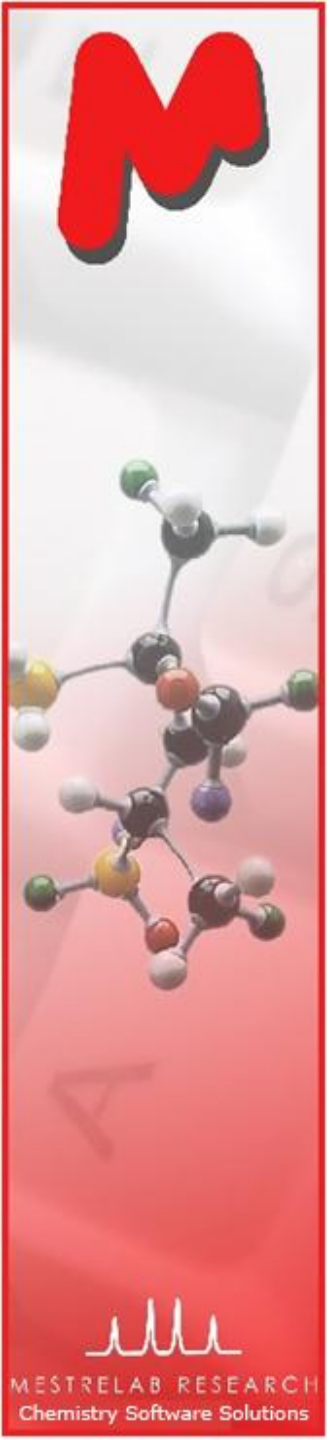

mnova 7

Efficient Desktop Tools for Processing, Analyzing, Reporting and Managing NMR and MS Data for Chemistry

Version 7.0
June 2011

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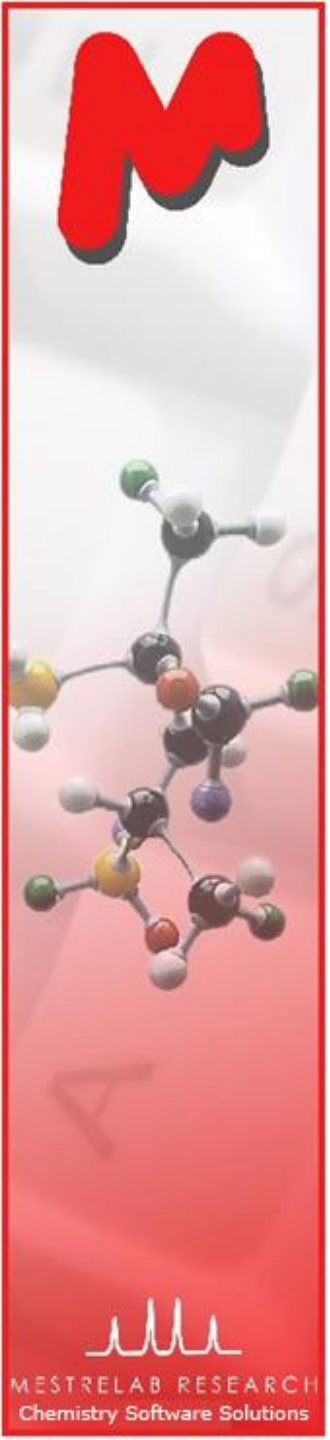
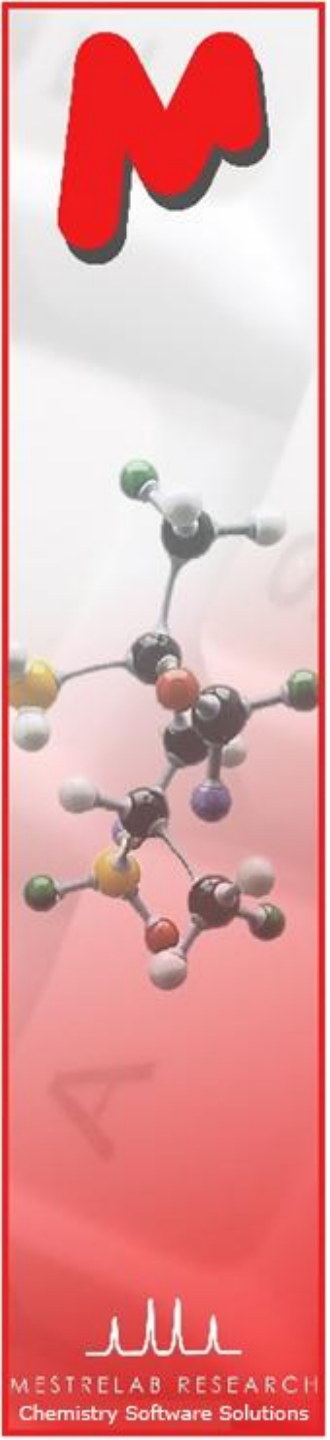


Outline

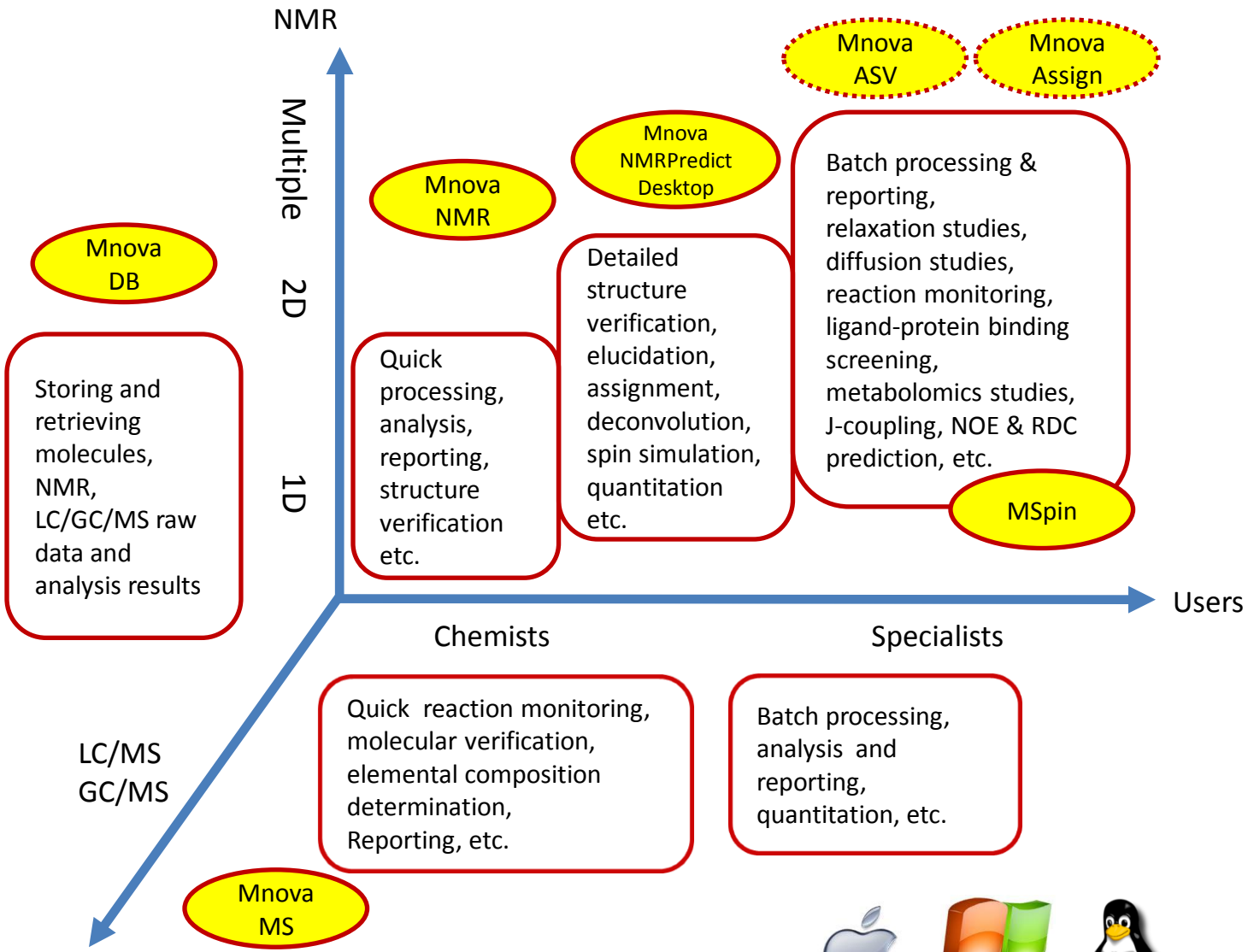
- The Company and Products Overview
- Mnova NMR
- Mnova NMRPredict Desktop
- Mnova MS
- Mnova DB



About Mestrelab Research

- 1996: A research project in University of Santiago de Compostela, Spain, developed free **MestReC** software for NMR processing
- 2004: **Mestrelab Research** incorporated in Santiago de Compostela
- 2004: New **MestreNova (Mnova)** platform and **NMR** plugin released
- 2006: **NMRPredict Desktop** plugin released with Modgraph
- 2009: **LC/GC/MS** plugin released with Sierra Analytics
- 2009: Global Spectral Deconvolution (**GSD**) algorithm released with ExtraByte
- 2011: **DB** plugin for Database Management
- 2011: **ASV** plugin for Auto. Structure Verification - to be released.
- 2011: Auto. 1D and 2D **Assignment** - to be released
- An **R&D company** with ~20 people and 70,000+ registered users

Products and Applications



Mnova is compatible with Mac, Windows and Linux

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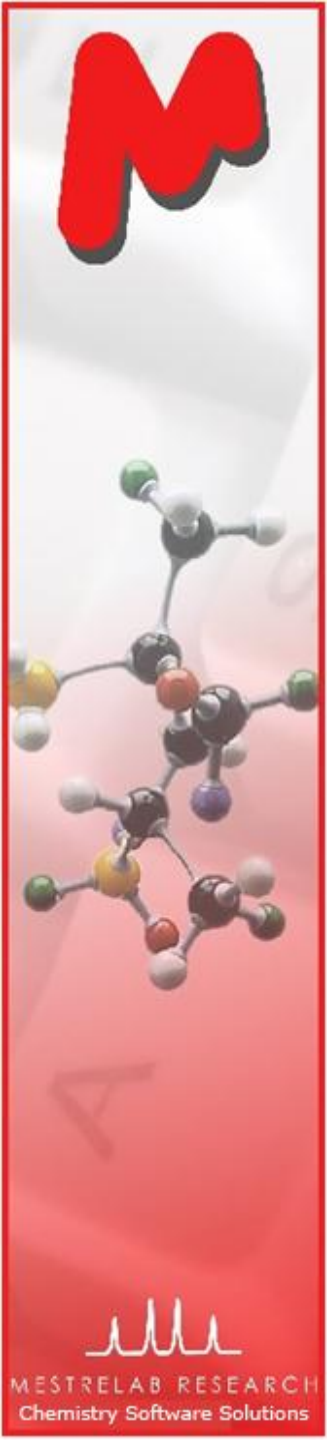


Mnova NMR

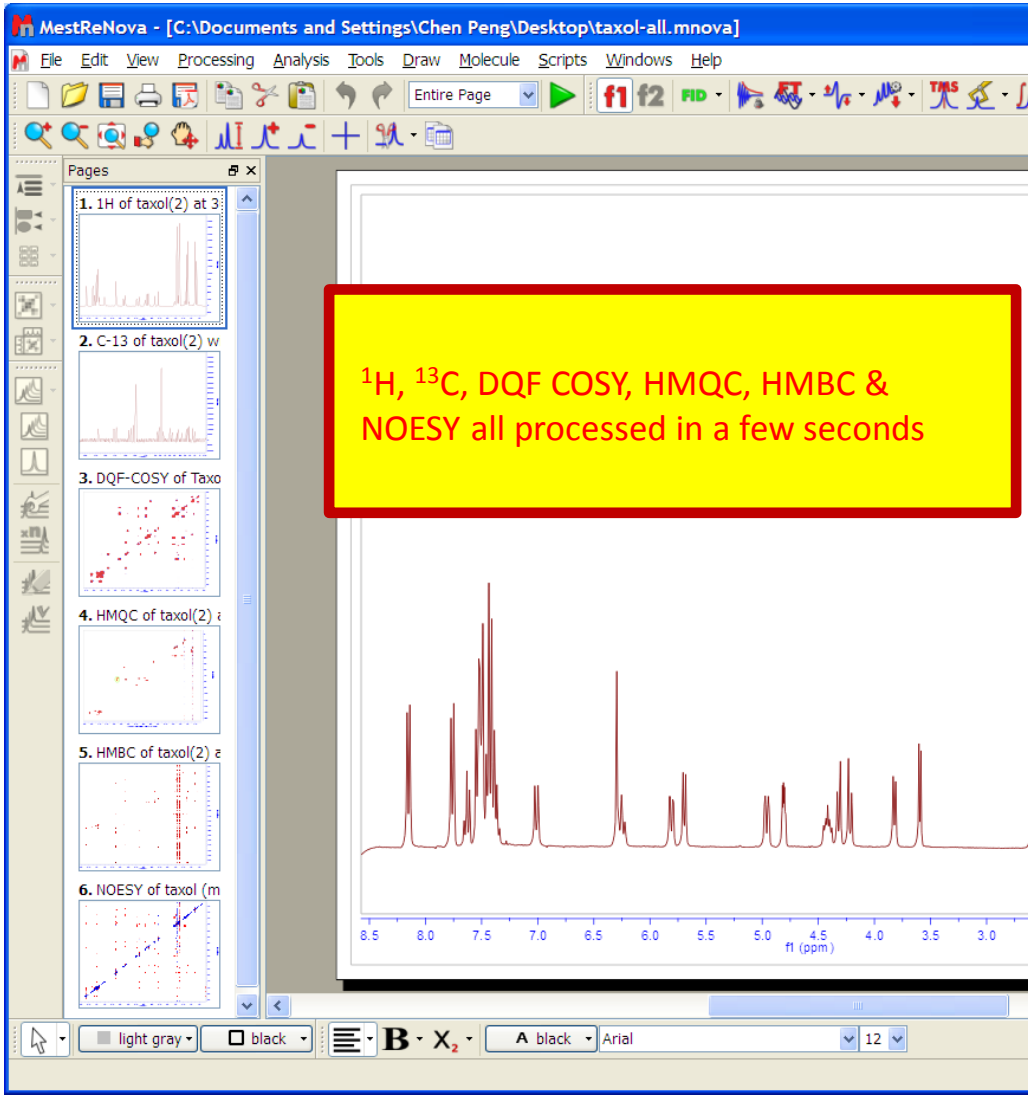
- Efficient tools for routine 1D and 2D NMR analysis and reporting
- Advanced tools for automation, quantitation, reaction monitoring, diffusion & relaxation, protein-ligand binding screening, metabolomics etc.

Fully Automated Processing of 1D or 2D spectra

Data acquisition

- Bruker
  fid, ser
- Varian
  fid
- JEOL
  .jdf
- JCAMP
  .jdx

Drag & drop



^{1}H, ^{13}C, DQF COSY, HMQC, HMBC & NOESY all processed in a few seconds

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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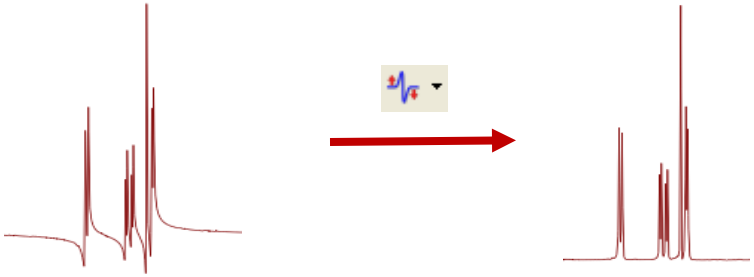
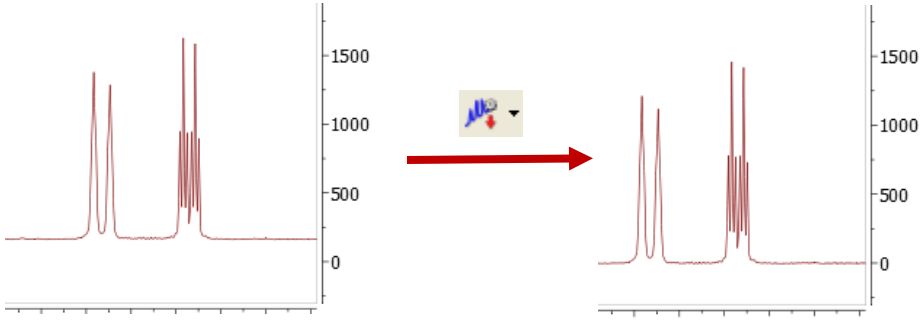
To correct phasing, baseline & reference

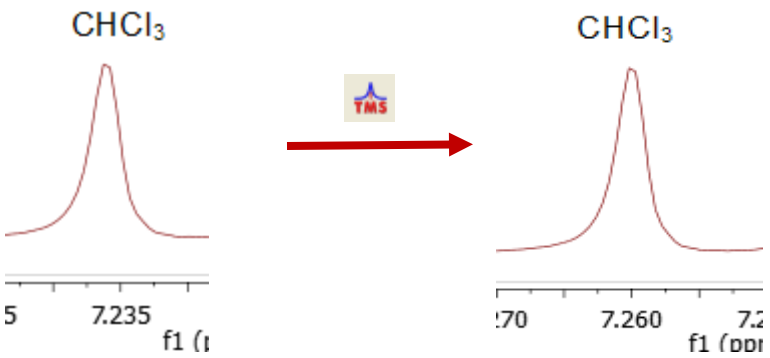
- Click  for **phase correction** if peaks are not symmetric*



- 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*

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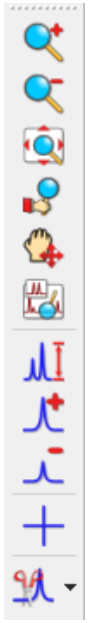
To visualize your spectrum



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 Height (or press H)

Increase Intensity (or rotate mouse wheel)

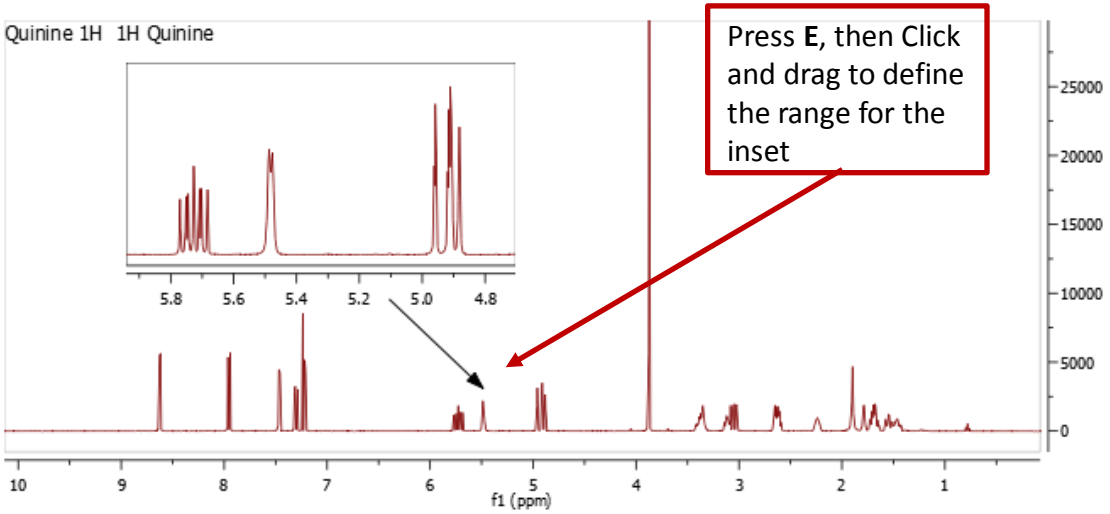
Decrease Intensity (or rotate mouse wheel)

Crosshair Cursor (or press C) for measuring *J*-couplings

Cut (or press X) to hide parts of the spectrum

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

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



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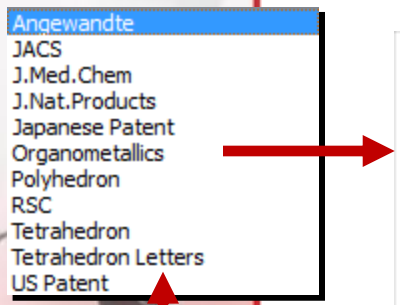
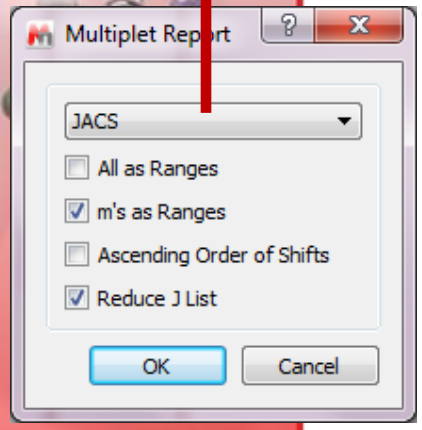
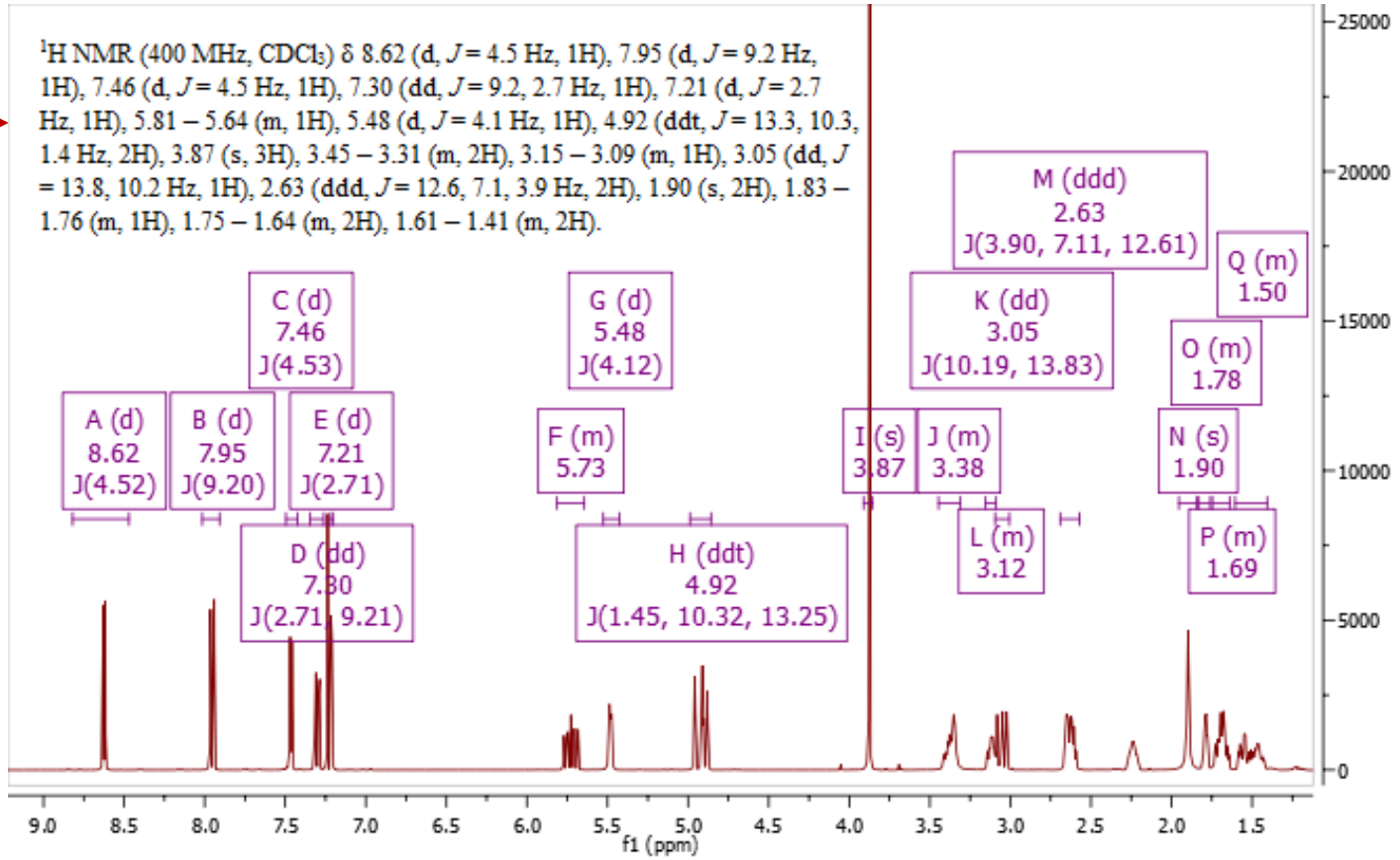
To analyze and report multiplets in H-1 NMR

- Mnova provides several approaches for multiplet analysis and reporting
  - Manual: click-and-drag to pick each multiplet interactively
  - Fully automatic multiplet analysis (with global spectral deconvolution, auto recognition of solvent peaks and estimation of num. of nuclides)
- In either case you can refine the results interactively, and report them in selected journal or patent formats



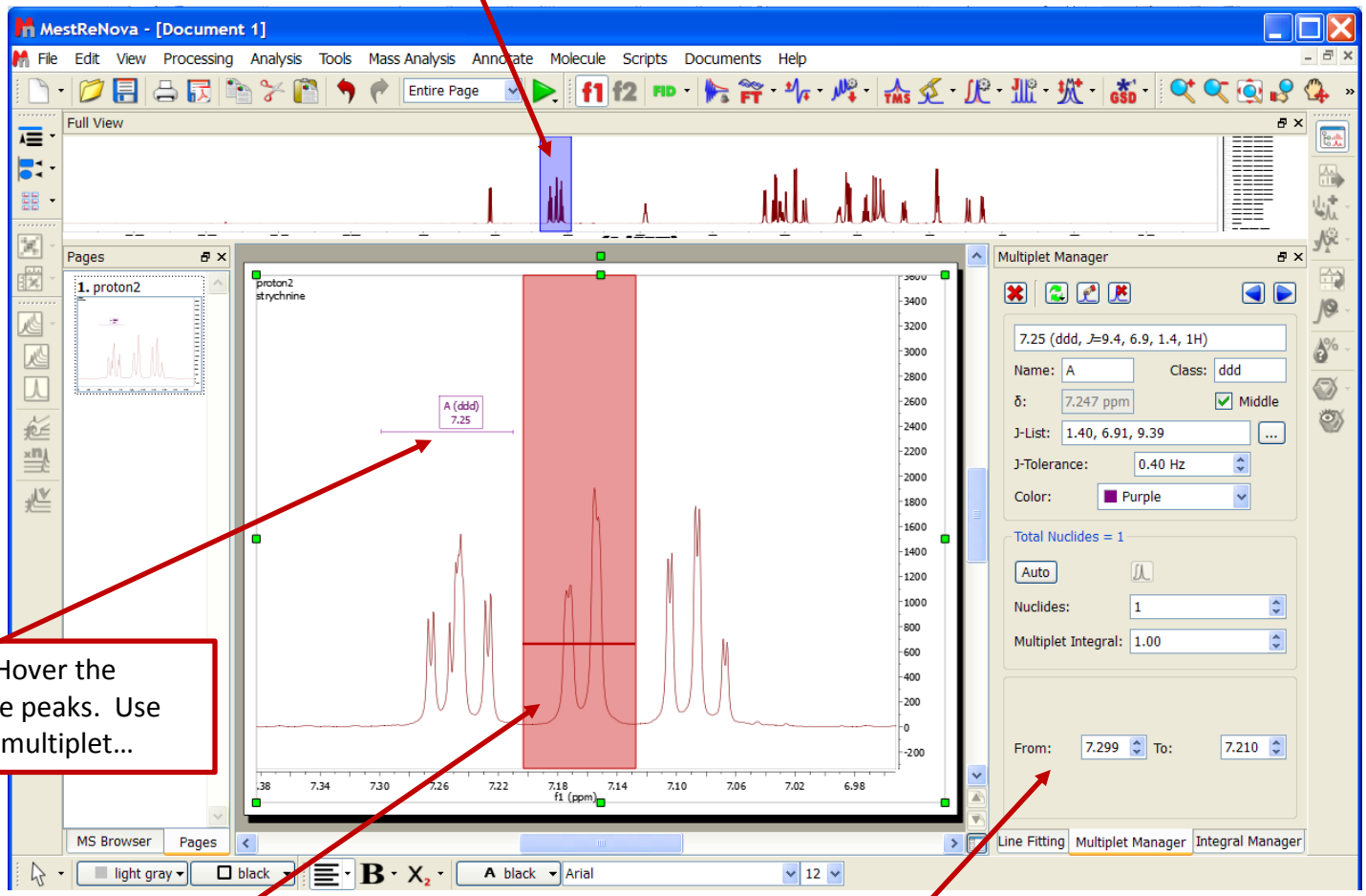




Tip: The contents in the multiplet label can be changed: Right-click on the spectrum and select Properties, choose the Multiplets tab and select an option for Label.

Tools for verifying and refining multiplet analysis results

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



Multiplet label: Hover the cursor on it to see peaks. Use the bar to split a multiplet…

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)

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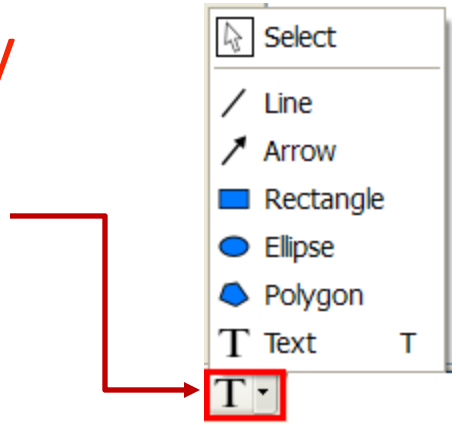
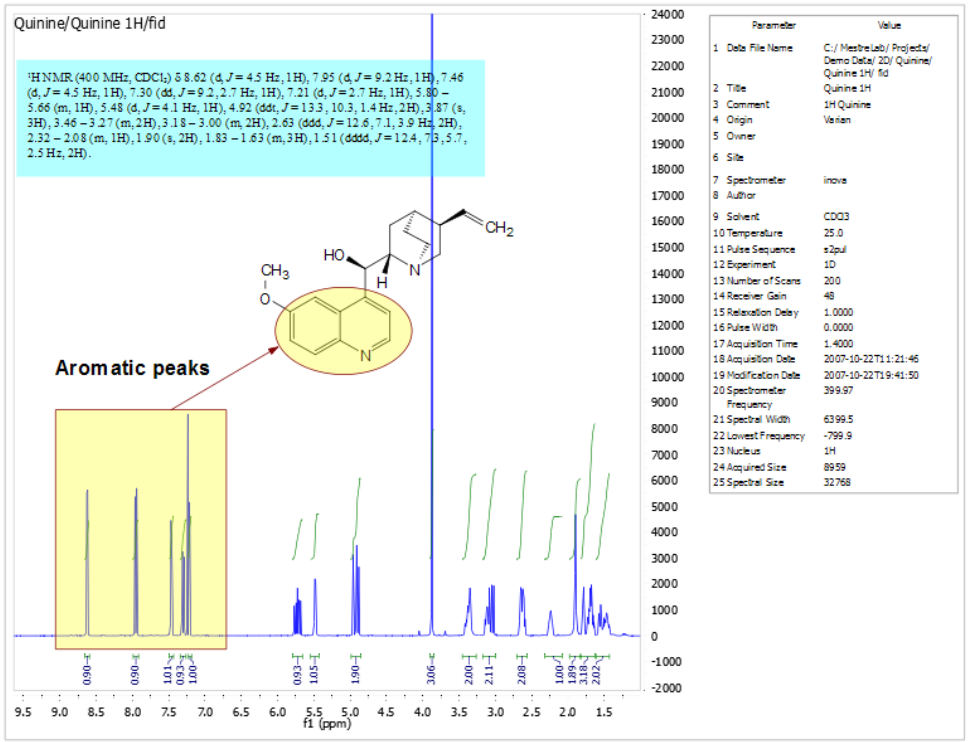
To annotate and report manually

- 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 a .mol,.sdf or .cdx file.*
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*

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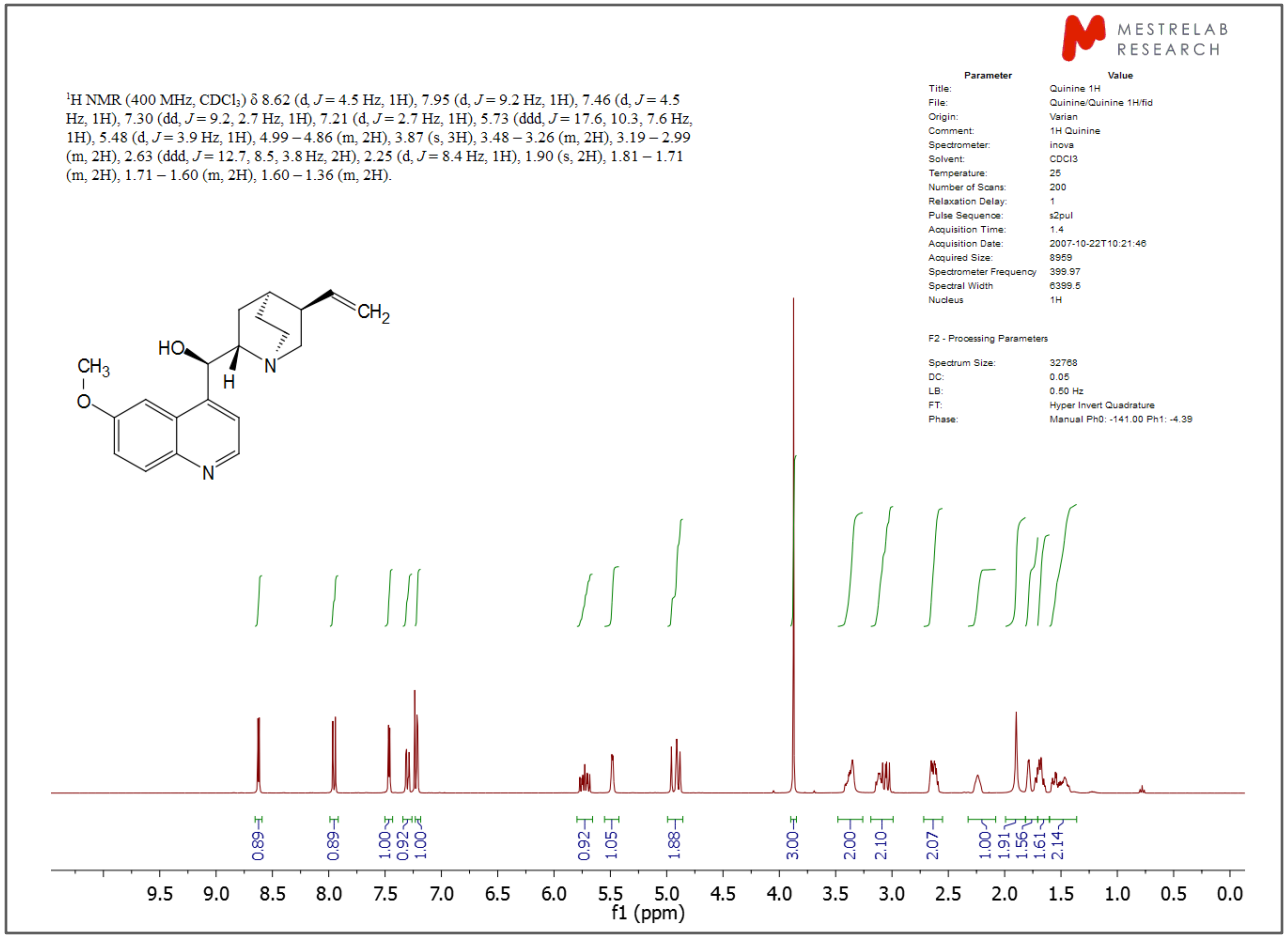
To report automatically using the **R** script*

- You can write scripts to automate processing, analysis and/or reporting
- In this example, the logo, parameters and multiplets texts are automatically reported and formatted by running a R script:



** You need to install R script. We can customize scripts for batch processing, pick peaking, multiplet analysis and reporting based on your requirements.*

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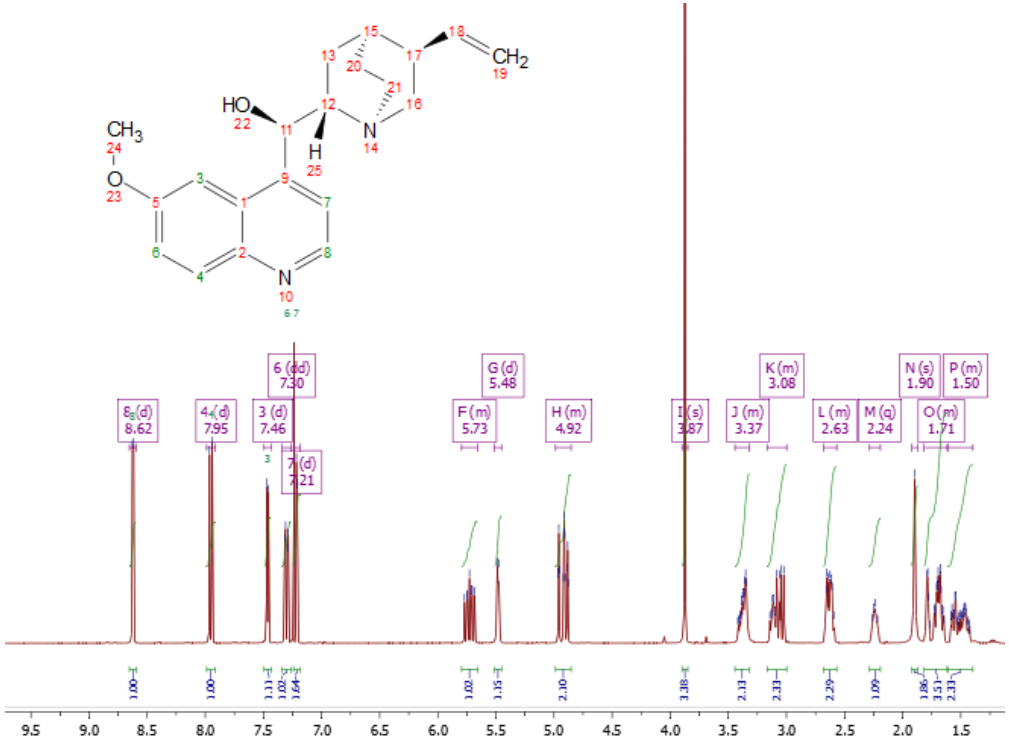
To assign a 1D ^{1}H spectrum

- Click **A** key (or choose **Analysis | Manual Assignment**) to enter Assignment mode.

- Click on an **atom** in the structure. Then choose the **peak** you want to assign. There are 3 ways to do it:
  - A picked **multiplet**, by clicking on the multiplet label, or
  - A **peak top**, or any point in the spectrum by clicking on it, or
  - A **range** in the spectrum, by click-and-dragging to cover it
- You can predict the ^{1}H spectrum to assist your assignment*



**Needs a separate license for Mnova NMRPredict Desktop*

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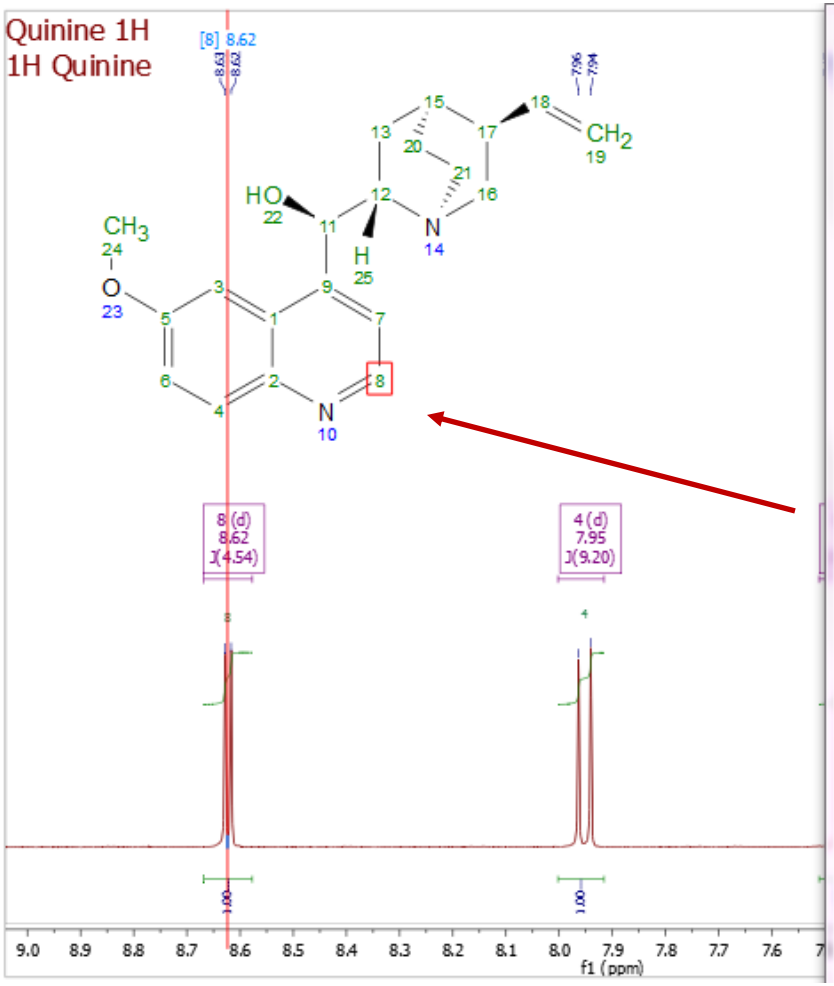
To display and browse assignment results

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



Assignments

Report | Copy | Delete | Expand | Collapse

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	

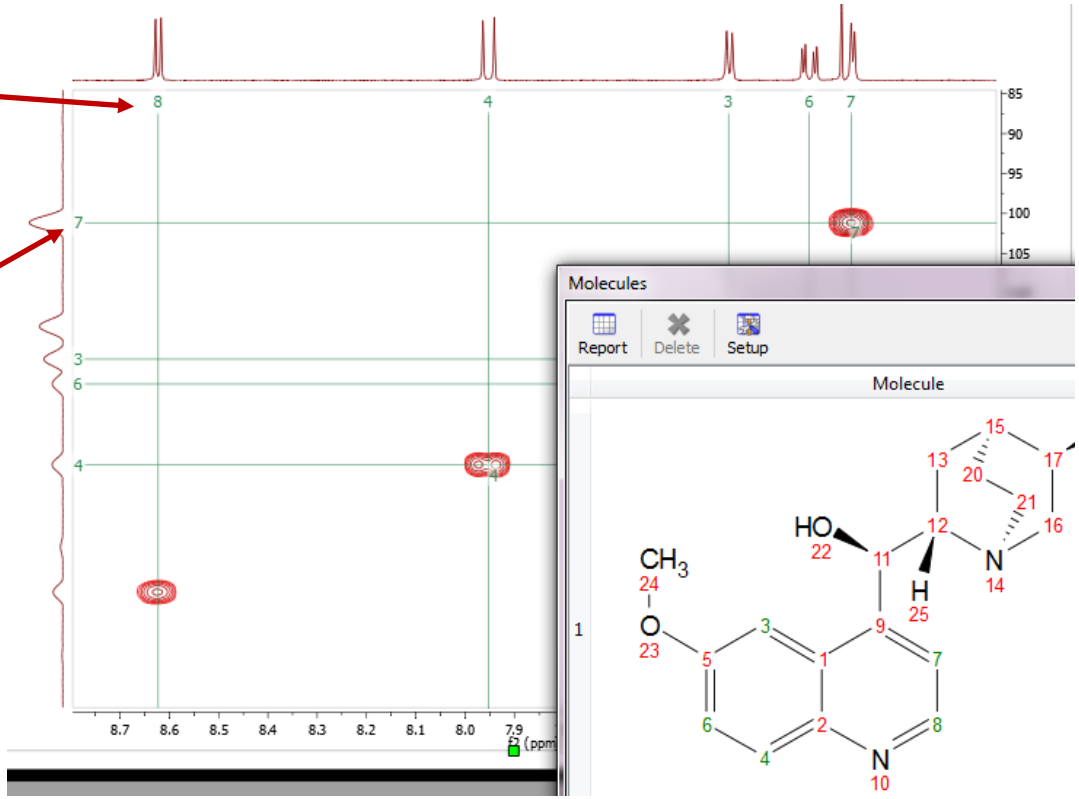
** You can right click on an atom and choose **Edit Atom Data** to change its label. Changed labels will be used in Assignments Table and other relevant reports.*

If you have 2D HSQC

- You can either first assign 1D H-1 peaks, and then assign HSQC cross peaks, or the opposite
- Assignments in one spectrum is carried over to all other spectra in the same document: All spectra in the same document are “correlated”
- To assign in HSQC, click **A** key to enter Assignment mode. Click on an **atom** in the structure. Next click on the cross peak to assign to it*

H-1 assignments from 1D spectrum or HSQC

C-13 assignments from HSQC



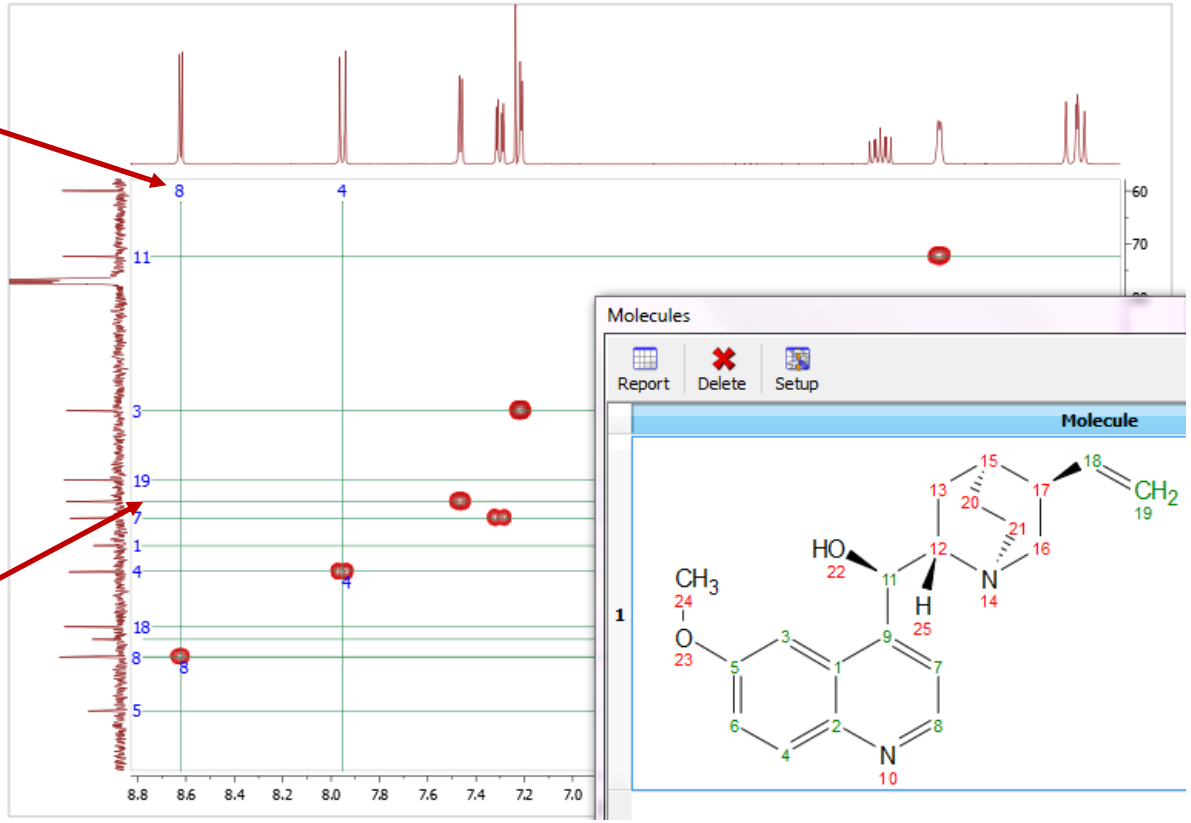
*By Default, Mnova automatically snaps to a peak top (with interpolation). Click **Shift** key one time to toggle it off if you want to manually locate the peak center.*

If you have a C-13 spectrum

- You can first assign the C-13 peaks, possibly with the help of Predict and Compare
- Next you can switch to the HSQC, and easily assign the HSQC peaks, and get most of the H-1 shift assigned.
- Finally you can switch to the H-1 spectrum, and assign all H-1 peaks *

H-1 assignments from HSQC peaks

C-13 assignments from C-13 spectrum



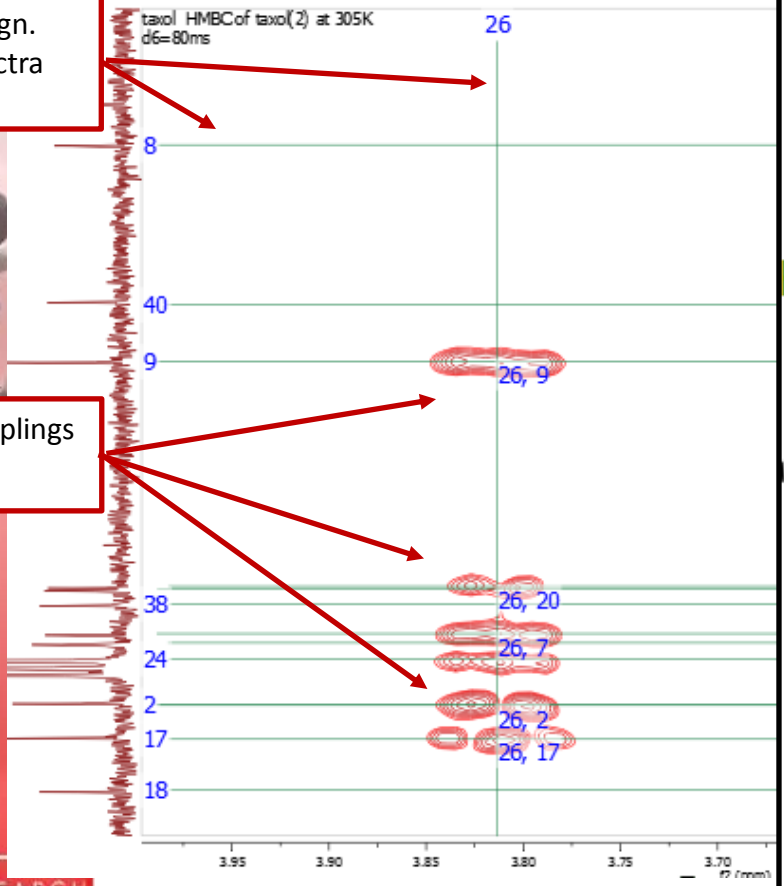
** If you assign a H-1 chemical shift to the same atom multiple times (e.g. first from HSQC, and then from H-1 spectrum), the last one is taken. It is possible to assign multiple atoms to the same peak. To remove an assignment, delete the assigned chemical shift from the Assignments Table*

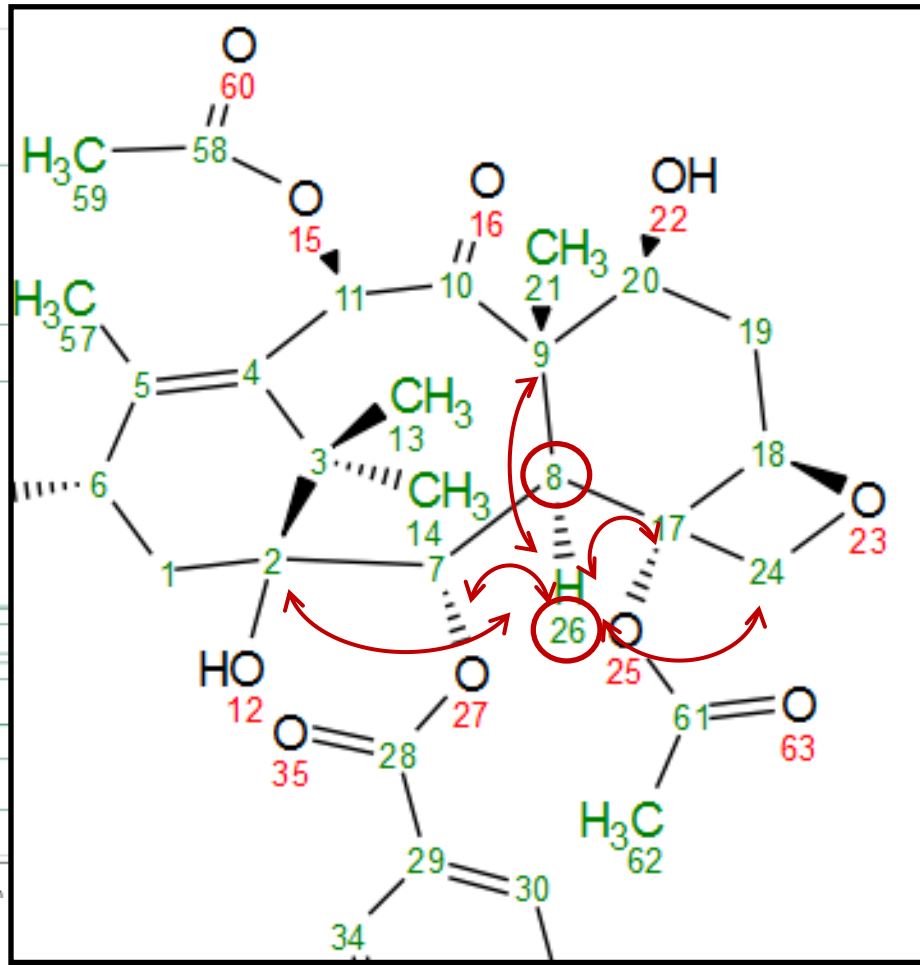
If you have 2D HMBC

- The assignments of both H-1 and C-13 shifts are displayed on HMBC, making it easy to identify 2-3-bond long-range correlations between them.
- To assign an HMBC peak, click on an **atom** in the structure, next click on the cross peak to assign. Choose the other atom from the dialog.

H-1 & C-13 assign. from other spectra for H26-C8

Long-range couplings to H26





To superimpose HMBC and HSQC

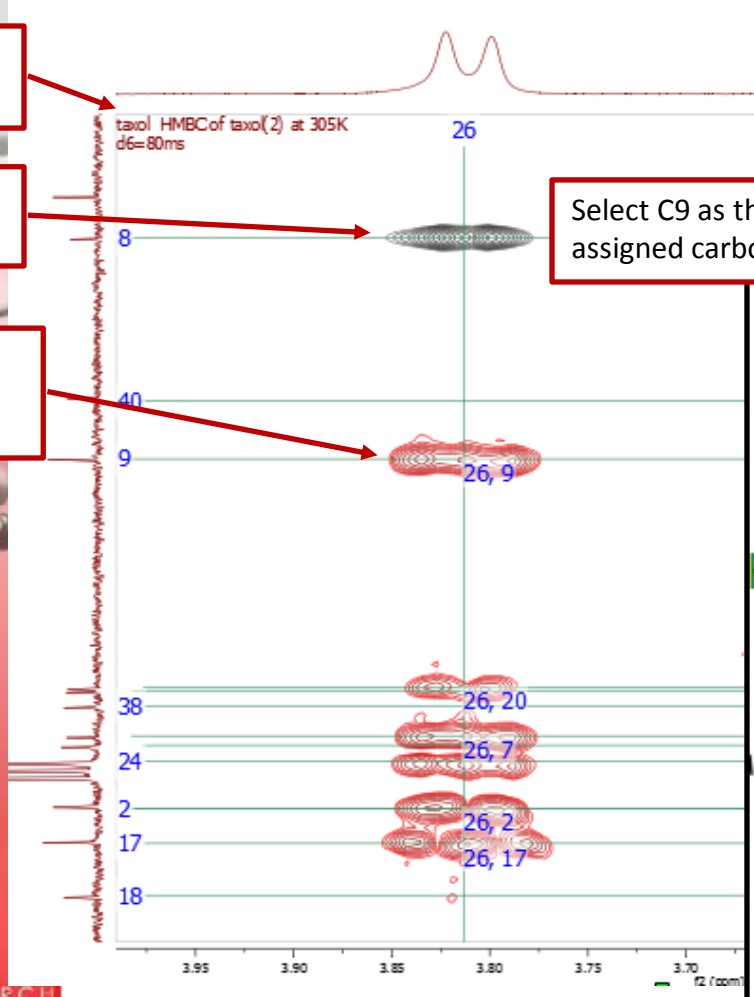
- Select both HMBC and HSQC from the Pages View, click  to superimpose them. Use **Shift+Up Arrow** keys to toggle the active spectrum. Change their contour colors (e.g. Grey for HSQC, Red for HMBC)*
- Make sure HMBC is the active one. In the assignment mode, click on a peak and then on one of the atoms. Choose the other atom from the dialog.

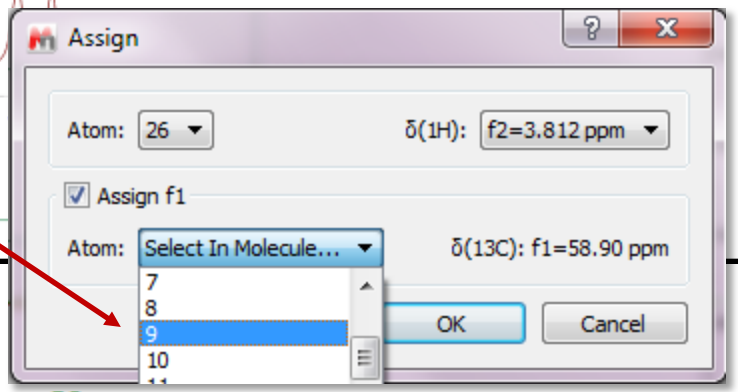
Title of the active spectrum

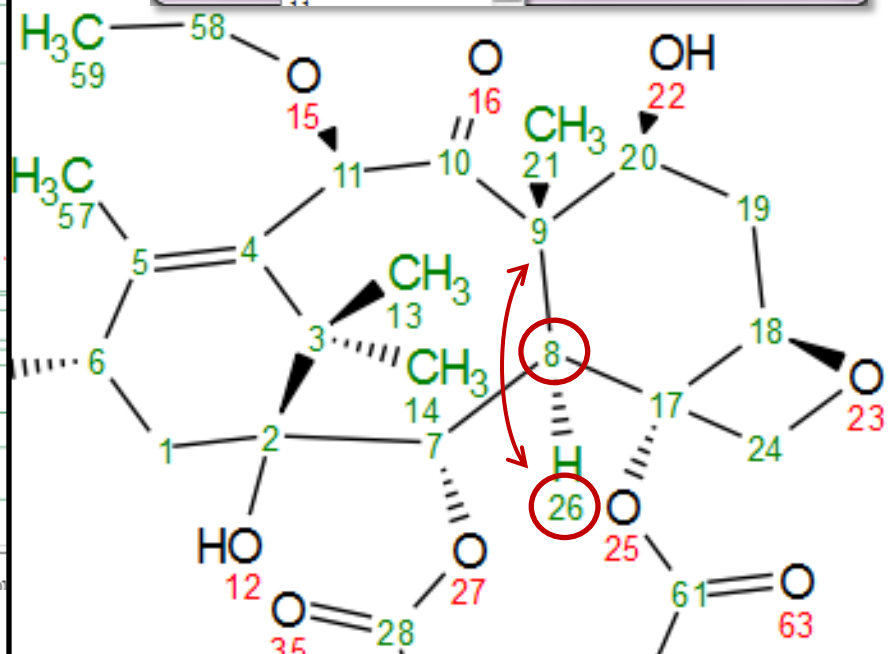
HSQC peak between C8-H26

Click on this peak and then click on H26 in structure

Select C9 as the assigned carbon

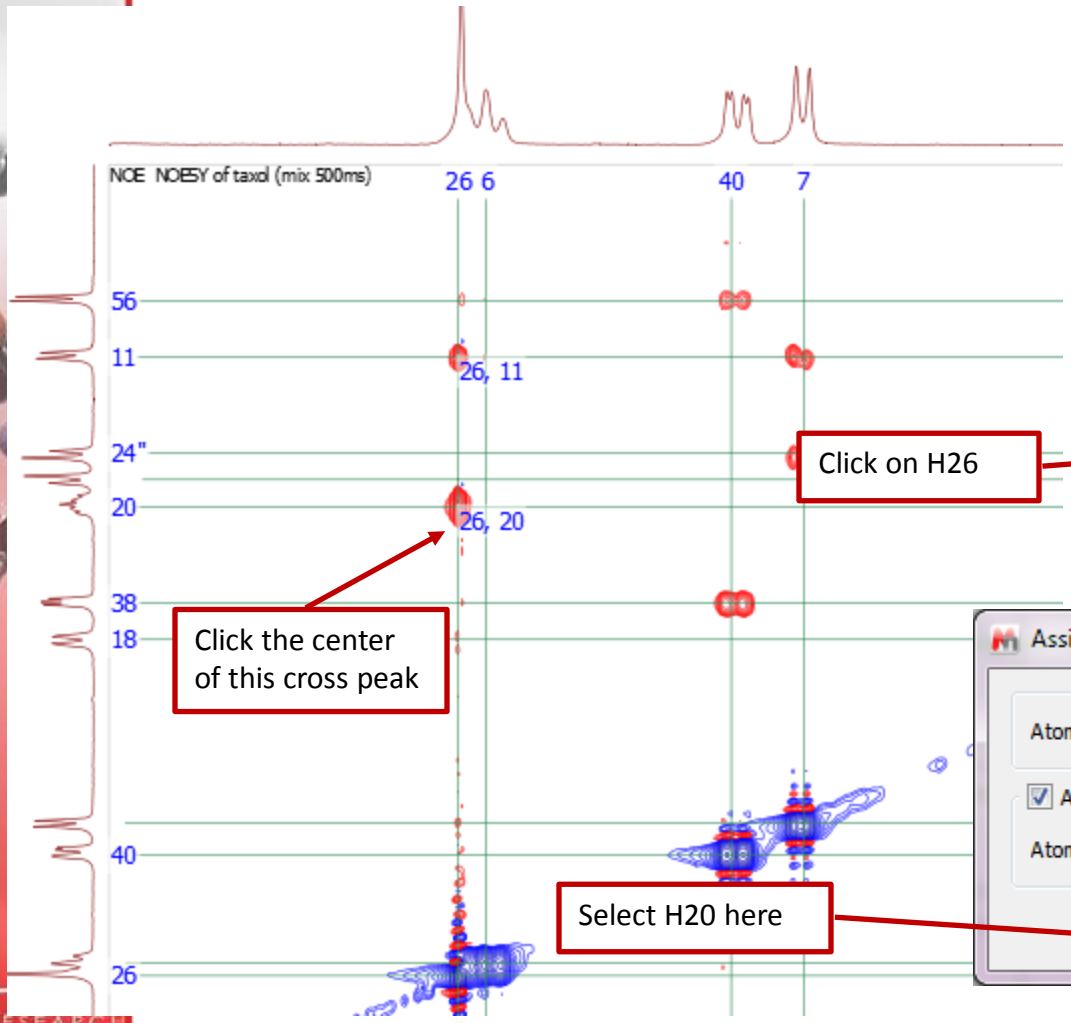


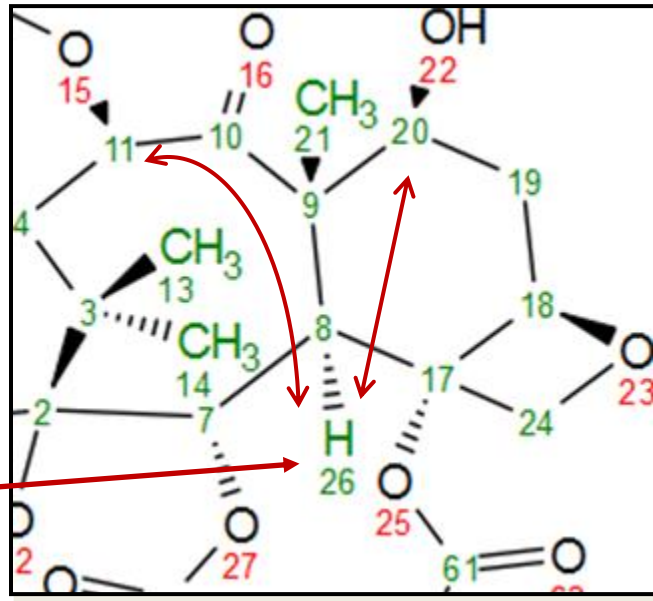


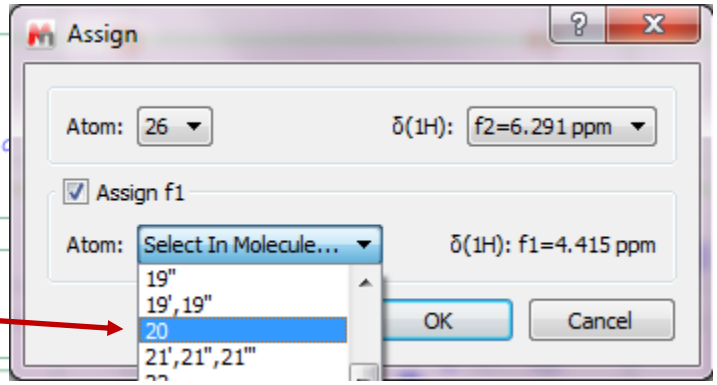


If you have NOESY, ROESY etc…

- Locate the cross peaks at the intersections of the assignment grids. Click on them and the corresponding atoms to do the assignments
- The assignment of two NOESY peaks are shown below







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The Assignment Table for multiple spectra

- Choose **View | Tables | Assignments** to open the Assignments Table if not yet
- The Table lists all assignment results, which can be copied to other documents

Assignments

Report | Copy | Delete | Expand | Collapse | Setup

Atom	Chemical Sl	Predicted S	COSY	TOCSY	HSQC	HMBC	H2BC	NOESY
1 C	36.08				1', 1"	7		
H'	2.35				1			
H"	2.29				1			
2 C	79.42					7, 26		
3 C	79.40					13', 13", ...		
4 C	133.54					57', 57", ...		
5 C	142.27					57', 57", ...		
6 C	72.46				6			
H	6.24				6			
7 C	75.13				7	26		
H	5.68		26		7	1, 2, 9, 28		
8 C	45.84				26			
9 C	58.92					7, 26, 21...		
10 C	203.84					11, 21', ...		
11 C	75.68				11			
H	3.82				11	10		26
12 O								
H								
13 C	27.02				13', 13", ...			
H3	1.25				13	3		
14 C	21.95				14', 14", ...			
H3	1.15				14			
15 O								
16 O								
17 C	81.46					24', 24", ...		

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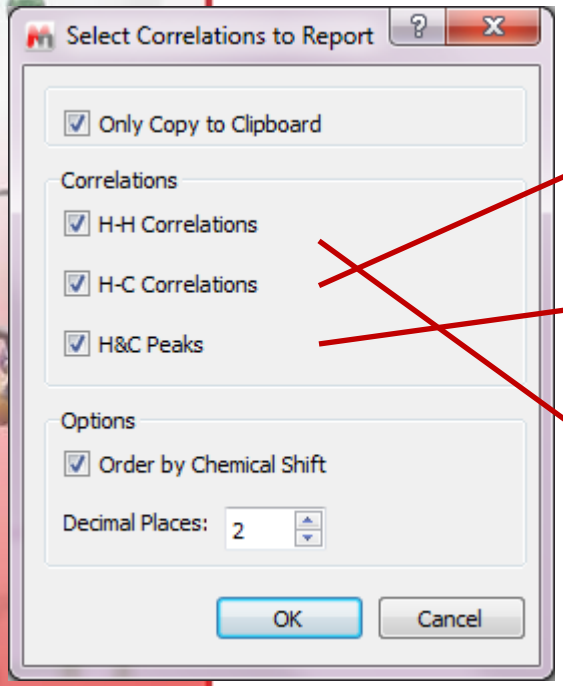
To export assignment results

- The **Assignment Table** can be copied to other documents such as MS Excel
- For more sophisticated reports, highlight the structure, then choose **Scripts | Report | Assignments**, and select the options. Next paste the reports to a MS Word or other documents directly



Number	δ (ppm)	HSQC ($^{1}J_{CH}$) Correlations (ppm)	HMBC Long Range ($^{1+n}J_{CH}$) Correlations (ppm)
3	7.22	101.16	
4	7.95	131.51	
6	7.46	118.25	
7			
8			

Number	^{1}H-Chemical Shift	Multiplicity (*J*-couplings)	^{13}C- Chemical Shift
8	8.62	d, *J*=4.54 Hz	147.42
4	7.95	d, *J*=9.20 Hz	131.50
6	7.47		118.25
7	7.30	dd, *J*=9.25,2.68 Hz	121.52

Number	δ (ppm)	COSY Correlations (ppm)	NOESY Correlations (ppm)	TOCSY Correlations (ppm)
30	8.14			
45	7.50			
43	7.49		7.01(41')	
47	7.49		5.80(38'), 4.80(40'), 3.59(56')	
44	7.43			
46	7.43			
52	7.38			
54	7.38			
41	7.01		7.49(43'), 7.01(55')	
55	7.01		7.01(41')	
26	6.29			
6	6.24			
38	5.80	3.59(56')	7.49(47')	
7	5.68			
18	4.95			

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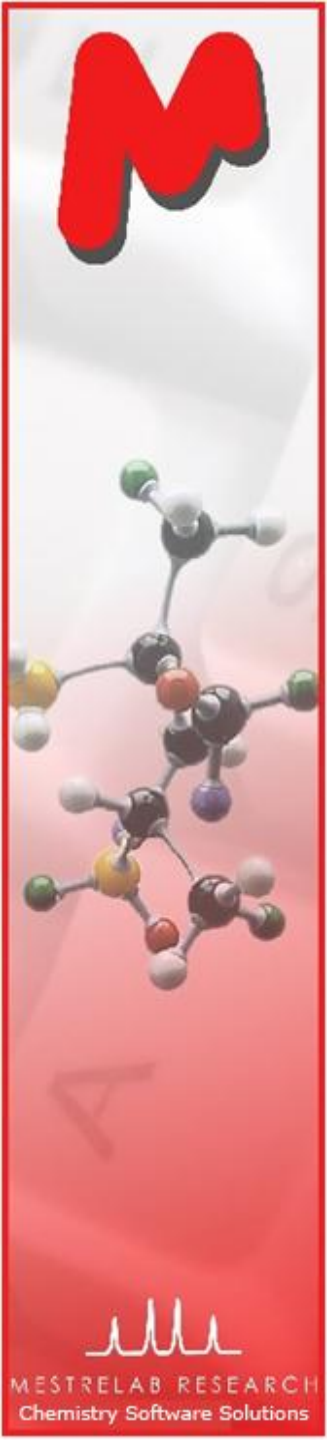
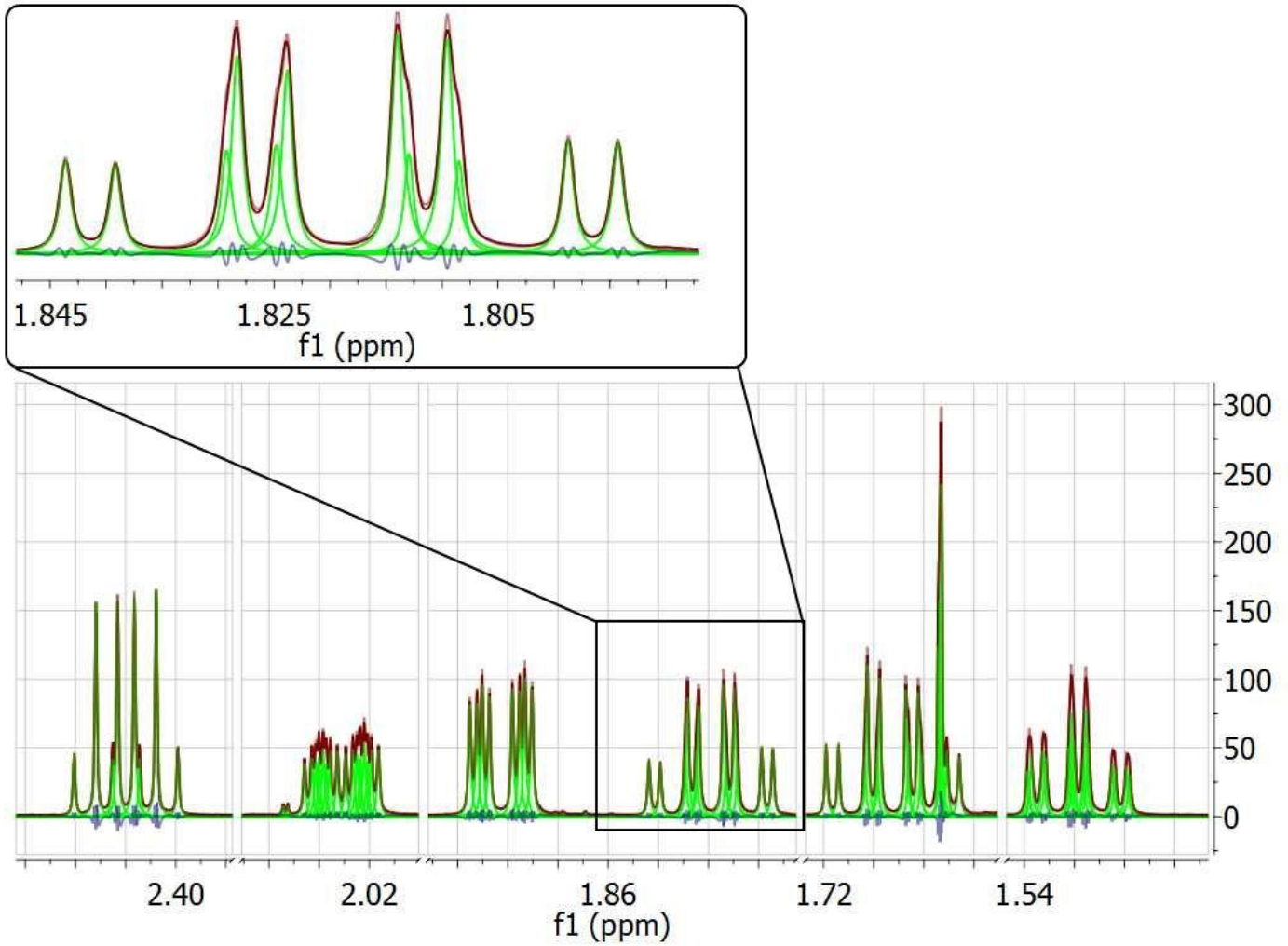
Chemistry Software Solutions



GSD: Global Spectral Deconvolution

- Many applications require a reliable and comprehensive analysis of experimental ^{1}H-NMR data. Main problems are:
  - Global artifacts, in particular baseline distortions which will affect integral values
  - Solvent peaks
  - Lack of sufficient spectral resolution, etc.
- GSD is a novel algorithm developed by Prof Stan Sykora at ExtraByte exclusively for Mestrelab
- Fully automatic multiplet deconvolution for the whole spectrum to recognize and extract all peaks and recognize artifacts
- The results are
  - List of peaks (center, height, width, class etc)
  - Synthetic spectrum
  - Array of residues
- In version 7.0, GSD is embedded in peak picking by default. So GSD is automatically done and the deconvoluted peaks are picked

GSD: Global Spectral Deconvolution



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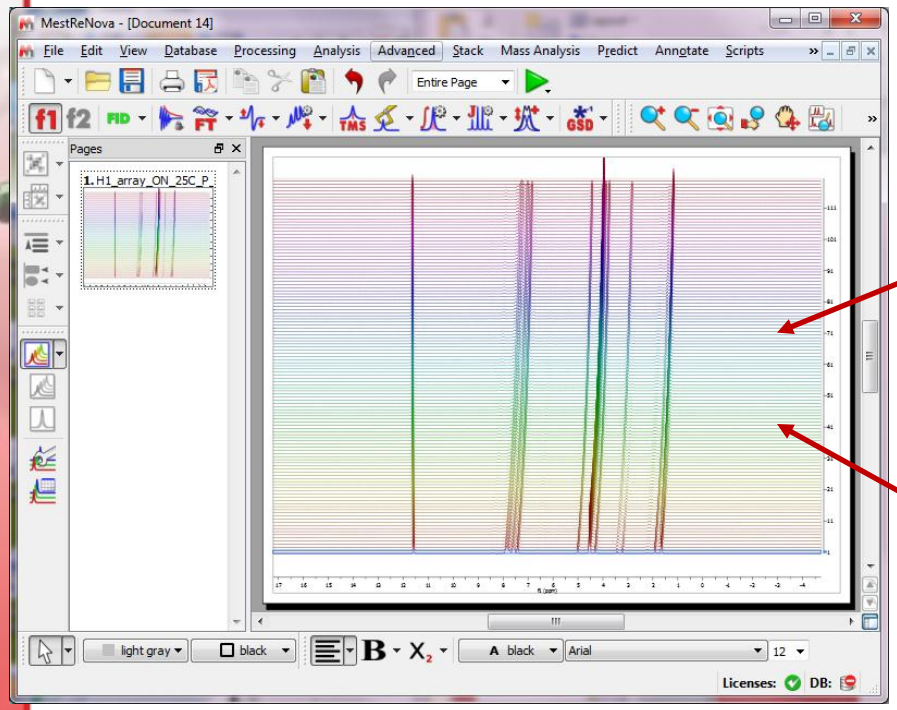
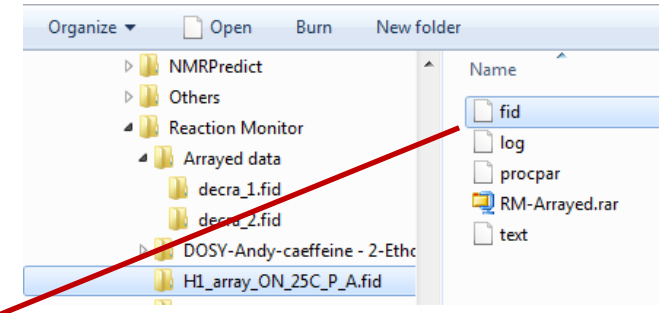
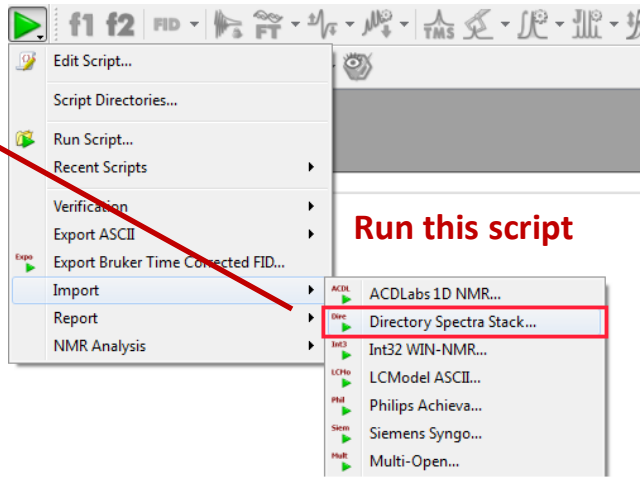
To process and stack multiple spectra

- For multiple spectra acquired in **arrayed mode**: Just open the FID (Varian) or SER file (Bruker), and the individual spectra will be processed and stacked.
- For multiple spectra acquired on **individual basis**: Run the Directory Spectra Stack script to open and stack all spectra under a base directory:





Drag & drop



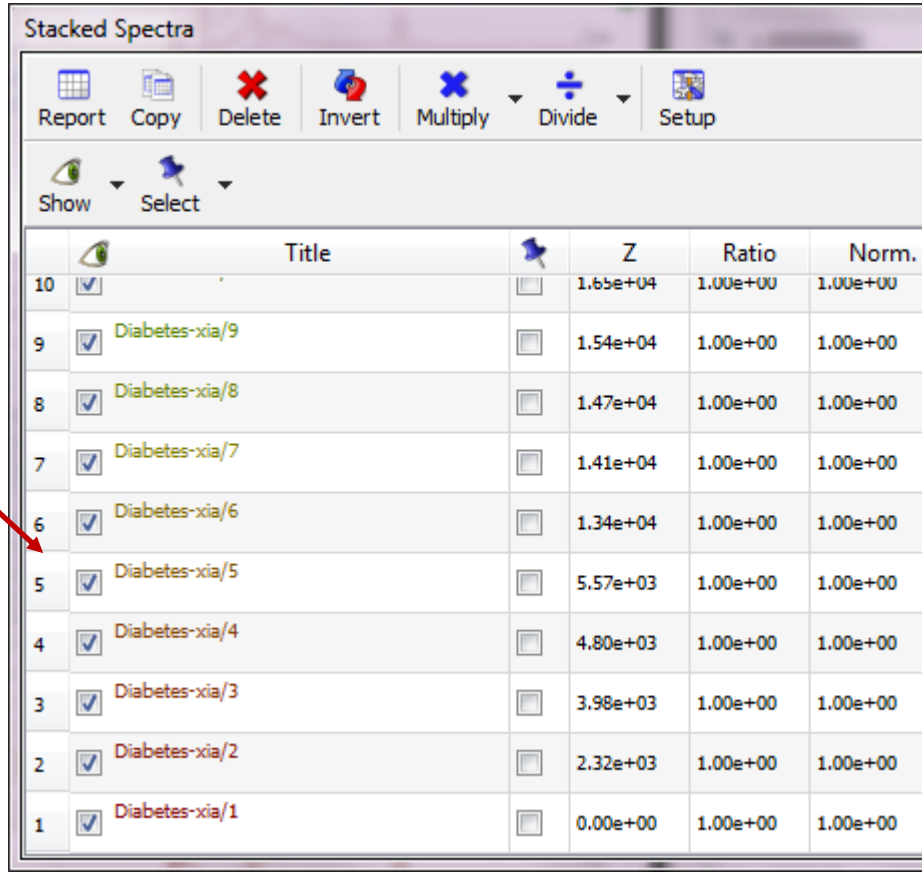
Run this script

** If you have only a few 1D spectra to stack and compare, just open them in the same document, select all of them from the Page View, and use the Stack menu commands to stack or superimpose them*

To re-process 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
  - Change which ones to display
  - Change which ones to re-process, such as phasing, baseline correction etc.

Click and drag here to change the order of a spectrum in the stack



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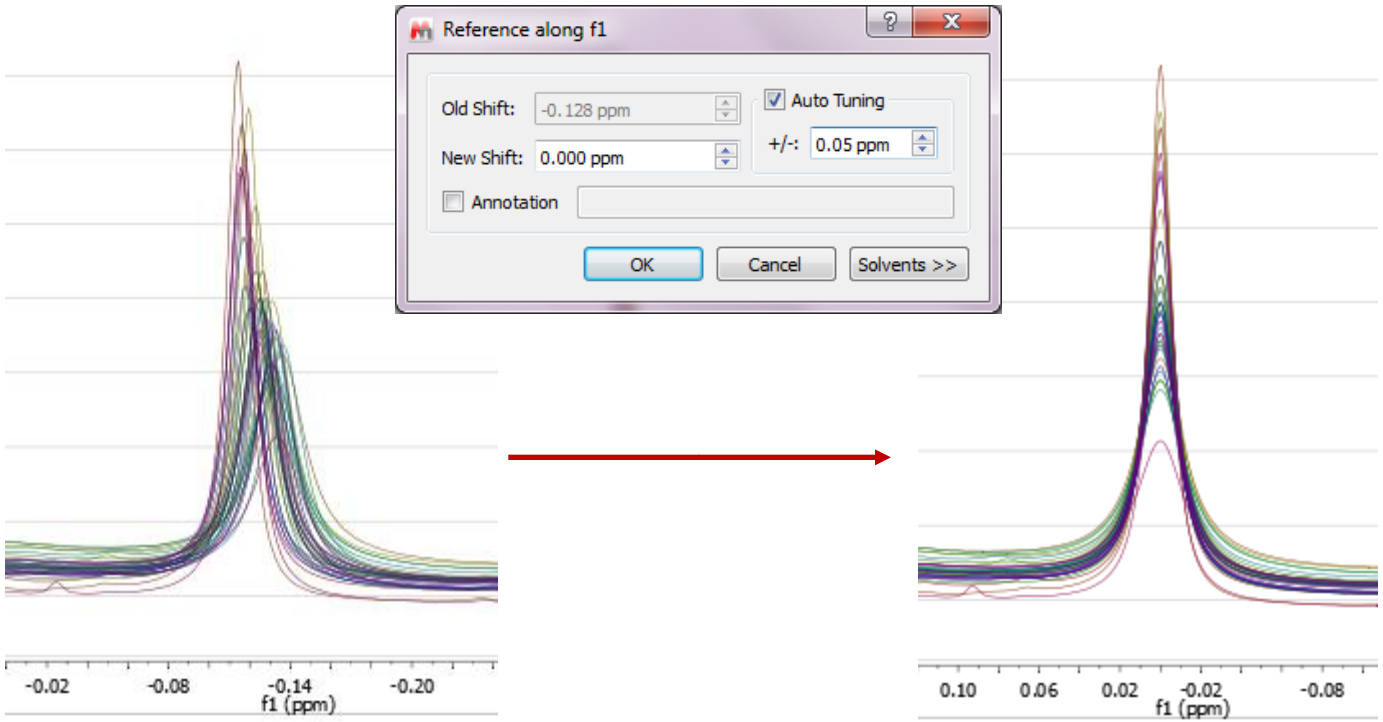
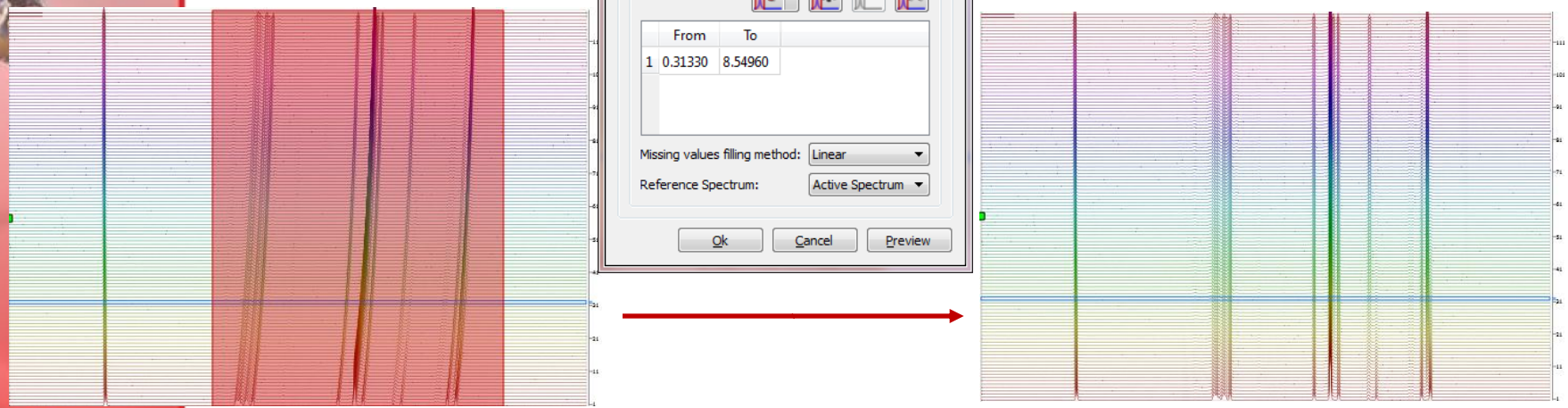
To align multiple spectra by correcting reference

- Systematic errors of chemical shifts can be corrected if there is an internal reference peak, e.g. TSS peak.
- Click TMS and then click on the reference peak in the active spectrum
- In the following dialog, set the proper chemical shift for the reference peak, check Auto Tune, and define a tuning range (e.g. +/- 0.05 ppm):



To correct local peak misalignment*

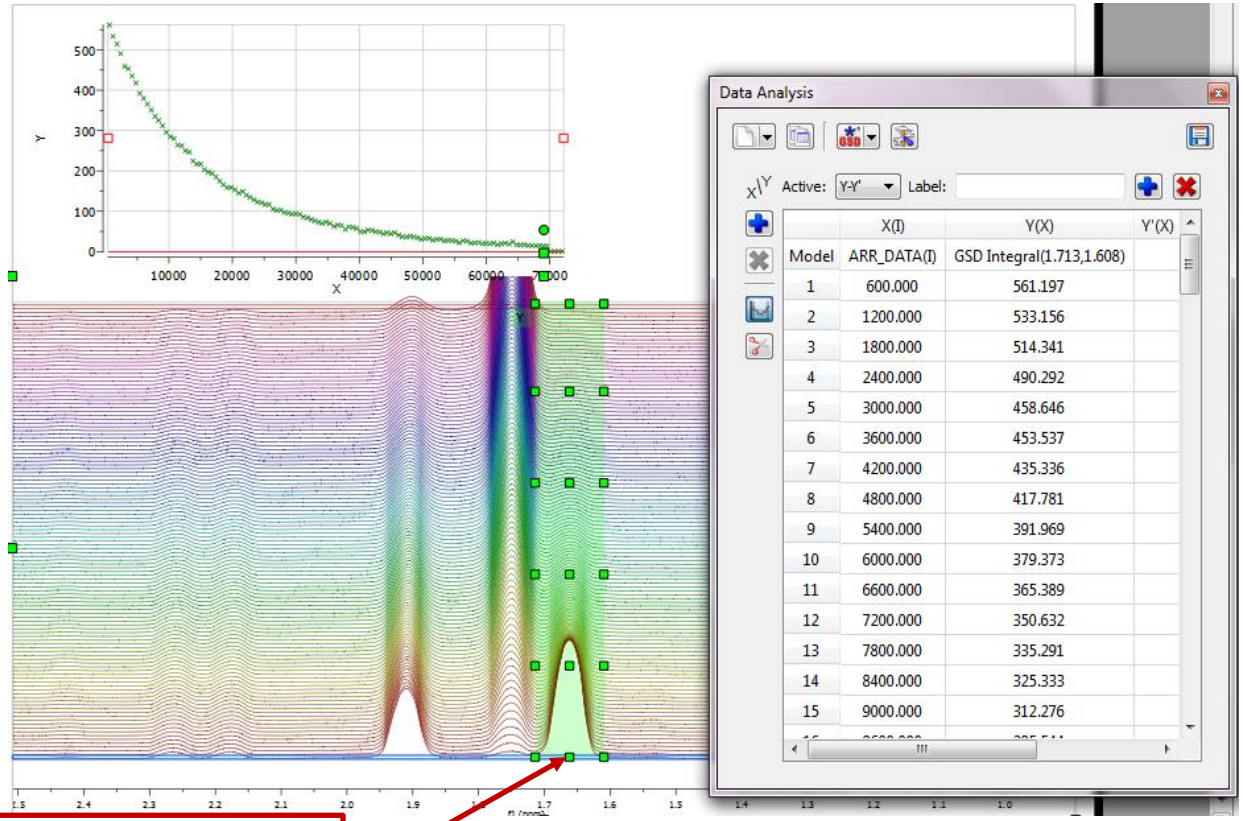
- Zoom into the region of interest, select **Advanced | Align Spectra**.
- Click  , then click-and-drag to cover the peaks to align. Click Preview to see the alignment result. Adjust other parameters until satisfactory.
- Move to other regions to continue this process until done.
- Click OK to accept the results



** When there is peak cross-over, it may not be good idea to use local peak alignment. Instead, use the UI feature to change the integration regions so that they follow the change of the peak locations. See later slides.*

To extract data using the Data Analysis Panel

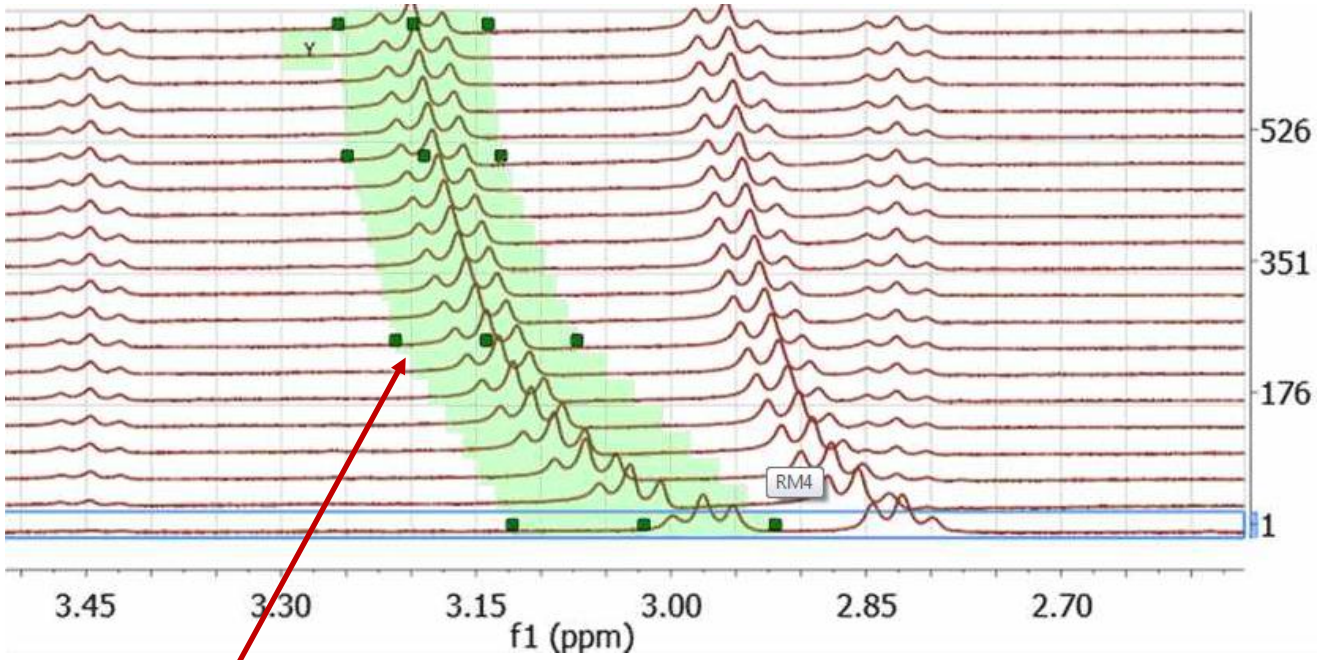
- The areas of the GSD peaks in the defined region are filled in the Y(X) column, and also plotted in the X-Y graph.



The region within which GSD peaks are integrated as Y(X) values

To extract data from drifting peaks

- If the peaks drift over time, you can manually change the direction of the integration regions :



Click & drag the handles to change the shape of the selection region.
Press Shift to move all points simultaneously

Tip: you can change the number of handles by clicking the Options button on the Data Analysis Panel: 

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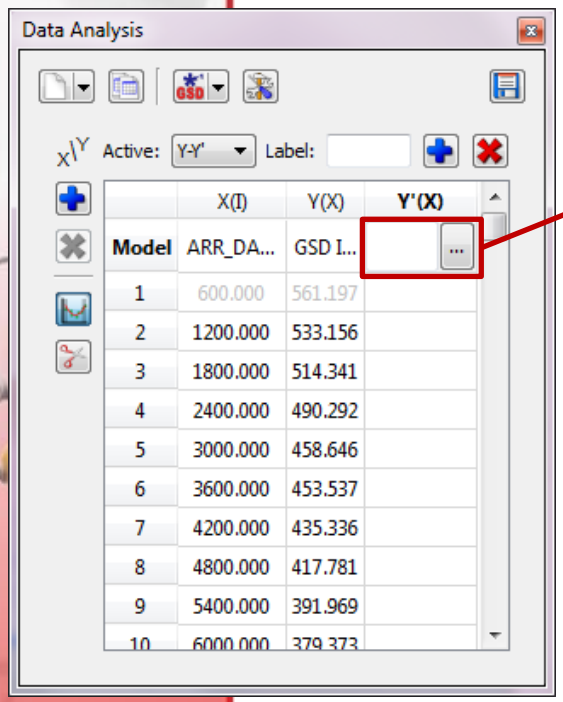
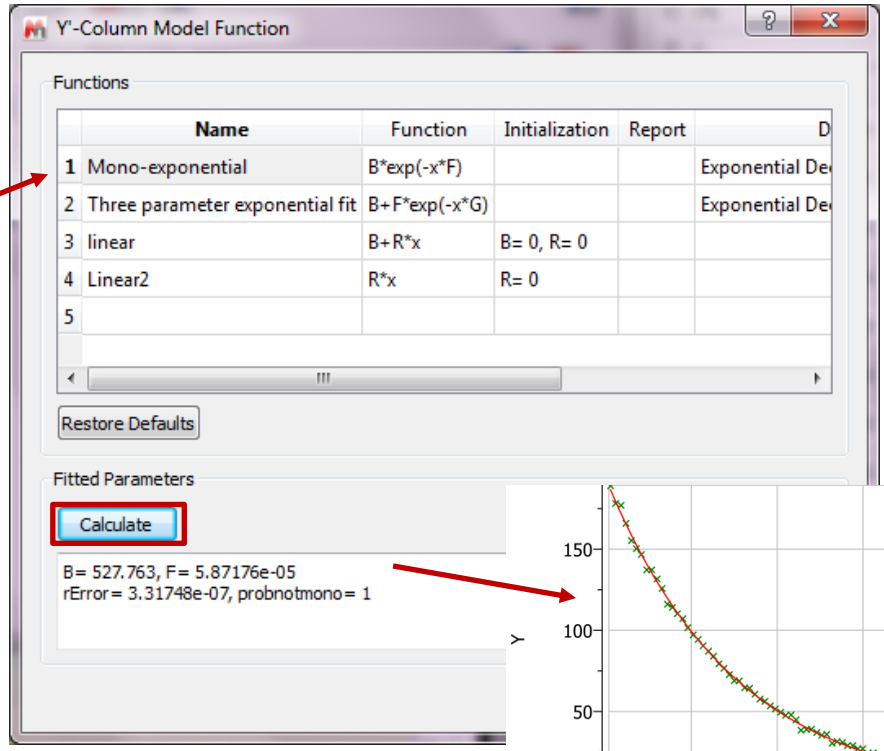
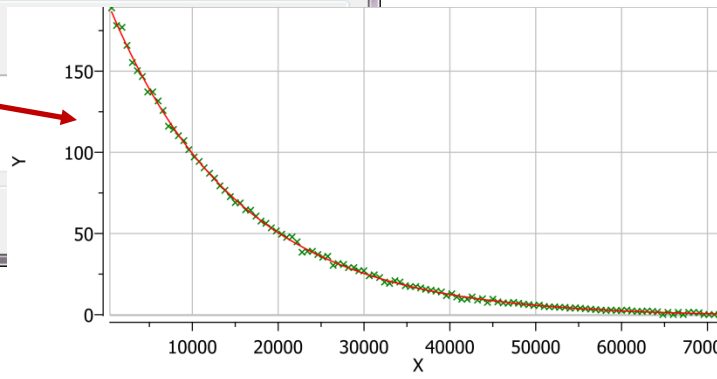
To fit the data to a function

- To fit the XY points to a function, double click the first cell in the Y'(X) column, and choose (or define) a function, and click Calculate to do the fitting. Click OK to accept the results:



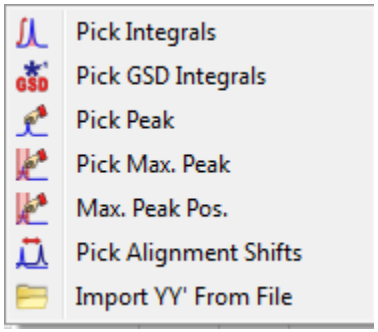


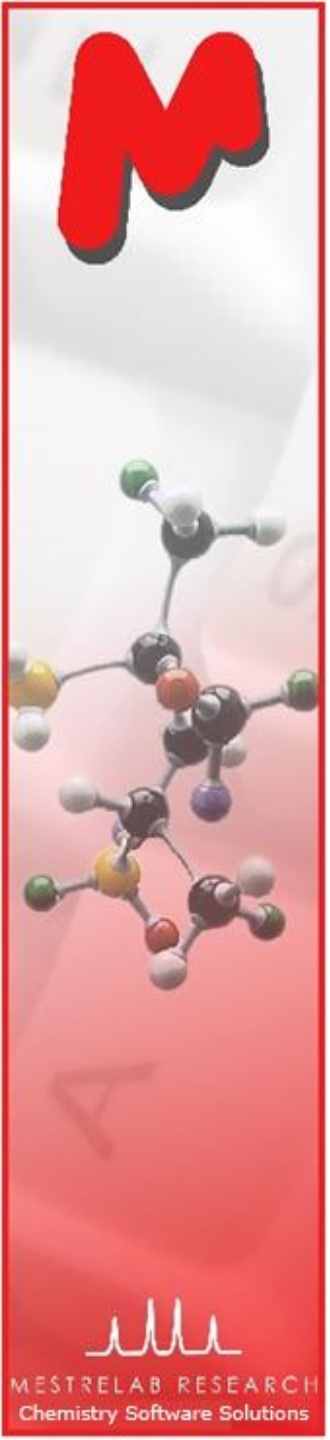


This example shows a first order reaction. F is the rate constant (k). The half-life $t_{1/2} = 0.693/F$

Applications of the Data Analysis Panel

- The Data Analysis Panel provides an elegant way to extract and analyze multiple spectral data, including:
  - Integrals: analog peak areas
  - GSD Integrals: areas of deconvoluted peaks
  - Peaks: intensities of the peaks near a defined location
  - Maximum Peaks: intensities of the highest peaks in a defined region
  - Max. Peak Positions: positions of the highest peaks in a defined region.
  - Pick Alignment Shifts: the shifts of peaks relative to the peak in the first spectrum
- It can be used for a variety of applications, such as
  - Relaxation studies
  - Diffusion studies
  - Reaction monitoring and kinetic studies
  - Protien-ligand binding studies



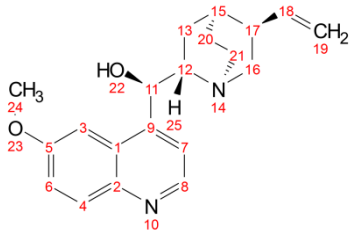


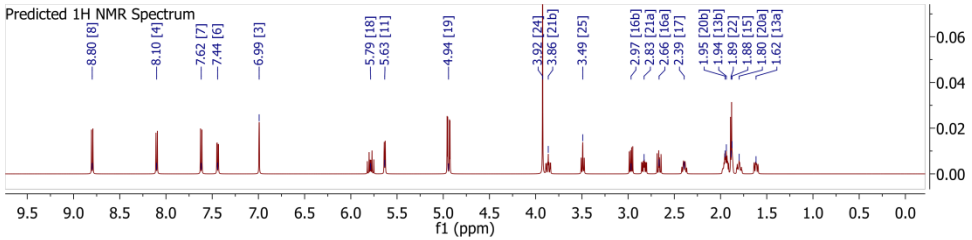
Mnova NMRPredict Desktop

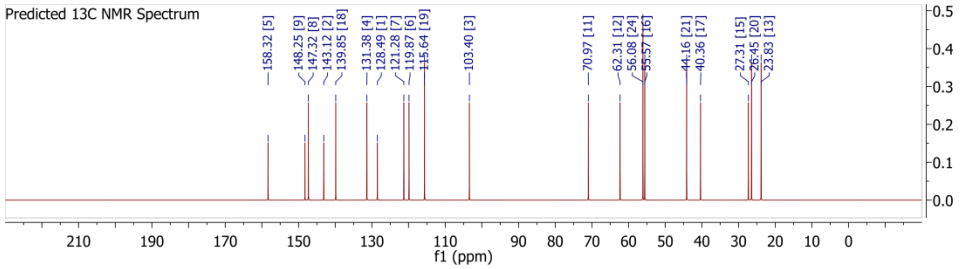
- Predict ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{29}Si, and ^{31}P spectra
- Predict and assist visual verification of a structure
- Predict and assist interactive peak assignment
- Mnova NMRPredict Desktop license required for prediction related tasks

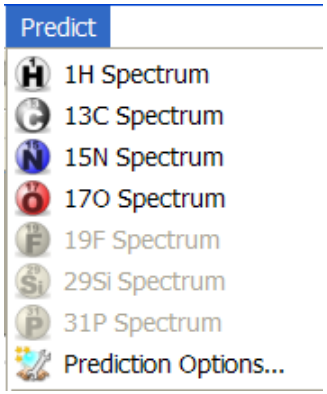
To predict NMR from a structure

- 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, .sdf or .cdx 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.

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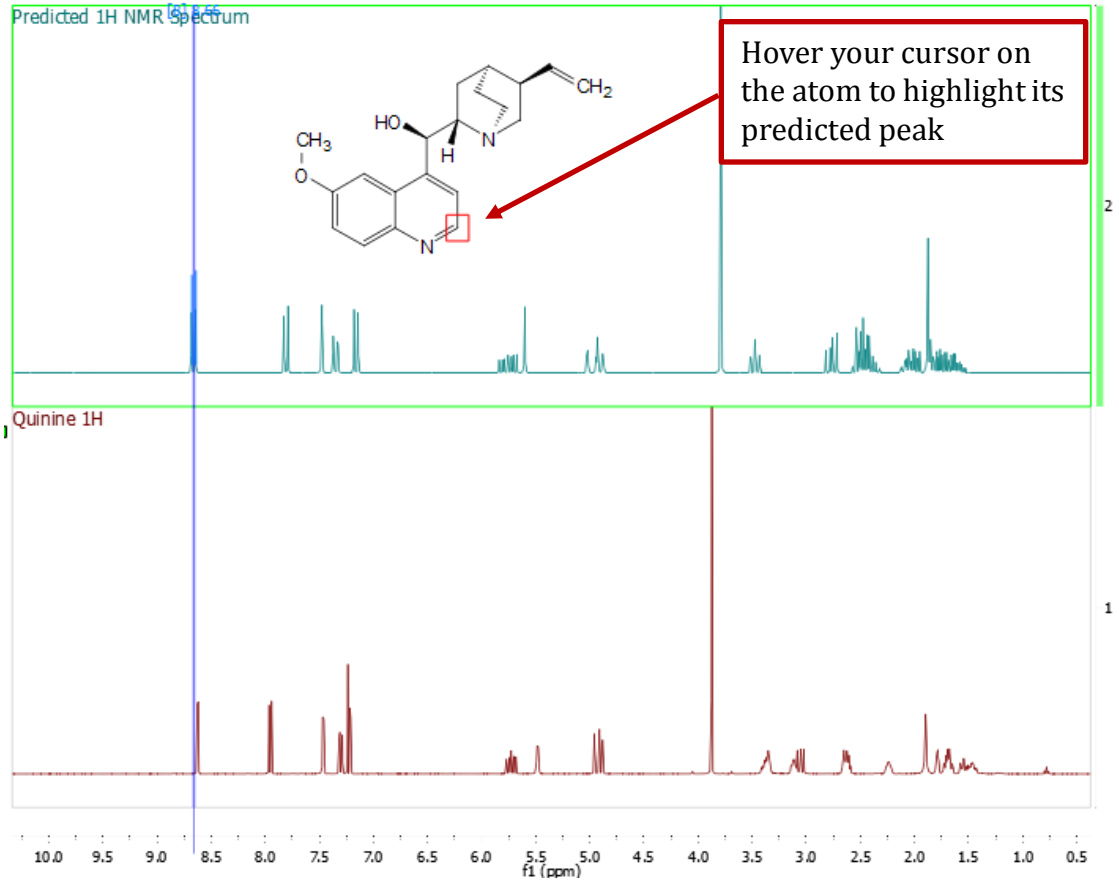
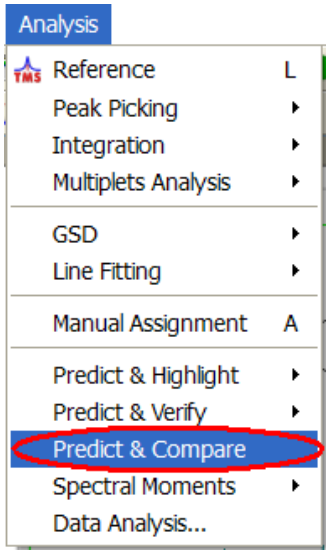
To predict NMR & verify your structure

- 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





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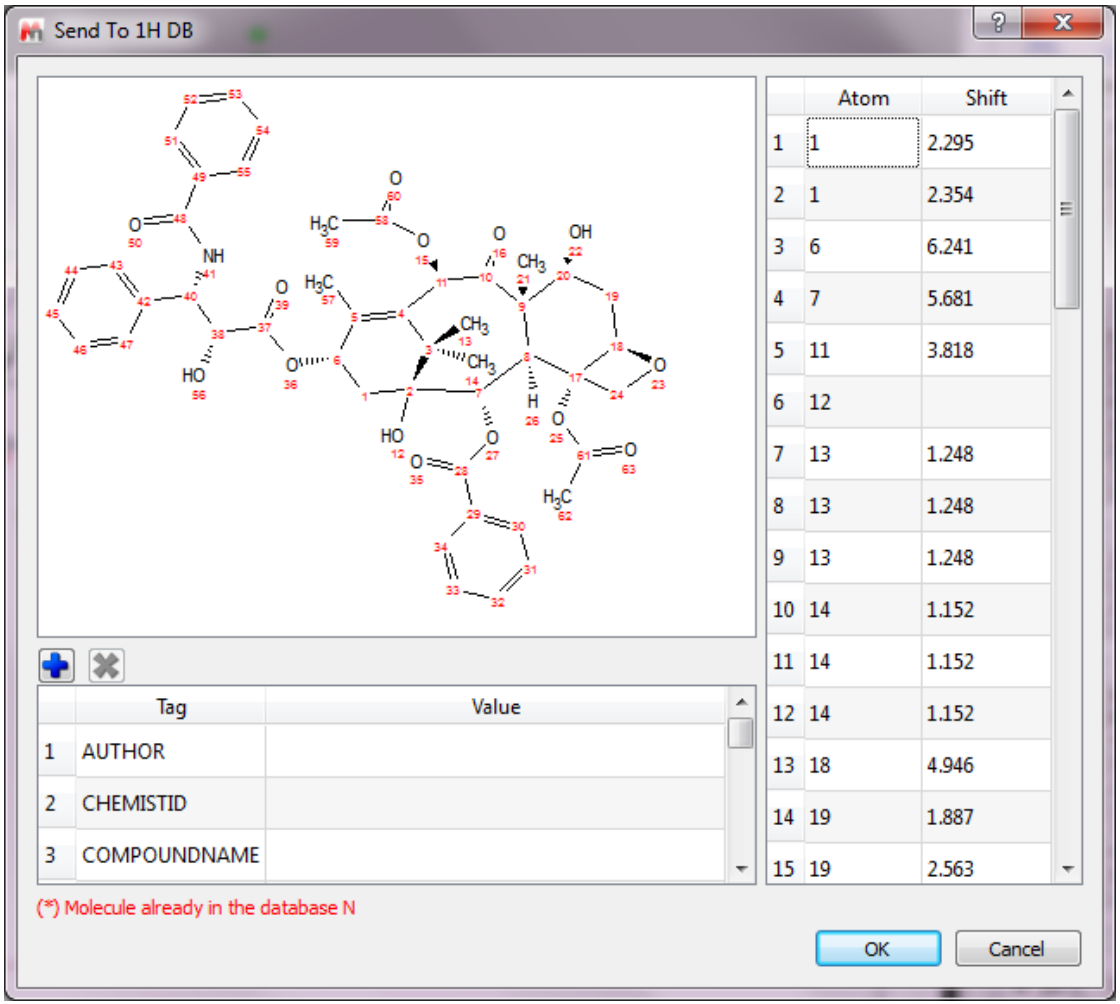
To improve NMR prediction using your assignments

- After you are done with the assignment of a 1D spectrum, choose **Predict | Update 1H User DB** to save it as a knowledgebase for H-1 prediction. This will improve the 1H prediction of similar structures



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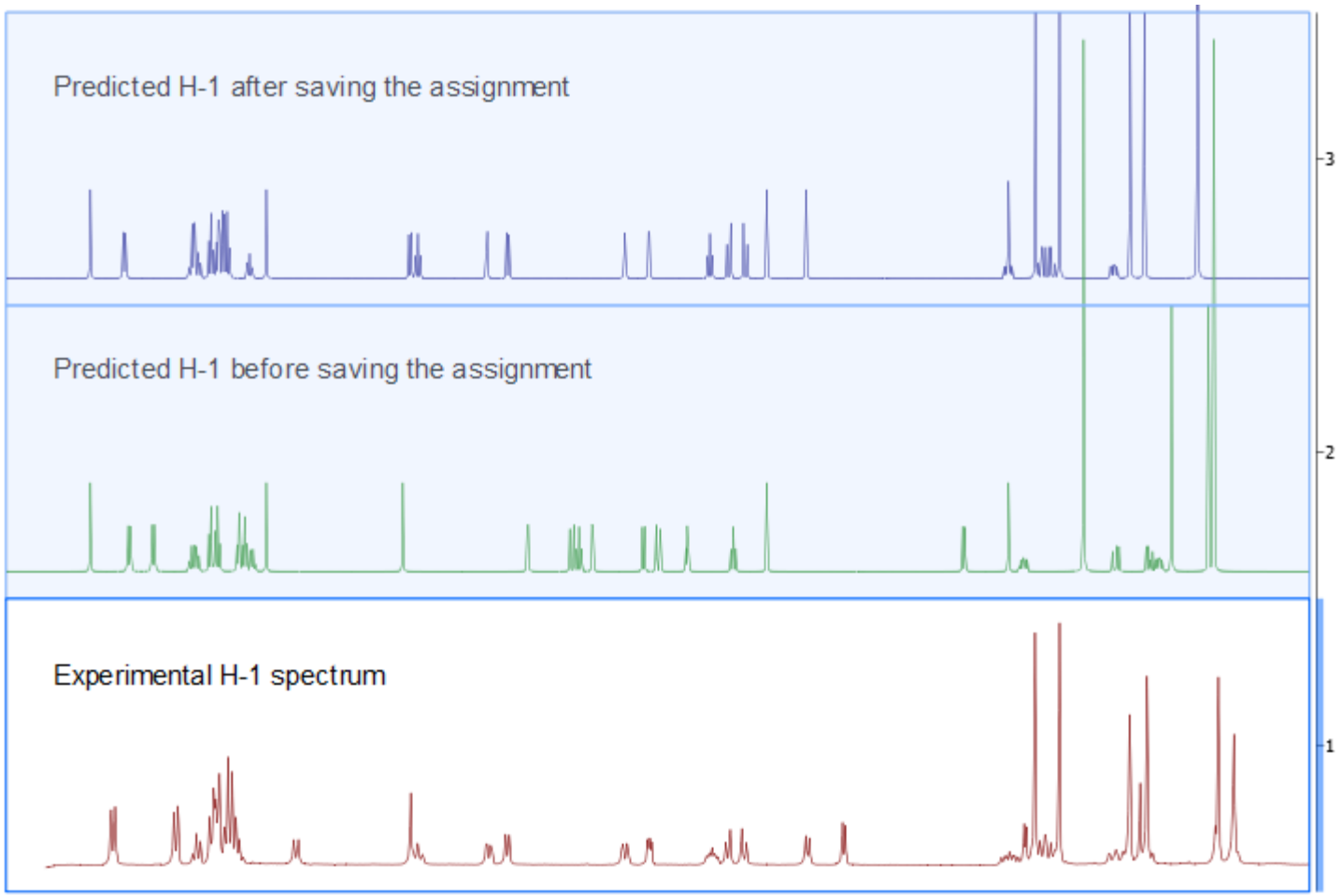
To improve NMR prediction using your assignments

- The prediction is usually improved after you save your assignments to Mnova NMRPredict Desktop



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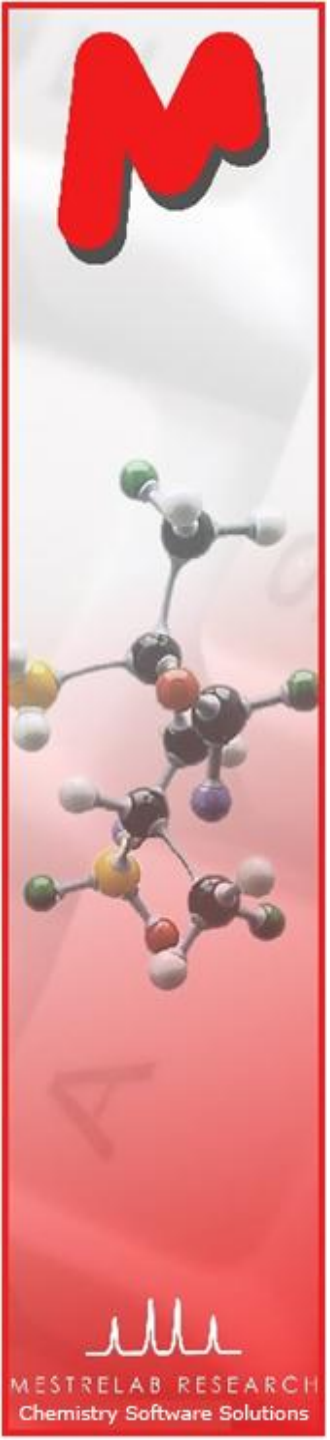


Mnova MS

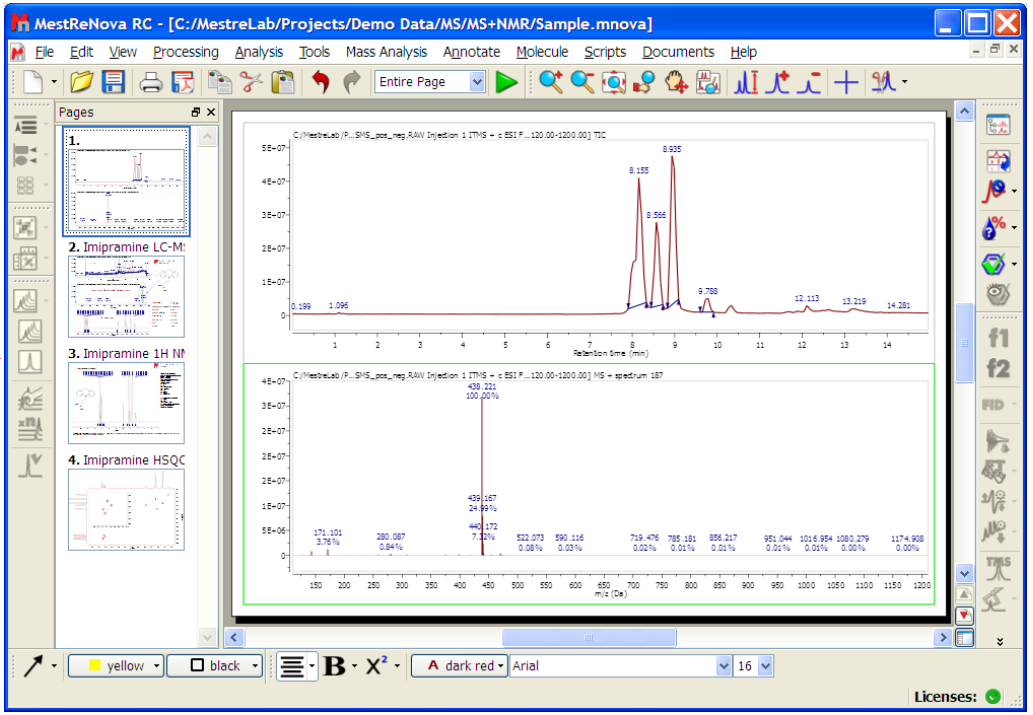
- Visualize your LC/GC-MS data and UV components from various vendors
- Integrate peaks automatically or manually with easy reporting
- Verify proposed structures by matching mol ion and isotope peaks
- Enumerate possible elemental compositions from a selected ion peak
- Mnova MS license required

Mnova MS: Open raw data automatically

Raw data

- Agilent
- Thermo
- Waters
- Bruker
- ABI/SCIEX
- JEOL
- Shimadzu

Drag & drop



NMR spectra can be opened in the same document. Molecular structures can be opened as .mol, .sdf or .cdx files, or be copied from ChemDraw, Isis/Draw and ChemSketch.

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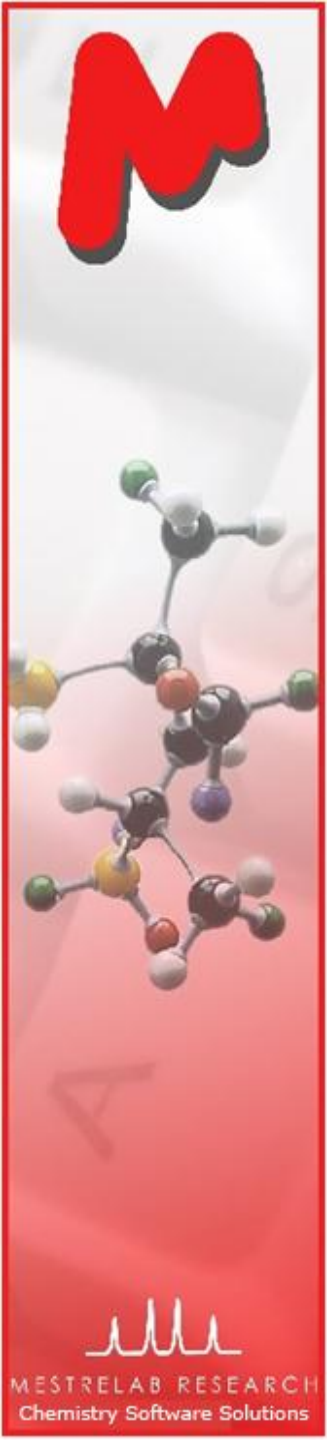


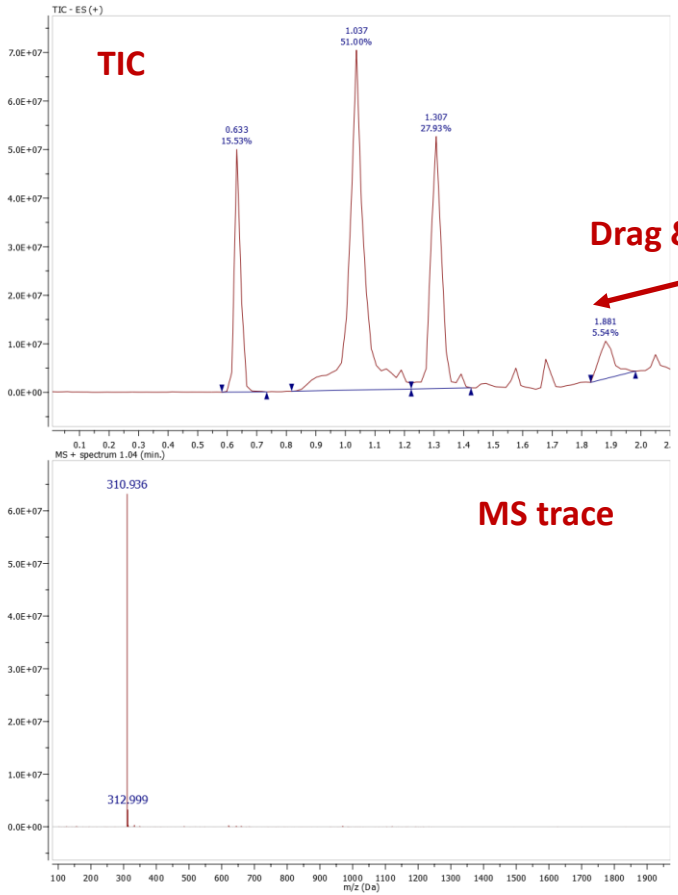
Supported data formats on different platforms

Vendor	Windows	Mac	Linux
Agilent	ChemStation, MassHunter, Ion Trap	ChemStation	ChemStation
Bruker*	XMass, Compass	XMass	XMass
Waters	MassLynx	MassLynx	
Thermo Scientific	Xcalibur		
JEOL	MSQ 1000, FastFlight		
SCIEX*	Analyst		
Shimadzu*	LabSolutions		
mzData, mzXML	mzData, mzXML	mzData, mzXML	mzData, mzXML
Midas	Midas	Midas	Midas
NetCDF ANDI-MS	NetCDF ANDI-MS		

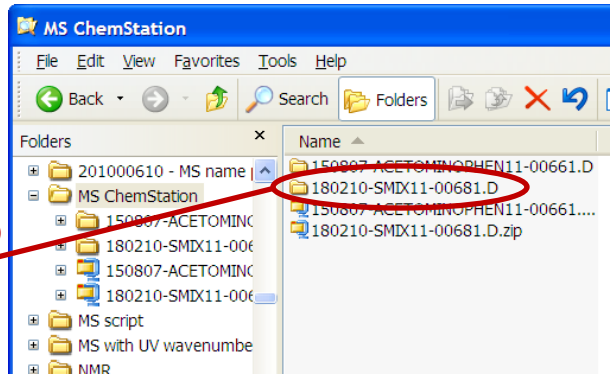
**The vendor software (Bruker, Analyst, or LabSolutions) is still required to be installed on the same computer for Mnova MS to import the raw data. However, we can provide scripts that do real-time or batch conversion of your raw data into Mnova binary files. Such Mnova binary files can be distributed to users who have only Mnova installed.*

To open your LC/MS data

- Choose **File | Page Setup | Orientation** and change the page orientation to portrait, if you prefer.
- Choose **File | Open** 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 integration.



Drag & drop



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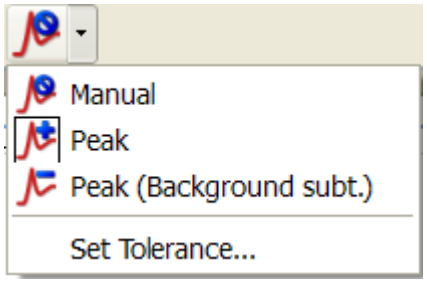
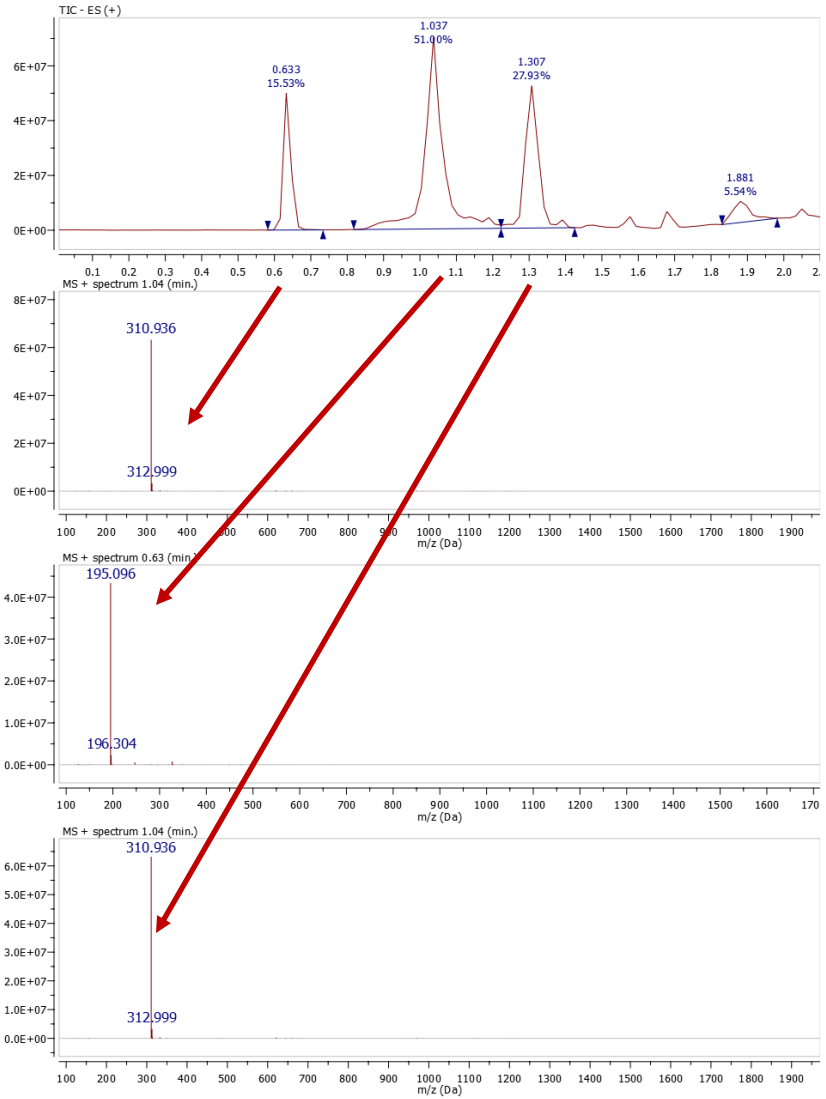
To browse the MS traces

- Click  to switch to crosshair cursor, and click on the TIC to display the MS trace at that retention time.
- Click  to change to appending mode if you want to display multiple MS traces
- Choose the Spectrum Selection Mode options to display co-added MS traces:





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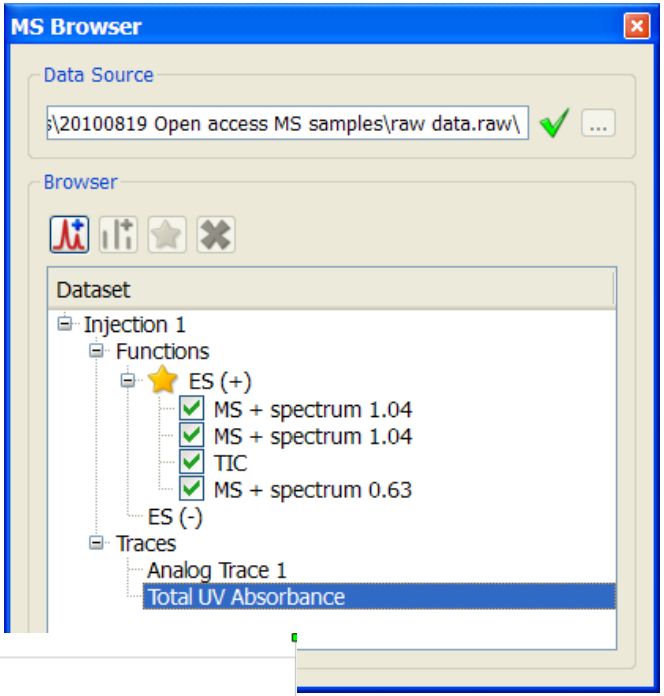
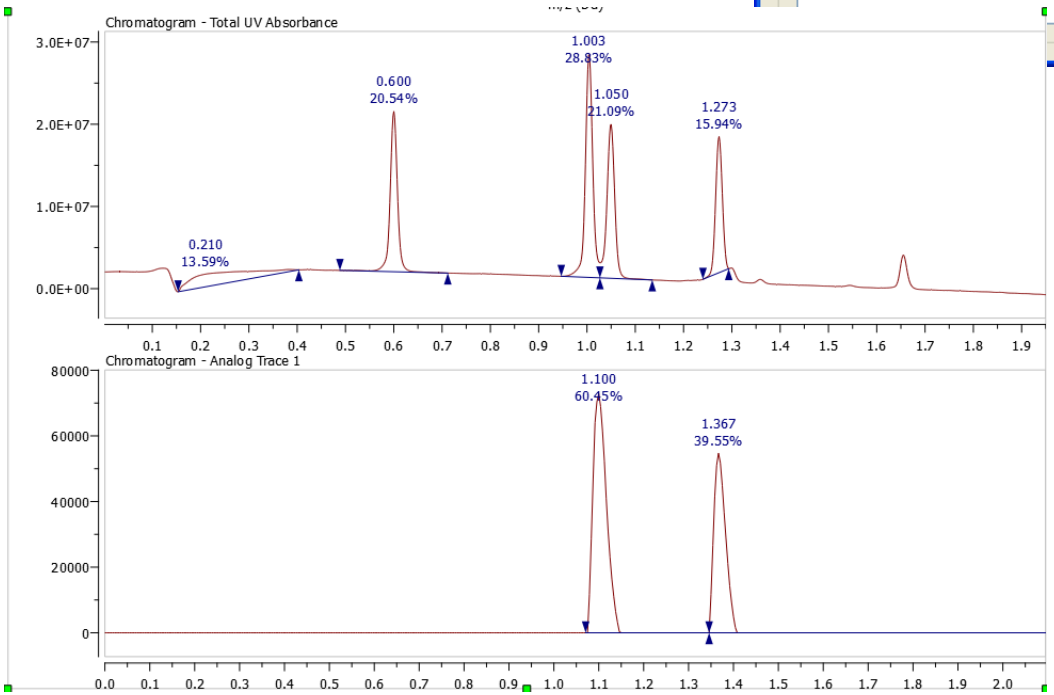
To browse the UV traces

- Click  to show the **MS Browser Panel**
- Choose the **Total UV Absorbance** under **Traces**, and Click  to display the UV TIC
- Repeat the above step to display the other UV components if any





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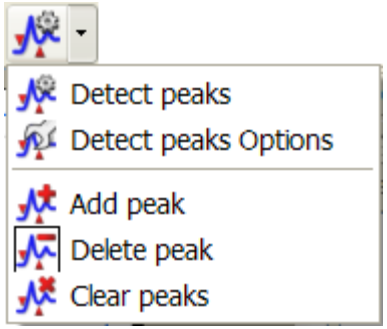
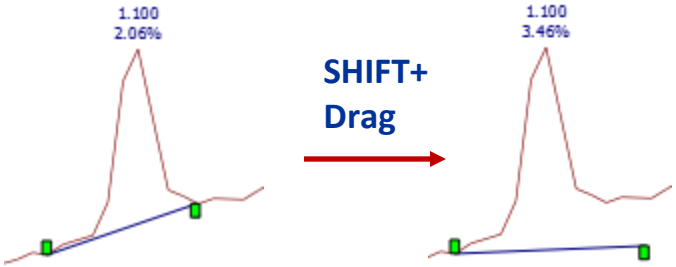
To edit and report peak integration results

- 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 on 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
- Choose **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	1.100	47	BB	3975.324	214.489	4.12	2.06	0.990	1.174
2	1.449	62	BB	5073.908	199.626	5.25	1.91	1.357	1.504
3	3.081	133	BB	71442.947	7866.334	73.95	75.41	2.787	3.429
4	3.539	153	BB	2165.626	171.022	2.24	1.64	3.429	3.612
5	3.814	165	BV	3666.850	252.017	3.80	2.42	3.722	3.832

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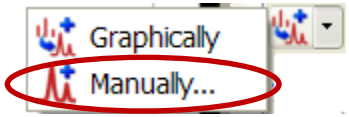
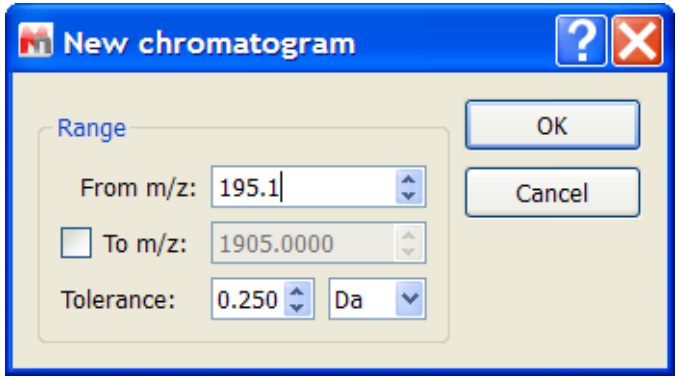
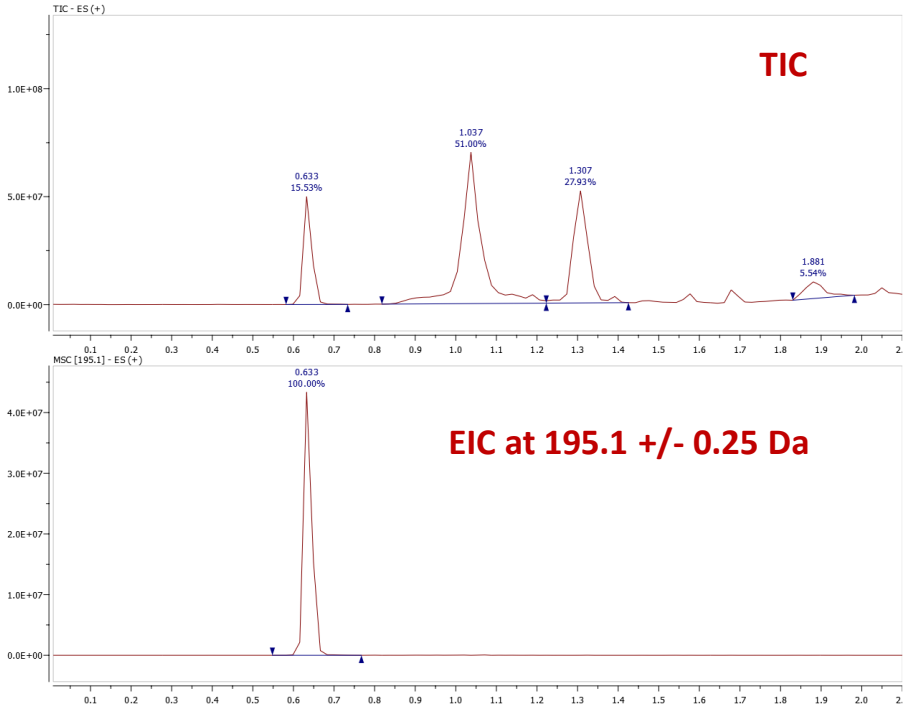
To display extracted ion chromatogram (EIC) from an m/z value



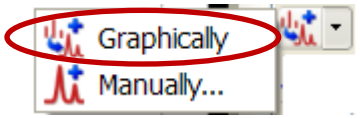
- Click  (or choose **Mass Analysis | New Mass Chromatogram | Manually**)
- In the New Chromatogram dialog, enter the m/z value that you are interested in, and a suitable Tolerance
- Press OK to display the EIC



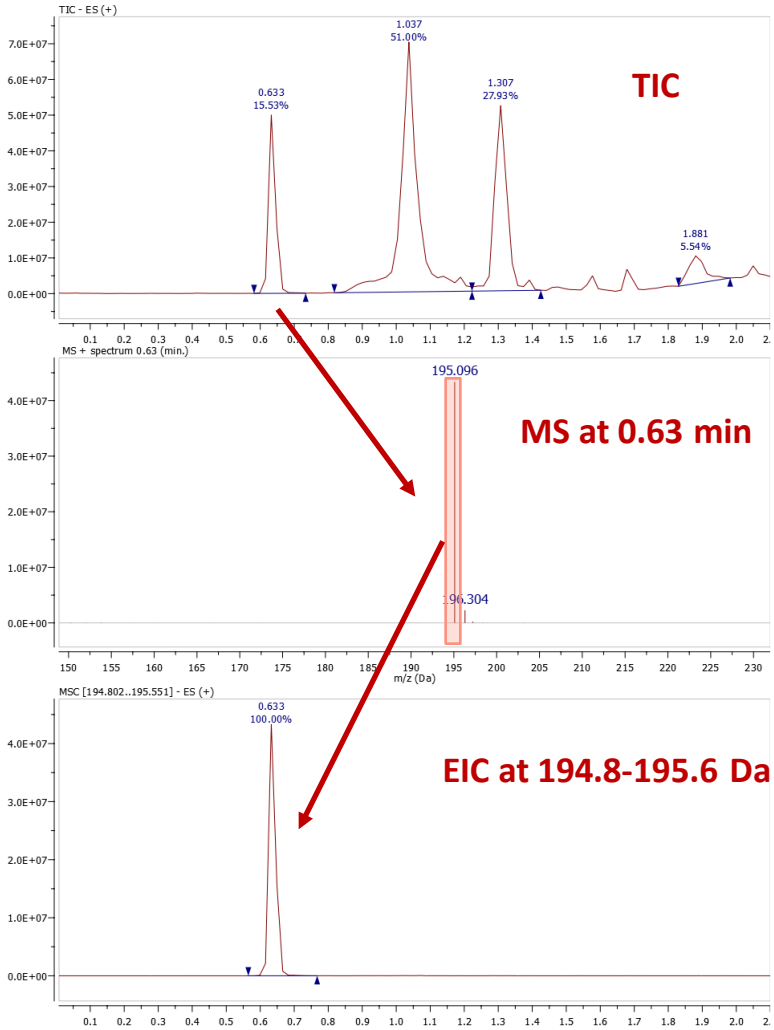


MESTRELAB RESEARCH
Chemistry Software Solutions

To display extracted ion chromatogram (EIC) for an MS peak



- First display the MS trace and zoom into the molecular ion peak that you are interested.
- Next select Click (or choose **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



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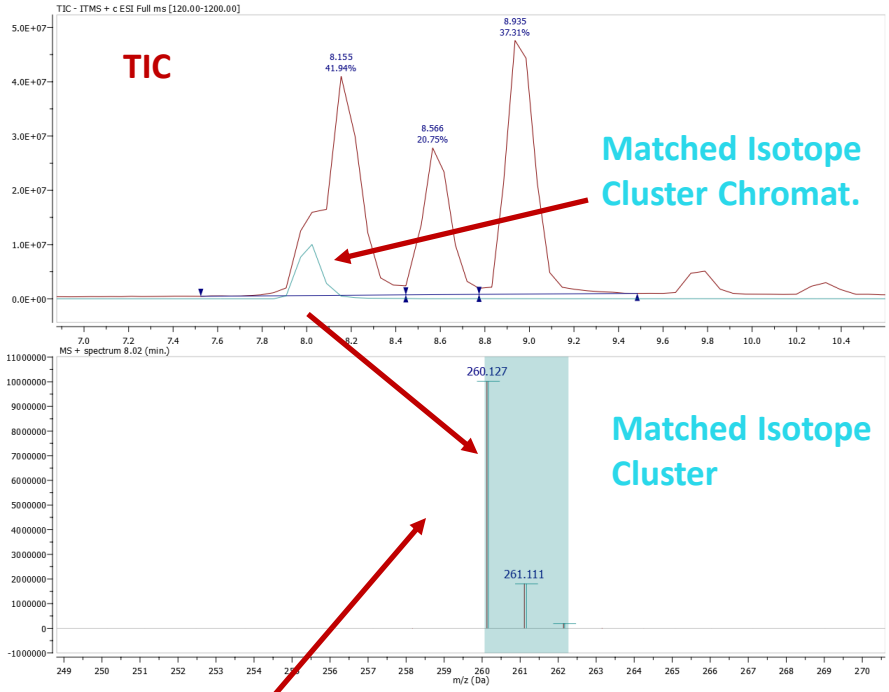
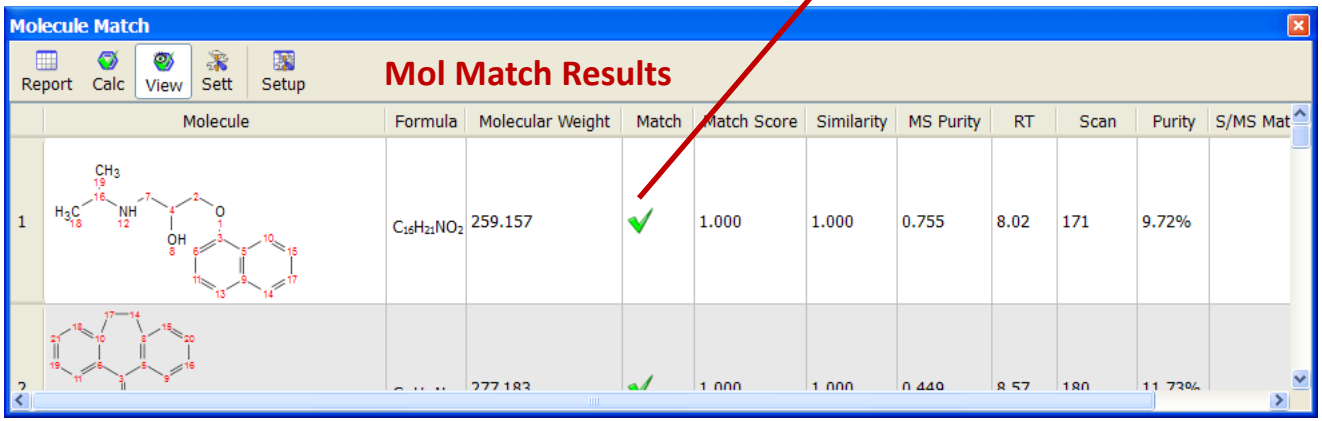
To confirm proposed structures using Molecule Match (1)

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





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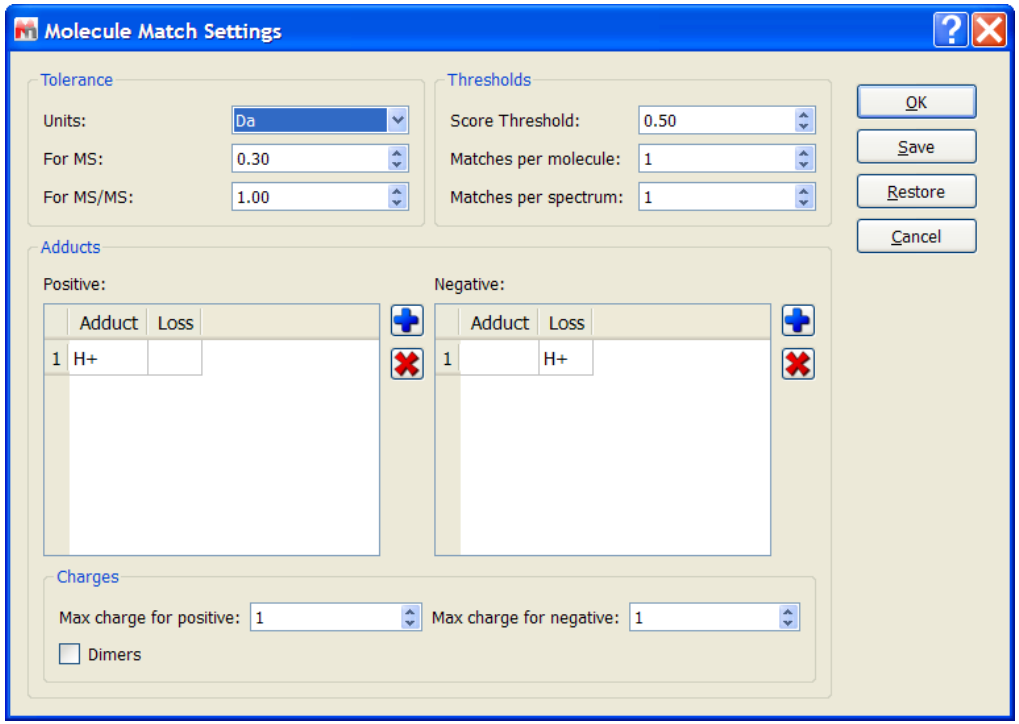
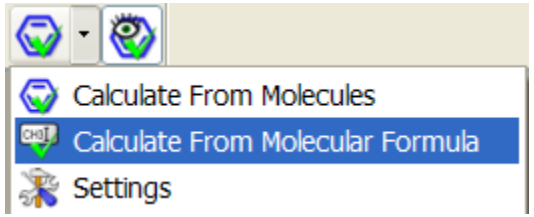
To confirm proposed structures using Molecule Match (2)

- You can choose **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** if you want.
- Click  to run the Molecule Match again

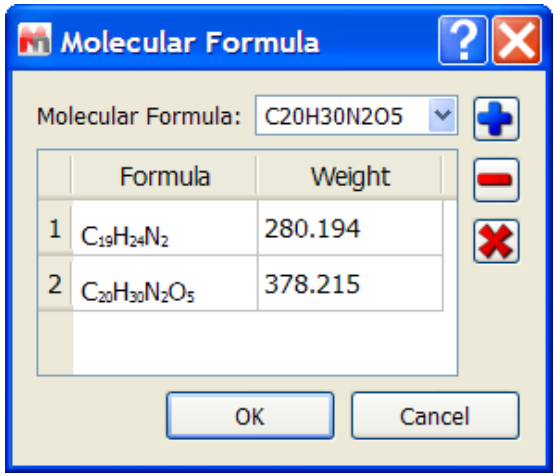


To confirm proposed molecular formula using Molecule Match

- If you don't have a structure but only a MF, choose the **Calculate From Molecular Formula** tool



- Enter one or more molecular formulas



- The results are displayed in Molecule Match Table

	Molecule	Formula	Molecular Weight	Match	Match Score	Similarity	MS Purity	RT	Scan	Purity
1		$C_{19}H_{24}N_2$	280.194	✓	1.000	1.000	0.830	17.64	299	100.00%
2		$C_{20}H_{30}N_2O_5$	378.215	✗	0.000	0.000	0.000			

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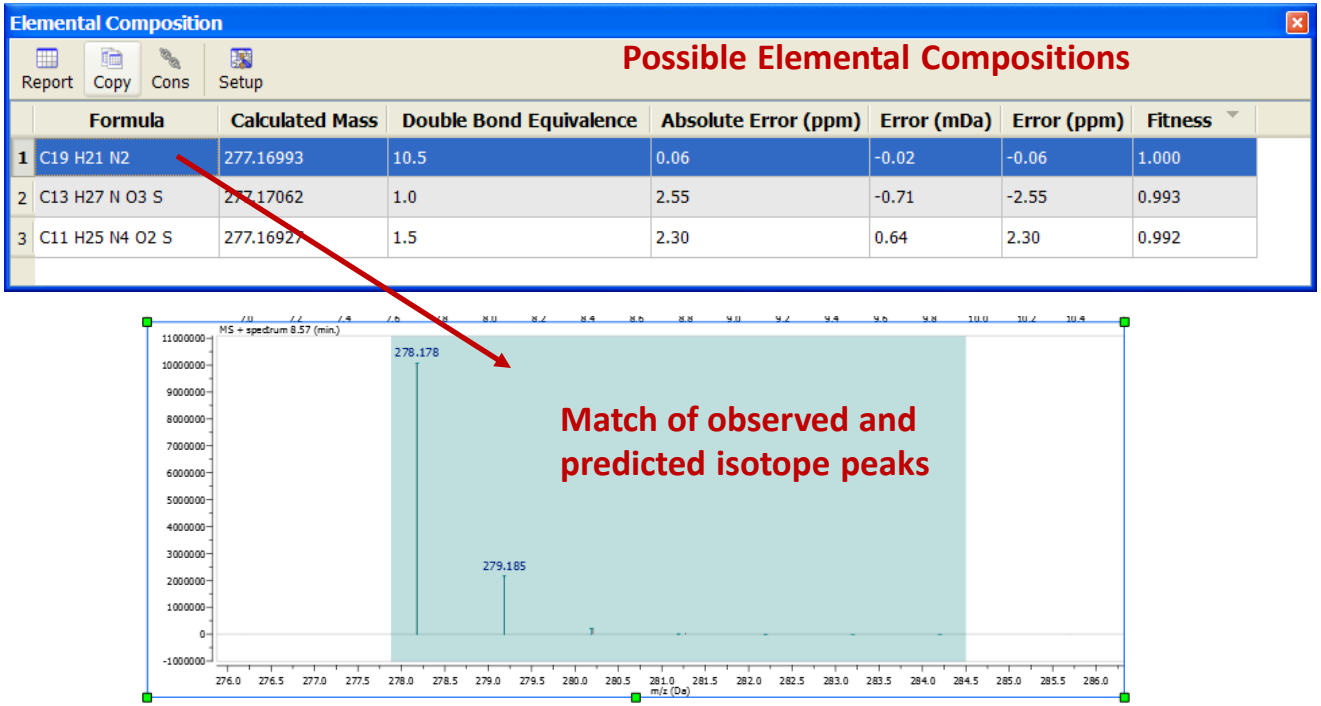
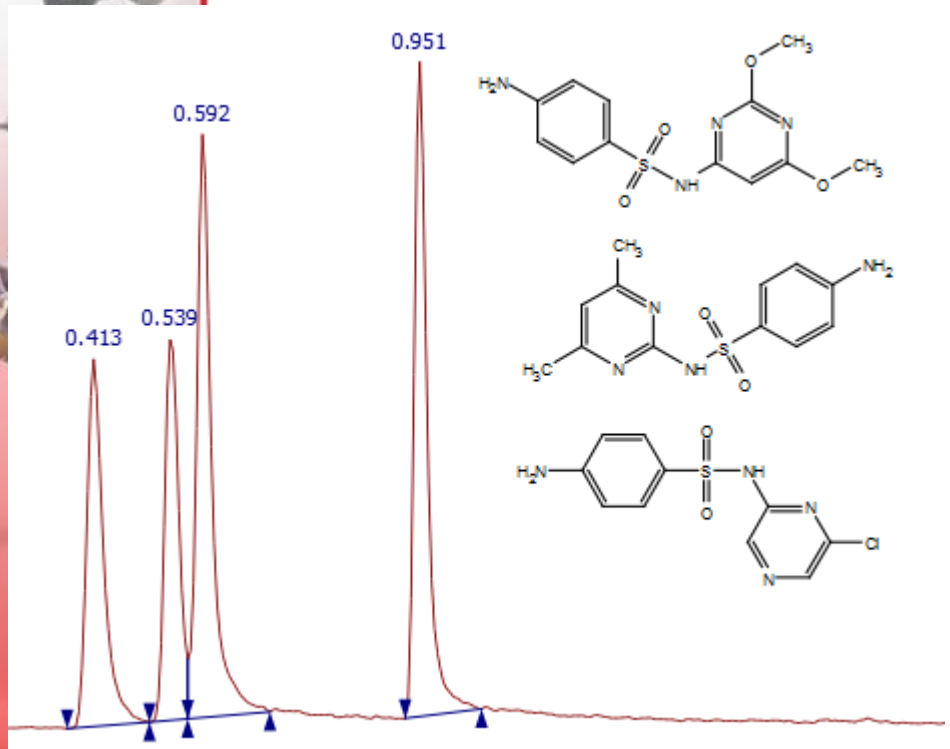
To calculate elemental composition

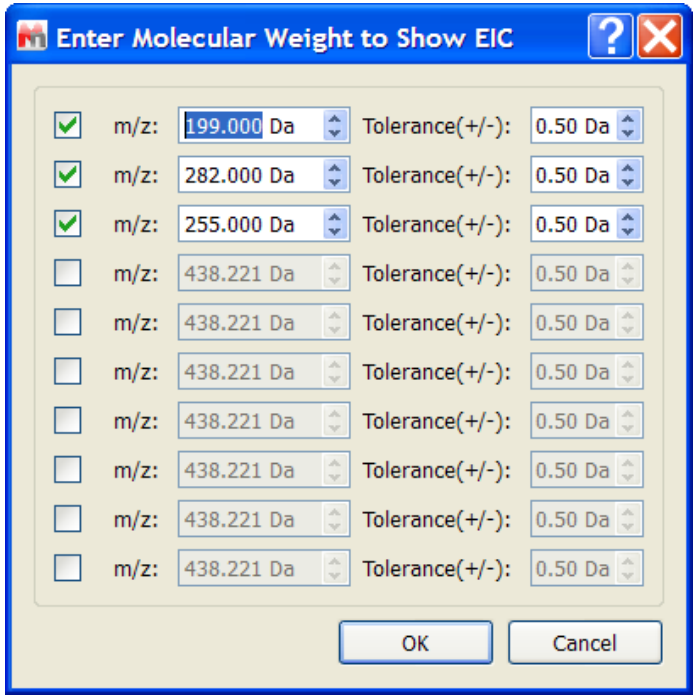
- Zoom into the molecular ion peak of a MS trace
- Click  or choose **Mass Analysis | Elemental Composition | Calculate**.
- Click on the molecule ion peak.
- An **Elemental Composition Table** is displayed
- Click on a row to see the match of observed and predicted isotope peaks
- Choose **Mass Analysis | Elemental Composition | Settings** to change the settings if necessary. Then click on the ion peak to recalculate.



“Push-button” analysis and reporting using a script M

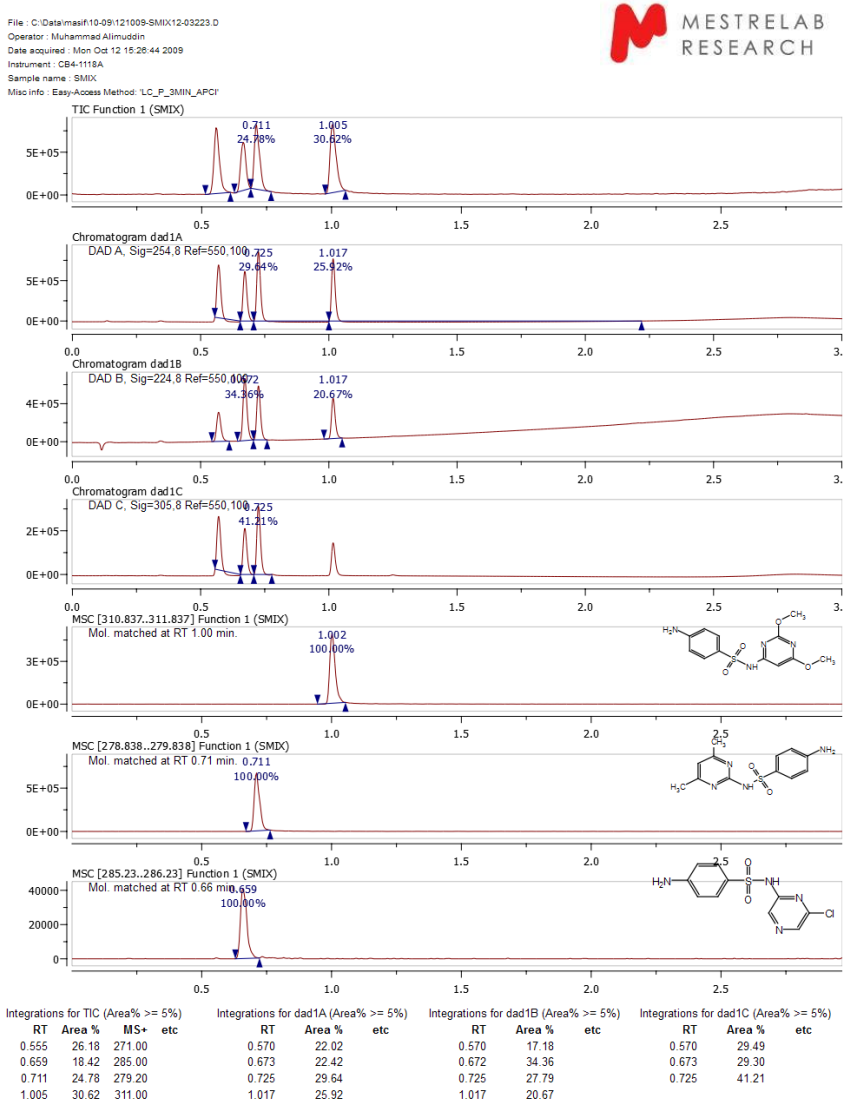
- In this example, you open an LC/MS dataset, and copy your structures (e.g. reactants and products) to it, if any. Then run the script.
- If there is no structure, Mnova asks for m/z values you are looking for. You can enter up to 10 m/z values





** We can write scripts to do automated analysis and reporting based on your requirements. The scripts can process data in either single mode or batch mode*

First page of the report by the script M



Integrations for TIC (Area% >= 5%)

RT	Area %	MS+	etc
0.555	26.18	271.00	
0.659	18.42	285.00	
0.711	24.78	279.20	
1.005	30.62	311.00	

Integrations for dad1A (Area% >= 5%)

RT	Area %	etc
0.570	22.02	
0.673	22.42	
0.725	29.64	
1.017	25.92	

Integrations for dad1B (Area% >= 5%)

RT	Area %	etc
0.570	17.18	
0.672	34.36	
0.725	27.79	
1.017	20.67	

Integrations for dad1C (Area% >= 5%)

RT	Area %	etc
0.570	29.49	
0.673	29.30	
0.725	41.21	

Header info

TIC

DAD traces

EIC and Molecular match results*

TIC and DAD peaks with integral ≥ 5%

Molecular match is based on the comparison of molecular ion and isotopic clusters (and fragmentation if such info is available.) See **Help > Contents > Mass Plugin for more details.*

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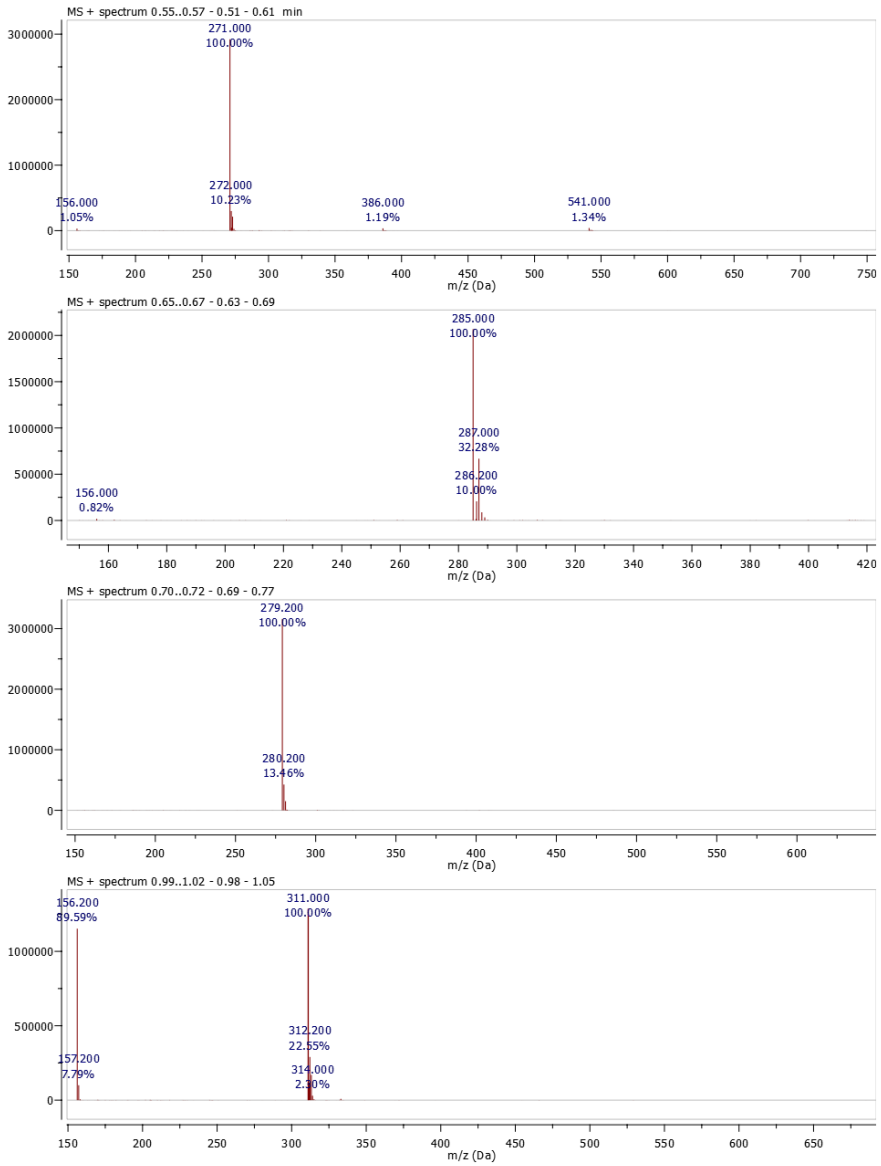
Other page(s) of the report by script M



Co-added mass spectra (with background subtracted) under each TIC peak reported in the first page

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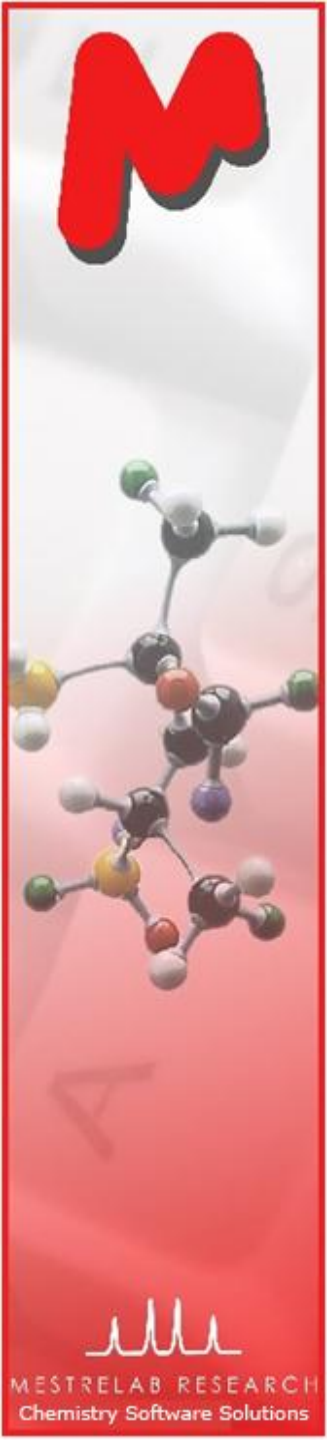
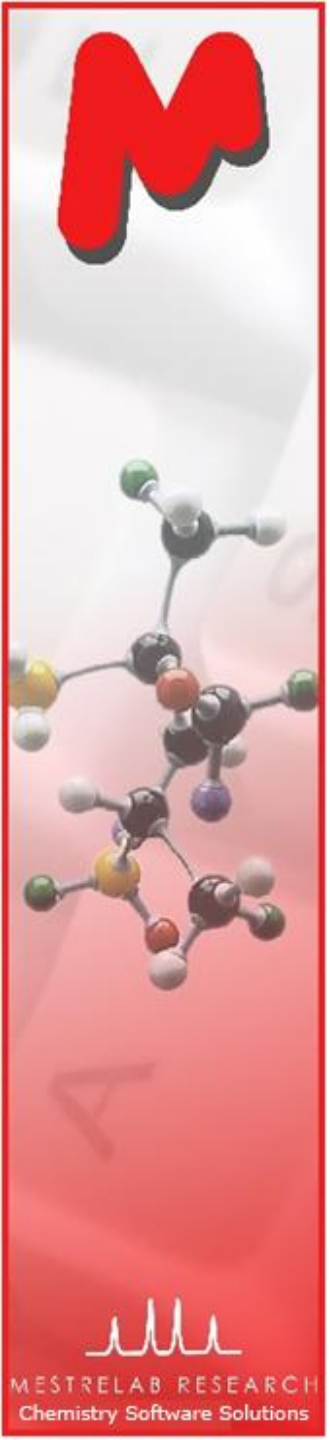


Batch mode or real-time data conversion, analysis and reporting

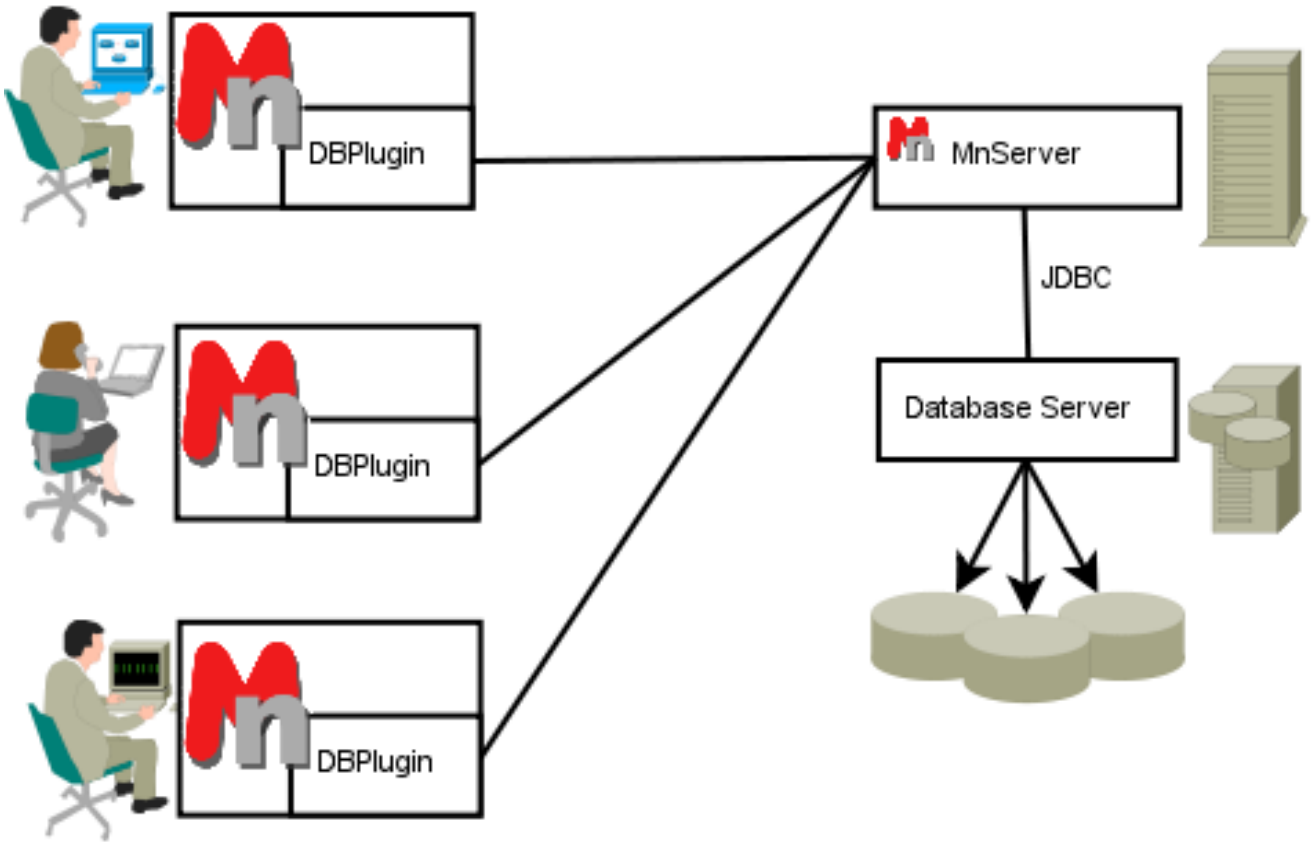
- With Mnova scripts, it is possible to analyze and report your data either in batch mode or in real-time
- The M script has a batch-mode version that opens all the LC-MS datasets (and their corresponding molecules) under a selected folder, and then do mol. match and generate a PDF report for each data set
- A Mnova script can be triggered by the addition of a new folder or file, and then load the dataset and do required analysis and reporting, such as:
  - Saving the dataset to a target folder in Mnova binary format
  - Generate a report and save it as a PDF (such as that by M script)
  - Email the report to a user
  - Archive raw data to other locations, or an Mnova database



Mnova DB

- An effective, fully integrated, multiplatform environment for storing, indexing and searching your analytical chemistry data
- Save everything on Mnova client (NMR and MS raw data and analysis results, structures etc) to your database
- Search and retrieve by peaks, text, (sub)structures etc.
- Platforms: Oracle, MySQL, Postgress
- Scriptable for automation and batching processing
- See more details at http://mestrelab.com/software/mnova-db/

Mnova DB: Architecture



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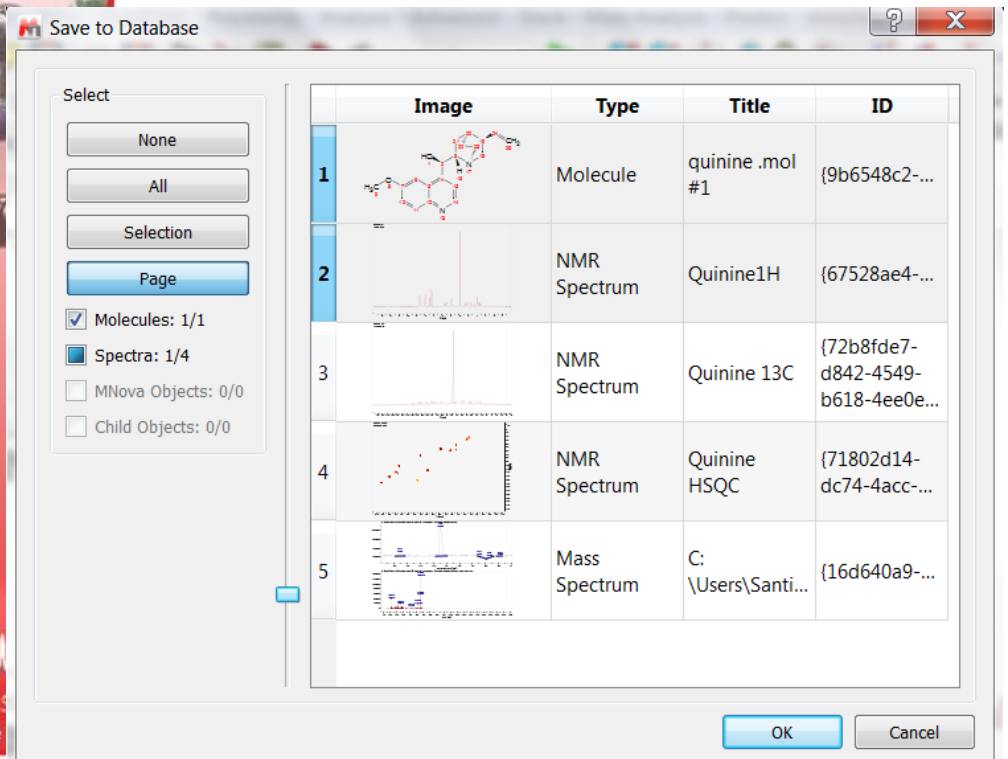
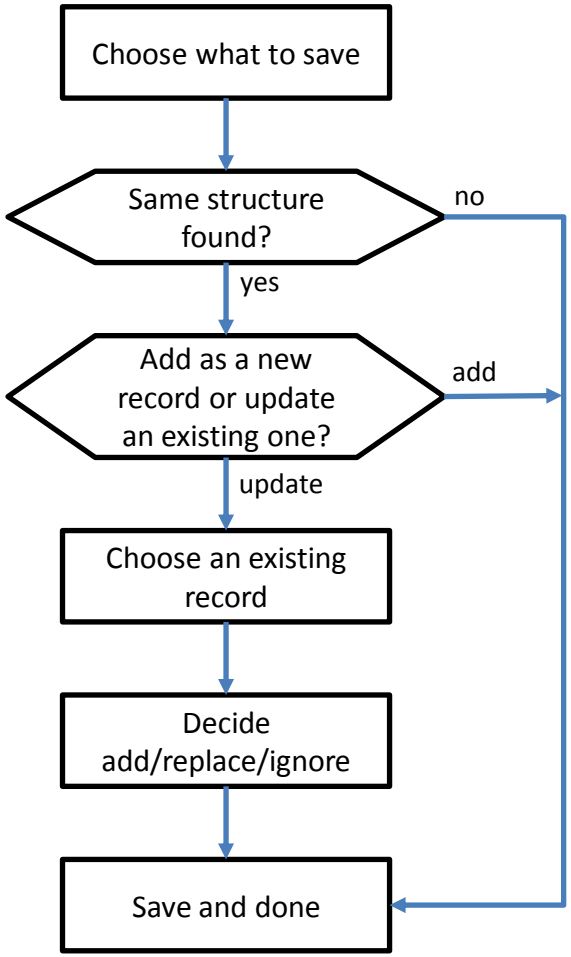
Save data as part of your workflow

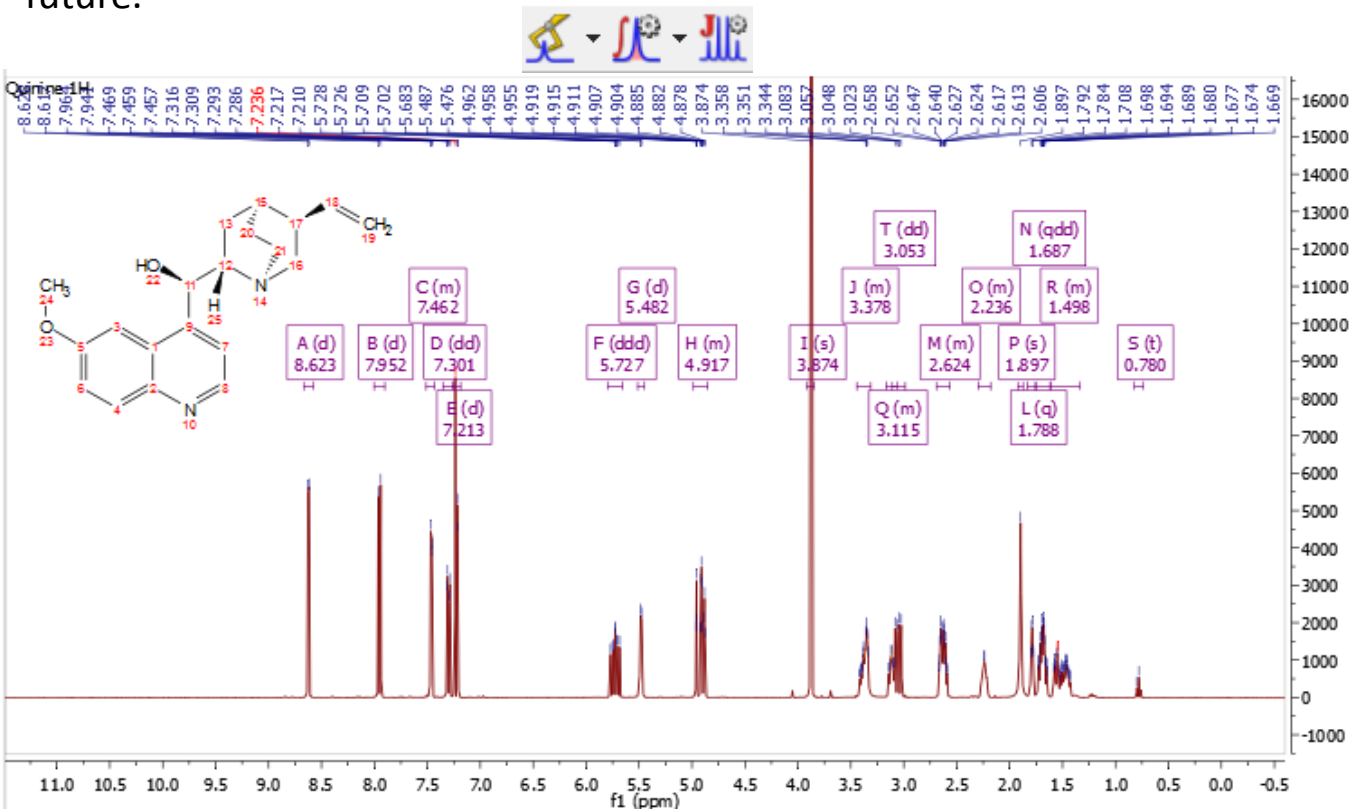
- At any stage of your data processing and analysis, you can choose **Database | Save** or click  to save the data in the current document to a database.
- Mnova shows a list of the data objects for you to choose to save
- Mnova compares the structure with the saved ones. If record(s) with the identical structure are found, you will select to add as a new record or update an existing one.





Save NMR spectra to a database

- You can save **multiple 1D and 2D** spectra into one record.
- The **raw data, processed spectra** and the spectral **parameters** are all saved.
- If you do not do a **peak picking**, Mnova does an automatic peak picking and saves the peak lists for later search. It is recommended that you pick a clean list of peaks using the Mnova peak picking tool before saving a spectrum to database. This will make peak search more efficient.
- For H-1 spectrum, it's recommended that you do a **multiplet analysis** before saving it to the database. This will allow you to do multiplet search in the future.



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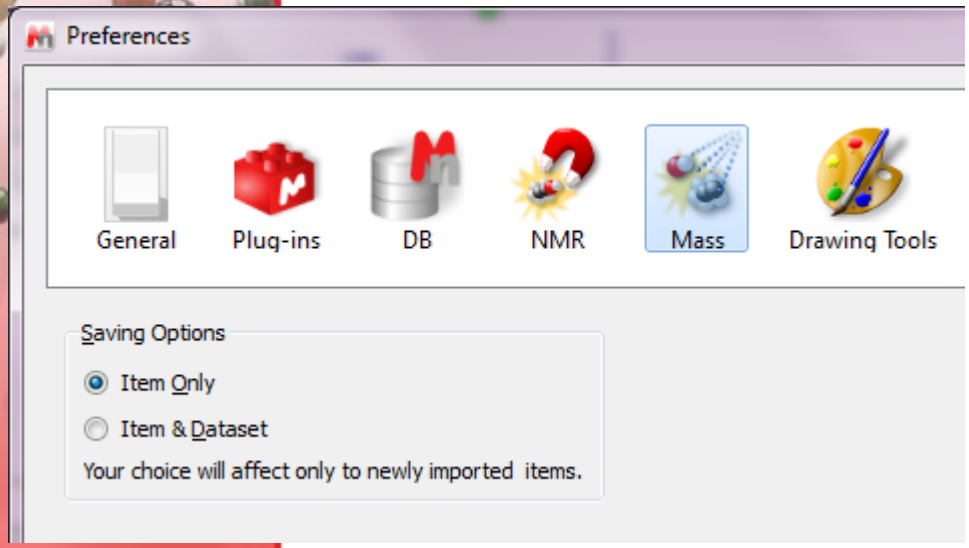
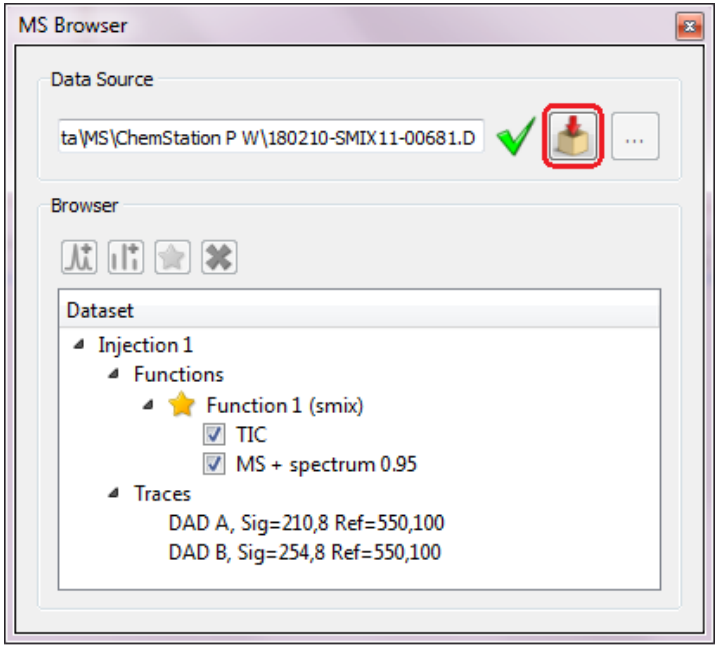
Save LC/MS or GC/MS to a database

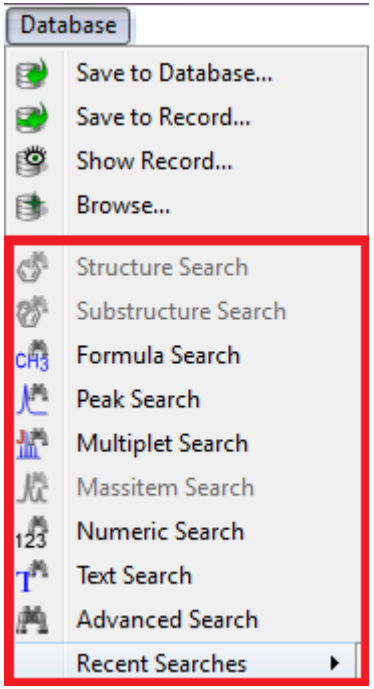
- Unlike for NMR, due to the potential large size of an LC/GC/MS dataset, Mnova does NOT save the whole dataset to database by default. Instead, it saves only the displayed chromatograms and mass spec to the database, together with the path to the original dataset (which means you have to keep the original data files if you want to access to the remaining data components, such as other mass spec, UV traces etc.)
- You can change this setting by **Edit | Preferences | Mass**, and set the **Saving Options** to Item & Dataset, or you can use the **Fetch Full Dataset tool** in rgw MS Browser to load the full dataset to Mnova and save it subsequently.

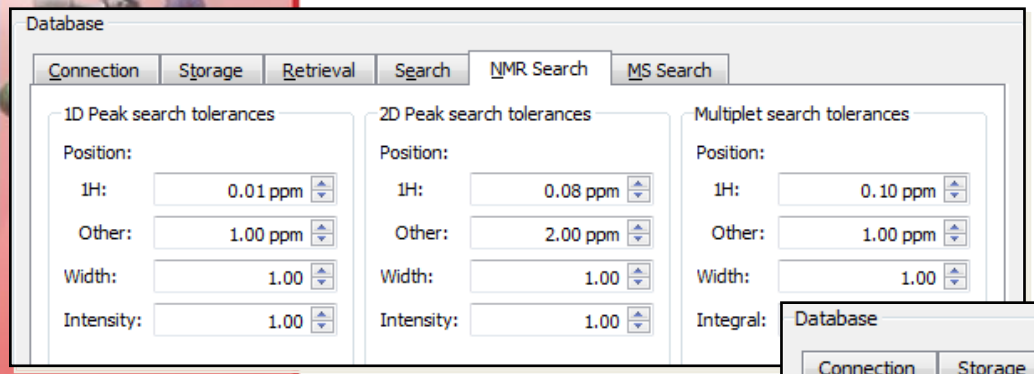


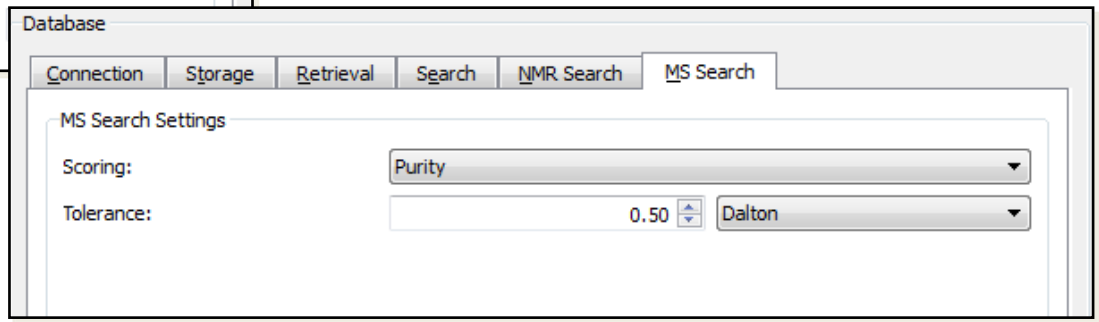


Search Mnova database in your workflow

- Mnova allows you to **search the database** by
  - Structures, substructures
  - Molecular formula
  - 1D or 2D NMR peaks
  - 1D NMR multiplets (shifts and coupling patterns)
  - Mass spec m/z values
  - Numerics
  - Text strings
  - Combined search of any of above categories (Advanced Search).
- Note many of the search parameters can be adjusted in **Edit | Preferences | DB**:







Note: *The peak Width and Intensity are normally not used for NMR peak search*

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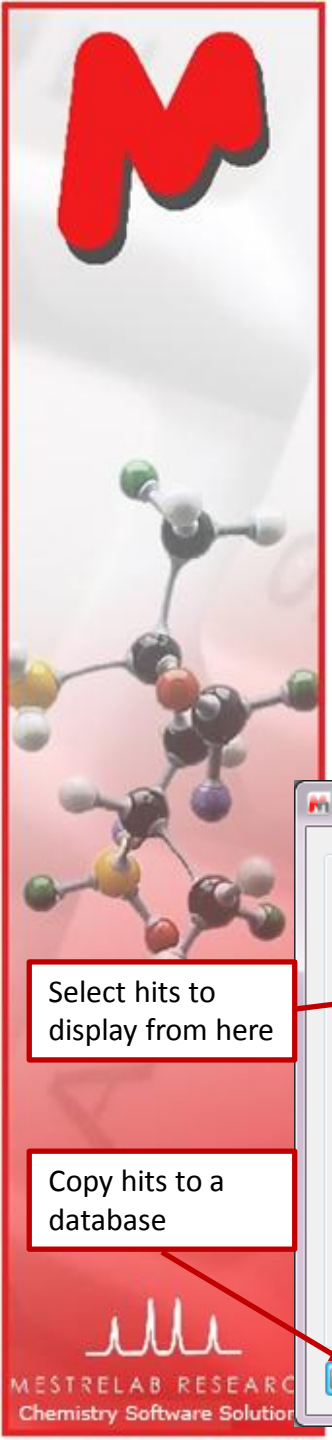
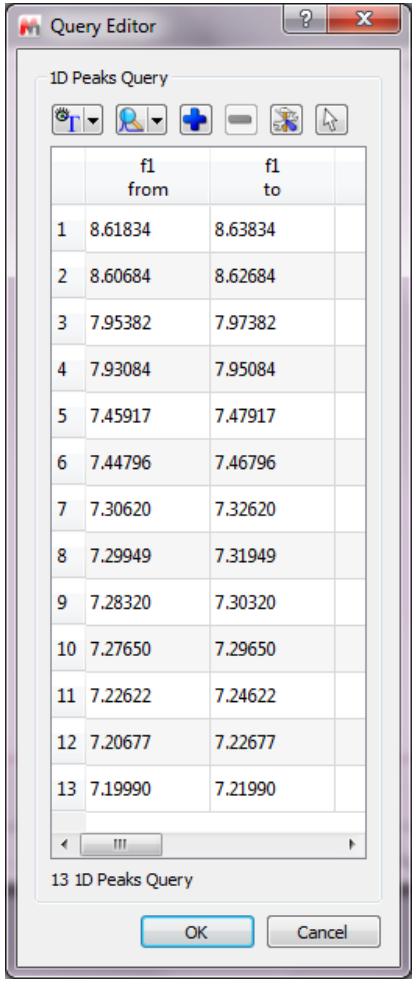
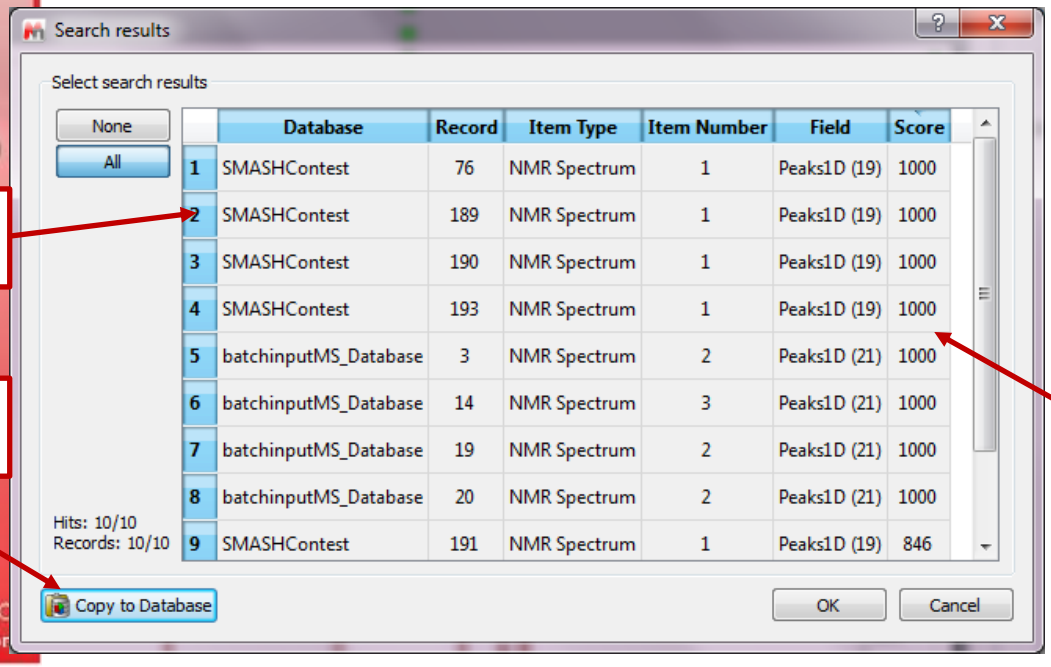
Search by NMR peaks

- Pick all or some peaks from a 1D (or 2D) NMR. Right click and select **Peak Search**.
- Mnova prompts you to select one or more **databases to search against**.
- A **Query Editor** is displayed for you to edit the peaks to search. Here you have several options:
  - Show spectrum or list of peaks (as a range including the tolerance).
  - Use only visible peaks or all peaks
  - When in the Text mode, add/delete/change peaks to search.
  - Change peak search tolerances
  - Select peaks from different spectrum in the document
- The **hit list** is like the following:







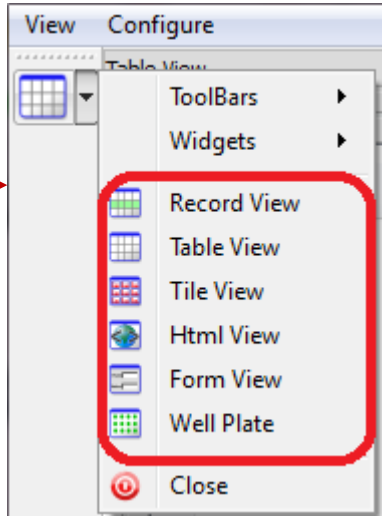
Select hits to display from here

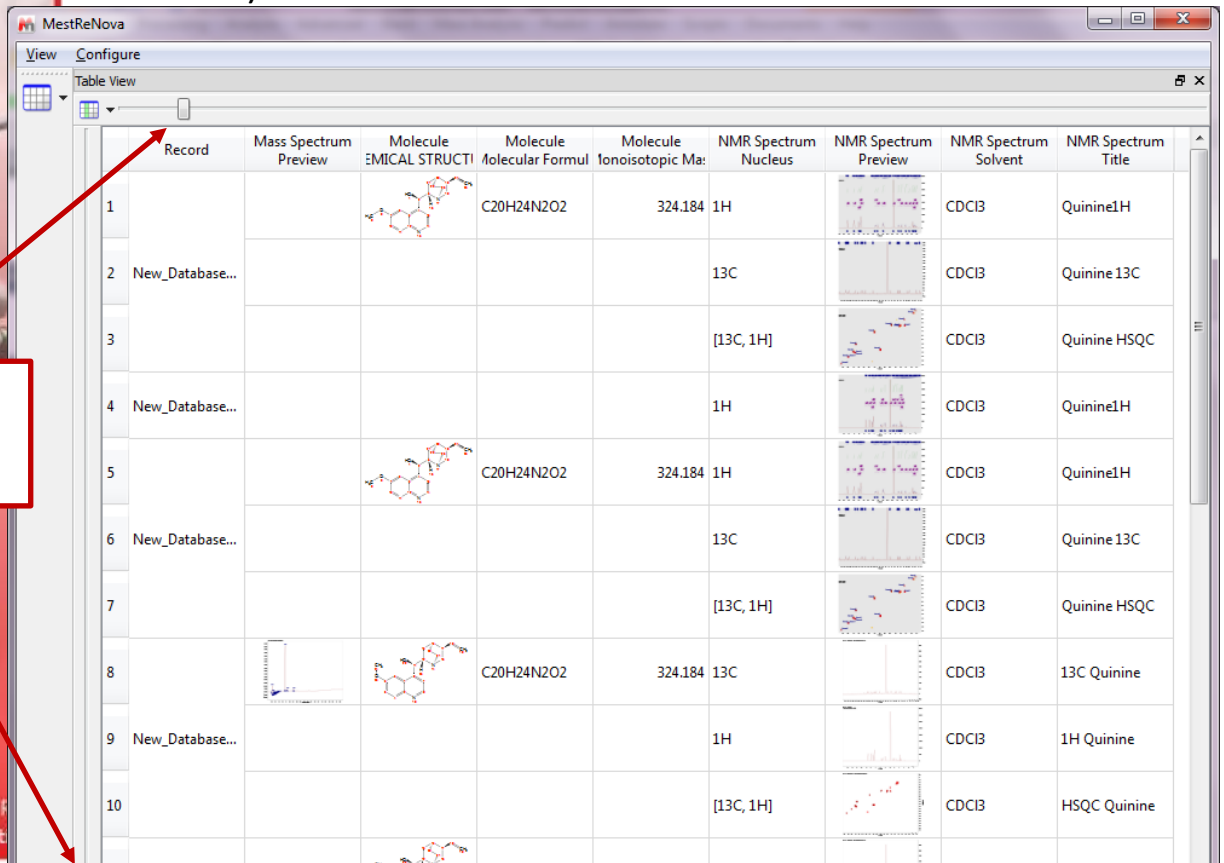
Copy hits to a database

Scores of hits: 1000 is the maximum

Visualize database contents

- Selected hits are displayed in a **Database View** so you can browse them and load selected ones to Mnova for further analysis.
- There are **6 ad hoc Views** for you to choose:
- You can customize any of them or add your own View, and save them.
- The following is a **Table View** (good for an overview of all hits):





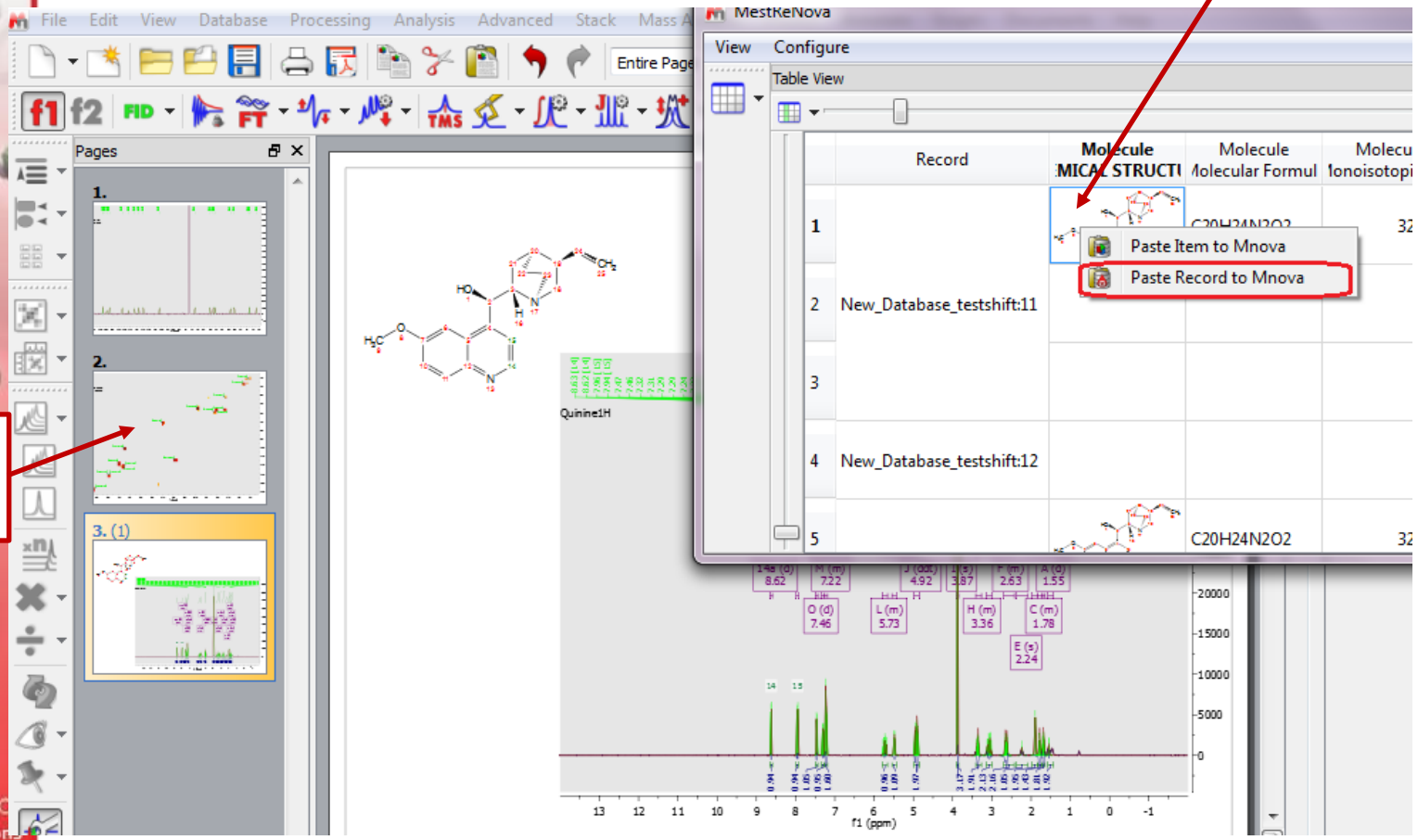
Use the sliders to change the size of the row/columns

Load an item or record to Mnova

- You can load part of or a whole record back to Mnova for further analysis.
- To load an item (such as a structure or one spectrum), right on it and select **Paste Item to Mnova**
- To load all items in a record, right on it and select **Paste Record to Mnova**

Right click and select Paste Record to Mnova

All items in the record are loaded to Mnova



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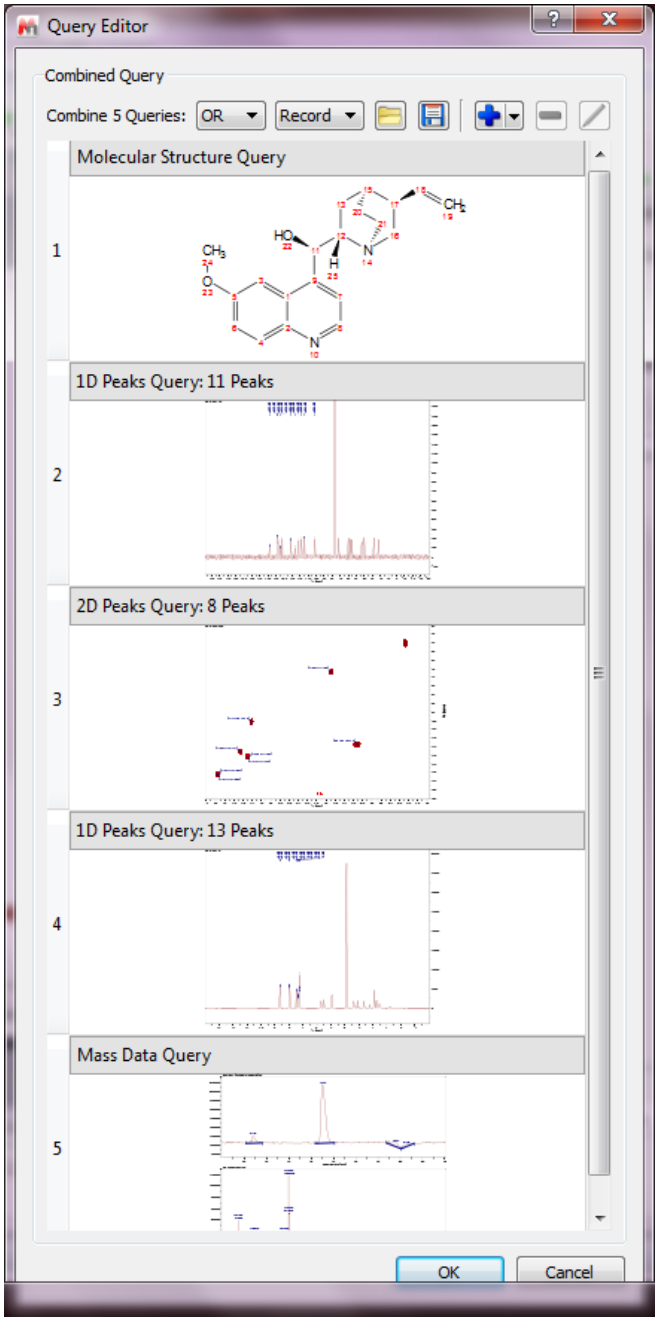
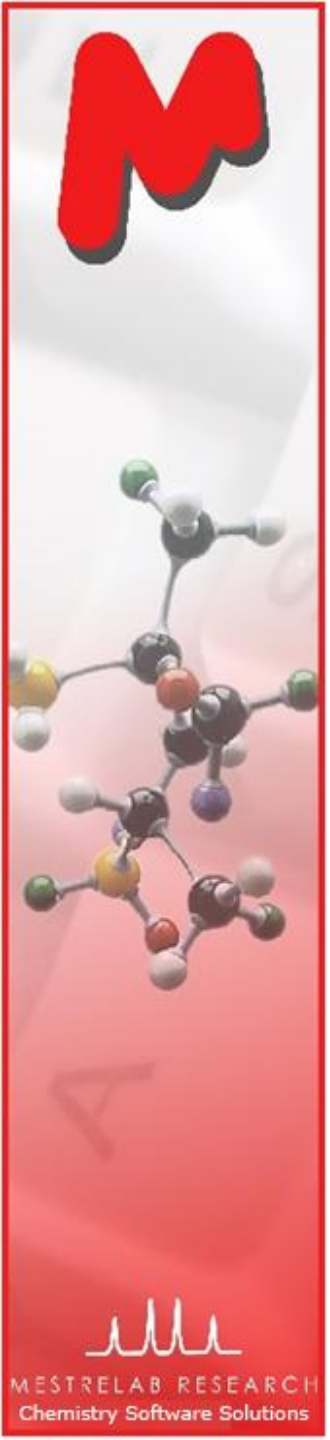
Advanced search

- To combine the search of different queries, choose **Database | Advanced Search**.
- The current NMR peaks, MS m/z values and structure, if any, will be listed in the Query Editor. You can add other queries (such as Text or Numeric) or delete items from the list, and choose the logical operator (OR/AND) .
- With **AND operator** you limit the search to a smaller list of hits.
- With **OR operator** you usually get a bigger list of hits.

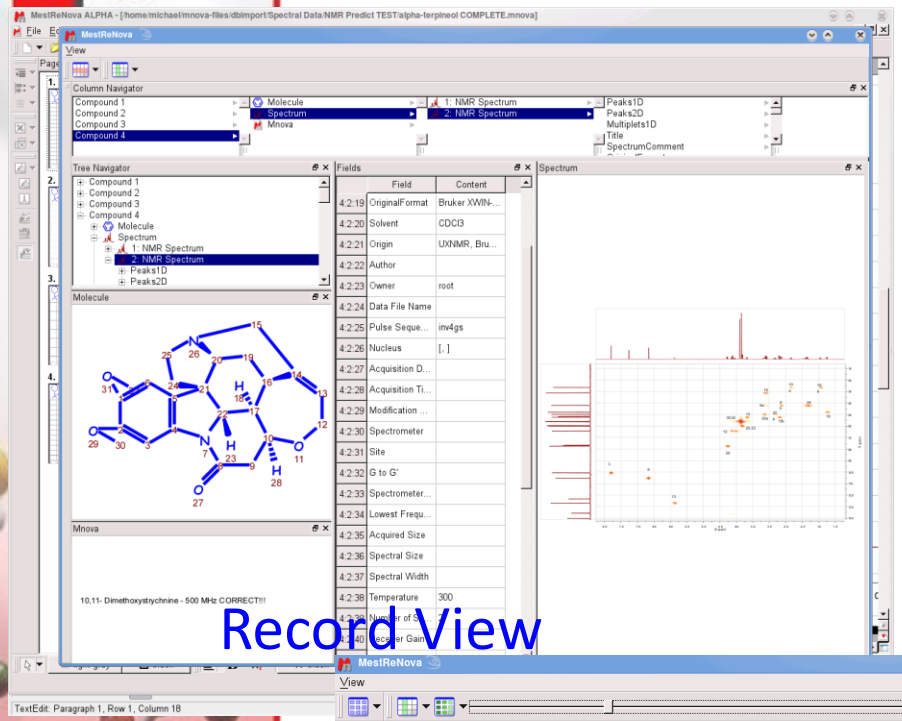


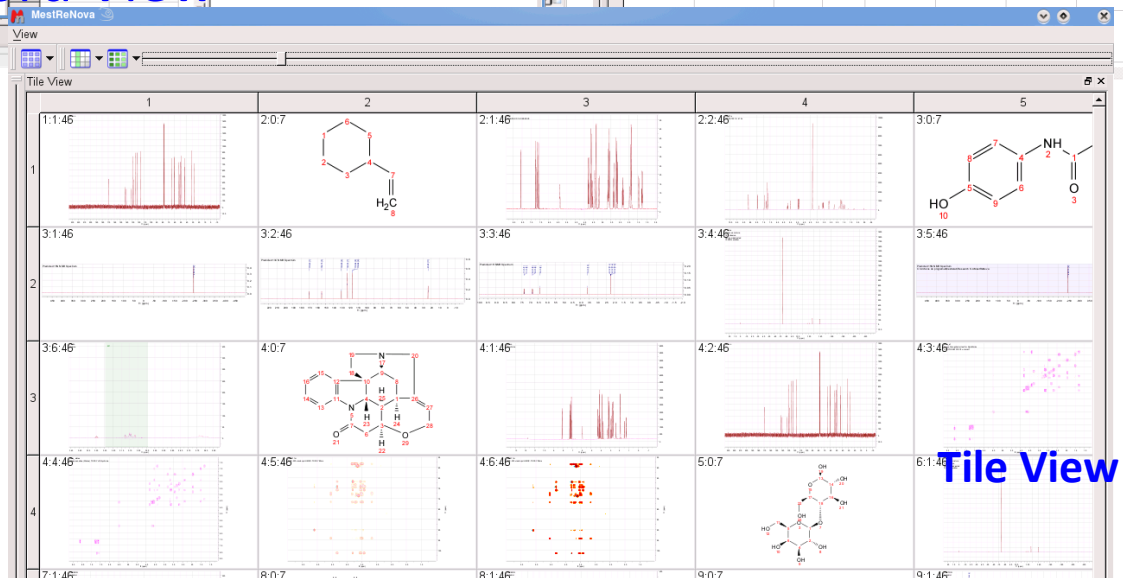


Application of Mnova DB: Some of the databases you may want to create

- Have databases for each group working on common chemistry, so that they can all benefit from each other's work
- Have **reference databases** for parent compounds so that chemists can easily compare their products with the parent, for quicker analysis
- Have **impurity databases** with fully characterized impurities which can be quickly matched (even automatically) to impurities observed in the current spectrum
- Have **databases of known compounds and materials** for quick (even automatic) random cross check when receiving new deliveries from suppliers (QC)
- Have **databases of final product** for quick (even automatic) check when a new batch of the product is synthesized (QC/QA)
- Use spectral DB as a **gateway repository** to other corporate systems such as compound registration, to allow final checks by Analytical Department to validate work (this can also be done with automatic verification)

Mnova DB: Different Views of Search Results





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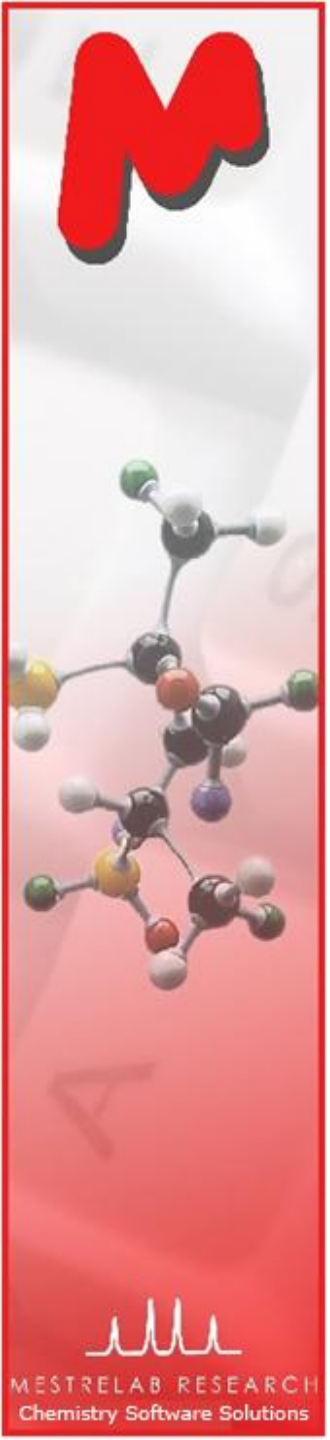

For more information…

- Visit www.mestrelab.com for free trial, manual, tutorials, prices etc
- Check **Help > Contents** in Mnova for help on specific topics
- Email to chen.peng@mestrelab.com or support@mestrelab.com for questions.