.L\MestReNova\examples\datasets.**

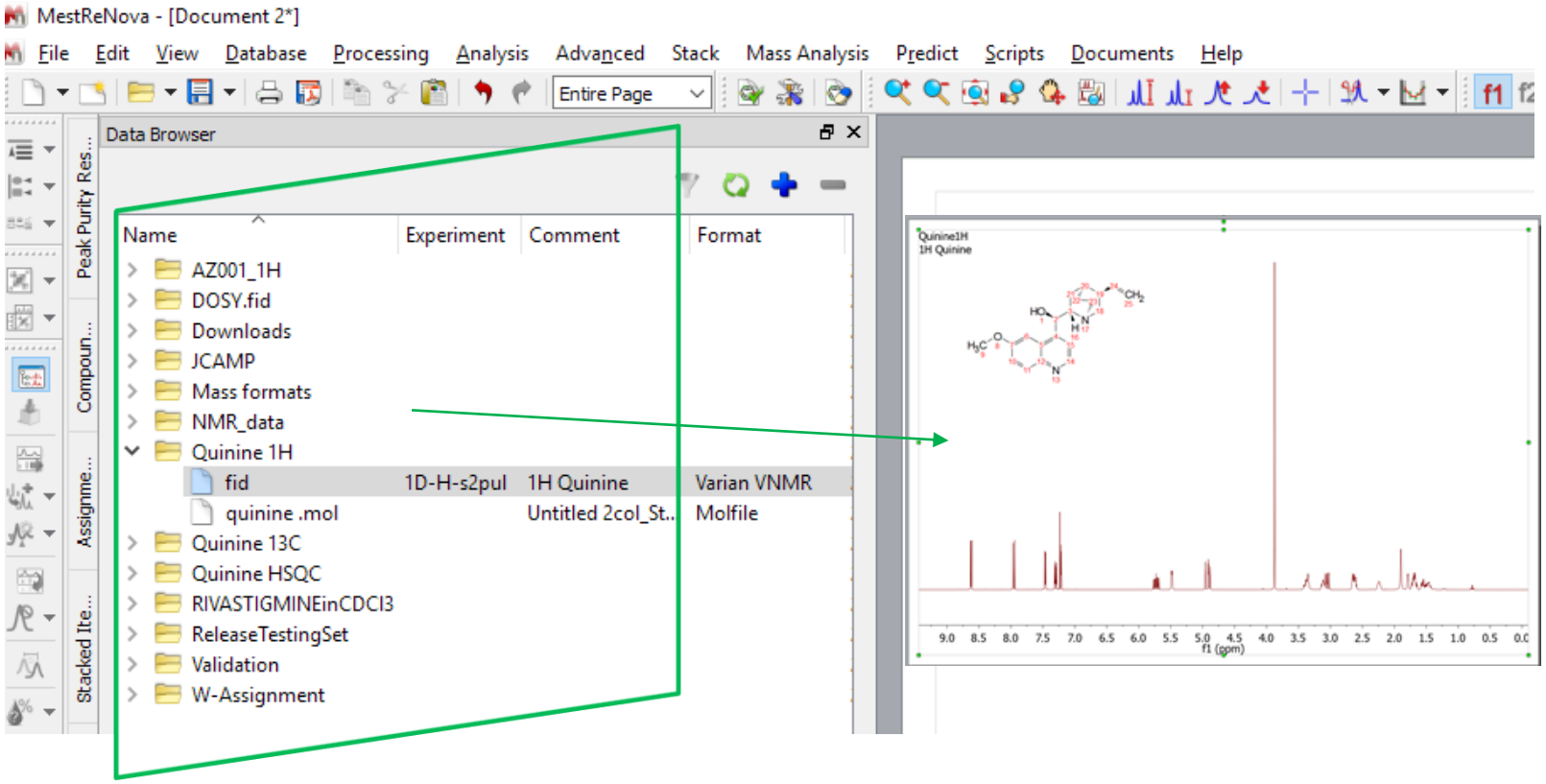
- Drag these folders or individual files into Mnova to open these practical examples.



Open and transform your NMR data

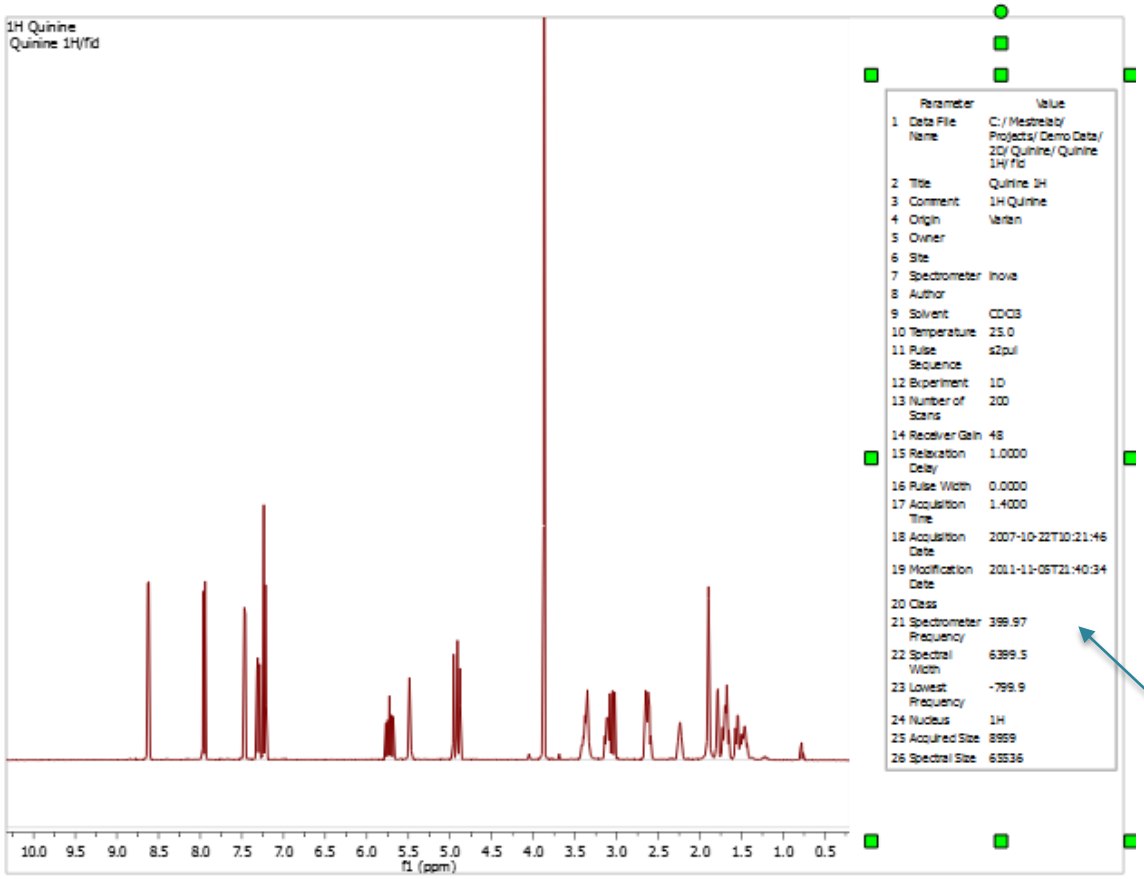
- Go to **File/Open** to open the **fid** (or **ser**) file from the raw data.
- Or drag an **fid** or **ser** file from a file browser into Mnova.
- Mnova automatically processes the spectrum.
- All data is brought in and depending on your preferences is processed to the desired extent. (manual or automatic).

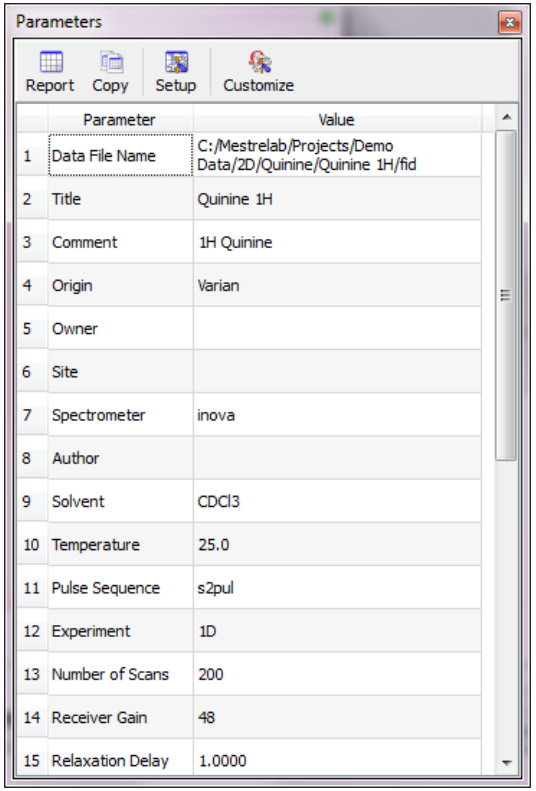
Available since Mnova 9:
Use the Data Browser to open spectra.
(View/Panels/Data Browser)



Display the parameters

- Go to **View/Tables/Parameters** to view the acquisition parameters.
- Press **Report** to report the parameters as a text box on the spectrum.



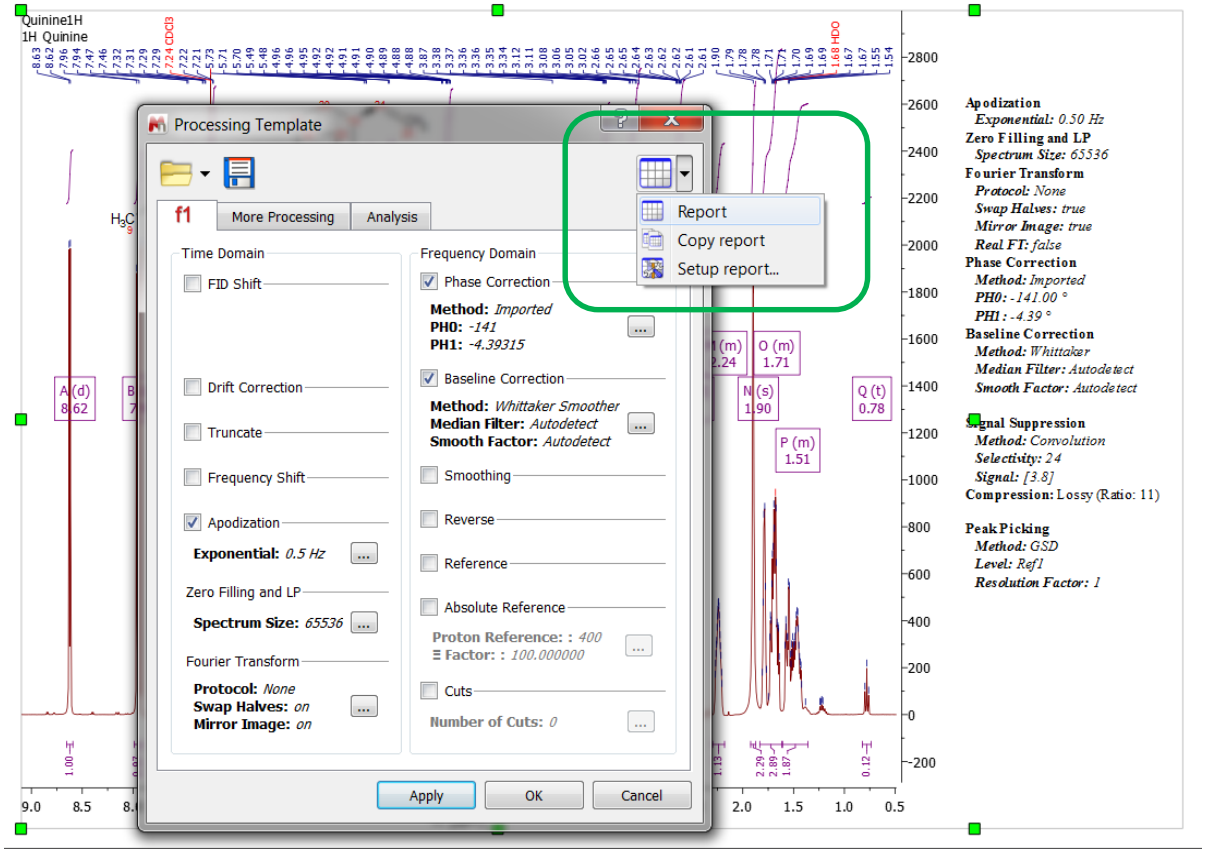


Use the green handles to move, rotate and resize the text box. Every object in Mnova can be relocated and resized.

Capability to report your 'Processing Template'

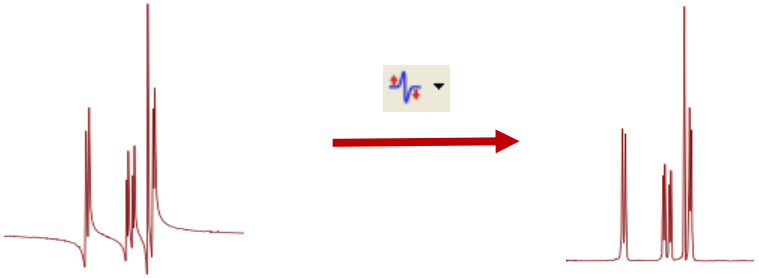
NEW ON MNOVA 11.0

- A report of the Processing Parameters can be generated using your preferred report template for 1D and 2D spectra. A customized template can be easily added.

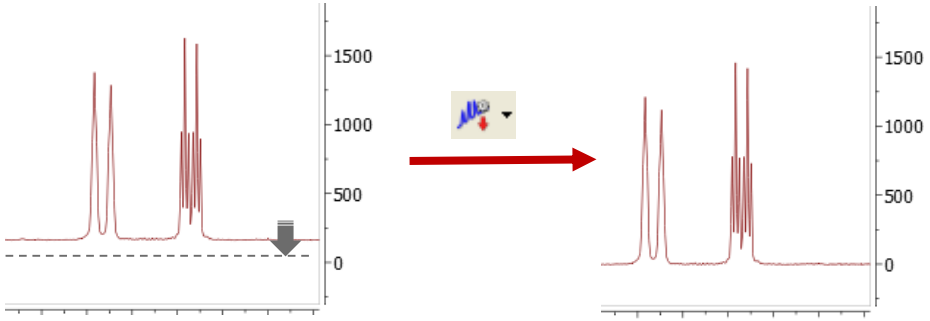


Phase, baseline correction & reference

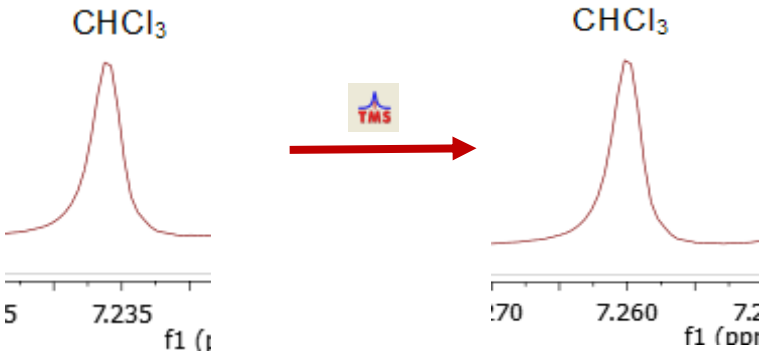
- Press  for **phase correction** if peaks are not symmetric.*



- Press  for **baseline correction** if baseline is not zero.*

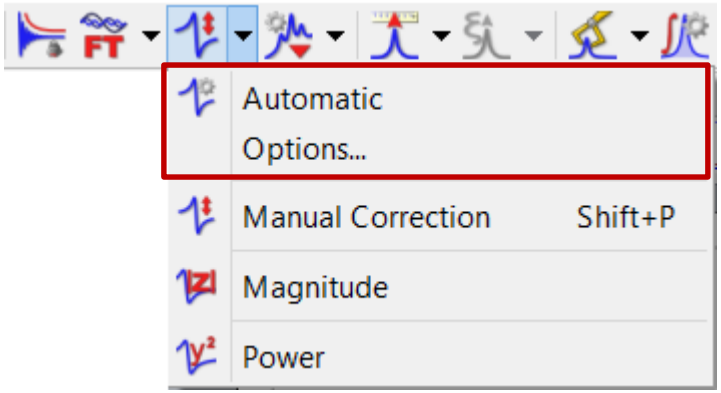


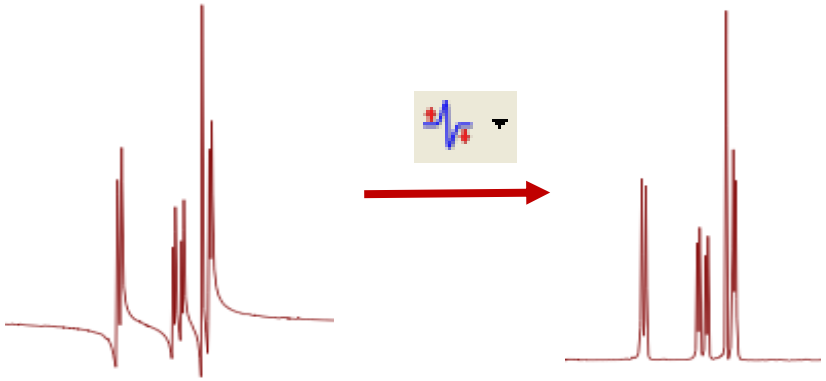
- Press  to calibrate the **chemical shift reference** if the solvent or TMS peak is not at the right ppm.

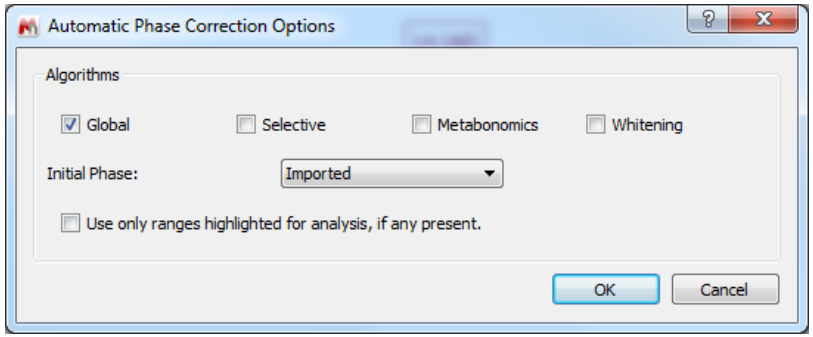


*Click the arrow next to the tool icon for options, such as manual phasing and manual baseline correction.
See **Help > Contents > Processing Basics** for more details.*

Automatic phase correction

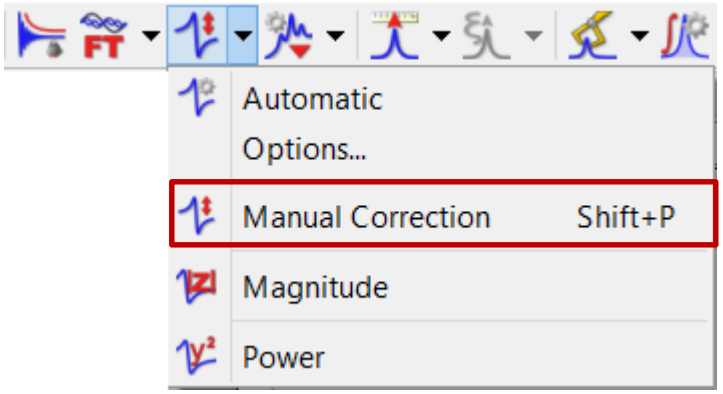


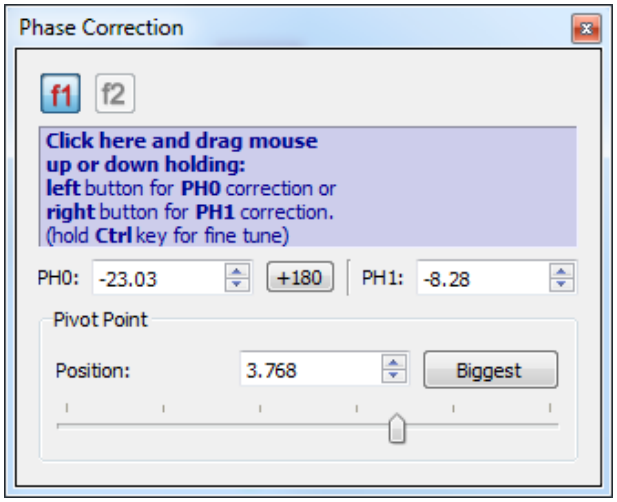


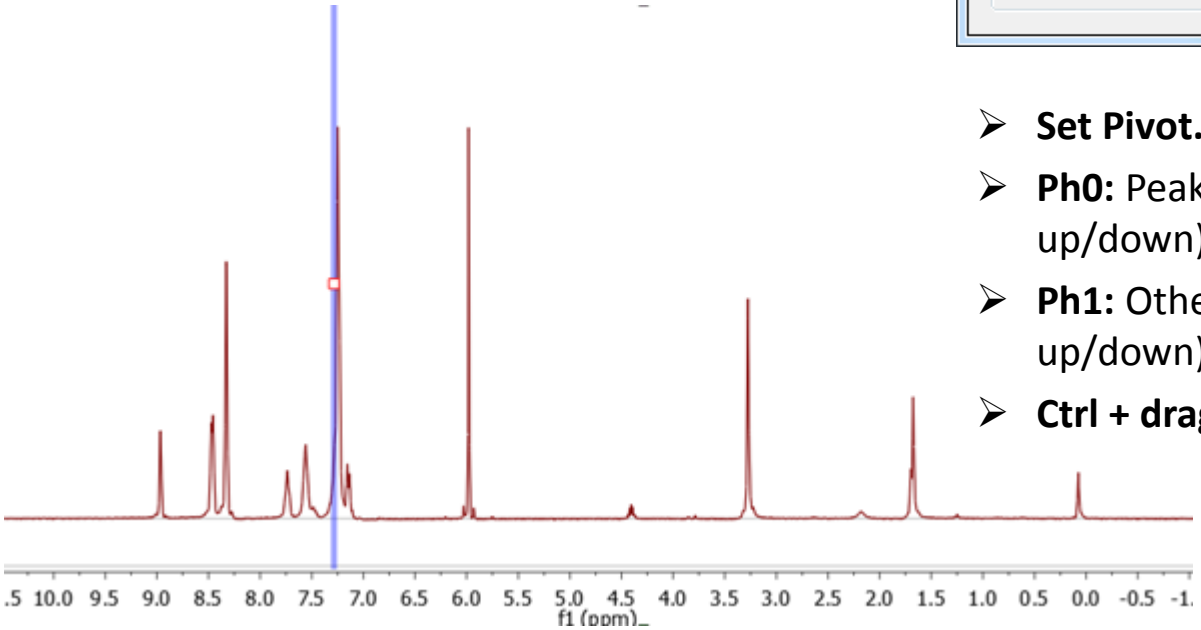


- **Global:** good for spectra without negative and big solvent peaks.
- **Selective:** DEPT type of spectra with negative peaks.
- **Metabonomics:** spectra with big solvent peaks.
- **Whitening**: usually for 2D.

Manual phase correction

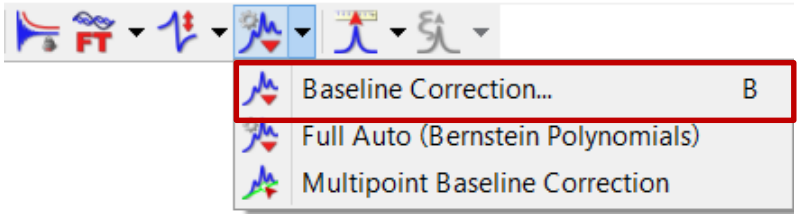


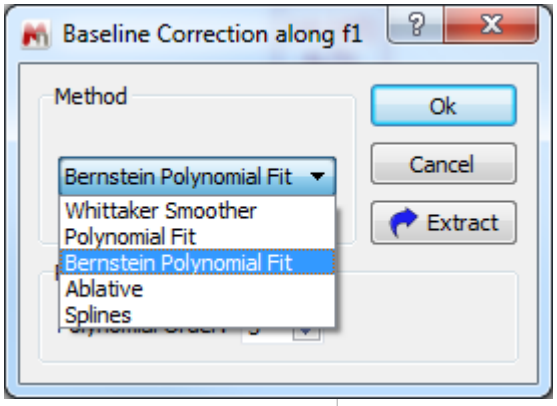




- **Set Pivot.**
- **Ph0:** Peak at pivot (left mouse button + up/down).
- **Ph1:** Other peaks (right mouse button + up/down).
- **Ctrl + dragging:** Fine tuning.

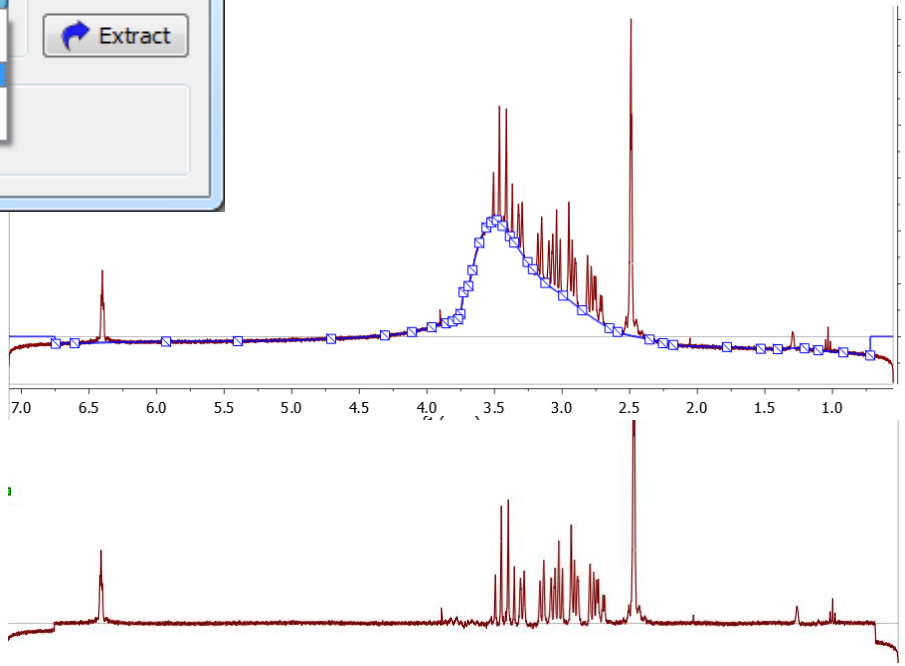
Baseline correction





Choose a function to model the baseline:

- **(Bernstein) Polynomial Fit:** Small base errors.
- **Splines or Ablative:** in between.
- **Whittaker:** Make sure peak base is not cut.
- **Multipoint B.C.**: Manually define base points. (next slide)

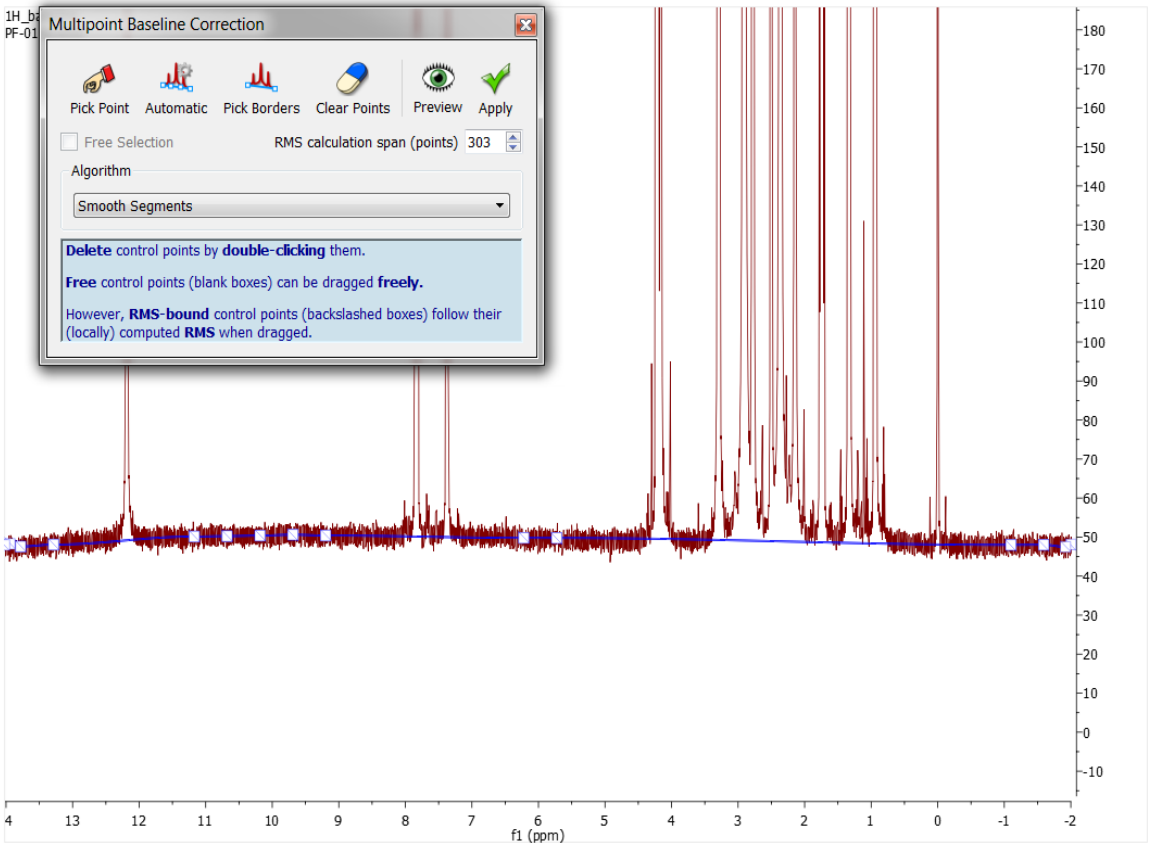


Multipoint baseline correction

NEW ON MNOVA 11.0

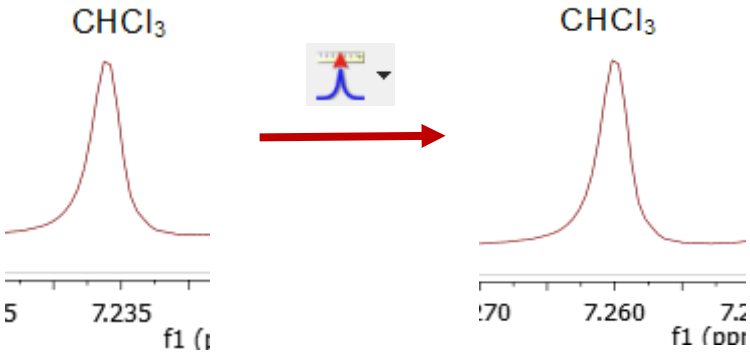
Improvements in the automatic detection of the control points have been done.

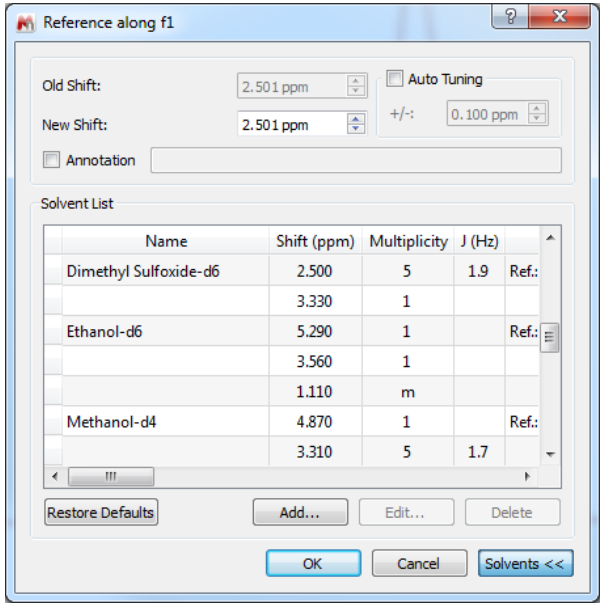
It estimates the noise regions and finds a lower number of control points for them.



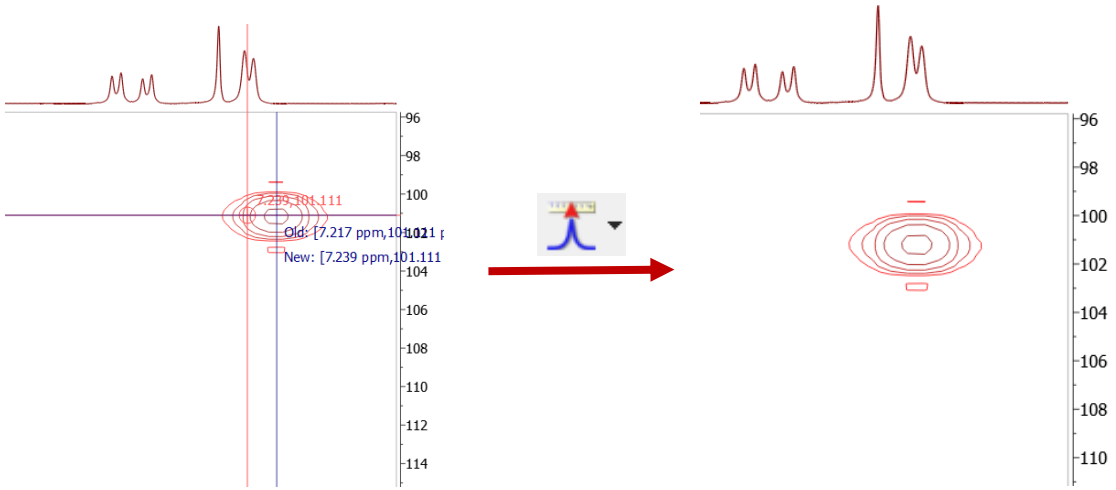
Referencing chemical shifts

Reference by entering the value



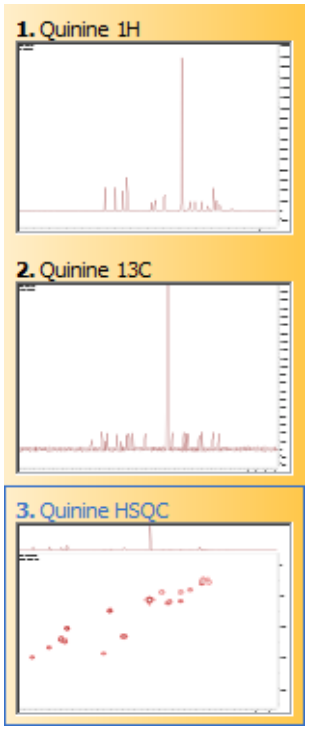


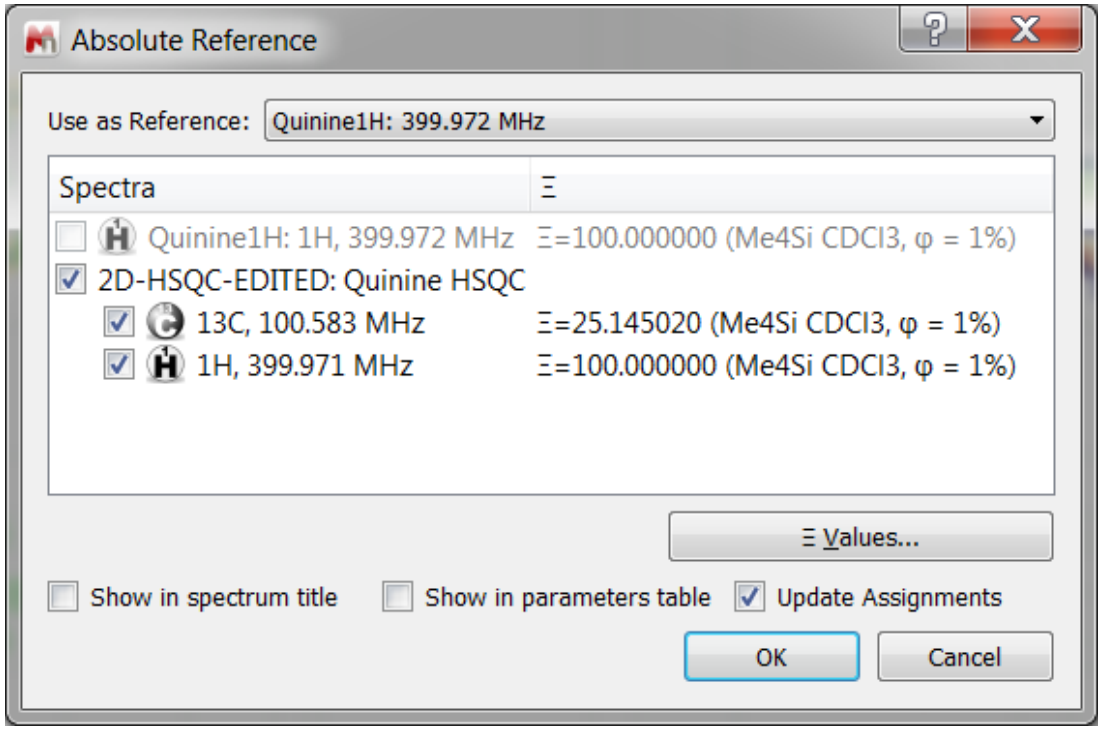
Graphic Reference
(two clicks)



Absolute Reference for automatically referencing multi-spectra/nuclei

- Use a referenced ^{1}H from the same instrument/probe/solvent/temperature.
- Auto references other nuclei.
- Auto references other spectra (1D and 2D).
- Saves such info in **Preferences** to do it automatically.





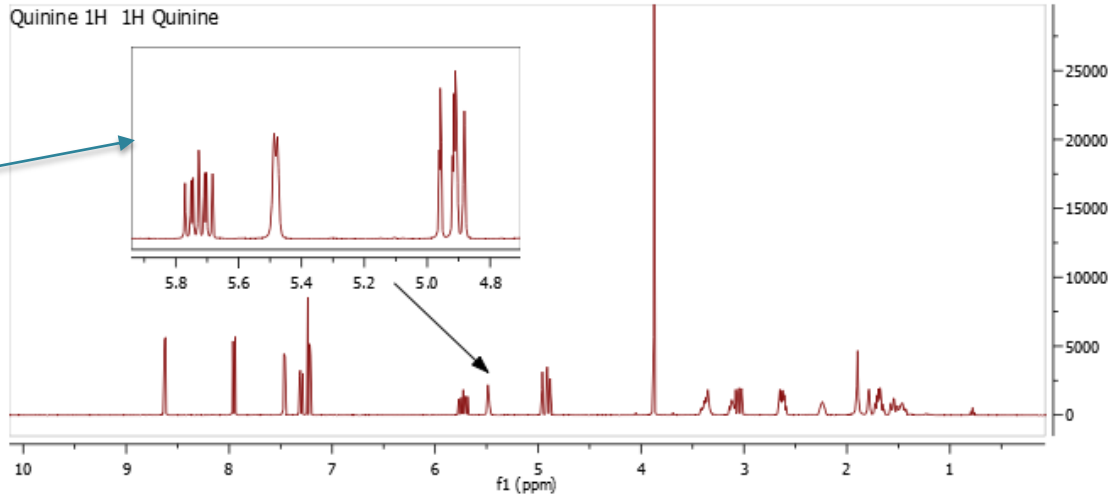
Visualize your spectrum

DISPLAY OPTIONS

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

Press **Z several times to toggle between horizontal/vertical/box zoom.*
*** Press **P** several times to toggle between free/horizontal/vertical panning.*

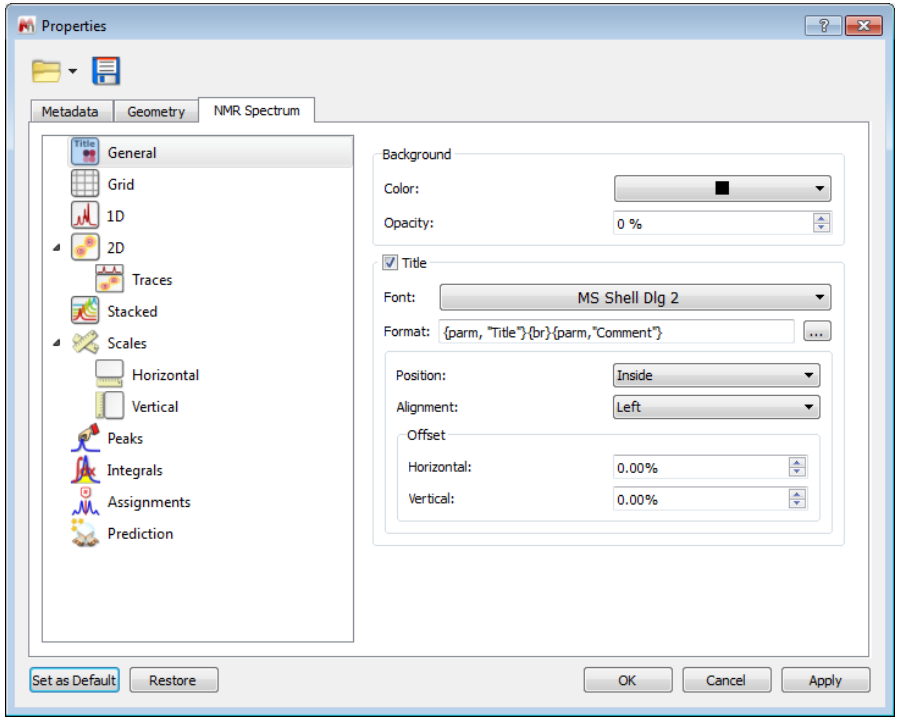
Press **E**, then click and drag to define the range for the inset



Change the display properties

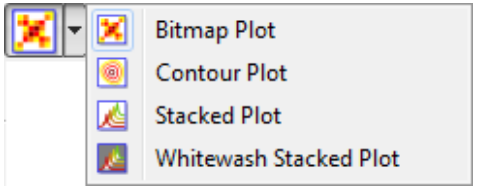
- Double click on a spectrum to open the **Properties** dialog.
- A lot of display properties can be customized.
- You can click on **Set as Default** to save the settings for spectra opened in the future.

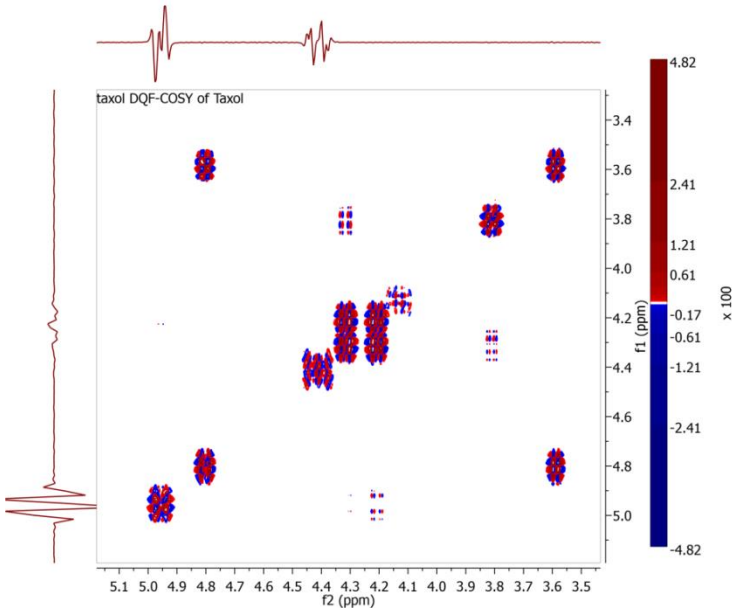
*Tip: Use the **Save** tool to save the properties to a file, and distribute it to other users for consistent display.*

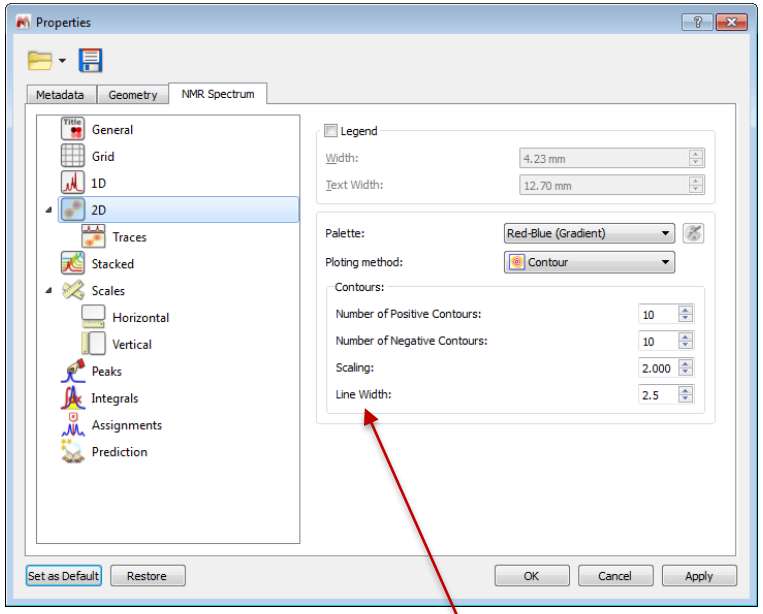


Display 2D spectra in the way you want

- Use the **Plot Mode** tools to change to bitmap or contour display etc.
- Change other display properties by double-clicking on the spectrum to open the **Properties** dialog:
  - Legend
  - Color Palette
  - Contours
  - Traces





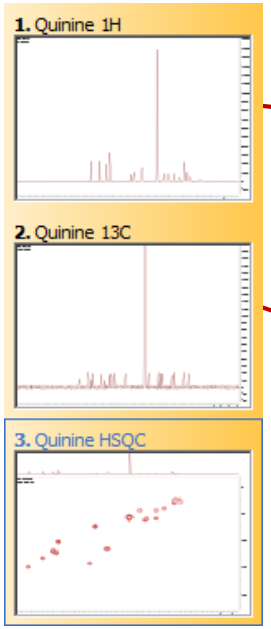


Tip: You can set a line width for 2D contours independent of that for 1D curves.

Attach 1D to 2D spectra

- Open 1D and 2D spectra in the *same* document. They are displayed in separate pages.

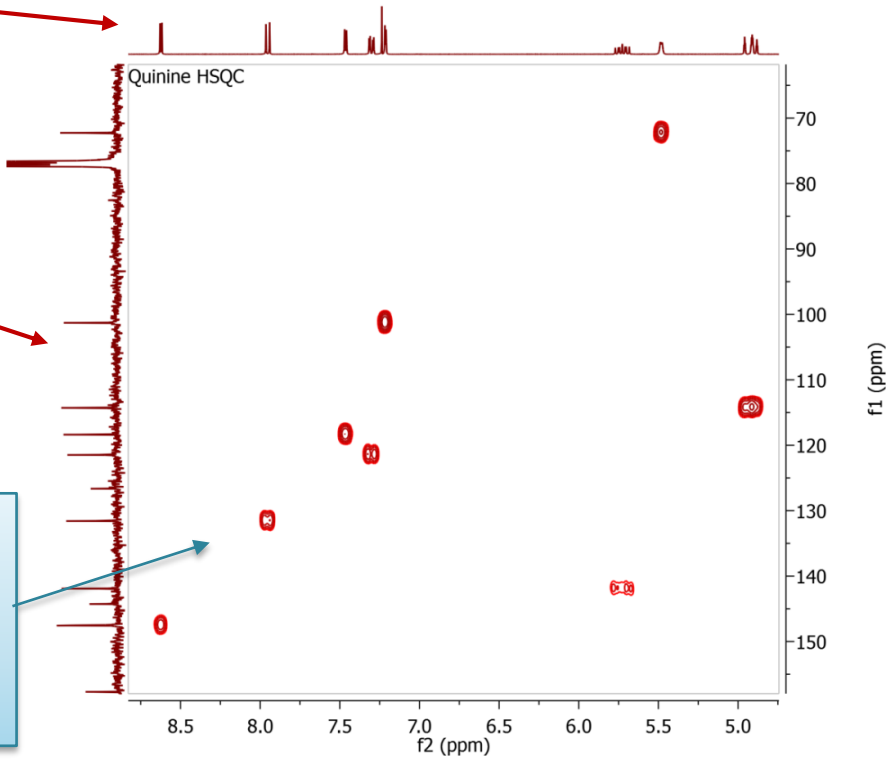
  If you don't see the Pages View, choose **View/Pages.**
- Display a 2D spectrum, drag a 1D from the Pages View to attach it to the 2D.
- It can be done automatically through **Edit /Preferences /NMR.**



Drag & drop

Drag & drop

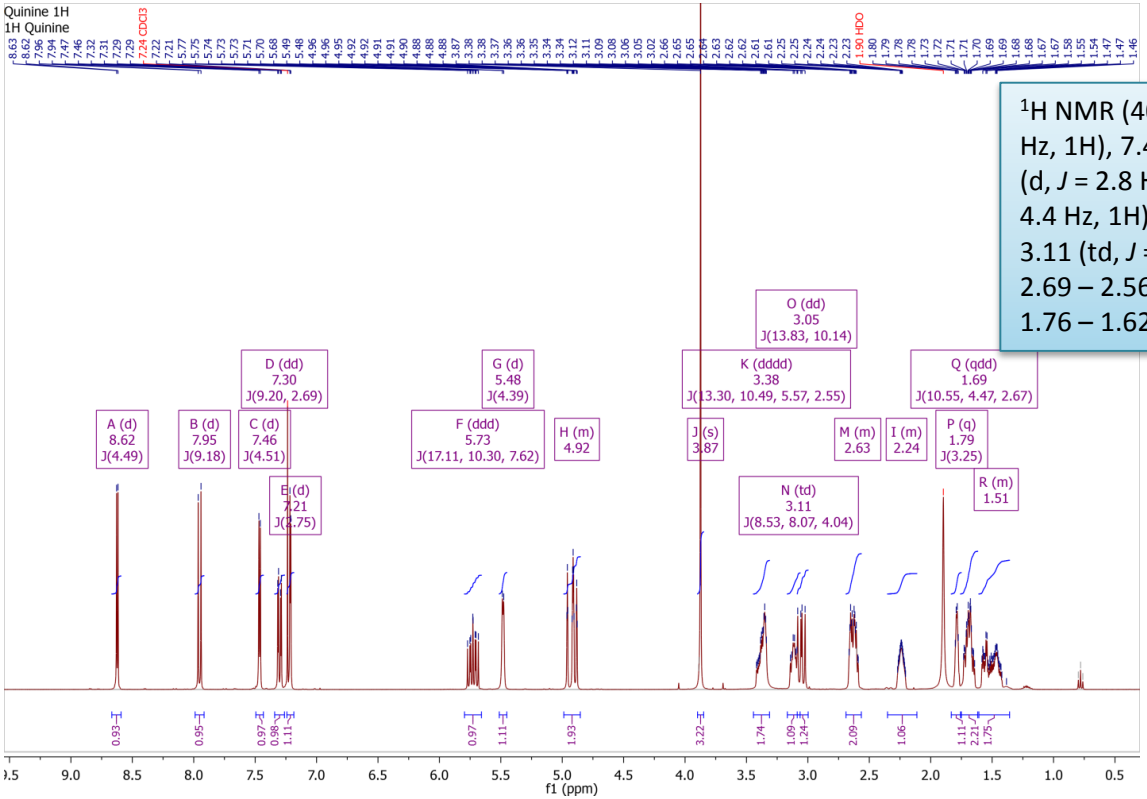
Try Absolute Reference to reference all 1D and 2D spectra with one click!



Change the Y intensity of the traces:
Place the cursor on the trace and scroll the mouse wheel, or click **Ctrl+Shift+arrow keys.**
Move the baseline of a trace: Shift + mouse wheel.
Change the space of the attached 1D's: Double click on the spectrum and open the **Properties** dialog.

Analyze and report multiplets of ^{1}H NMR

- Mnova provides two approaches to **multiplet analysis:**
  - **Fully automatic:** peak picking, integration and multiplet analysis *all done by one click*, with peaks deconvolved using GSD* and types classified.
  - **Manual**: click-and-drag to pick each multiplet interactively.
- In either case, you can refine the results interactively, and report them in the selected journal or patent formats.

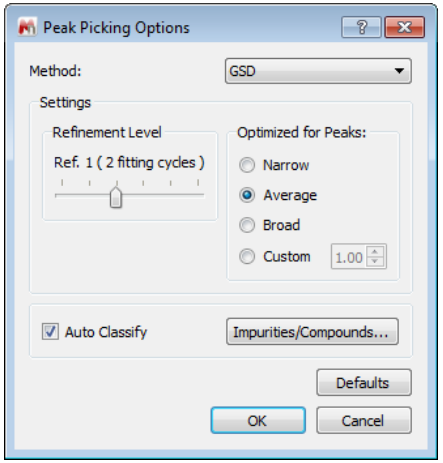


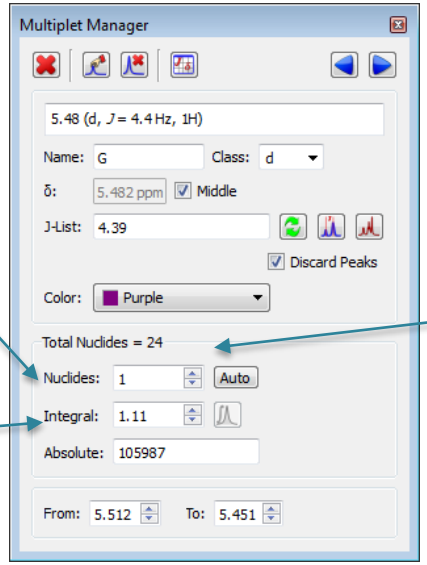
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.5 Hz, 1H), 7.95 (d, *J* = 9.2 Hz, 1H), 7.46 (d, *J* = 4.5 Hz, 1H), 7.30 (dd, *J* = 9.2, 2.7 Hz, 1H), 7.21 (d, *J* = 2.8 Hz, 1H), 5.73 (ddd, *J* = 17.1, 10.3, 7.6 Hz, 1H), 5.48 (d, *J* = 4.4 Hz, 1H), 4.99 – 4.85 (m, 2H), 3.87 (s, 3H), 3.44 – 3.31 (m, 2H), 3.11 (td, *J* = 8.5, 8.1, 4.0 Hz, 1H), 3.05 (dd, *J* = 13.8, 10.1 Hz, 1H), 2.69 – 2.56 (m, 2H), 2.35 – 2.11 (m, 1H), 1.79 (h, *J* = 2.7 Hz, 1H), 1.76 – 1.62 (m, 2H), 1.61 – 1.36 (m, 2H).

**GSD (Global Spectral Deconvolution): See Help > Contents > Analysis tools > Peak Picking > GSD for details.*

Fully automatic multiplets analysis

- Click  to do automatic multiplet analysis. By default, Mnova does the following automatically:
  - Picks peaks using GSD (if no peaks were picked) and classify their types (compound, solvent, impurity peaks etc.). Note these are controlled by the Peak Picking options
  - Groups the picked peaks into multiplets and fits them to J-coupling patterns, and calculates their integrals (depending on the Multiplet Analysis options). Note these are controlled by the Multiplet Analysis Options
  - Estimates the total number of nuclides (NN) and normalizes the integrals for each multiplet

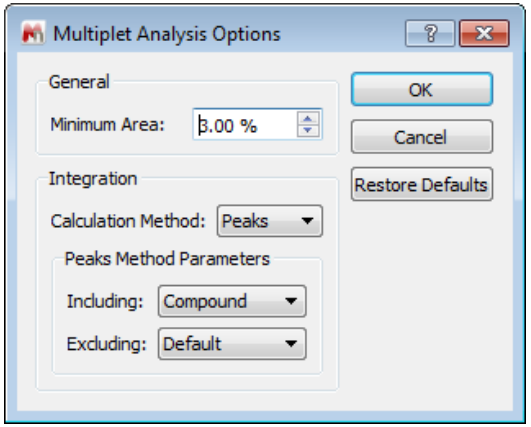




The number of nuclides (NN) of the multiplet

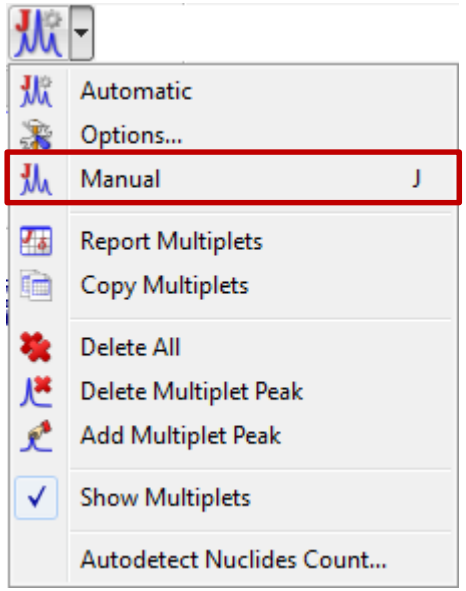
Normalized integral of the multiplet.

Total # of nuclides from all the multiplets and the # of protons in the molecule (if present)



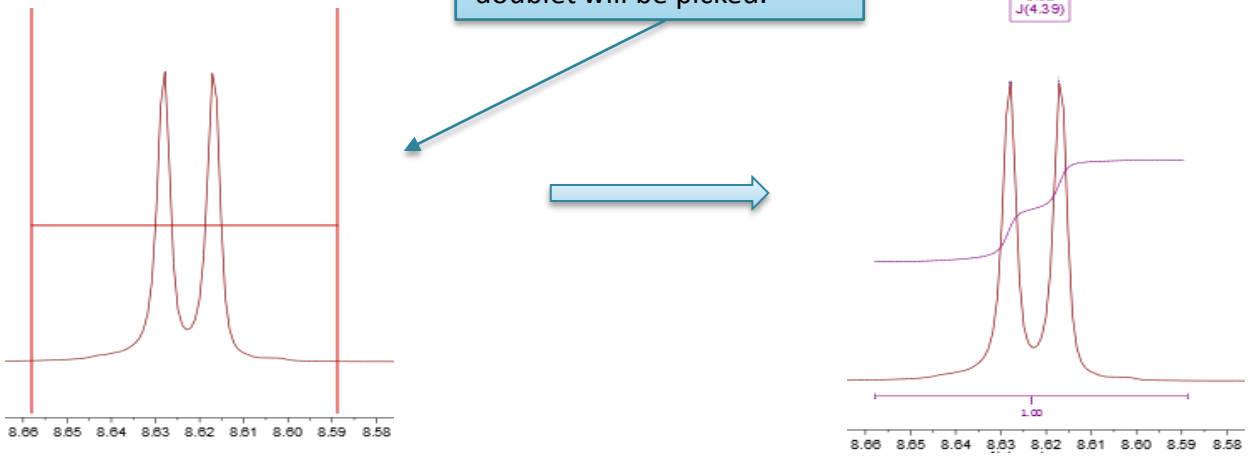
***GSD (Global Spectral Deconvolution):** See Help > Contents > Analysis tools > Peak Picking > GSD for details*

Pick multiplets manually



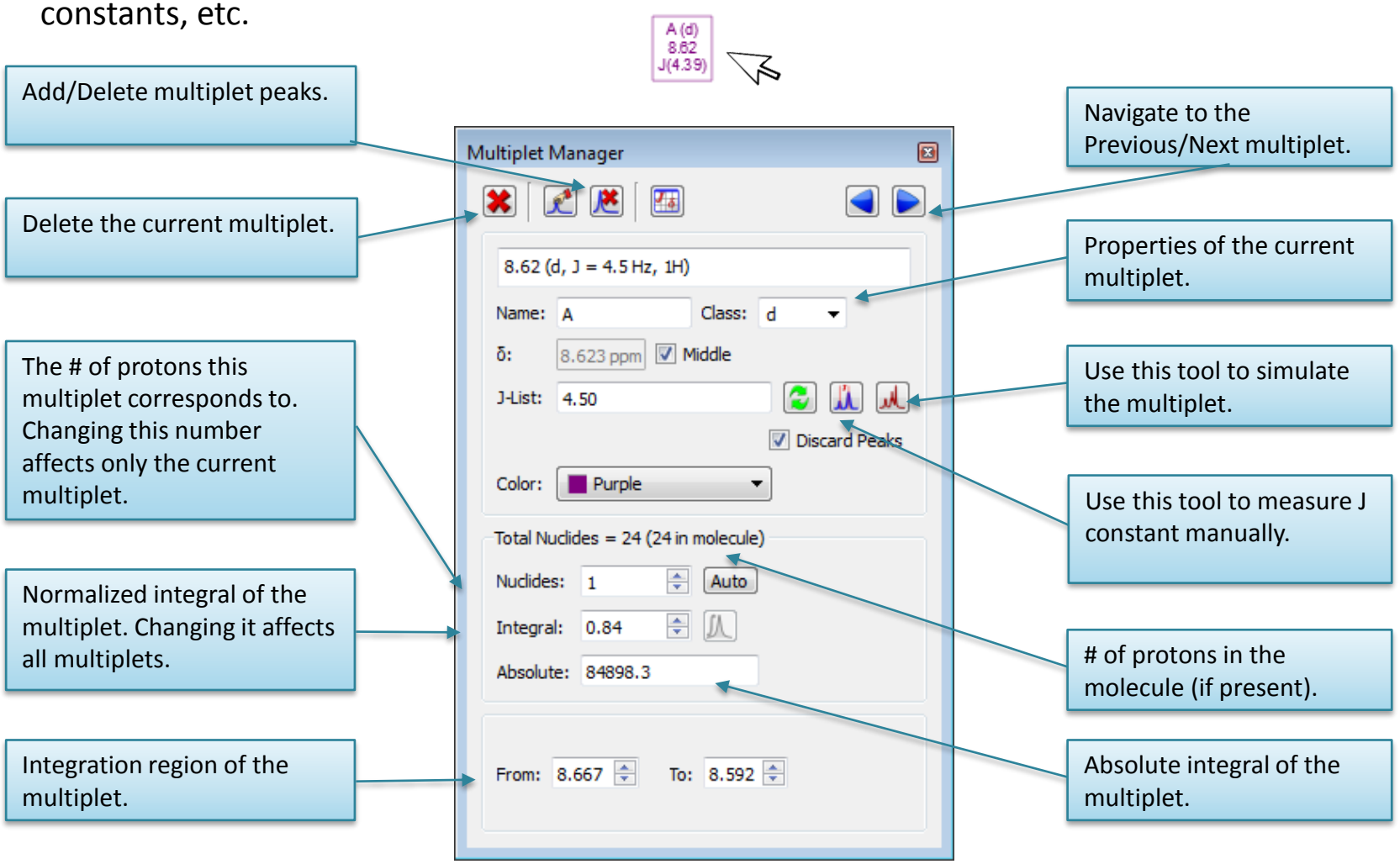
- Manual Multiplet Analysis allows you to have more control of the multiplet analysis (**J** is the shortcut key).
- You zoom into each multiplet, click and drag to define the following:
  - Peak picking threshold
  - Integration region*
- Mnova picks the peaks in the region, fits them to a *J*-coupling pattern and defines the multiplet in the same way as in automatic multiplet analysis.

Click and drag to define the **integration region** and **peak picking threshold** and a doublet will be picked.



Multiplet Manager

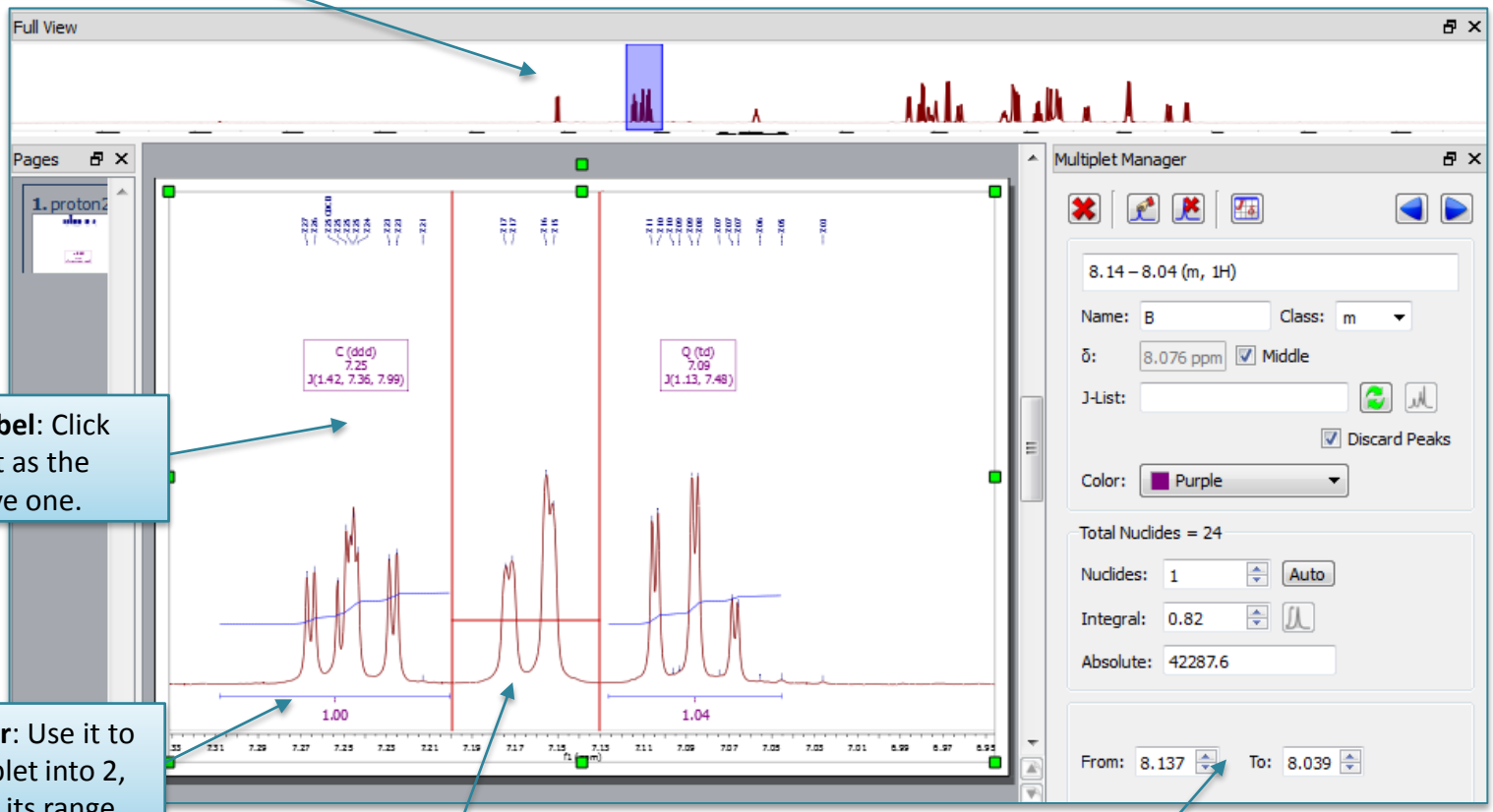
- Double click on a multiplet label to open the Multiplet Manager. Use it to inspect and change the properties of the multiplets, including the normalization of the integrals, *J*-coupling patterns and constants, etc.



Handy tools for multiplet analysis

Full View: The whole spectrum and zoom-in area. Drag the blue box to move to other multiplets. (Choose **View/Full View** to open Full View).

You can also use the **Auto Cut tool**, which will hide all noise-only regions of the spectrum. **View/Cuts/Auto Cut**.



Multiplet label: Click on it to set it as the current active one.

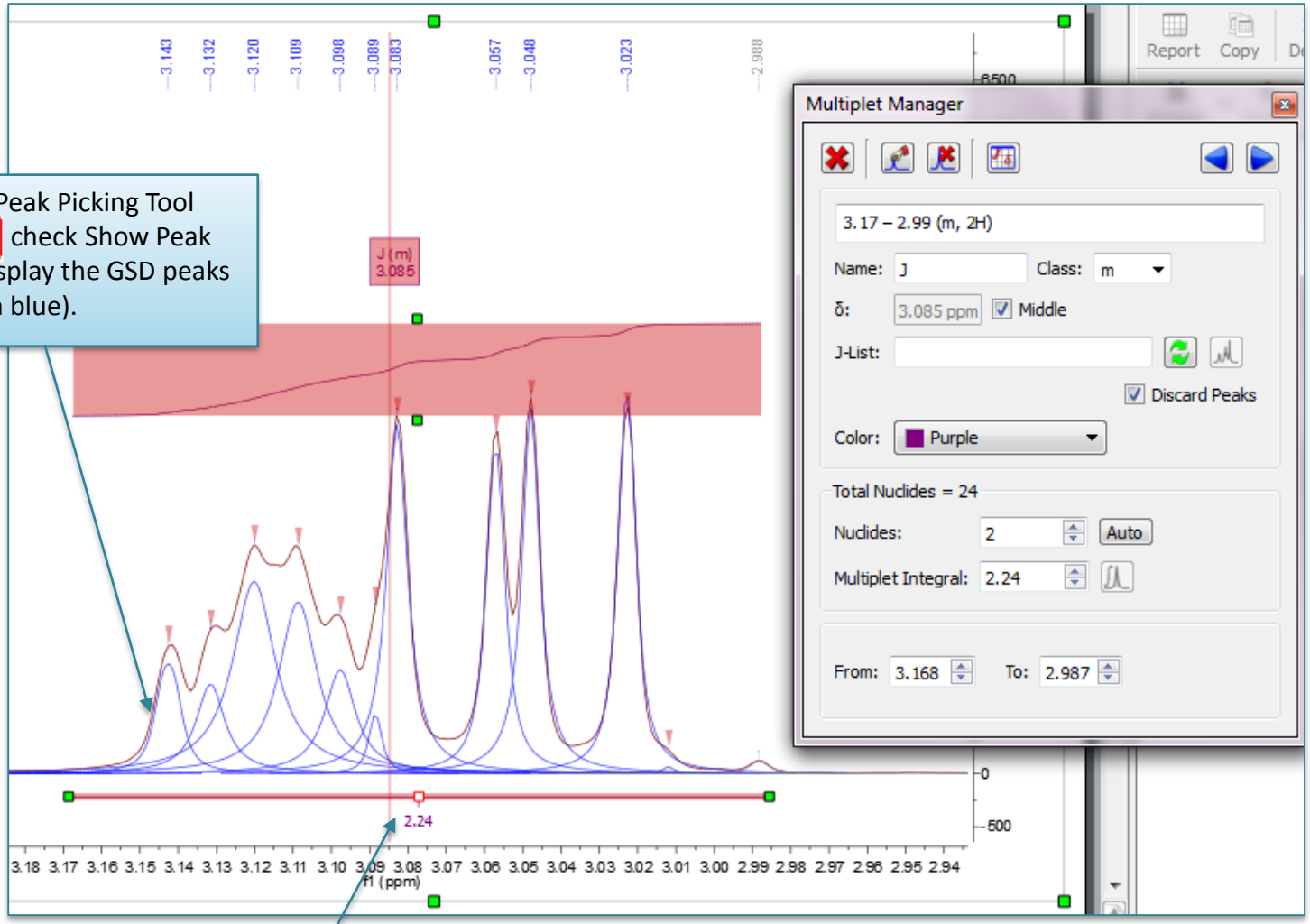
Multiplet bar: Use it to split a multiplet into 2, or to change its range.

Manual multiplet analysis: Press **J**, then click and drag to define the range and peak picking threshold for a multiplet.

Multiplet Manager shows the properties of the current multiplet picked. (Double click on a multiplet label to open it).

Split partially overlapping multiplets (1)

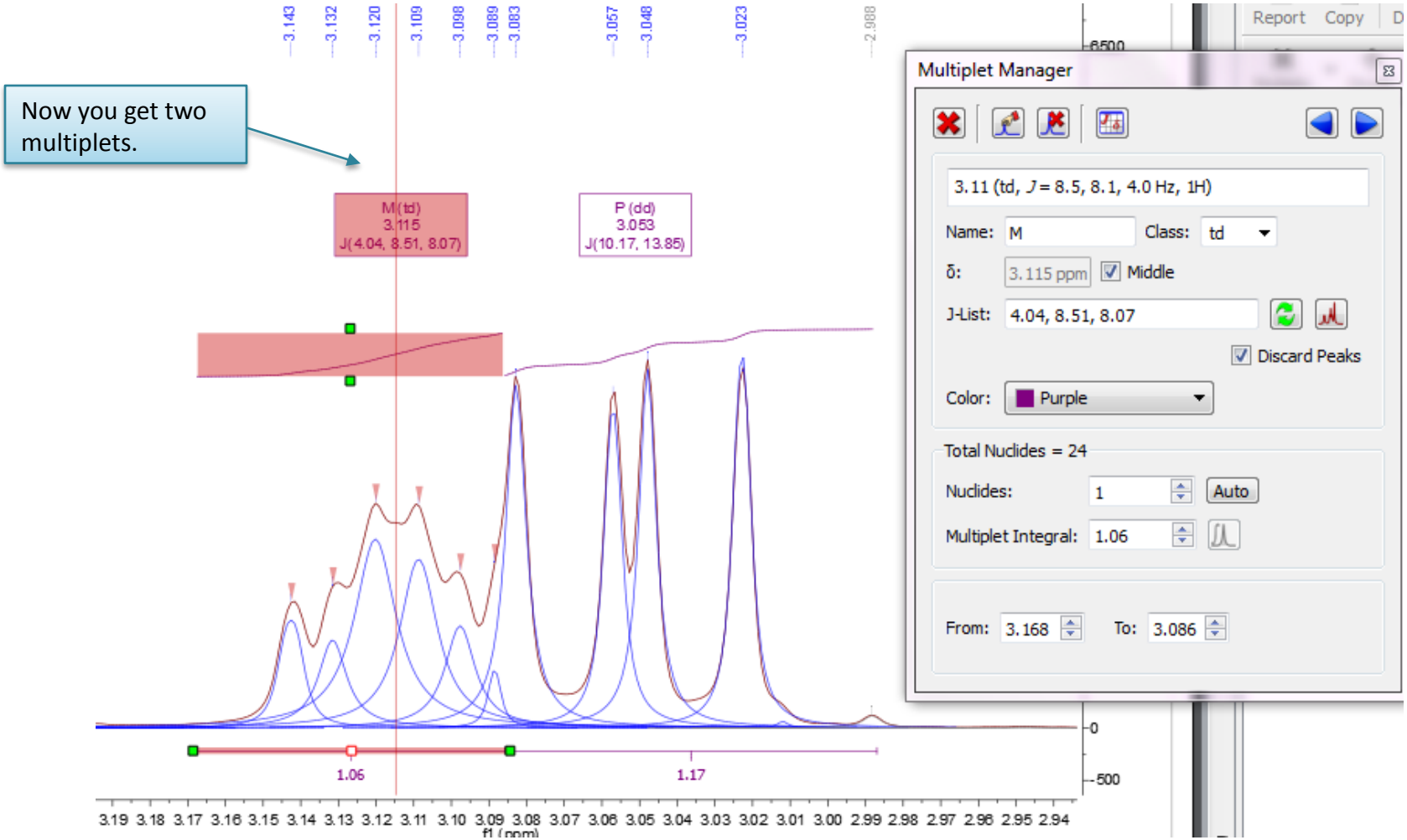
Expand the Peak Picking Tool menu, check Show Peak Curves to display the GSD peaks (displayed in blue).



Drag this red box to where you want to split the multiplet into two.

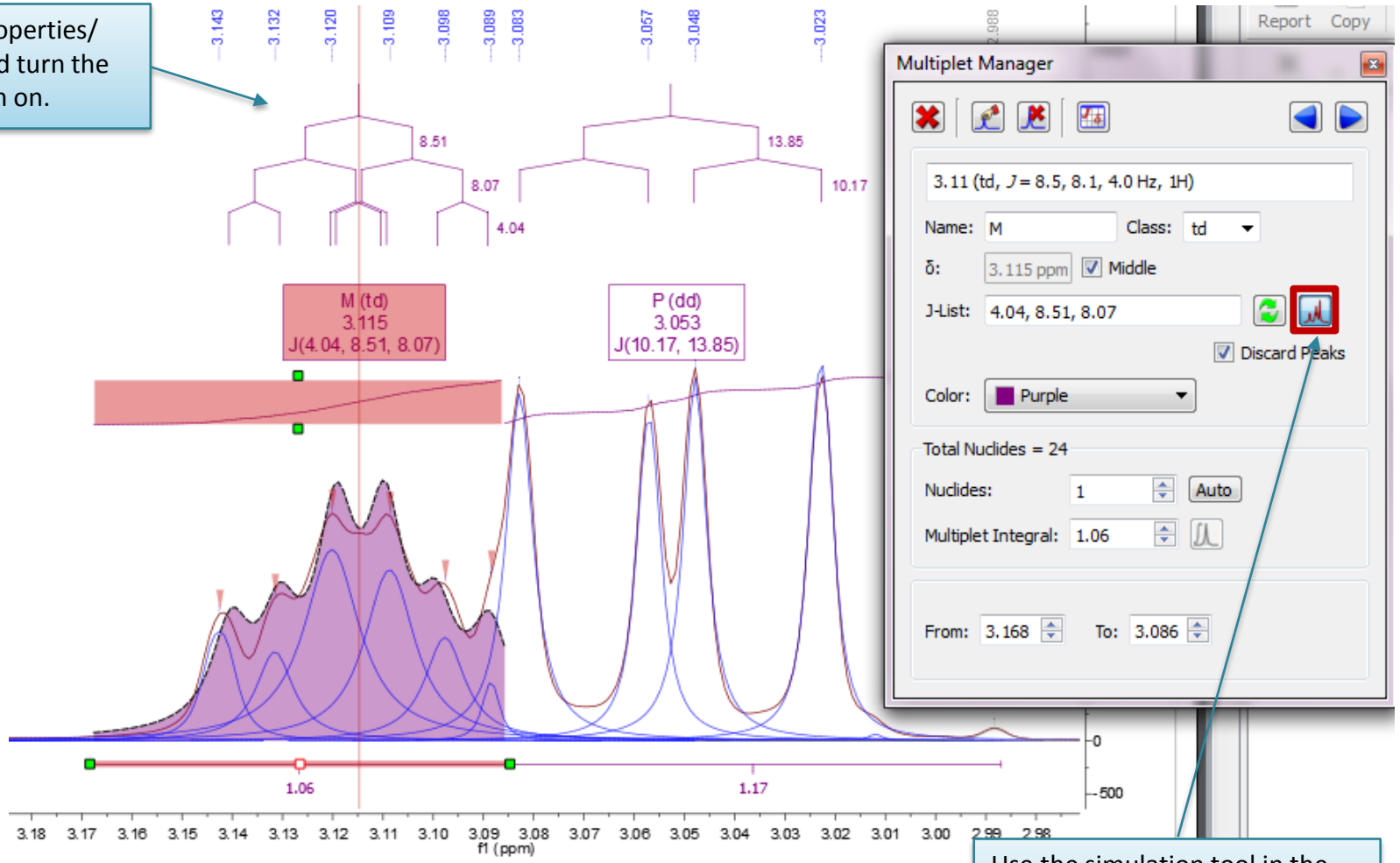
Tip: You can also change the display of the deconvolution peak curves in the Properties Dialog > Peaks > Curve tab.

Split partially overlapping multiplets (2)



Tools to verify multiplet analysis results

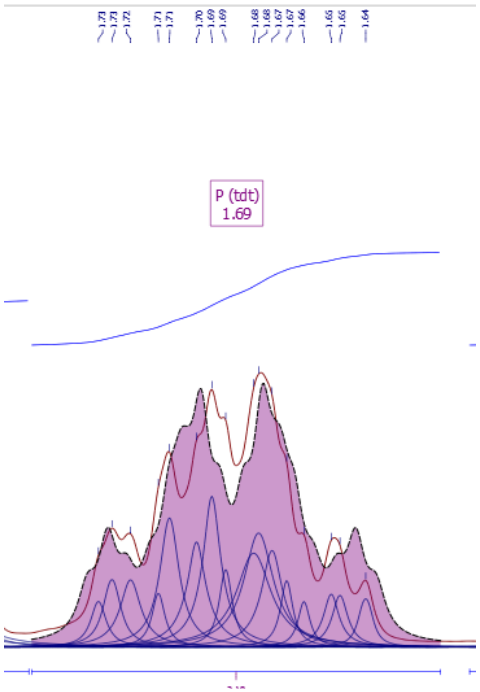
Go to Edit/Properties/ Multiplets and turn the J's Tree option on.

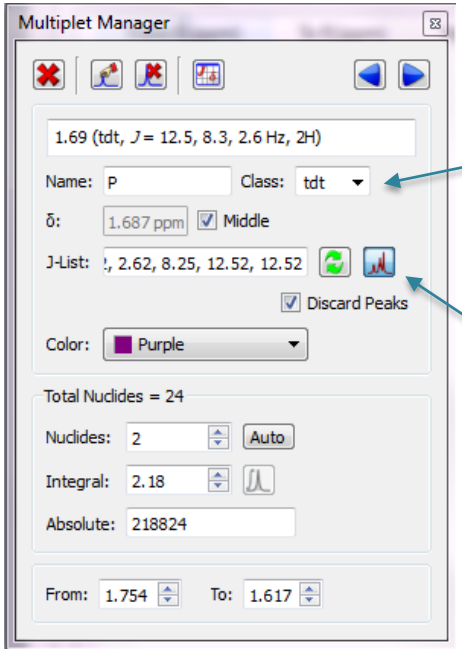


Use the simulation tool in the Multiplet Manager to simulate the multiplet and compare.

Override the multiplet results with the Multiplet Manager

- You can override the analysis results of a multiplet in Multiplet Manager.
- In this example, the multiplet was over-fit as a “tdt”. The simulated multiplet does not agree with the observed spectrum and hence it is wrong.
- Select “m” from the drag-down menu of Class to override it.



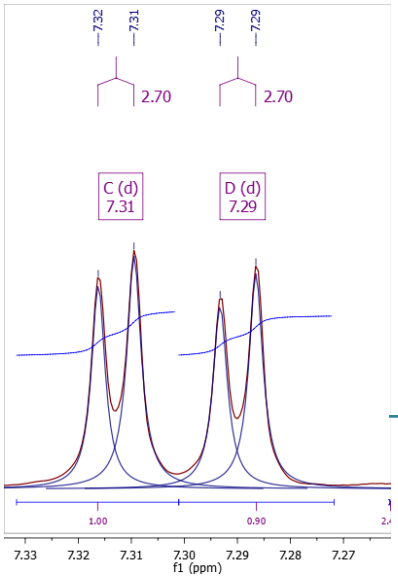


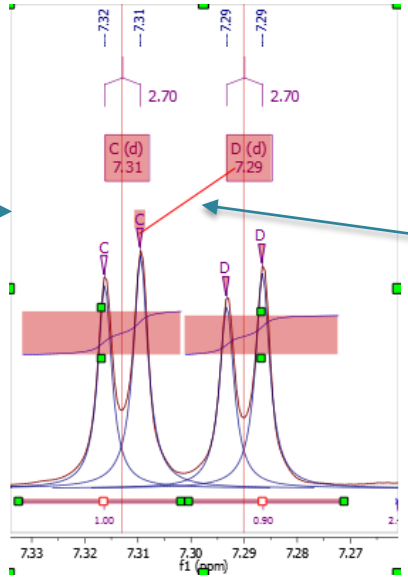
Choose “m” from the drop-down menu to override the results.

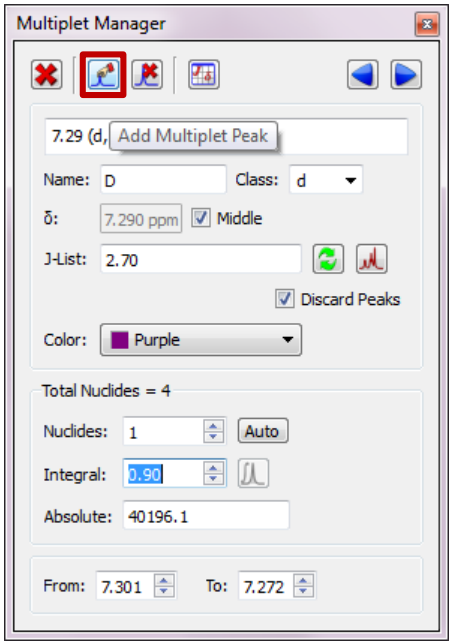
Use the simulation tool to simulate the multiplet and compare.

Re-assign peaks to multiplets

- If a peak is assigned to a wrong group, use the Add Multiplet Peak tool in the Multiplet Manager to re-assign it to a different group
- In the following example two peaks were re-assigned, forming a different pair of doublets:



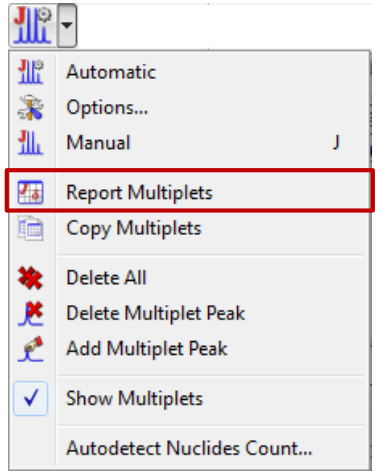


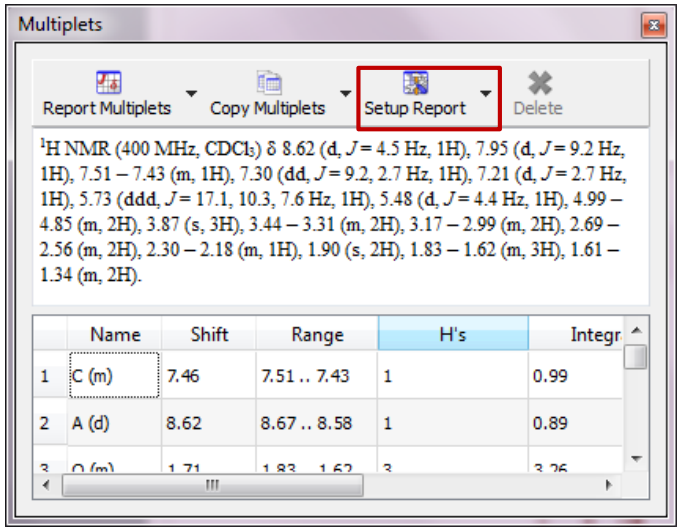


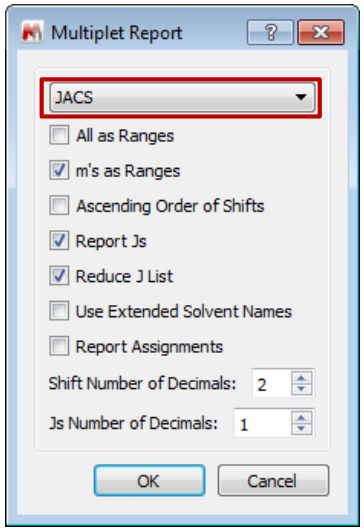
Click on the triangle mark on top of the peak, drag it to the multiplet label "D" to assign it to a different group.

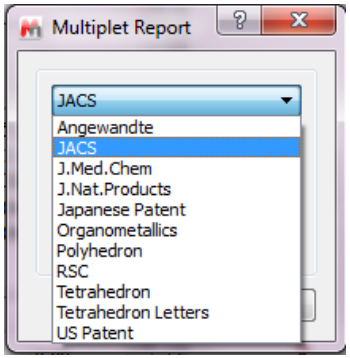
Report multiplets

- Click on **Report Multiplets** to report the results in a particular journal format.
- To change the journal format: Go to **View/Tables/Multiplets** to display the Multiplets Table. Then click on **Setup Report.**





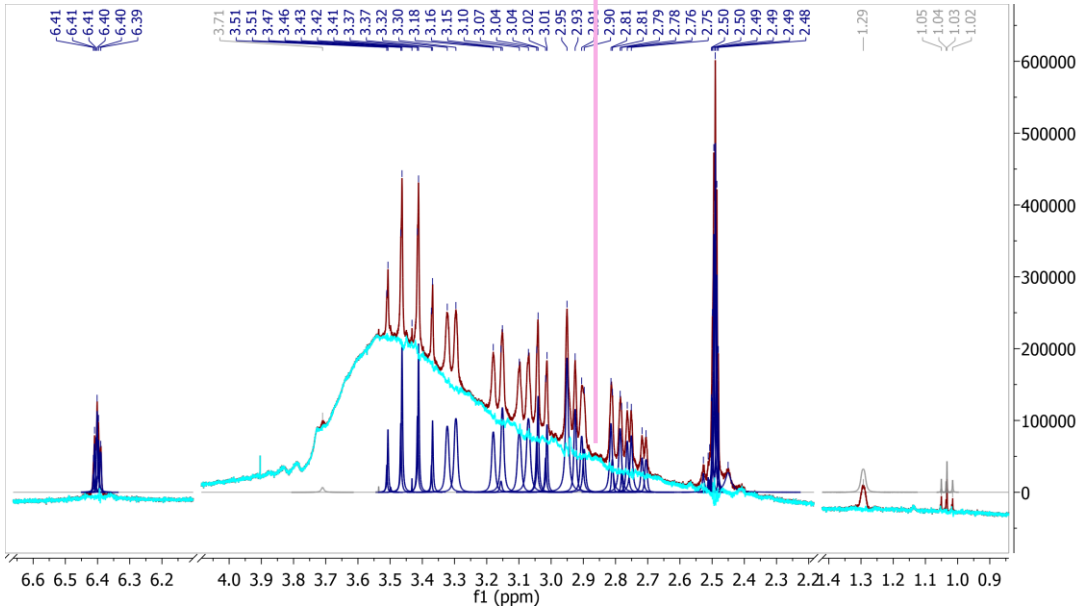


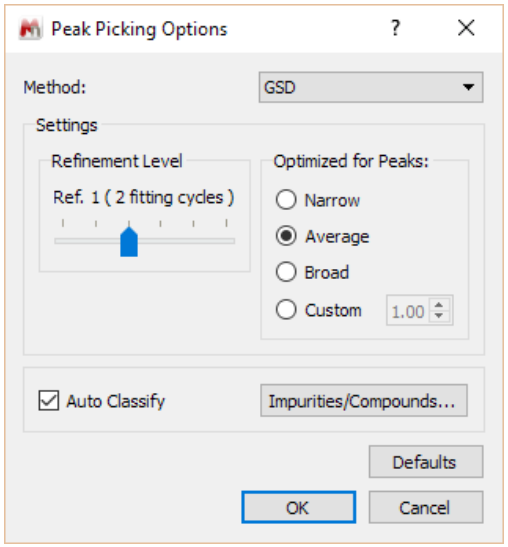


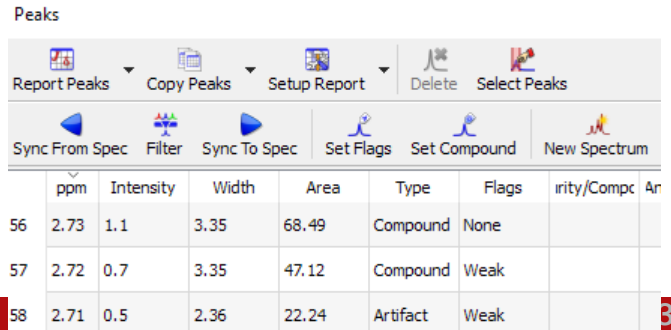
*Tip: From the Multiplet Table, click **Copy Multiplets** and then paste the texts to your document. Click on **Copy Table** and then paste the spreadsheet to your document. The table can be customized using **Setup Table.***

GSD Peak picking

- When you do peak picking or multiplet analysis , by default, Mnova does a global spectral deconvolution (GSD), and uses the deconvolved peaks as peak picking results.
- Go to **View/Tables/Peaks** to see the results in the Peaks Table.
- You can choose to display the deconvoluted peaks (blue) and the residuals (cyan) as shown below.





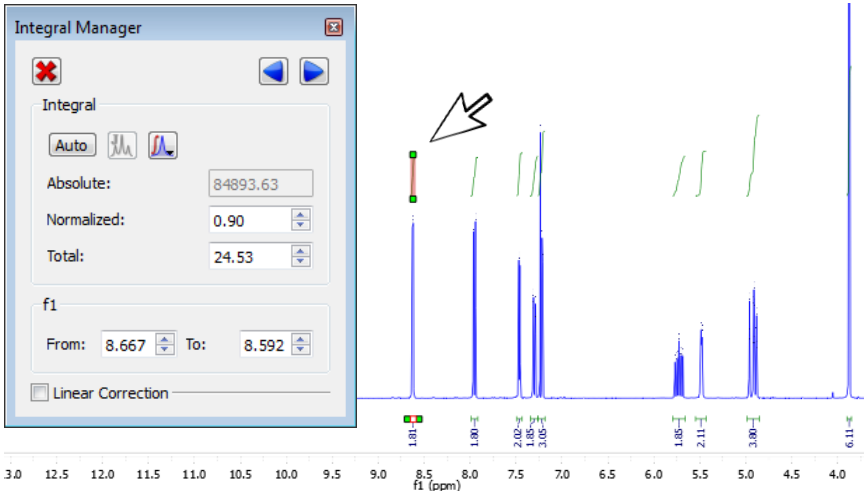


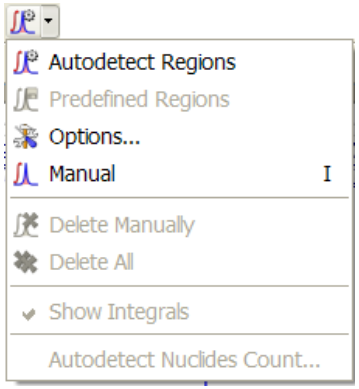
	ppm	Intensity	Width	Area	Type	Flags	
56	2.73	1.1	3.35	68.49	Compound	None	
57	2.72	0.7	3.35	47.12	Compound	Weak	
58	2.71	0.5	2.36	22.24	Artifact	Weak	

See more details about GSD:
http://mestrelab.com/resources/gsd

To integrate peaks independent of multiplet analysis

- Press  to do auto integration or press "**I**" to do it manually.
- Double click on an integral curve to popup the Integral Manager:

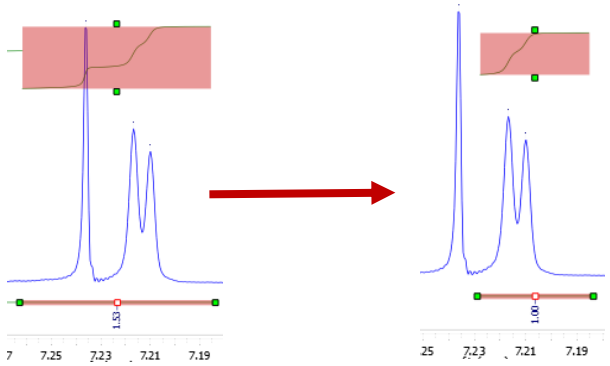




** Note: The results from Integration is independent of those from the Multiplet Analysis.*
Use Integration Options to change the method and other parameters.

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

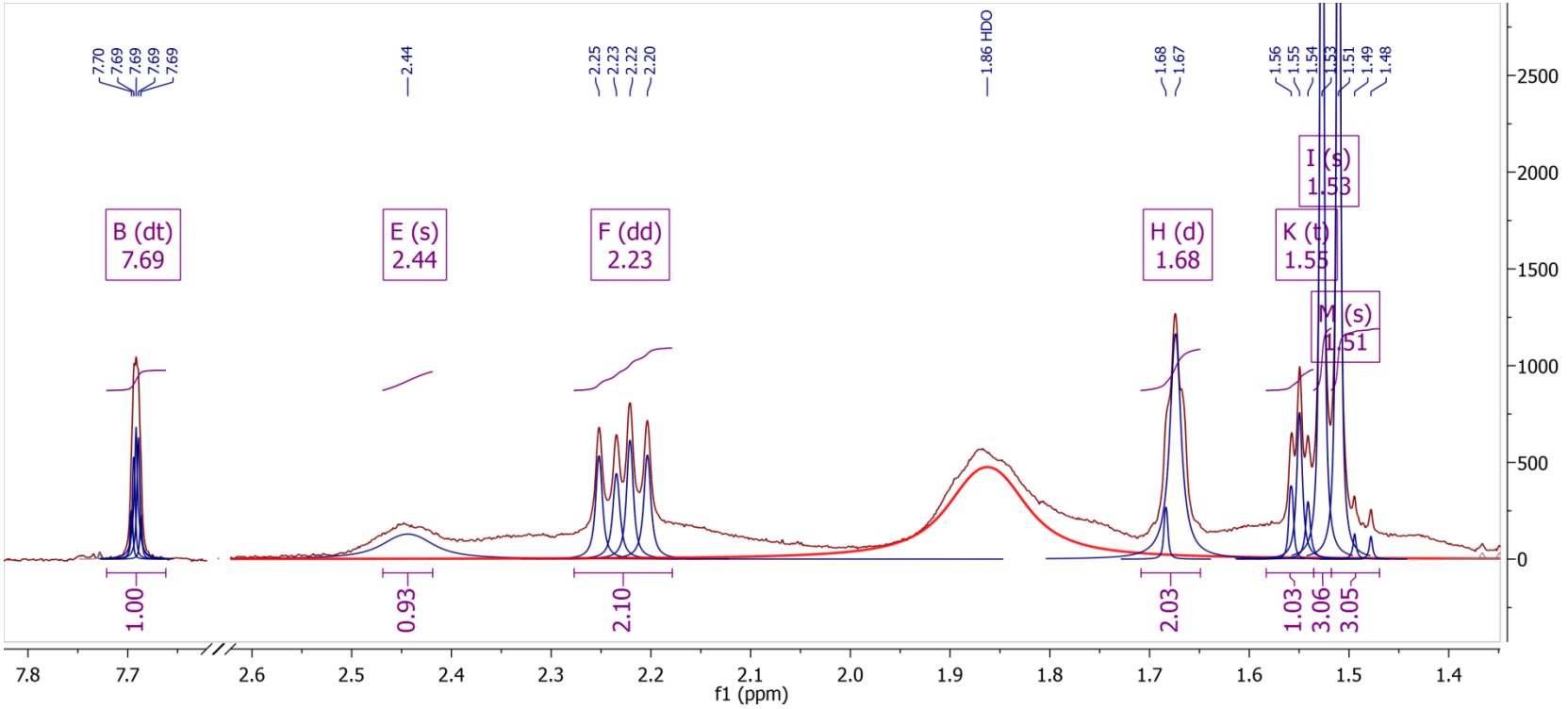
Click and drag the left green box to change the range of the integral.



Why are the integrals from multiplet analysis different from regular integration? (1)

(GSD) Peaks based integration when running multiplet analysis

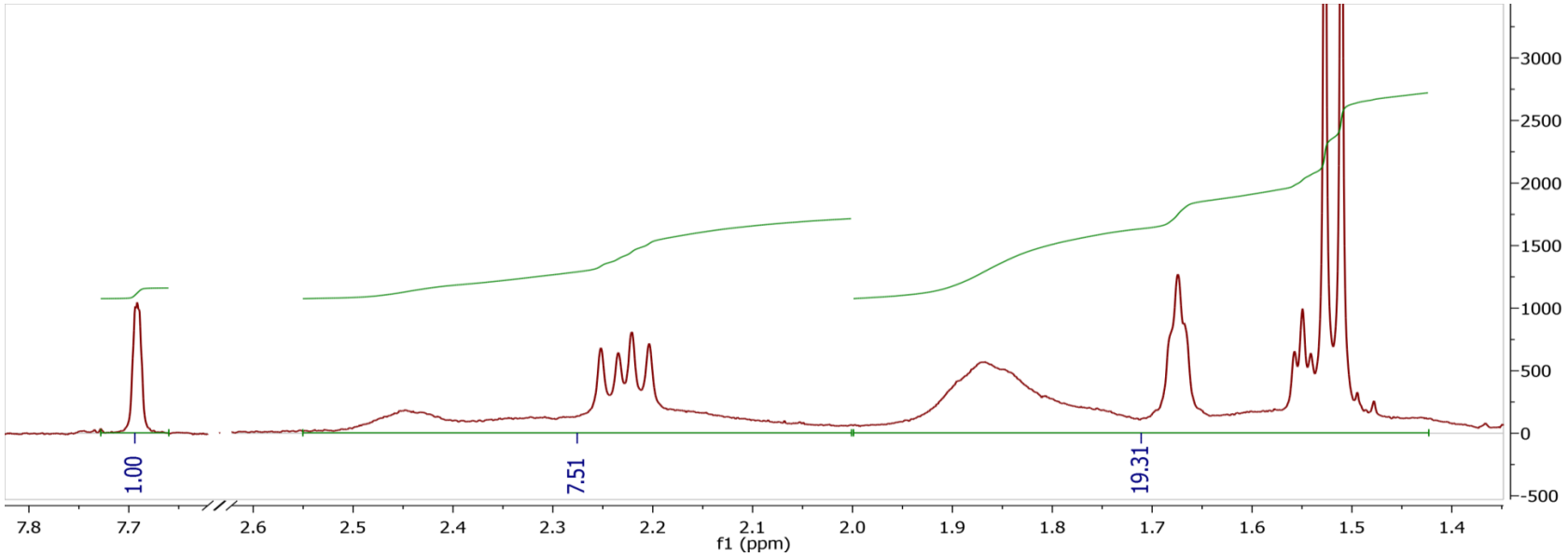
- When the peaks have irregular shapes, Peaks-based multiplet analysis may give significantly different integration results than regular (sum-based) integration.
- In the example below, Peaks-based multiplet analysis extracts the regular peaks but ignores the irregular ones usually due to exchangeable protons.



Why are the integrals from multiplet analysis different from regular integration? (2)

Sum-based integration when running multiplet analysis

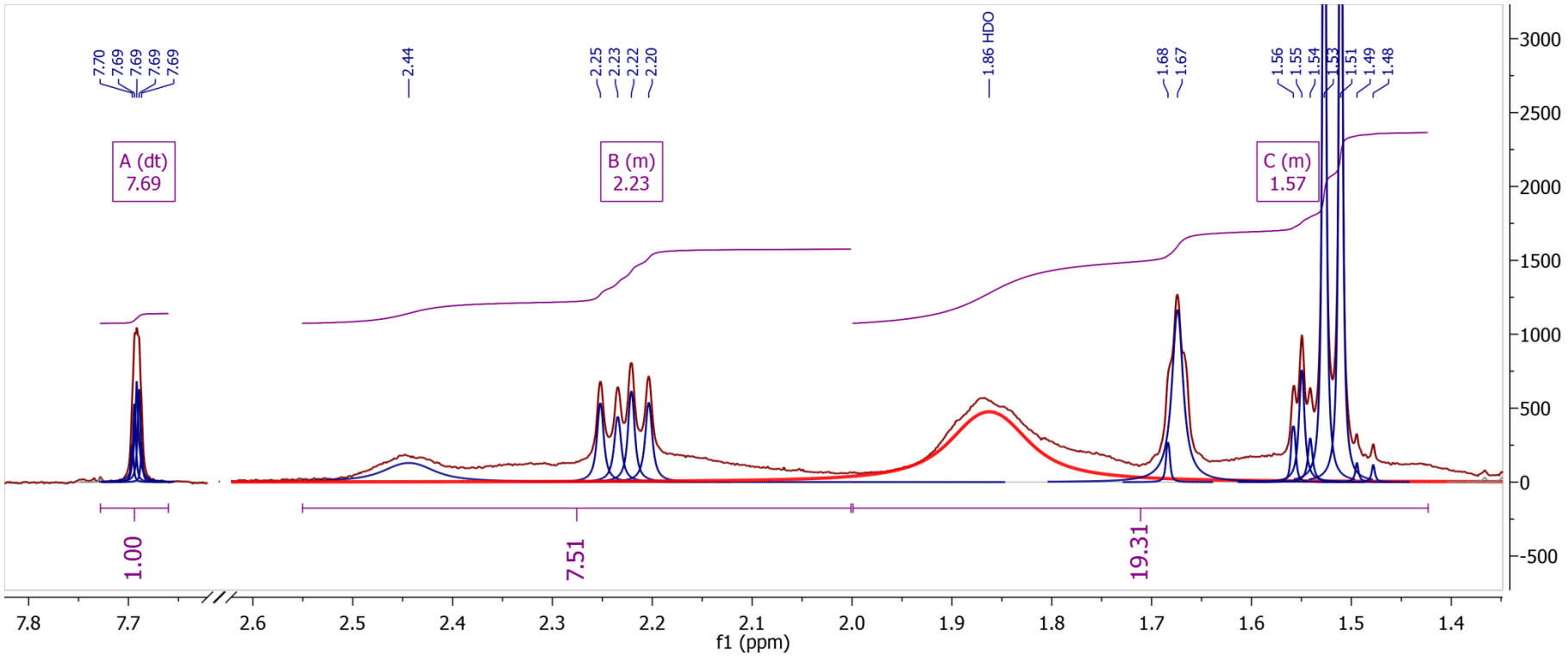
- When you do regular (sum-based by default) integration, all peaks are included by adding point by point within the integration region
- Depending on the goal of the analysis, users must choose the appropriate integration method



Force to use the regular integration results in multiplet analysis

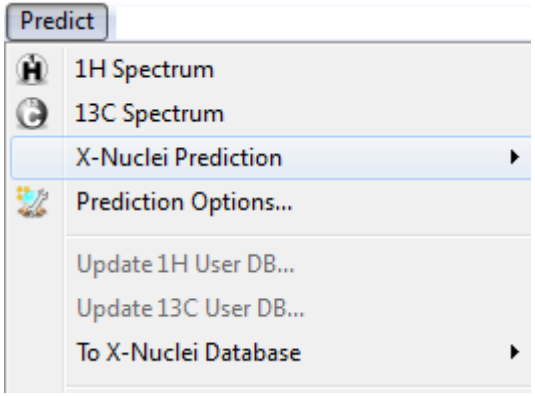
Combine Sum-based integration and multiplet analysis

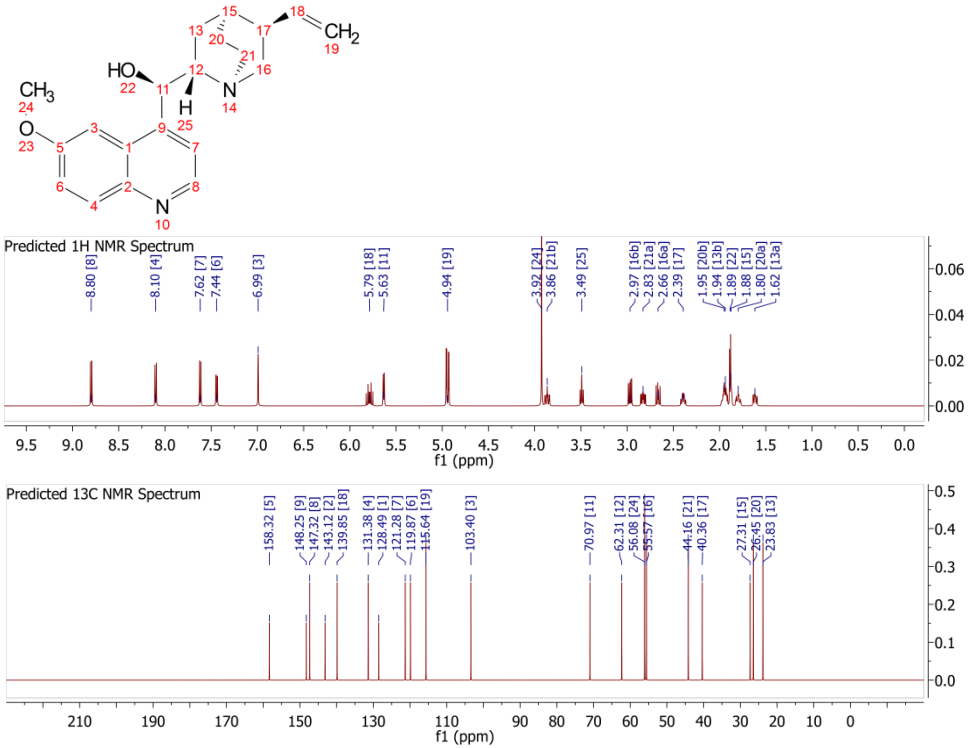
- If you do the regular integration prior to automatic multiplet analysis, the integration results (integration regions and integrals) will be retained for Multiplet Analysis.



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, .cdx or a .sdf file.
- Choose a command from the **Predict** menu.





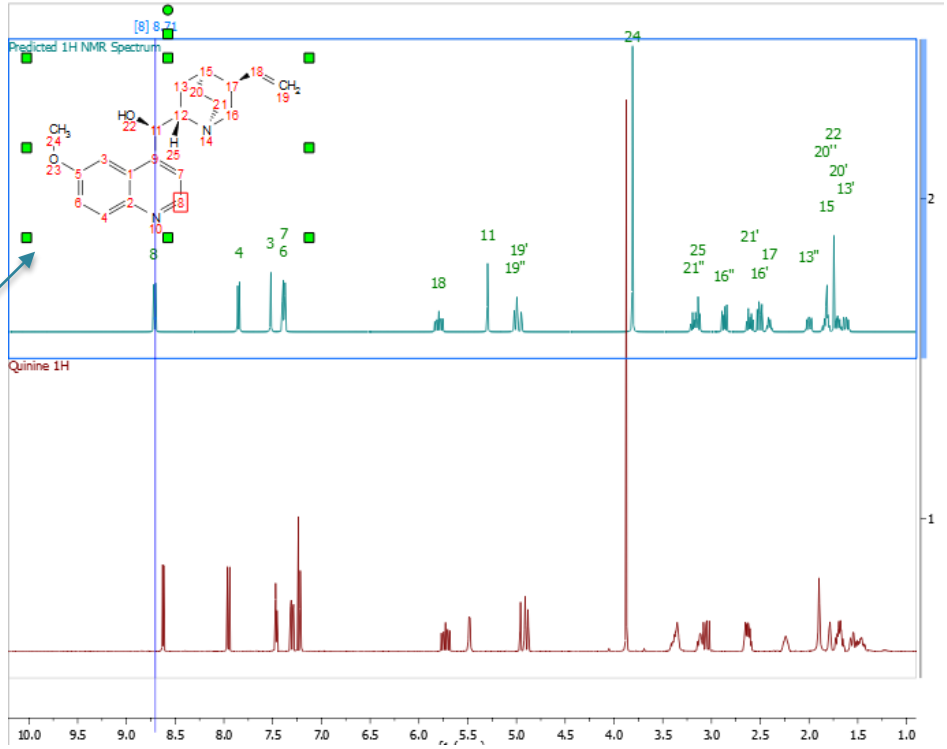
Tips:
*1. Choose **Predict|Prediction Options** to change settings.*
2. You can turn on/off the atom numbers by right-clicking on the structure and choose Properties.
*3. You can open the **Prediction Table** to list the predicted shifts and J-couplings, and manually change them.*

- *A separate license of Mnova NMRPredict Desktop is needed.*
- *The new Random Forest Prediction package is also available on Mnova 11.*

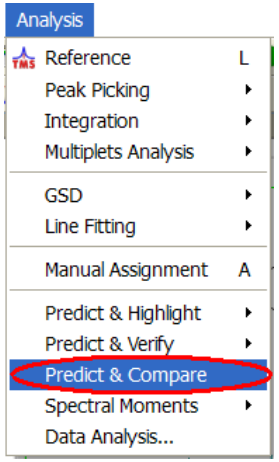
NEW ON Mnova 11.0

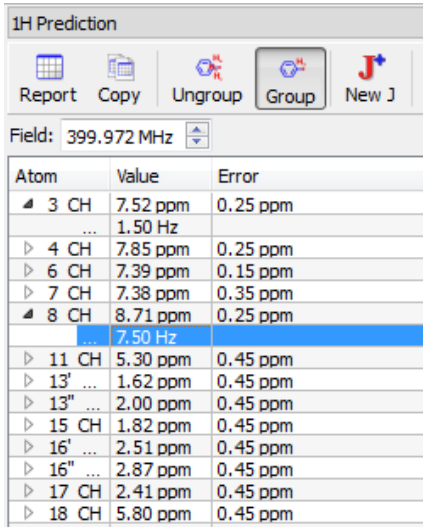
Predict NMR data & compare with your structure

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



You can drag the label of a predicted peak to change its chemical shift. You can also change the predicted *J*-couplings in the ^{1}H Prediction Table.

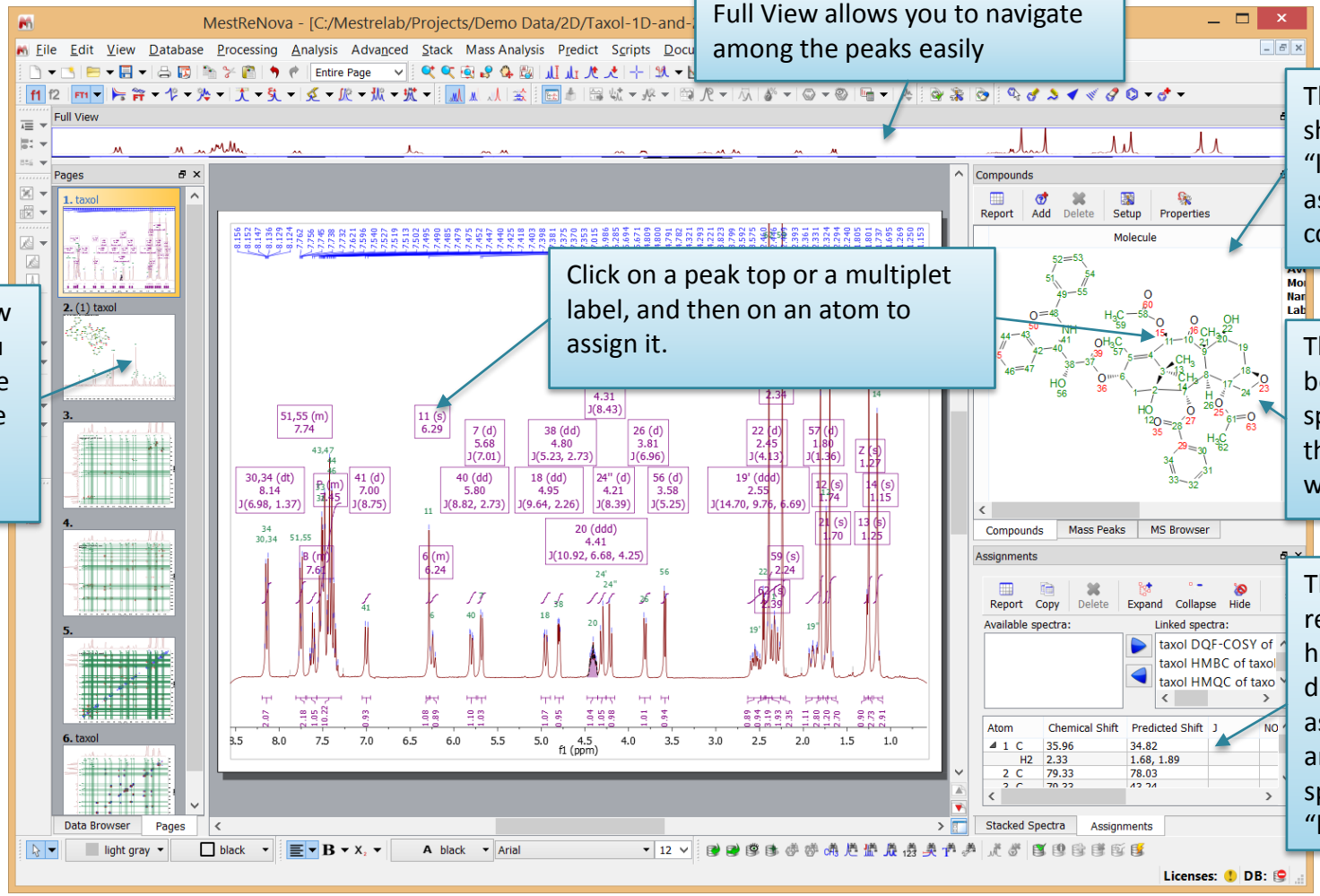




Mestrelab Research
chemistry software solutions

INTERFACE

Efficient working environment for peak assignment for multiple spectra



Full View allows you to navigate among the peaks easily

The structure(s) is shared for all "linked" spectra and assigned peaks are color coded

Pages View allows you to navigate among the spectra easily

Click on a peak top or a multiplet label, and then on an atom to assign it.

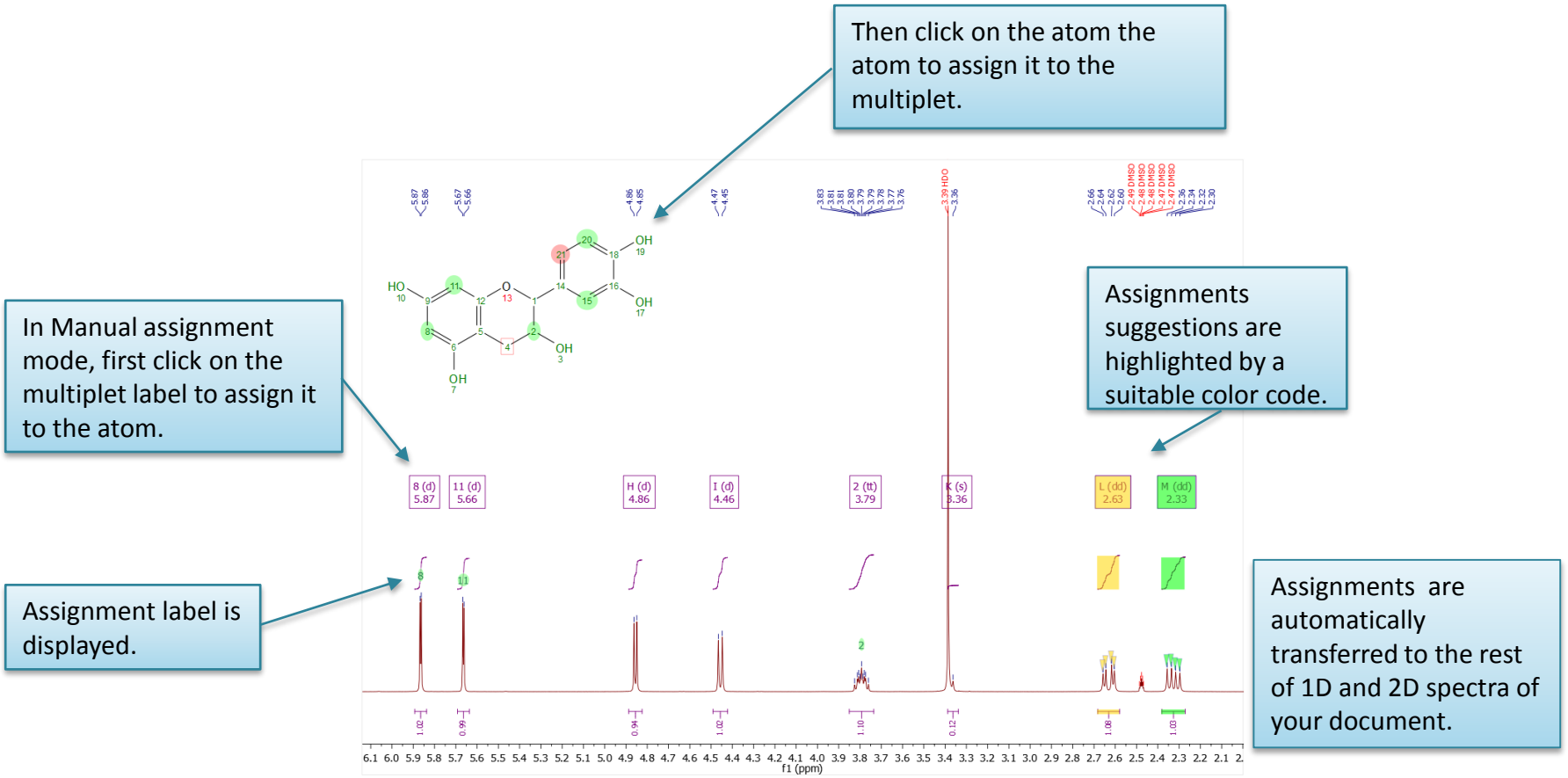
The structure can be shown on the spectrum plot or in the compound window

The assignment results are listed here. You can delete or change assignments here, and choose which spectra to be "linked"

Tip: Don't mix spectra from different samples in the same document. Don't open the same structure multiple times. Instead, use the Compounds Table to report the structure to the spectrum when needed. You can copy/paste and display multiple spectra side-by-side on the same page.

Assign a multiplet to an atom

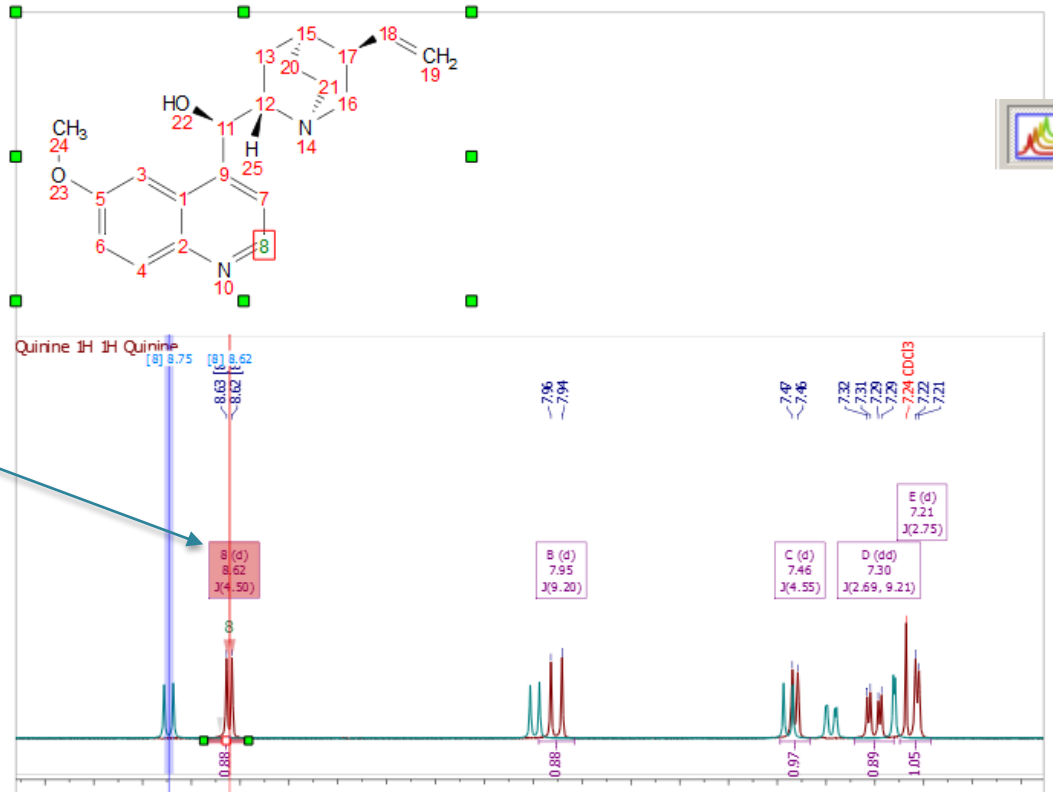
- Press the **A** key (or choose **Analysis/Manual Assignment**) to enter Manual Assignment mode:



Tip: After the assignment, the atom label is changed to green. The multiplet label shows the atom label. The multiplet label can be turned off by unchecking Analysis /Multiplet Analysis /Show Multiplets

Predict NMR & help you assign peaks

- Open your ^{1}H (or ^{13}C) **spectrum** in a new page, do multiplet analysis or peak picking as usual
- Copy your **structure** from ChemDraw or Isis/Draw.
- Go to **Analysis/Predict & Compare.** The predicted spectrum is stacked with the experimental one for visual comparison.
- Switch to **Superimposed Mode** so you can assign the multiplets/peaks guided by the predicted peaks.

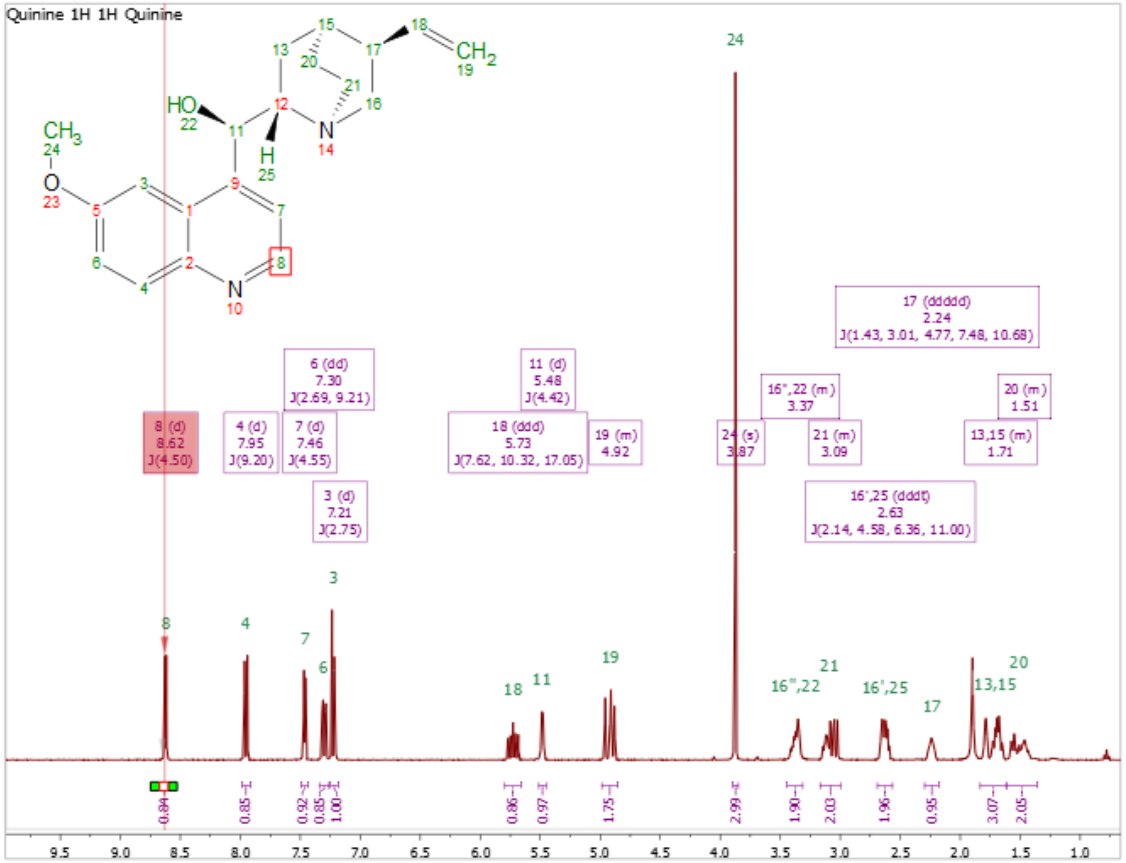


Use Shift + Up Arrow key to change the active spectrum and see the multiplet labels as well as predicted peak labels. In Assignment mode, click on a multiplet label and then on an atom to make the assignment.

Blue: predicted peaks
Red: observed peaks.

Automatic assignment of ^{1}H spectrum*

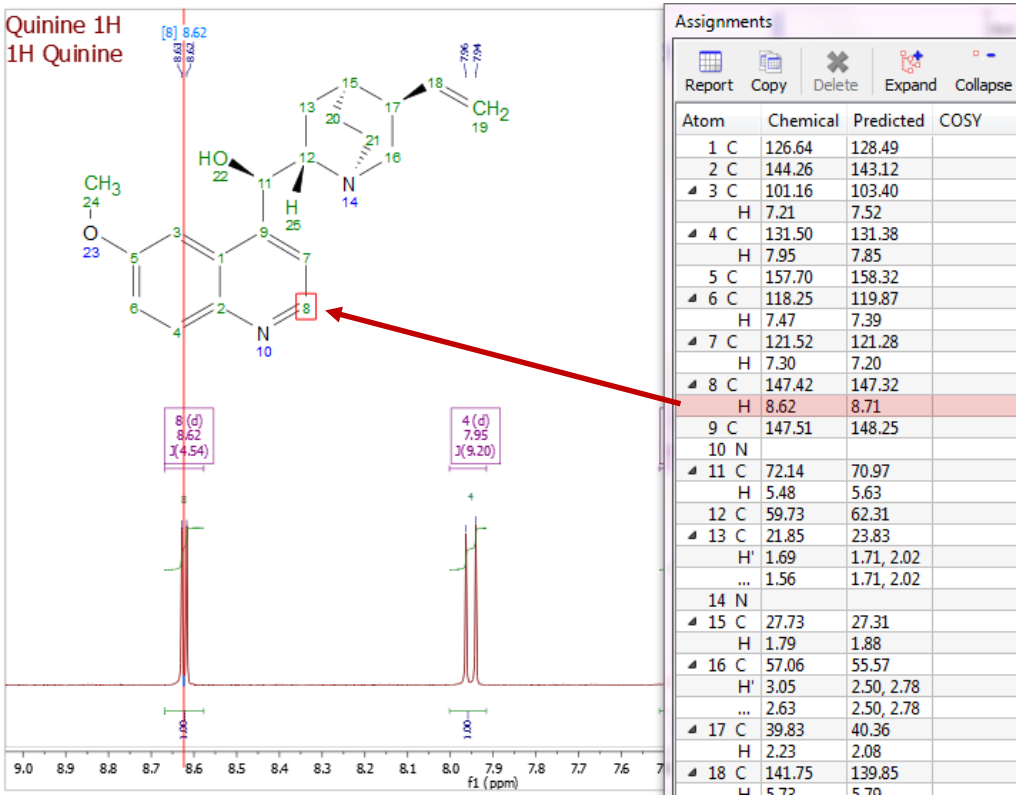
- Open your ^{1}H **spectrum** in a new page, copy your **structure** from ChemDraw or Isis/Draw.
- Go to **Analysis/Automatic Assignment.** Mnova does multiplet analysis (if not done yet), predicts ^{1}H spectrum, and automatically assigns ^{1}H peaks.
- Automatic assignment is also available for 2D HSQC and 13C spectra.



**A separated Mnova NMRPredict Desktop license is needed in addition to Mnova NMR. The new Random Forest Prediction package is now also available with Mnova 11.*
Tip: you can do multiplet analysis and clean them up prior to auto assignment. Also, try ***Mnova Verify*** *that automatically verifies your proposed structures (http://mestrelab.com/software/mnova-verify/).*

Display and browse assignment results

- Go to **View/Tables/Assignments** to open the Assignments Table.
- The Table and the structure are correlated: You can click on a row to highlight the atom (and its assigned peak), and vice versa.

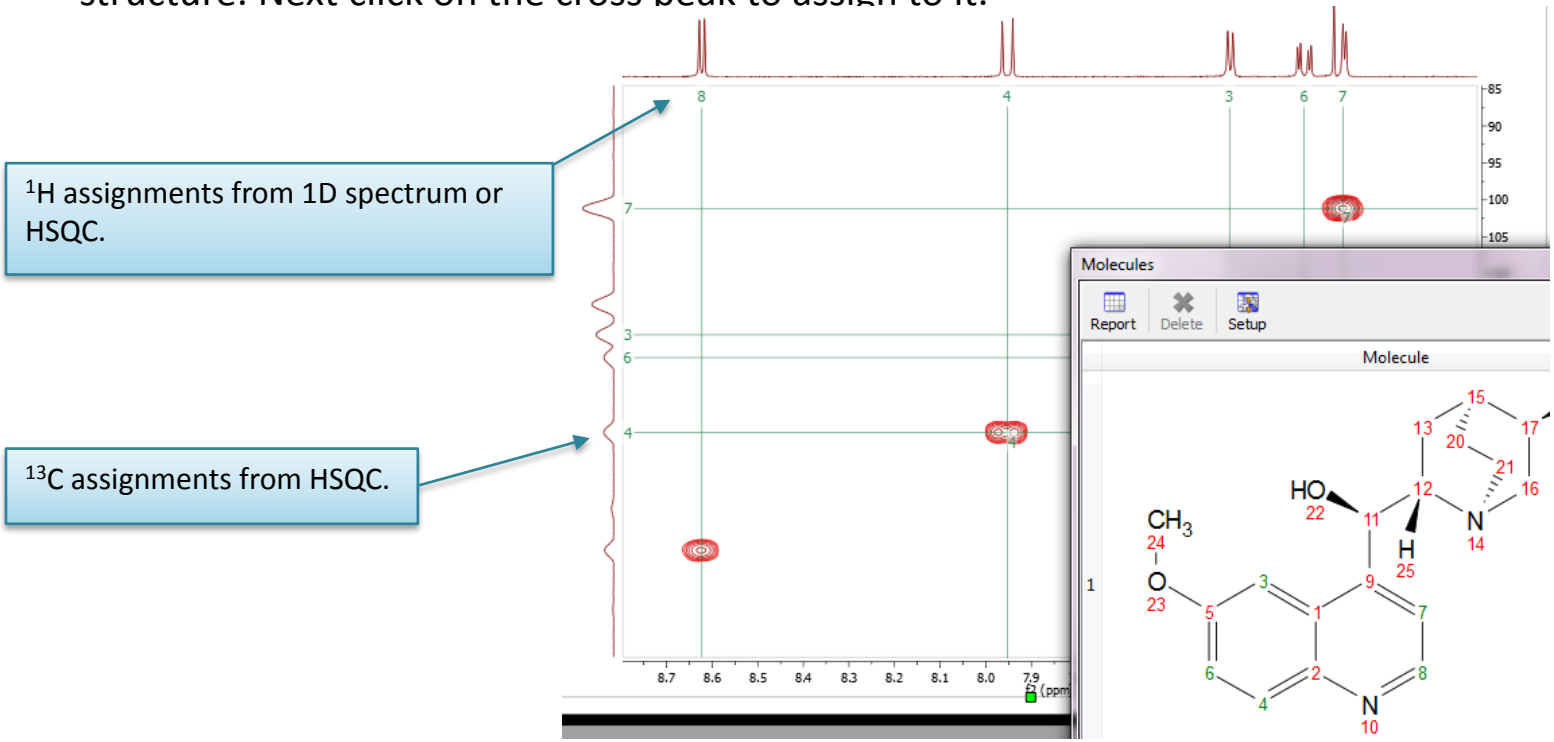


Atom	Chemical	Predicted	COSY
1 C	126.64	128.49	
2 C	144.26	143.12	
3 C	101.16	103.40	
H	7.21	7.52	
4 C	131.50	131.38	
H	7.95	7.85	
5 C	157.70	158.32	
6 C	118.25	119.87	
H	7.47	7.39	
7 C	121.52	121.28	
H	7.30	7.20	
8 C	147.42	147.32	
H	8.62	8.71	
9 C	147.51	148.25	
10 N			
11 C	72.14	70.97	
H	5.48	5.63	
12 C	59.73	62.31	
13 C	21.85	23.83	
H'	1.69	1.71, 2.02	
...	1.56	1.71, 2.02	
14 N			
15 C	27.73	27.31	
H	1.79	1.88	
16 C	57.06	55.57	
H'	3.05	2.50, 2.78	
...	2.63	2.50, 2.78	
17 C	39.83	40.36	
H	2.23	2.08	
18 C	141.75	139.85	

*Tip: You can right click on an atom and go to **Edit Atom Data** to change its label. Changed labels will be used in Assignments Table and other relevant reports.*

If you have 2D spectra

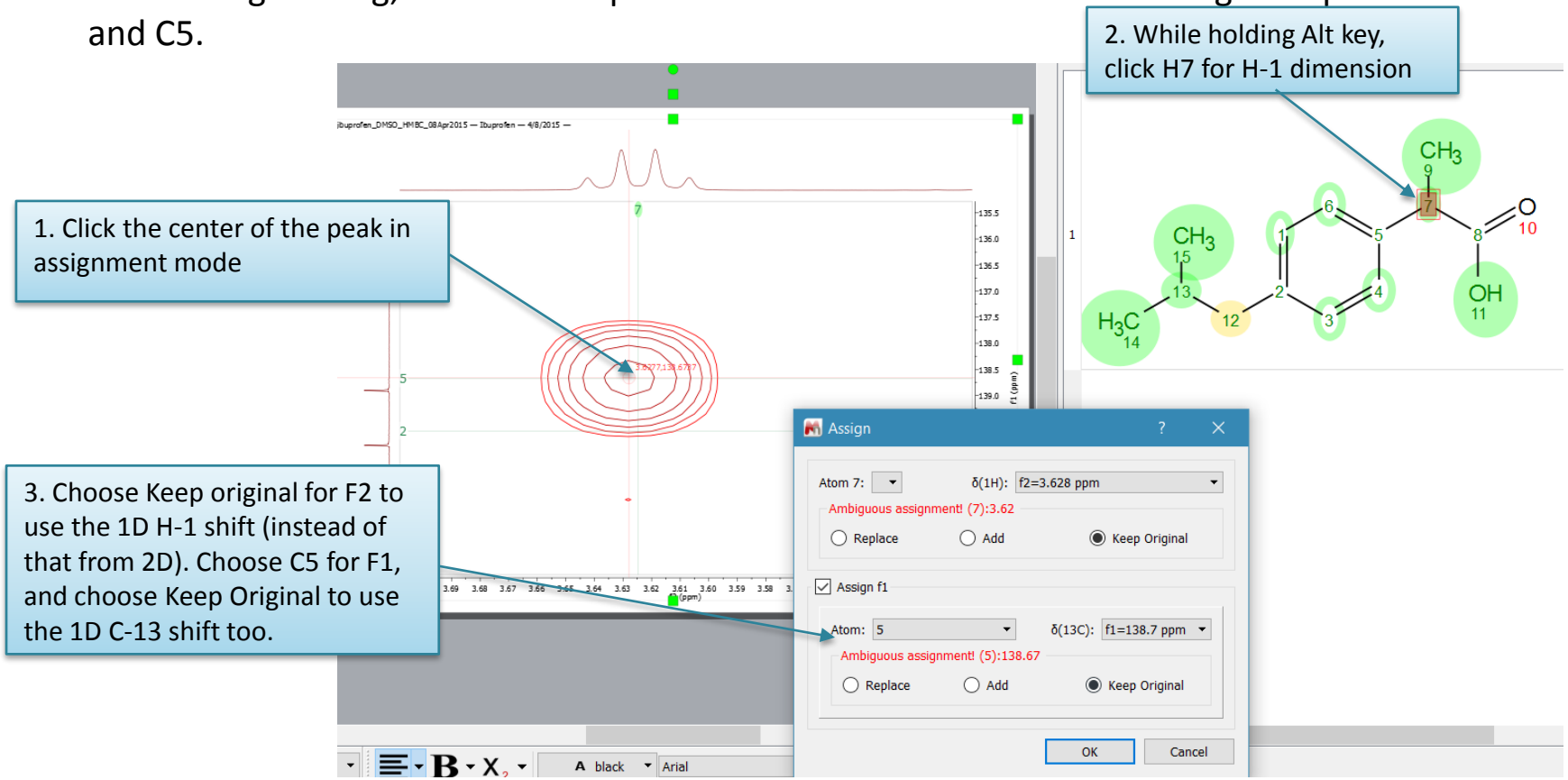
- You can first assign 1D ^{1}H peaks, and then assign for instance a HSQC cross peaks, or vice versa.
- Assignments in one spectrum are carried over to all other spectra in the same document:
  All spectra in the same document are "correlated" by default.
- To assign atoms in a HSQC, press the **A** key to enter in Assignment mode. Click on an **atom** in the structure. Next click on the cross peak to assign to it.*



*By Default, Mnova automatically snaps to a peak top (with interpolation). Press the ***Shift*** key one time to toggle it off if you want to manually locate the peak center. To see more choices, press and hold ***Alt*** key while assigning a peak (New in Version 11).*

Assigning a HMBC peak

- In assignment mode, click the center of the HMBC peak shown below, and then click on H7 while *holding Alt key*. *
- In the Assign dialog, choose the options as shown below. Click OK to assign the peak to both H7 and C5.

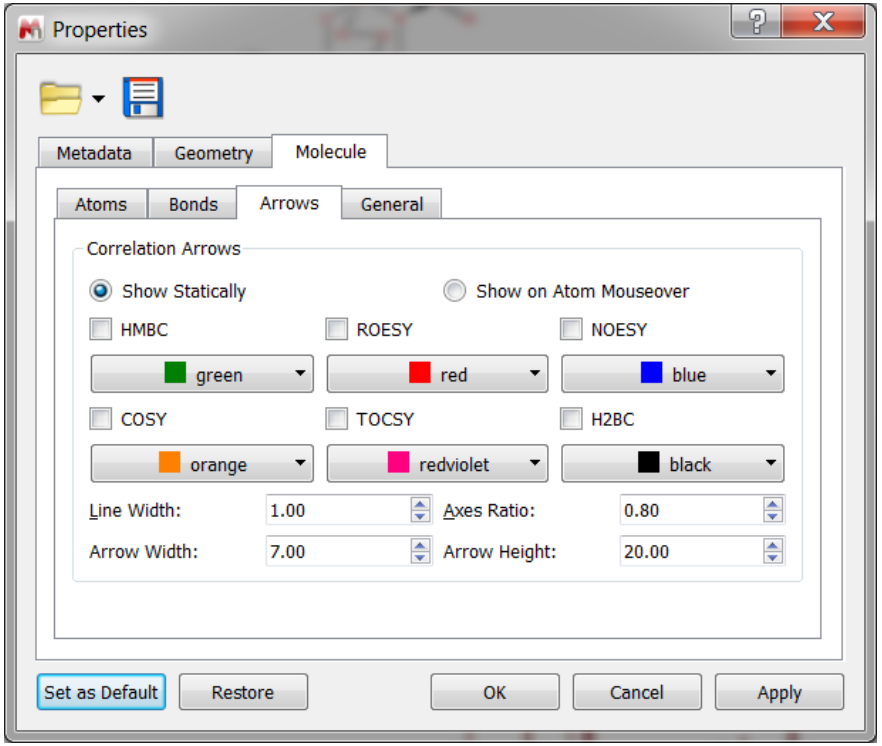


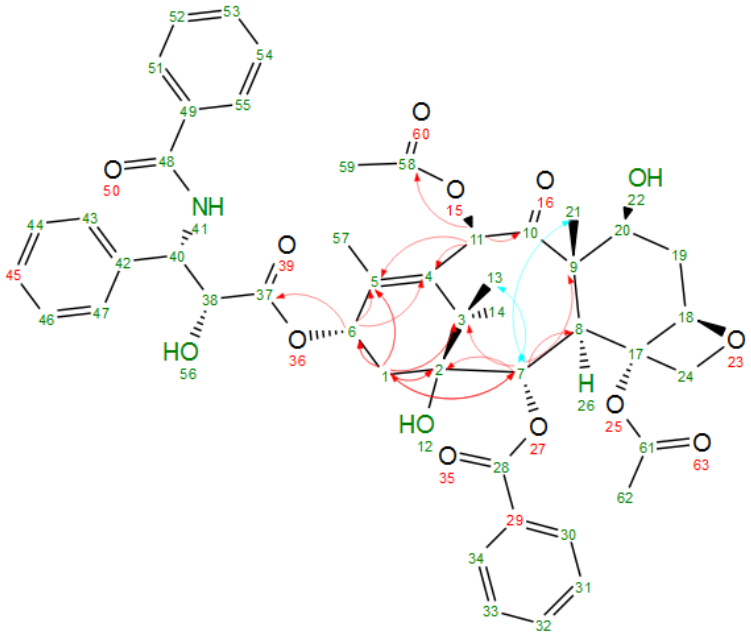
Since chemical shifts from 1D NMR is usually of higher resolution than 2D, we recommend you to use 1D shifts whenever possible. To access such choices, press and hold **Alt key while assigning a peak (New in Version 11).*

Display HMBC and NOE assignments

NEW ON MNOVA 11.0

- Report the structure from the **Compounds Table** *
- Edit/Properties to change the **display properties** of the structure
- Choose to display the **HMBC/ROESY/NOESY connectivities** for assigned atom pairs.

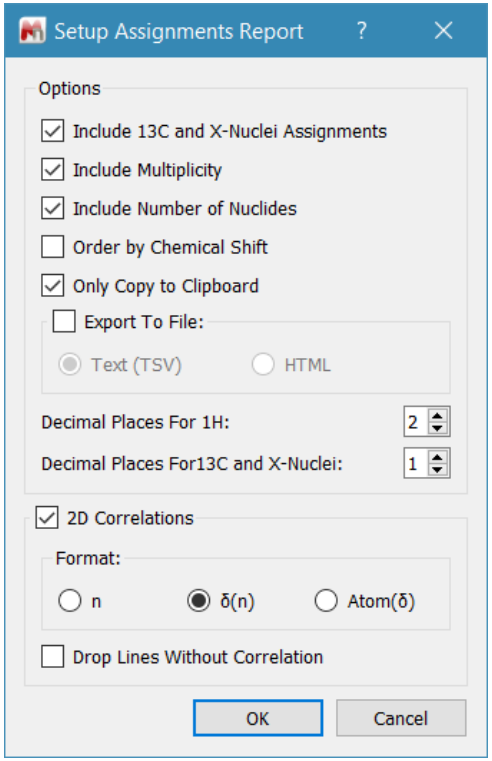




**Don't open the same structure multiple times. Instead, use the Compounds Table to report the structure to the pages where needed.*

Report peak assignment in journal format

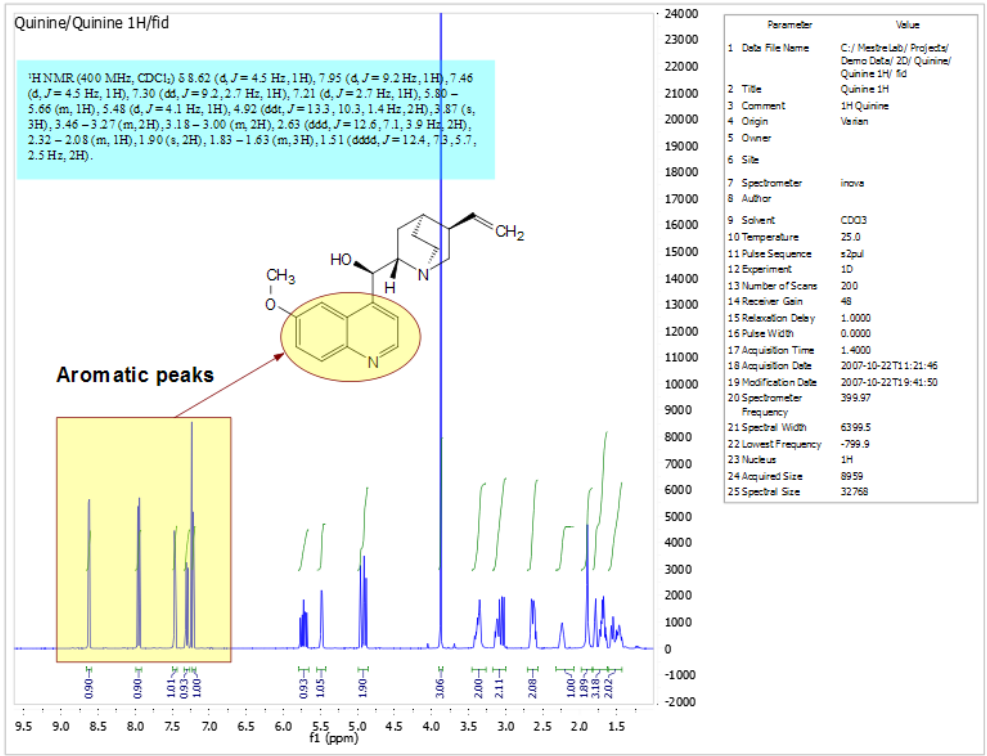
- Go to **Script/Report/Peak Assignments** to report the assignment results in journal format.
- The report can be pasted to an MicroSoft Word or Excel document.

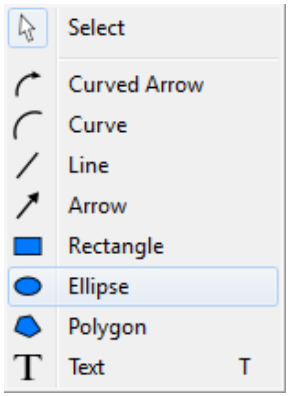


No	δ_H	Multiplicity, *J* (Hz)	δ_C	HSQC	HMBC	NOESY
1	2.33		35.96	35.96(1)	72.58(6), 75.23(7),79.33(2), 79.33(3), 142.19(5)	
2			79.33			
3			79.33			
4			133.45			
5			142.19			
6	6.24	m	72.58		133.45(4), 142.19(5), 172.90(37)	
7	5.68	d,J=7.01 Hz	75.23	75.23(7)	35.96(1), 45.90(8), 58.88(9), 79.33(2), 79.33(3)	3.81(26)
8			45.90			
9			58.88			
10			203.81			
11	6.29	s	75.80	75.80(11)	133.45(4), 142.19(5), 171.41(58), 203.81(10)	3.81(26)
12	1.74	s				
13	1.25	s	27.11	27.11(13)		
14	1.15	s	22.03	22.03(14)		
17			81.42			
18	4.95	dd,J=9.64,2.26 Hz	84.64	84.64(18)		3.81(26)

Annotate and report manually

- Press the **Annotation Options** button at the bottom-left corner of Mnova window and use the annotation tools there.
- The display of the objects can be customized by right clicking on it and then selecting **Properties.**
- **Tables of Peaks, Integrals, Parameters** etc. can be opened by **View/Tables.** Contents in the tables can be reported or copied to other documents.

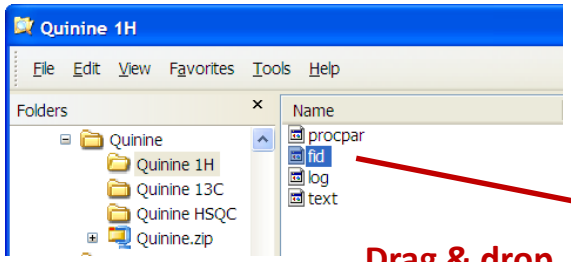




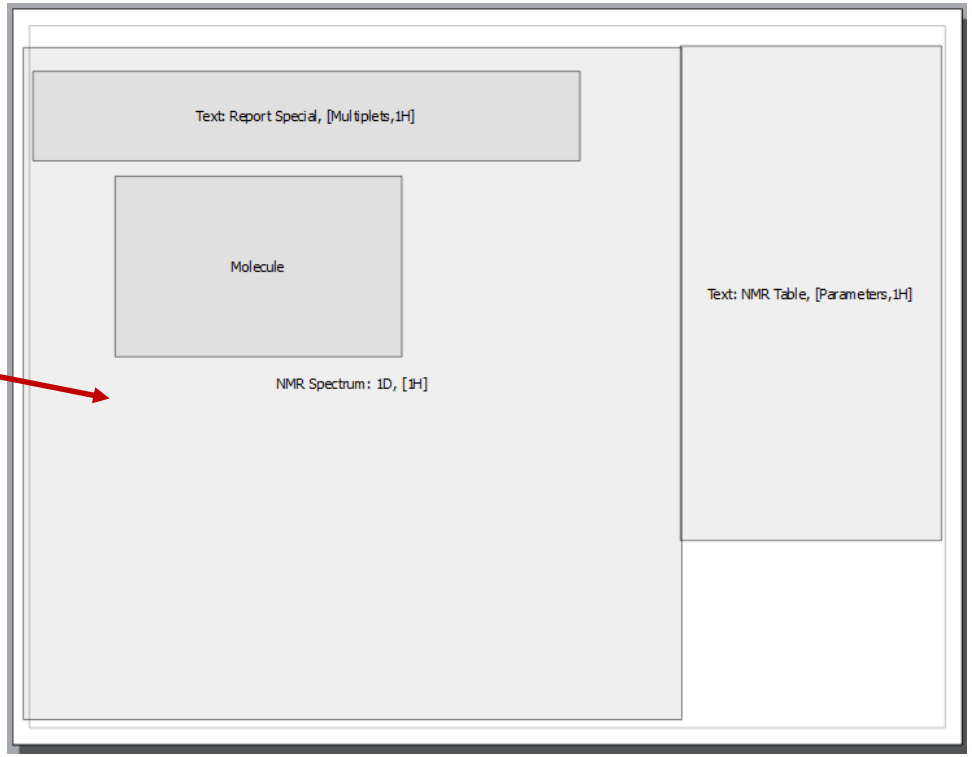
Tips:
Copy a **molecule from ChemDraw or Isis/Draw, or open .mol or .sdf files.*
Use **View /Layout Templates menu to generate and apply layout templates, or request an auto **formatting script** from Mestrelab.*
****Copy/paste** any object(s) to your document with high resolution.*
Click to export **PDF.*

Create a layout template

- Once you are satisfied with the layout, choose **View/Layout Template/Create Layout Template Document**, and save the layout.
- You can continue to edit the template.
- Once ready, open a new FID or structure to the template, and they will be auto formatted to the desired size and location.
- If you have a spectrum already opened, choose **View/Layout Template/Apply Layout Template Doc** to format it.



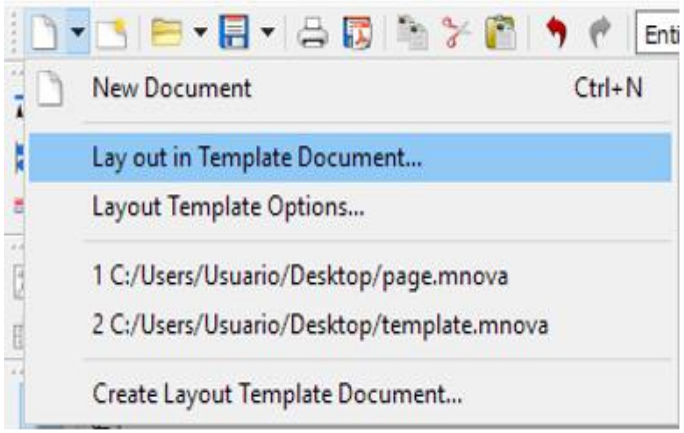
Drag & drop

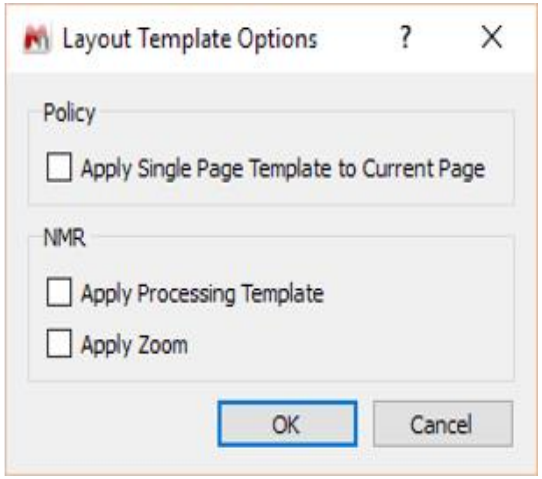


Apply layout templates to specific pages of a document

NEW ON MNOVA 11.0

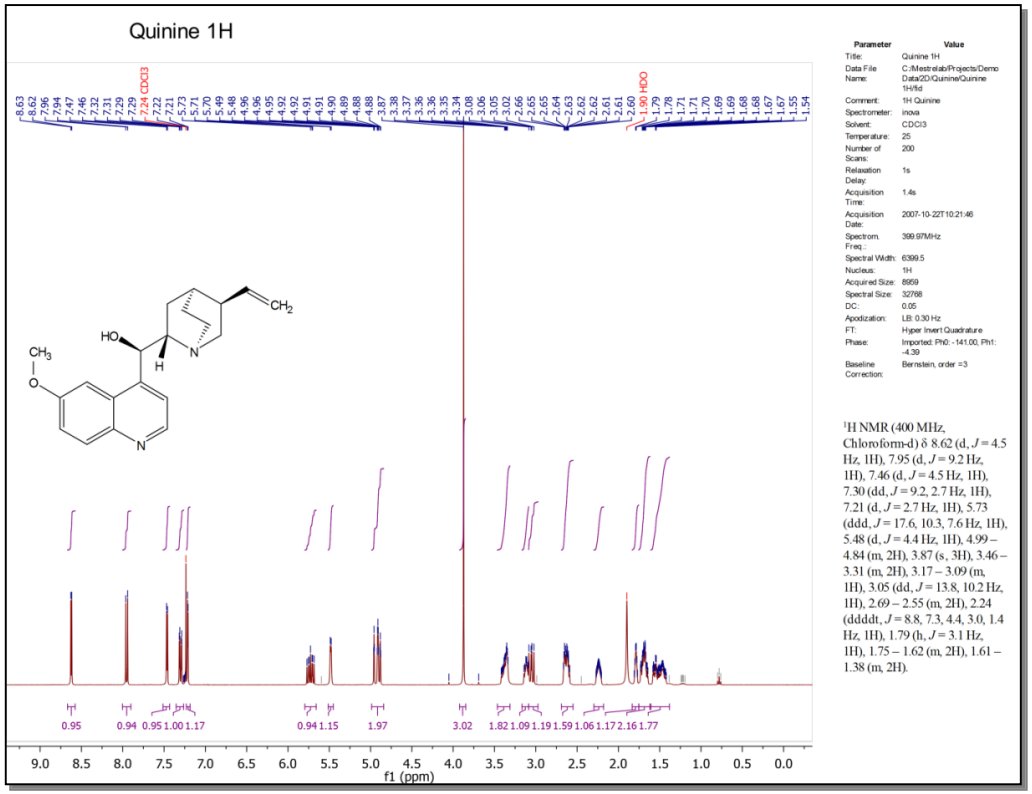
- A layout template can now be applied to a specific page of a document with several pages. The zoom ranges can also be set in the template.





Auto format using Mnova script*

- Mnova has a powerful scripting engine that allows you to automate many operations, including processing, analysis and reporting.
- The following is a sample output by running a Mnova script.



** Click http://mestrelab.com/scripts/ to download free formatting scripts. We also provide development service for more complex batch processing and reporting requirements.*

Auto Process, Analyze and Report

Example: Auto Process, Analyze and Report a 1D spectrum using an Mnova script (PAR.qs)*

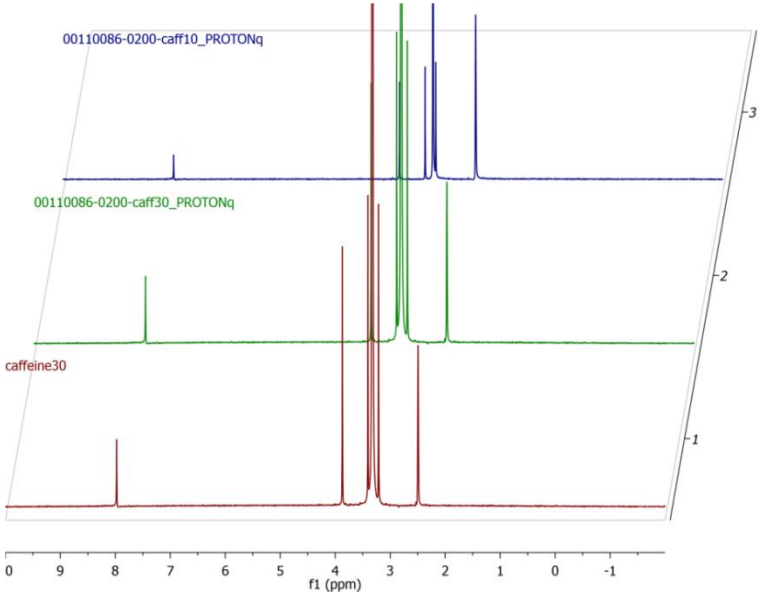
- Open a 1D ^{1}H spectrum, run this free script* for the first time. It does the following: **
  - Re-processing the spectrum with line broadening of 0.3 Hz, enhanced correction for Bruker Group Delay if applicable, zero-filling to double the data size or at least 64K points, and baseline correction using 3rd order Bernstein Polynomial.
  - Automated peak picking and multiplet analysis using the current options.
- Manually verify and correct the multiplet analysis results.
- Run the script *again*, and it generates a report similar to the one in the previous slide.
- You can easily customize the processing, analysis and reporting options by editing the script.
- This script also works for ^{13}C and other nucleus, in slightly different way (e.g., it picks and reports peaks instead of multiplets).
- This script does formatting only if it is a 2D NMR.

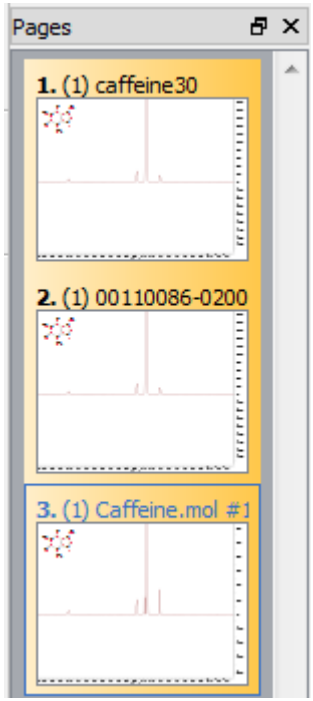
- *Write to support@mestrelab.com and ask for PAR.qs. It's free for academia. To run the script, first save it on your computer.*
- *Next choose Scripts > Run Script, and open it.*

*** You can edit the script and customize the settings.*

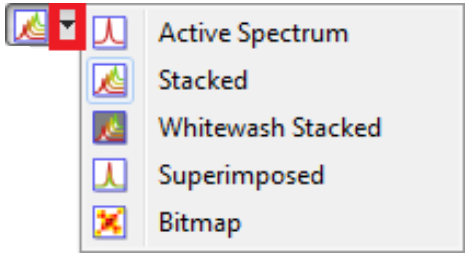
Open and stack multiple 1D spectra

- Open several 1D spectra in the same document.
- Select some or all of them in the Pages View.
- Press  to stack them in a new page:





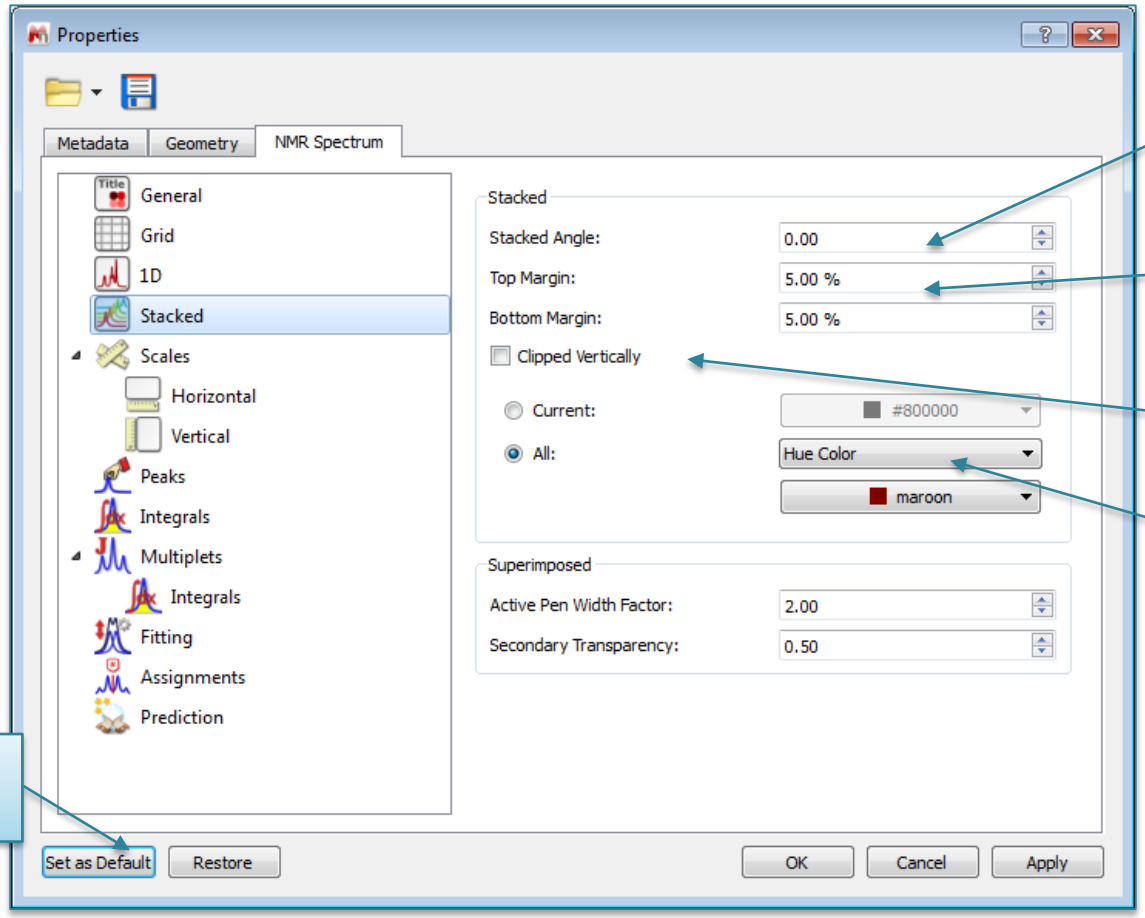
- Click  to change the display to another Stack Mode, such as the Superimposed mode.



Tip: - You can also drag a 1D from a different page to stack it to the current paae using the Pages View.
- When multiplet pages are selected, you can choose the ***Superimposed*** *tool*  *to superimpose them directly.*
- If you want to stack all the 1D spectra under a certain folder, use ***Scripts > Import > Directory Spectra Stack.***

Change display properties of stacked spectra

- Right click on it and select **Properties**:



Enter 0 here if you don't like the tilt angle.

Enlarge the top/bottom margins for better 3D effects.

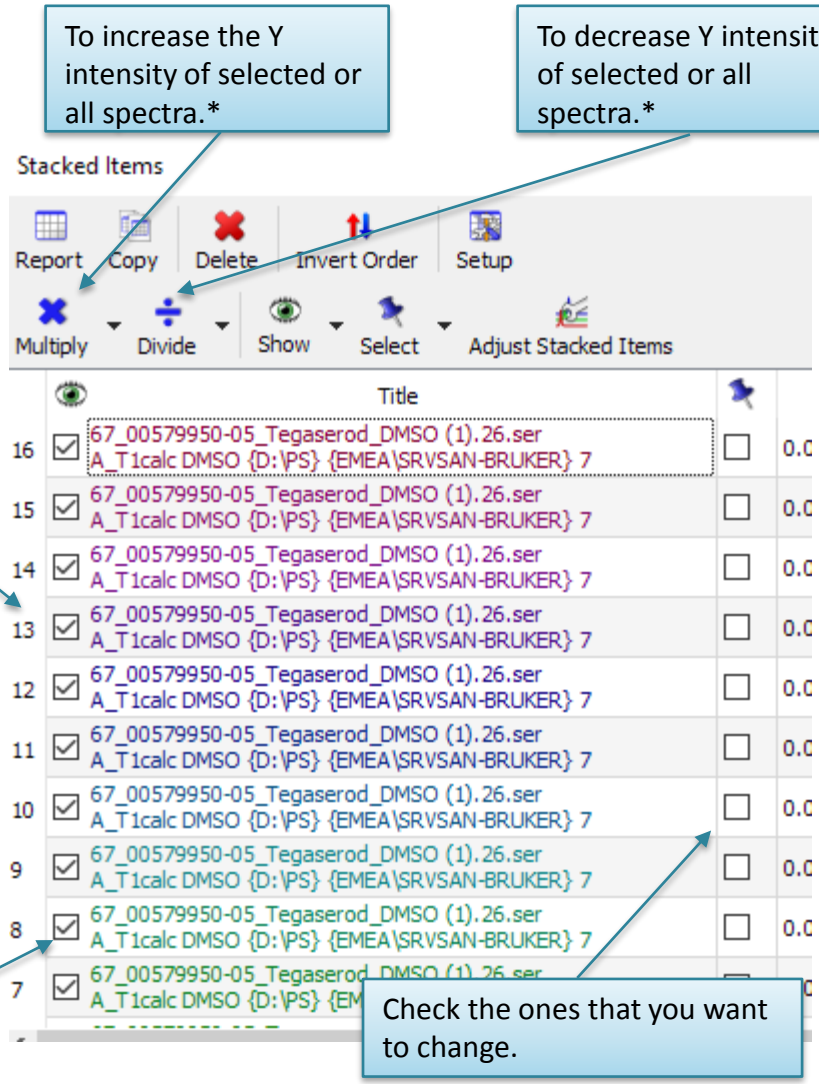
Check here if you want to clip the peaks.

Change colors of spectra.

Click here to set the changes as default.

Handle the stacked spectra

- Click  to toggle on the **Stacked Spectra Table.**
- Use this table to do the following:
  - Delete spectra from the stack
  - Change order of the spectra in the stack
  - Change the Y-intensity of selected spectra
  - Choose which ones to display
  - Choose which ones to adjust



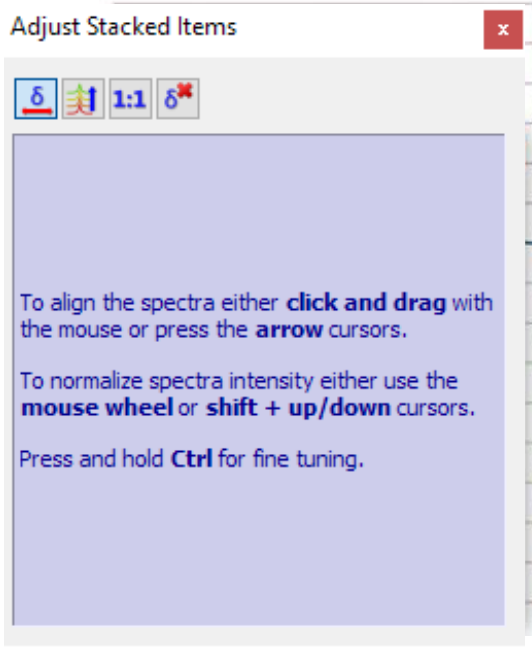
Tip: Read Help > Contents on more advanced data analysis, such as reaction monitoring, metabolomics, relaxation studies, DOSY processing etc.

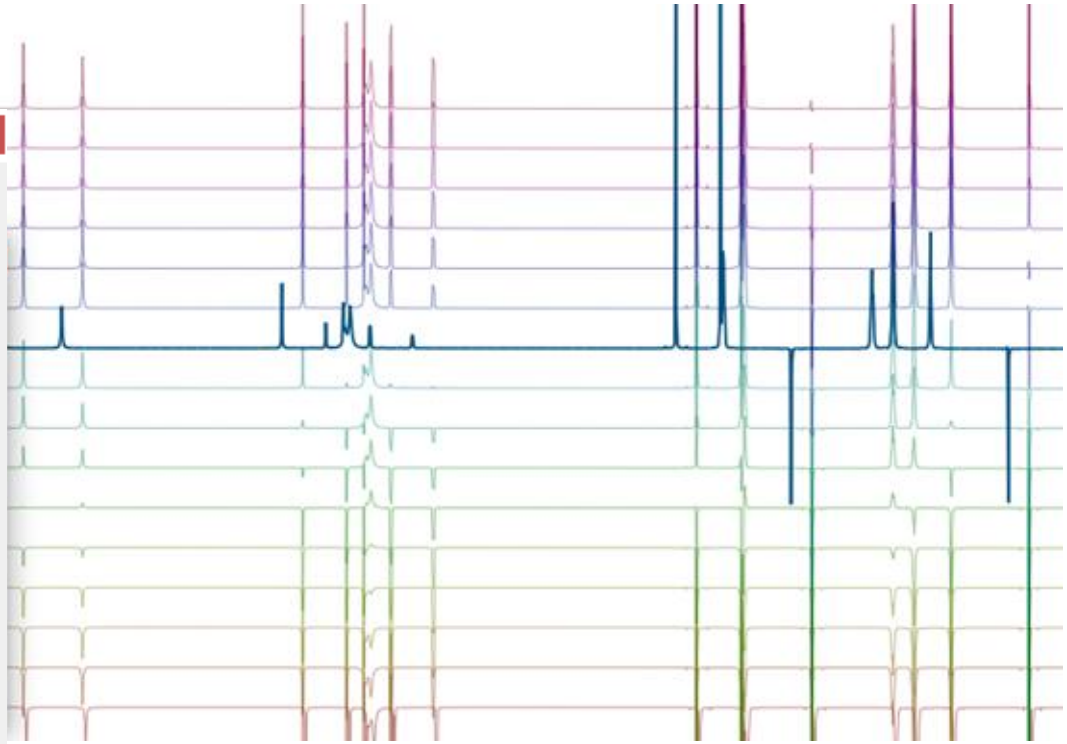
Handle the stacked spectra (2)

- Adjust Stacked Items 

It works like the phase correction panel: The cursor has to be inside the blue dialogue box

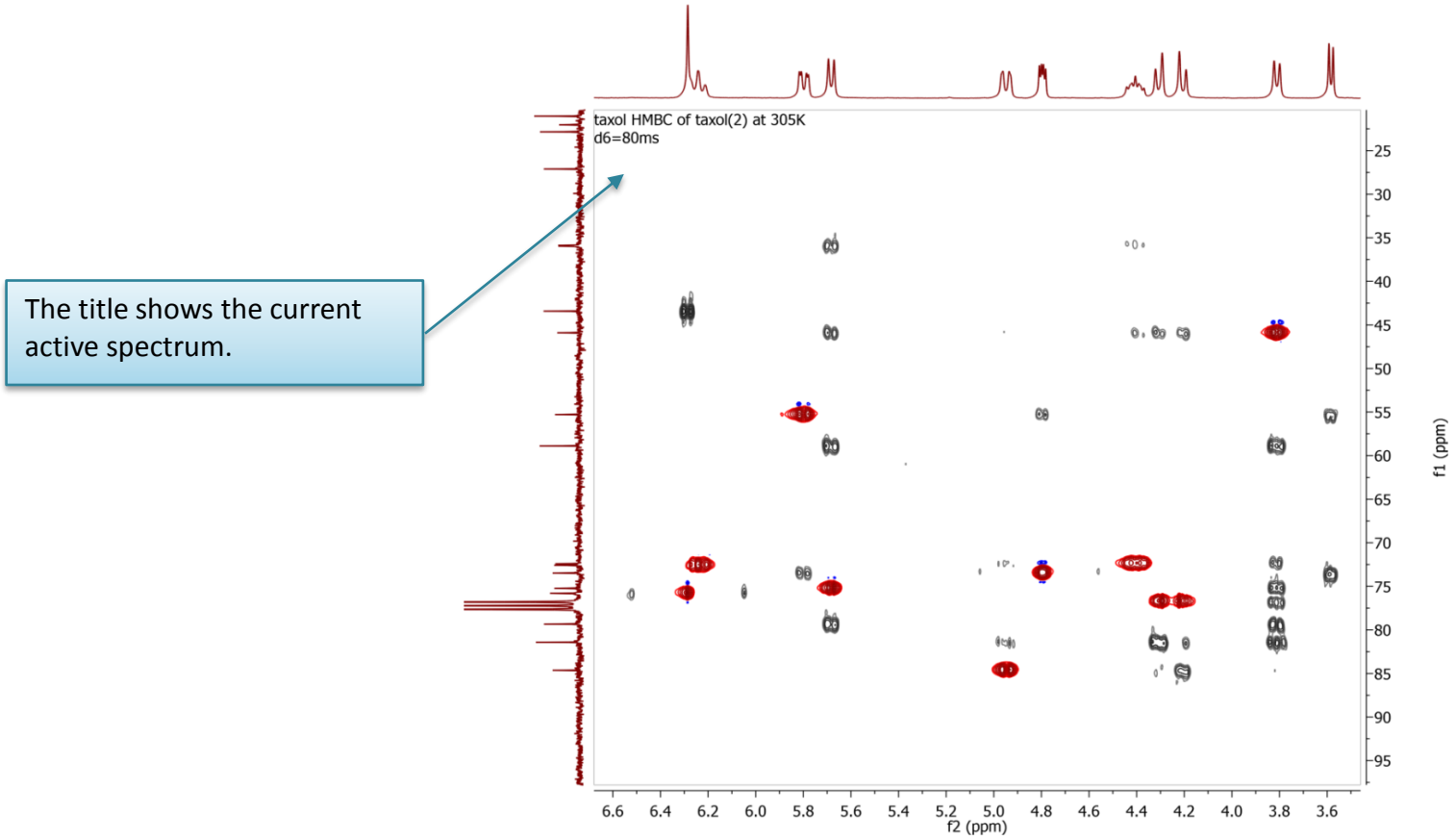
-  Click&drag to shift a spectrum horizontally.
-  Click&drag to adjust the vertical offset between stacked spectra.
-  Reset intensities.
-  Reset shifts.





Superimpose multiple 2D

- Multiple 2D can be stacked or superimposed in the same way as 1D.
- Press the **Shift + Up Arrow** key to change the active spectrum.
- Right click on it and select **Properties** to change the color of the contours for the active spectrum.



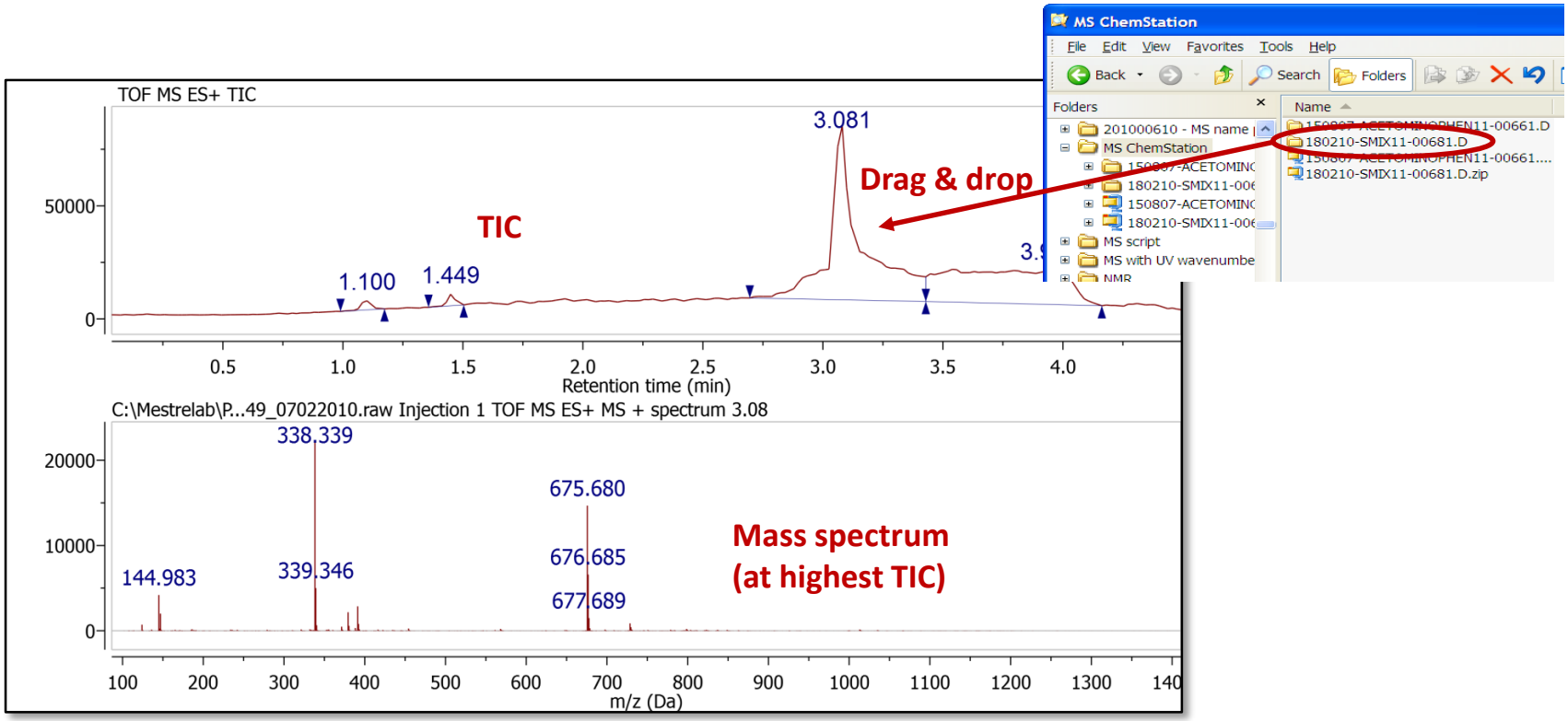
LC/MS data formats compatibility

Vendor	Windows			Mac	Linux
Agilent	Chemstation	MassHunter	Ion Trap		
Waters	MassLynx	Compass	Openlynx	MassLynx	MassLynx
Thermo	Xcalibur	Exactive	Q-Exactive		
Bruker[1]	XMass	Compass		XMass	XMass
JEOL	MSQ 1000	FastFlight			
AC SCIEX	Analyst	Data Explorer			
Shimadzu[2]	LabSolutions v3	Labsolution v5			
mzData, mzXML	mzData, mzXML			mzData, mzXML	mzData, mzXML
NetCDF ANDI-MS	NetCDF ANDI-MS				
Advion Expression	Data Express				

[1]Bruker software is required to be installed on the same computer (or users can download and install CompassXtract, as instructed in http://mestrelab.com/resources/bruker-compass-mnova-ms/).
[2]LabSolutions software is required to be installed on the same computer
Note: In all the cases above, you can open a raw dataset in Mnova on a computer with the vendor software installed, and then convert it to a Mnova binary file and send it to other users with Mnova only. This can also be done in batch mode or in real-time using an Mnova script.

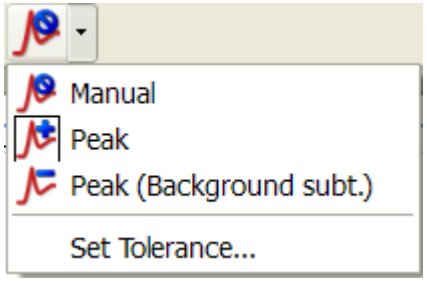
Open your LC/GC/MS data

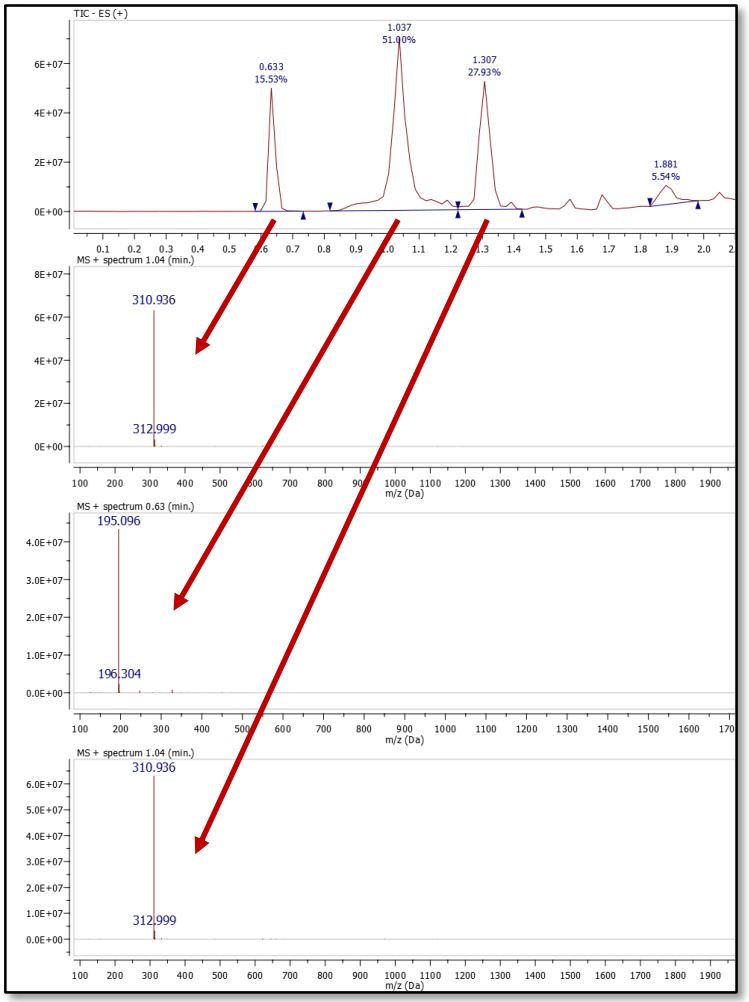
- Go to **File/Page Setup/Orientation** and change the page orientation to portrait if you wish.
- Go to **Data Browser** to open any file in the folder containing the raw data, or **drag&drop** the folder from Windows Explorer to Mnova.
- Mnova automatically converts your data and does peak picking.



Browse the mass spectra

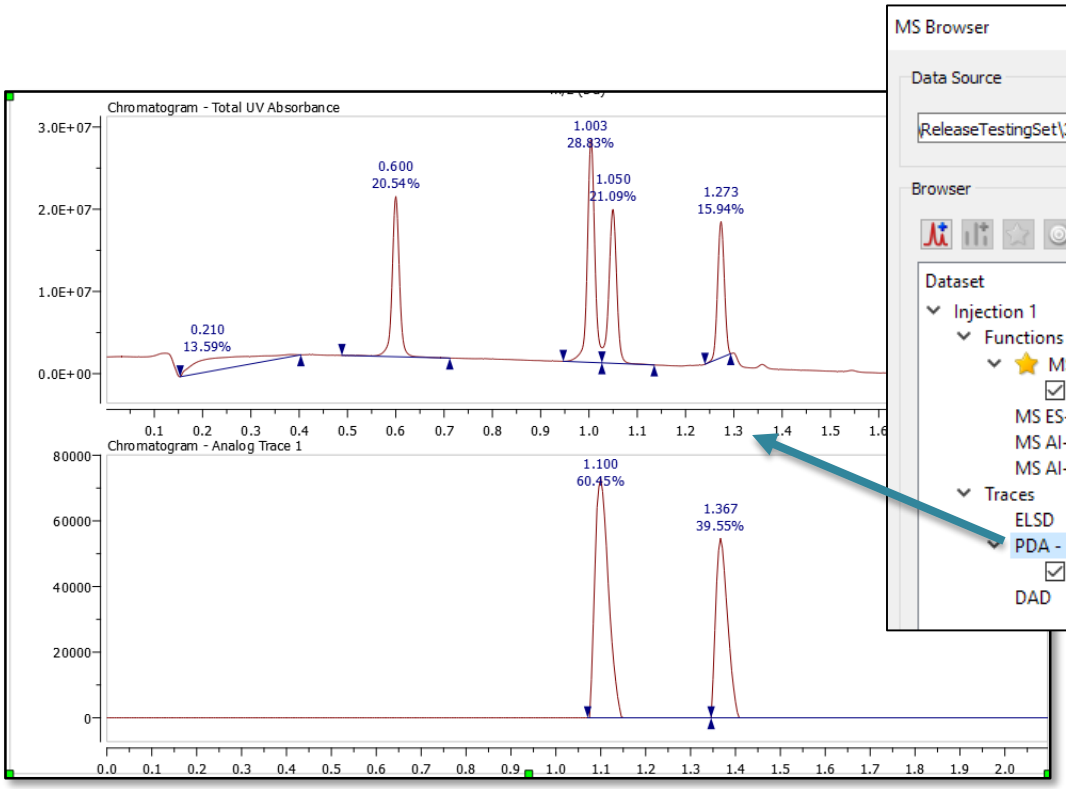
- Press  to switch to crosshair cursor, and click on the TIC to display the mass spectrum at that retention time, or click-and-drag to display co-added spectra.
- Press  to change to appending mode if you want to display multiple mass spectra.
- Choose the **Spectrum Selection Mode** to display mass spectra conveniently:
  - **Manual mode**: Click to display a single MS, or click-and-drag to co-add multiple MS.
  - **Peak mode**: Click on a peak to display the co-added MS within the peak range.
  - **Peak (Background subtraction) mode**: Click on a peak to display the co-added MS within the peak range with the background subtracted.

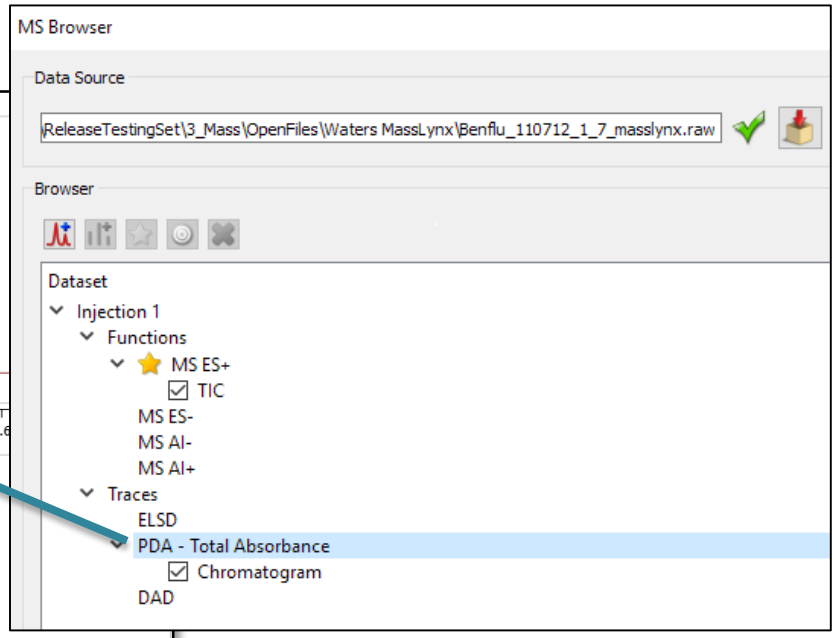




Browse the UV traces

- Press  to show the MS Browser dialog.
- Highlight the Total UV Absorbance under Traces, and press  to display it.
- Repeat the above step to display the other traces if any.



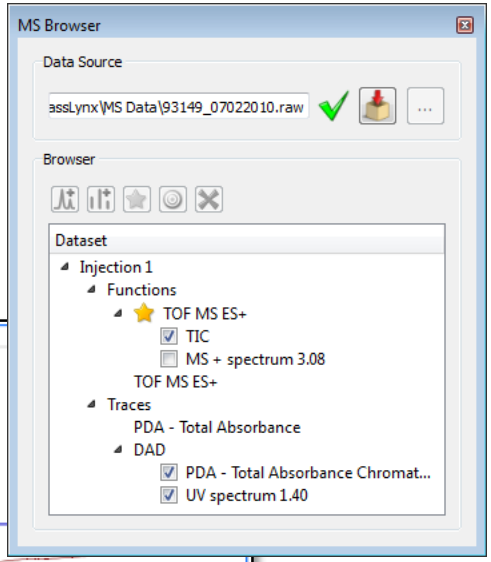


Extract a UV trace at selected wavenumber

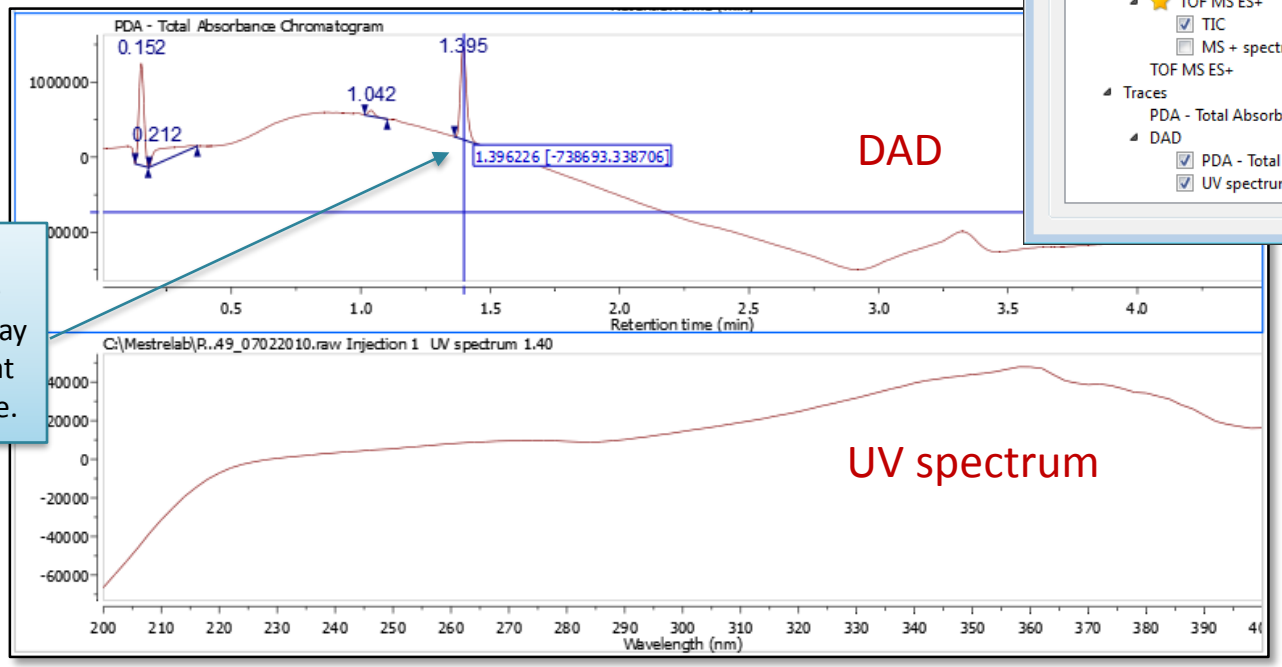
- Highlight the DAD in the MS Browser.
- Press  to display it.
- In the New Chromatogram dialog, choose Wavelength, and enter a wave length and a tolerance to display the extracted UV trace.

Display a UV spectrum at selected retention time

- If available, highlight the DAD Trace in the MS Browser and press  to display it.
- Press  for Crosshair cursor, press and hold Alt key, click on the DAD trace to display the UV spectrum at that retention time.

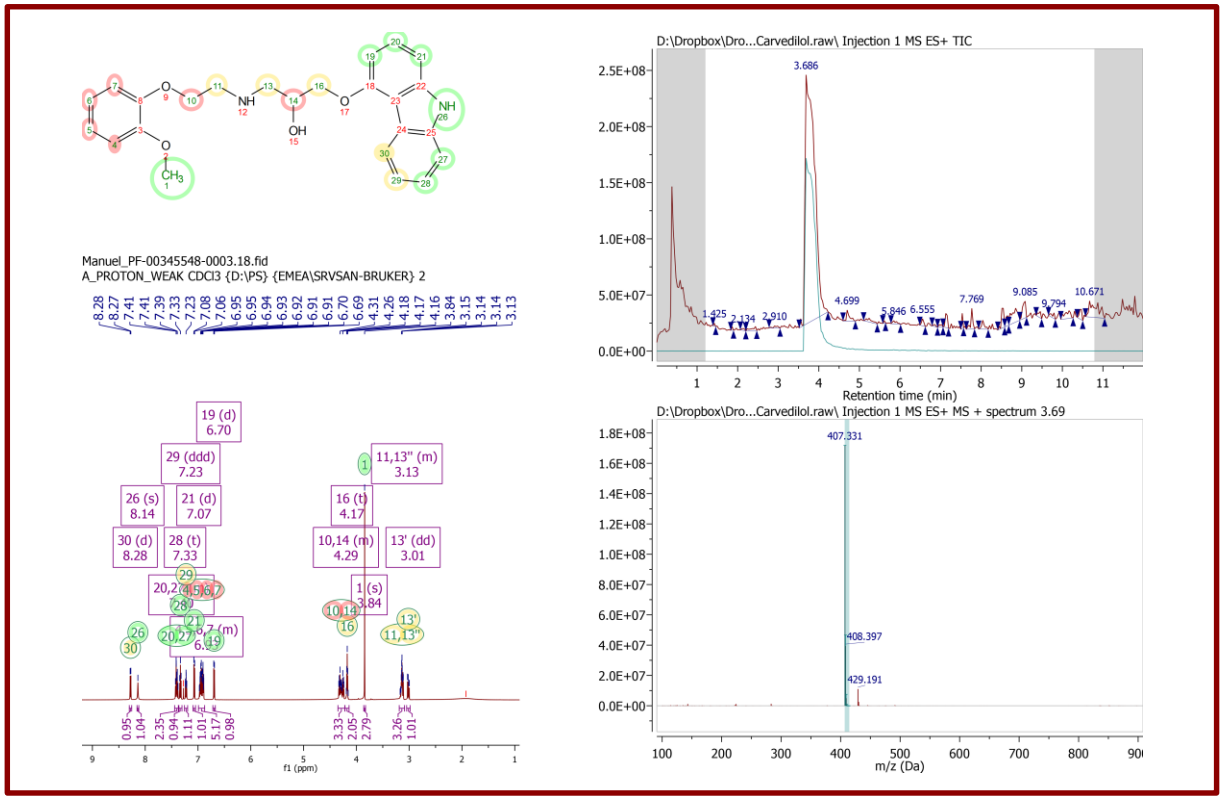


In crosshair cursor mode, click on the PDA curve to display the UV spectrum at that retention time.



Common interface for all analytical techniques

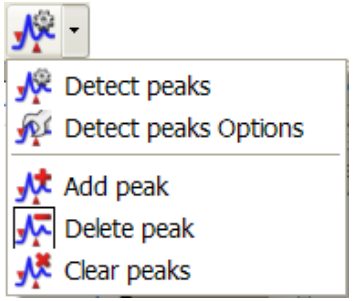
Easily combine your MS and NMR data in the same page using Mnova.



Note: When you open multiple spectral objects, they go to separate pages. You can copy (or cut) and paste them to the same page.
Tip: Use the Bring to Back/Front, Align and Tile tools to arrange the objects nicely.

Edit and report peak integration results

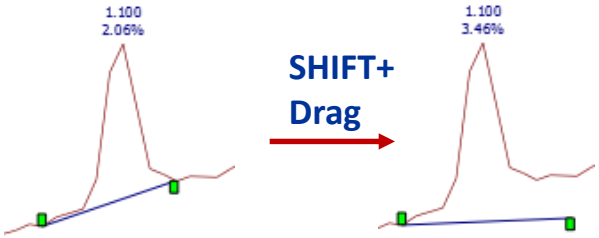
- Peaks are automatically integrated when you open a chromatogram.
- Use the Peak Detection tool menu to re-detect peaks, add, delete or clear peaks.
- Hover your cursor over the wedges, click and drag the green boxes to change the range of a peak.
- Or press Shift, click and drag the green boxes to change the baseline of a peak.
- Go to **View/Tables/Mass Peaks** to display or report the Mass Peaks Table.



Mass Peaks

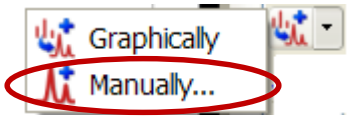
Report Copy Setup

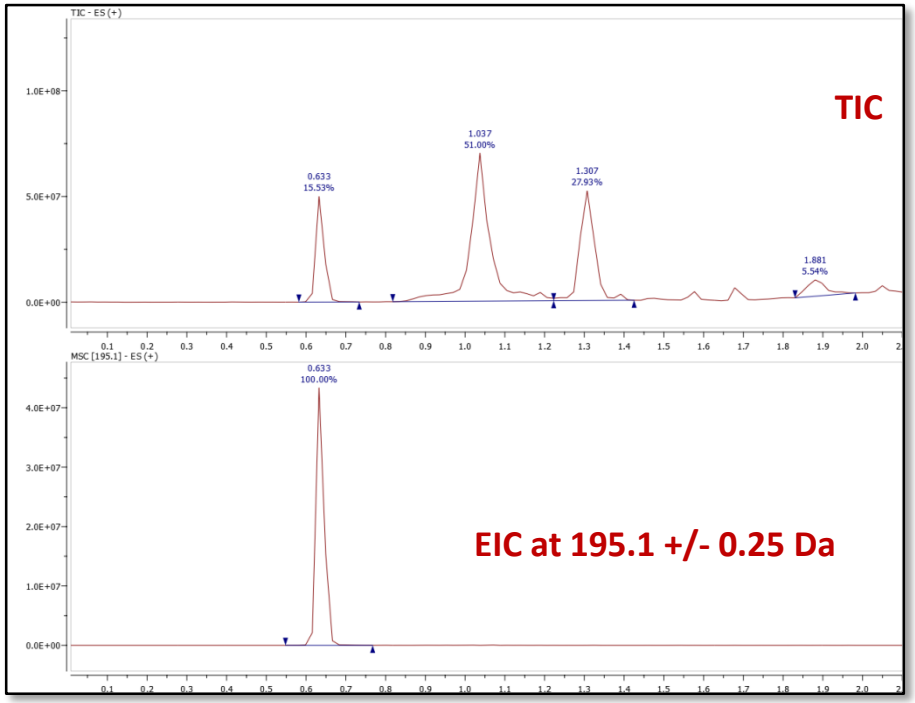
	RT	Scan	Type	Height	Area	Total Height %	Total Area %	Start time	End time
1	14.281	278	VB	81225.226	534185....	0.06	0.14	14.169	14.696
2	13.219	260	VV	1304763...	7794466...	1.02	2.04	13.023	13.843
3	12.488	248	VV	1081035...	6887554...	0.85	1.80	12.359	12.964
4	12.113	242	VV	2214036...	5056029...	1.74	1.32	12.040	12.300
5	11.926	239	VV	528807....	1541438...	0.42	0.40	11.811	11.982
6	11.693	235	VV	457133....	1284582...	0.36	0.34	11.516	11.811
7	11.280	227	VV	12229.133	28628.710	0.01	0.01	10.988	11.457

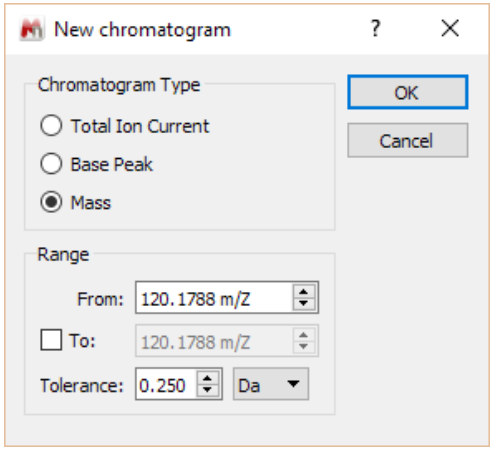


Display extracted ion chromatogram from an *m/z* value

- Press  (or go to **Mass Analysis/New Mass Chromatogram/Manually**).
- In the New Chromatogram dialog, enter the m/z value that you are interested in, and a suitable Tolerance.
- Press OK to display the EIC.

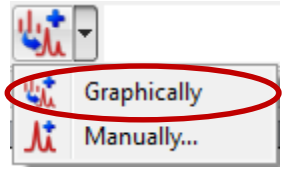




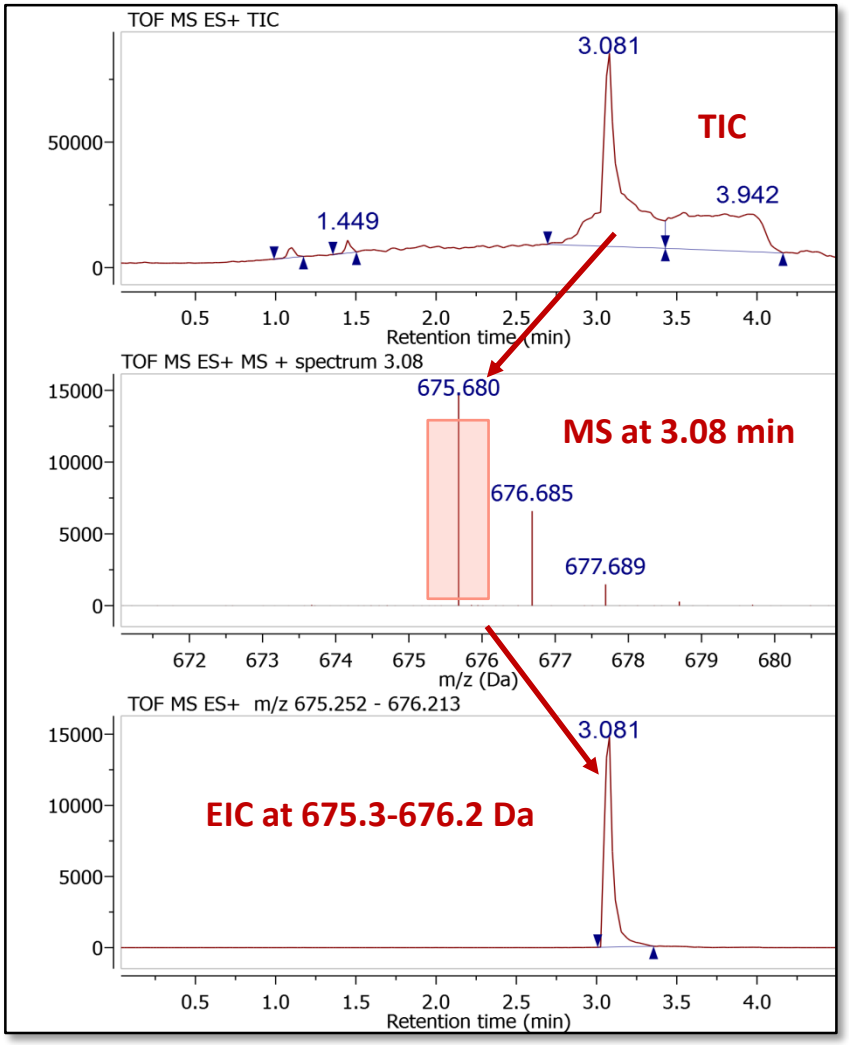


Tip: You can also go to Mass Analysis/Spectrum Prediction to run a mass prediction from a molecular formula.

Display extracted ion chromatogram for an MS peak

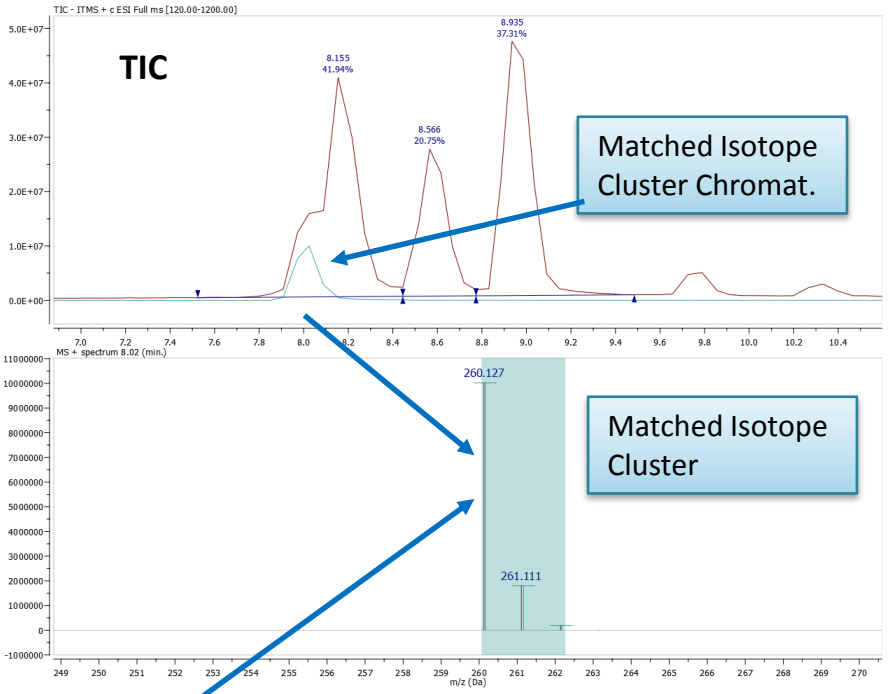


- First display the MS trace and zoom into the molecular ion peak that you are interested.
- Next press (or go to **Mass Analysis/ New Mass Chromatogram/Graphically**), click-and-drag around the peak to define a mass range.
- An EIC will be displayed within the mass range.



Confirm proposed structures using Molecule Match (1)

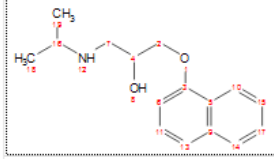
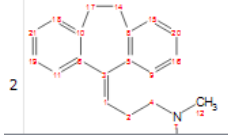
- Import one or several structures by copy/pasting from ChemDraw, Isis/Draw or ChemSketch, or by opening .mol or .sdf files.
- Press  (or go to **Mass Analysis/ Molecule Match/Calculate**).
- In the Molecule Match Table, click on a molecule to see the matching results.



Molecule Match

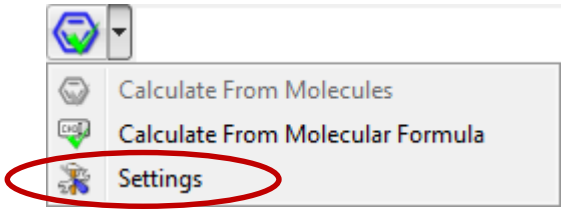
Report | Calculate | View | Settings | Setup

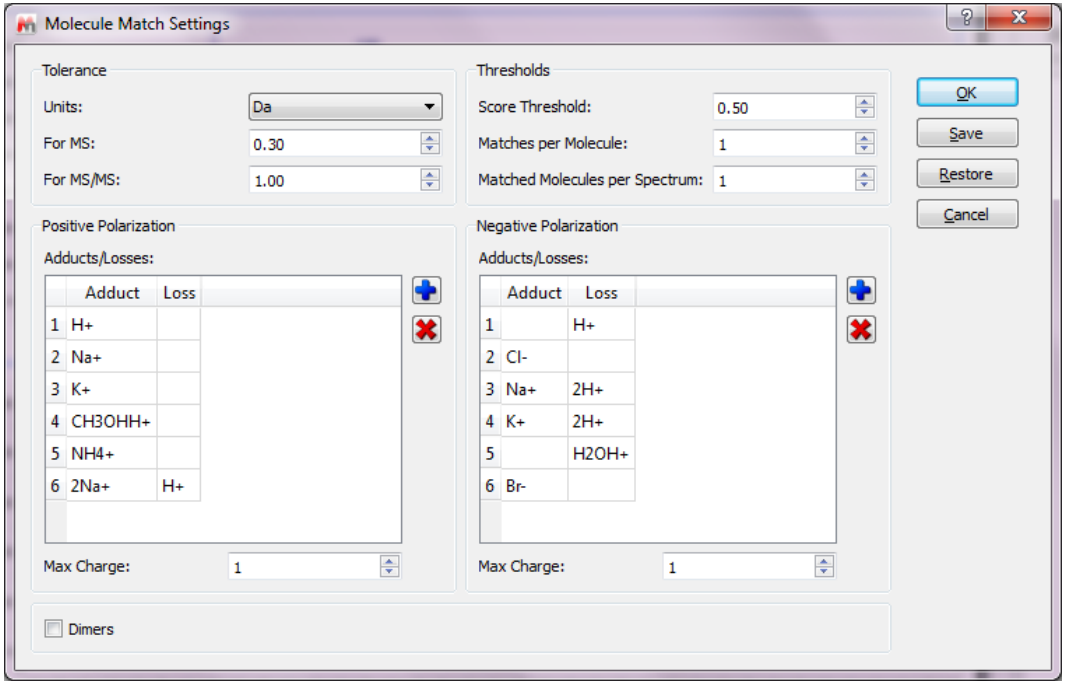
Mol Match Results

	Molecule	Formula	ecular Wei	Match	latch Score	Similarity	MS Purity	RT	Scan	Purity
1		$C_{16}H_{21}NO_2$	259.157	✓	1.000	1.000	0.756	8.02	171	10.00%
2		$C_{20}H_{23}N$	277.183	✓	1.000	1.000	0.450	8.57	180	11.39%

Confirm proposed structures using Molecule Match (2)

- You can go to **Mass Analysis/Molecule Match/Settings** to change the settings for Molecule Match.
- The default settings are for low-resolution MS. Change Tolerance to 5-10 ppm if you are using high-resolution MS.
- Edit the Adducts or Losses and other parameters if you want to.
- Press  to run the Molecule Match again.

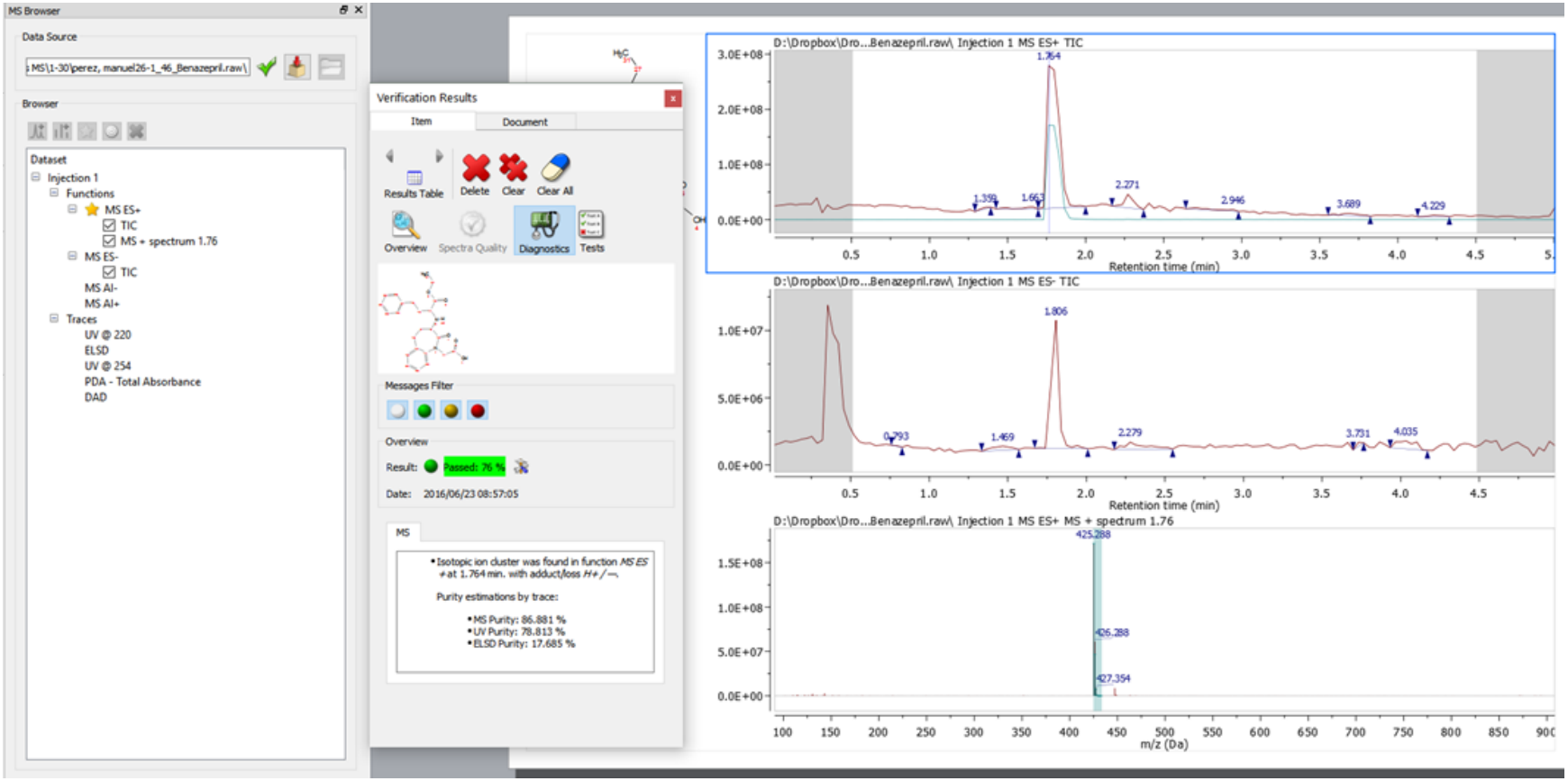




Tip: Click the "+" buttons to add a new adduct. Enter "+" for a radical cation. Highlight one and click the "x" button to remove it. Click Restore to reset to the default or previously saved settings.

MS driven structural verification

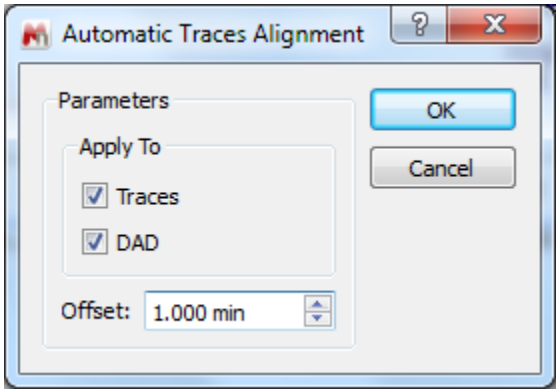
You can combine your MS data with NMR data to improve your results in structure verification process.

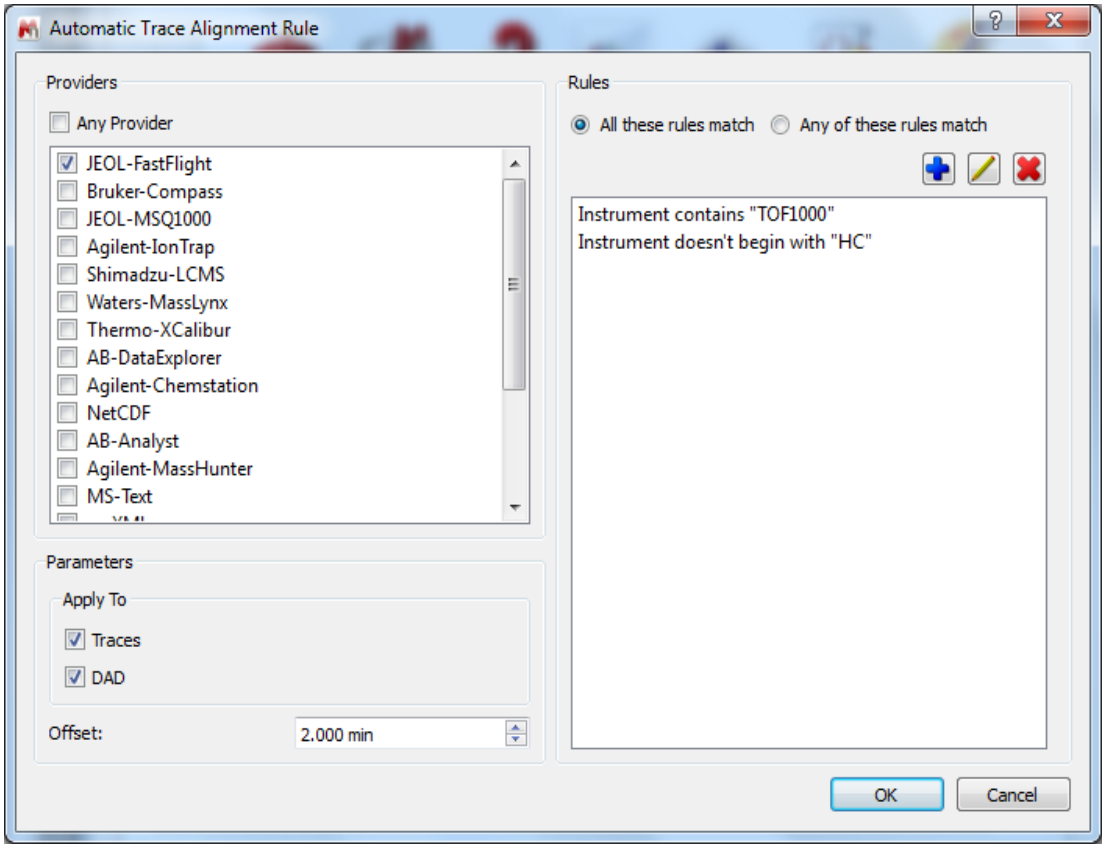


Automatic trace alignment: Instrument specific

Align your DAD or another trace to the TIC one using the auto-alignment settings.

Set the rules to specifically identify the instrument and apply the correct alignment automatically.

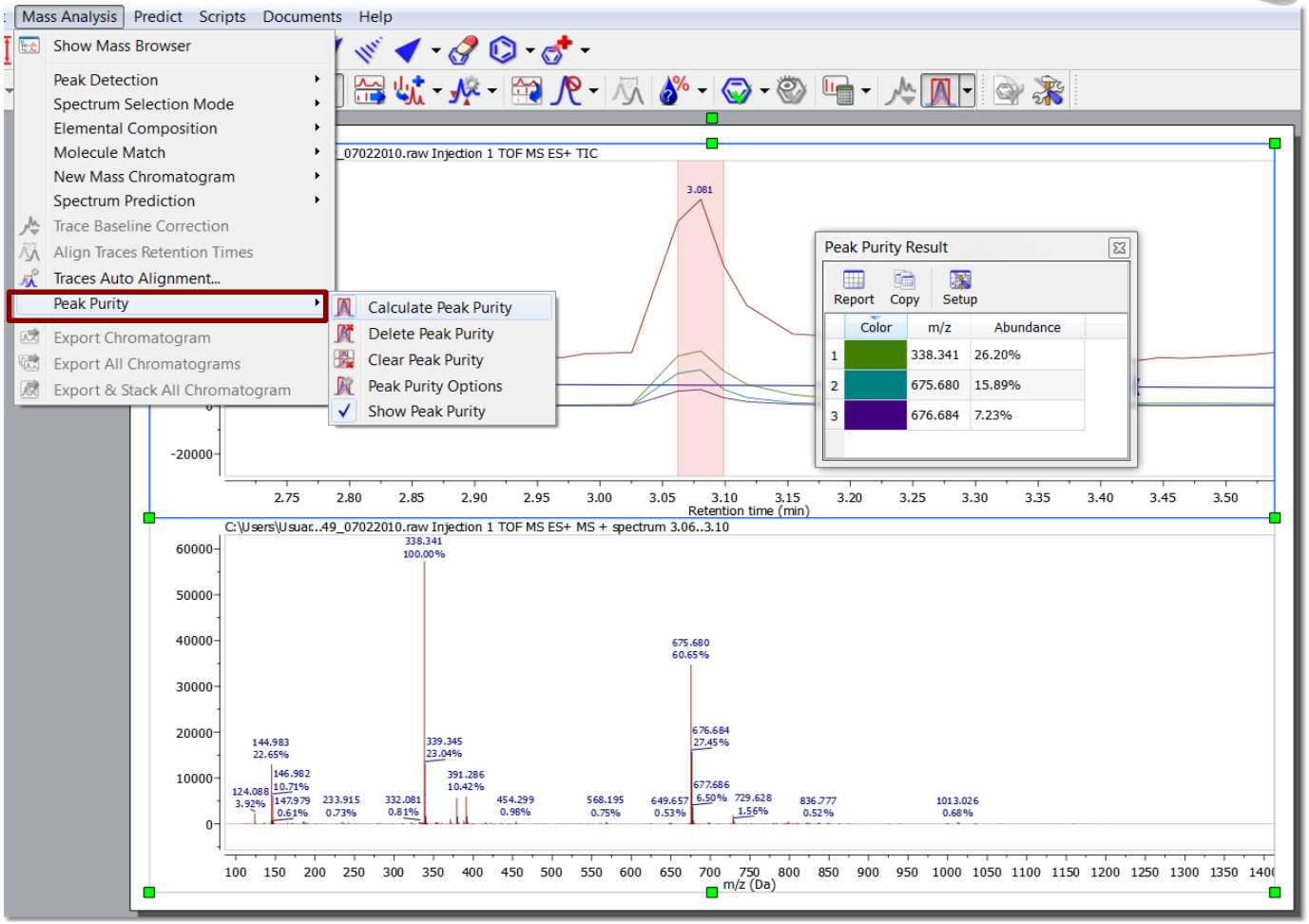




Peak purity calculation

NEW ON MNOVA 11.0

It shows the curves associated to the most abundant mass peaks under the selected chromatogram peak.



Just the tip of the iceberg!

Thank you for your time!

For more information:

- Visit www.mestrelab.com for manuals, tutorials, and many more Mnova plugins.
- Check **Help > Contents** in Mnova for help information.
- Email to support@mestrelab.com for technical questions.
- Email to chen.peng@mestrelab.com for sales related queries.

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Mnova 11 – Starting guide

Thank you for trusting our software solutions!