



Mestrelab Research
chemistry software solutions

Mnova 15 Quick Guidelines





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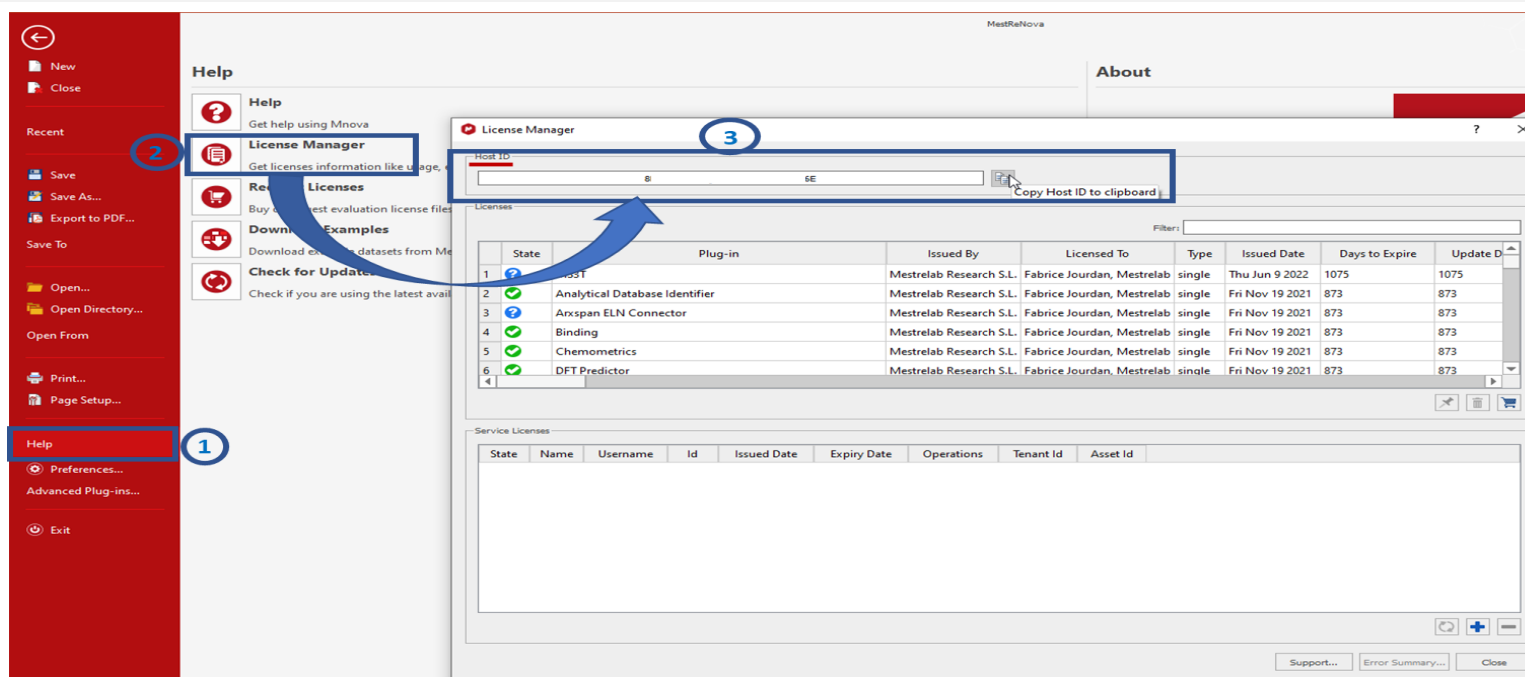
These quick guidelines are not meant to substitute the Mnova user's manual available [here](#)

INSTALLATION AND ACTIVATION

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❑ Downloading and Installing Mnova

- Mnova can be downloaded for [here](#). Once installed the software can be activated with a license file provided purchase of licenses from Mestrelab sales office (sales@mestrelab.com).
- The license file will be sent to the user(s) upon supply of the hostID of the installed Mnova software. This license file can be saved and needs to be drag&dropped into Mnova to activate the licenses.
- The hostID can be found from the File>Help>License Manager menu as indicated below:

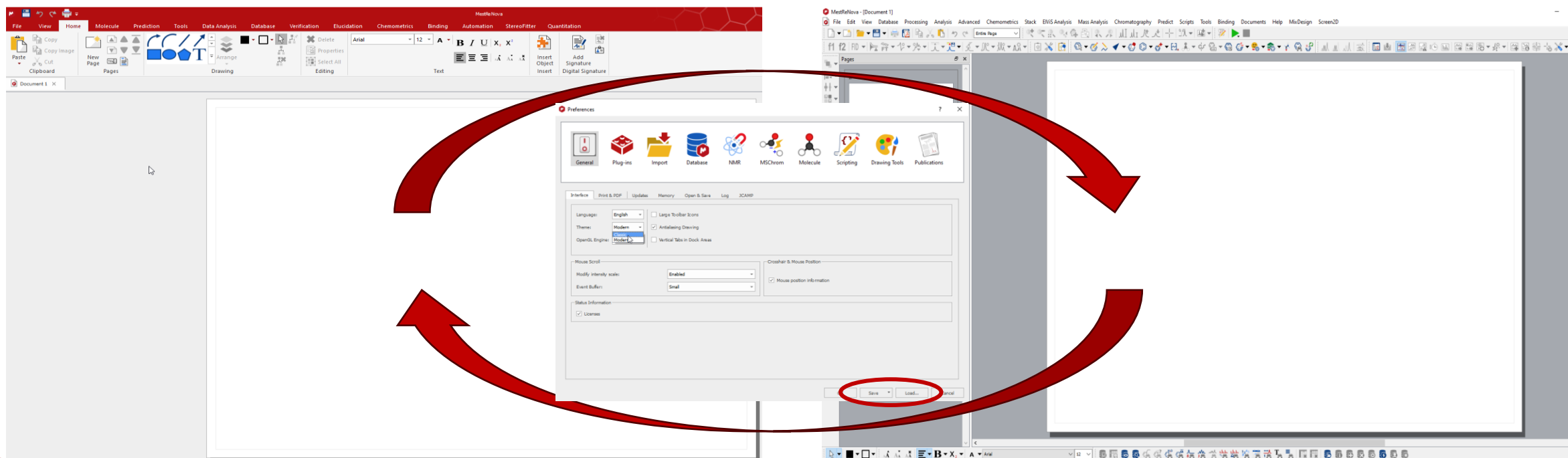


MNOVA USER INTERFACE

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MODERN AND CLASSIC USER INTERFACE

- When opening Mnova for the first time, users will be experiencing the Modern interface.
- User may wish to move to an alternative “classic” interface by going to **File>Preferences>General>Interface**, setting the theme to “Classic” (see below). The reverse operation can be done via the menu Edit>Preferences>General>Interface
- A series of other parameters can be modified in the Preferences panel. These settings can then be **Saved/loaded** at any time



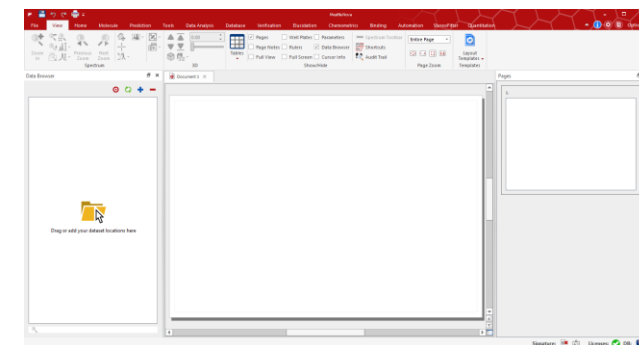
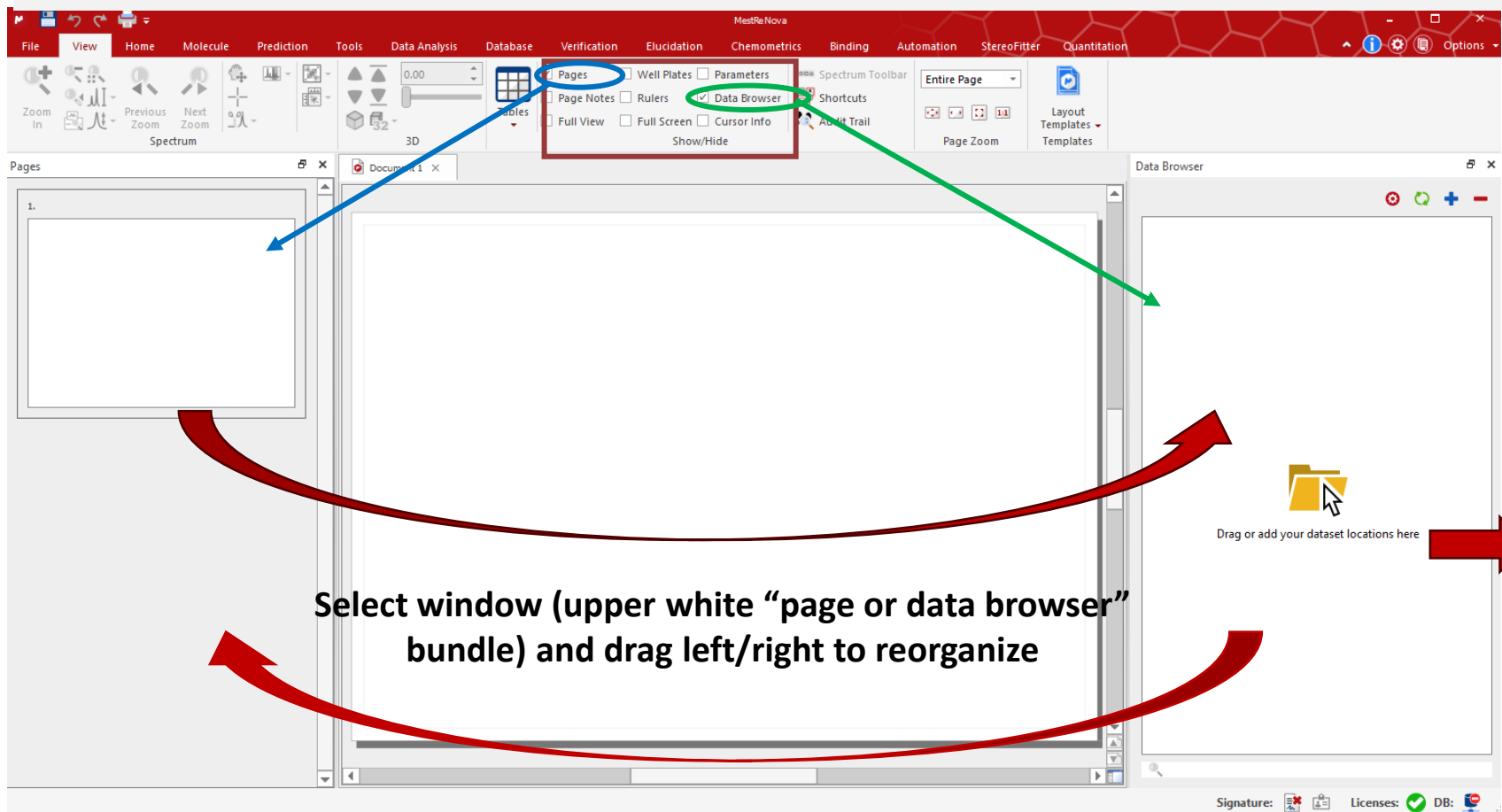
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MNOVA USER INTERFACE

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GENERAL OVERVIEW - SETTING-UP YOUR ENVIRONMENT

- Users can configure the interface with some preferred settings at any time. The last configuration will remain effective when reopening Mnova



OPENING DATA IN MNOVA



DATA OPENING FROM THE GENERAL MENU

- From **File>Open**. Then choose your data to open

DATA OPENING FROM THE DATA FOLDER

- Drag&drop the file/folder to open

The screenshot illustrates the MNOVA software interface with two methods for opening data highlighted by red arrows.

Method 1: Opening from the General Menu

The left sidebar shows the 'File' menu with 'Open...' selected. The 'Open' dialog box is open, showing a file explorer view of the 'QUININE(NMR&LCMS)' folder. The file list includes:

Name	Date modified	Type
Quinine1H	17/11/2021 19:55	File folder
Quinine13C	17/11/2021 19:55	File folder
QuinineHSQC	17/11/2021 19:55	File folder
QuinineMS.d	17/11/2021 19:55	File folder
quinine.cdx	19/07/2020 18:23	CS ChemDraw
quinine.mol	26/06/2020 12:29	MOL File

The 'File name' field is empty, and the file type is set to 'All Files (*.*)'. The 'Open' button is visible at the bottom.

Method 2: Opening from the Data Folder



The main window shows the 'Data Browser' panel on the right. A file explorer window is open, showing the 'QUININE' folder. A red arrow indicates dragging a file from this folder into the 'Data Browser' panel. The 'Data Browser' panel has a message: 'Drag or add your dataset locations here'.

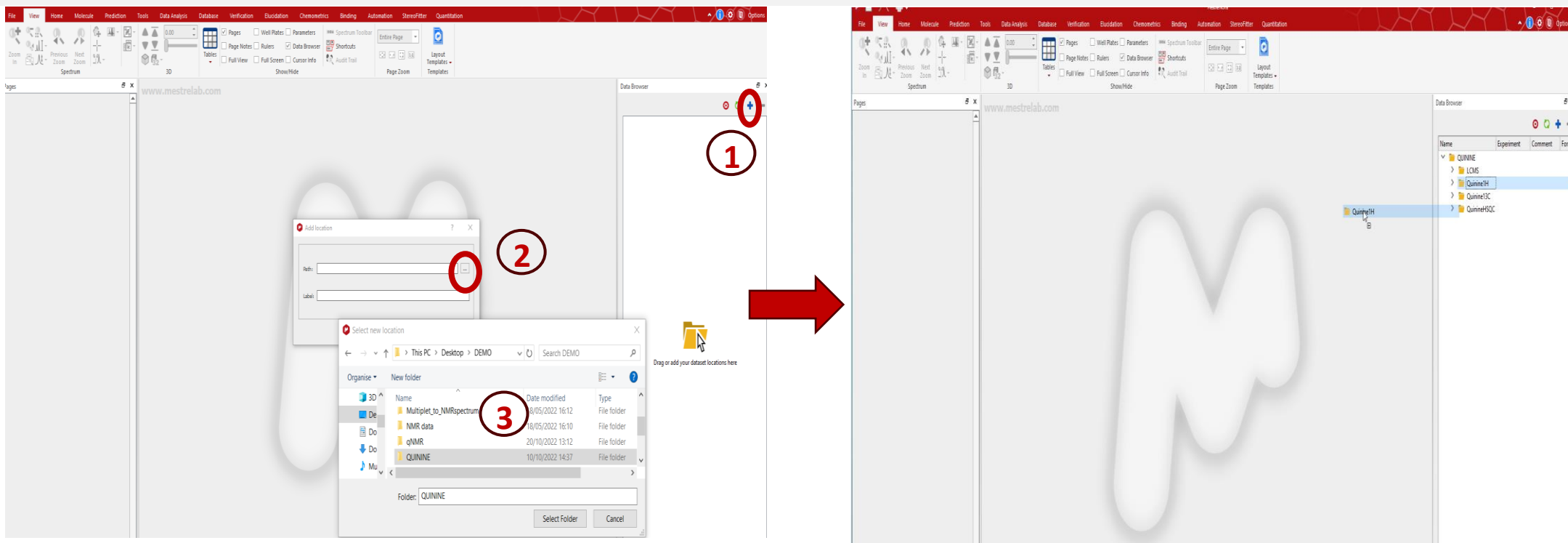
The background shows the MNOVA interface with various toolbars and a data plot at the bottom.

OPENING DATA IN MNOVA

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❑ DATA OPENING FROM THE DATA BROWSER:

- Configure the data browser: In the Data Browser, select the folders where your data can be found. Click , the  before selecting the folder containing your data.



- Data can now be opened from the Data browser by double clicking on a specific file/folder or drag&dropping the required file/folder





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Mnova NMR

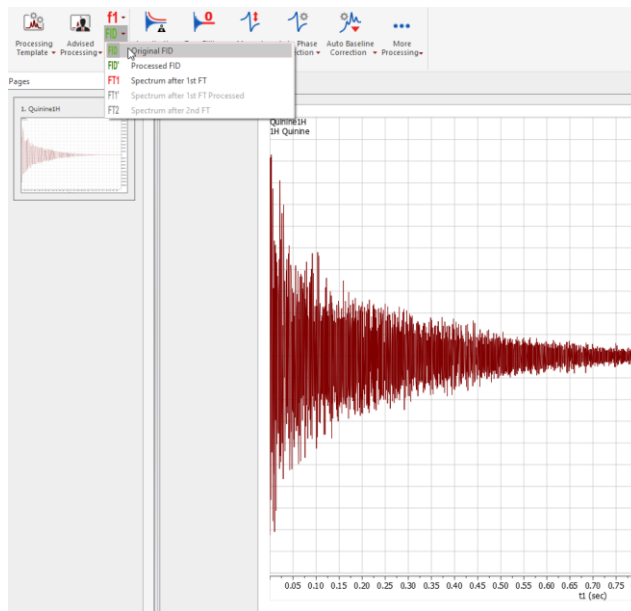


PROCESSING NMR DATA

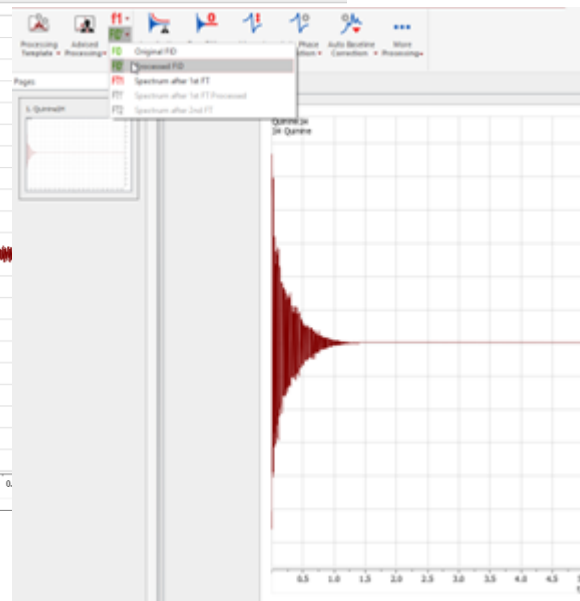
— ..

VIEWING NMR DATA

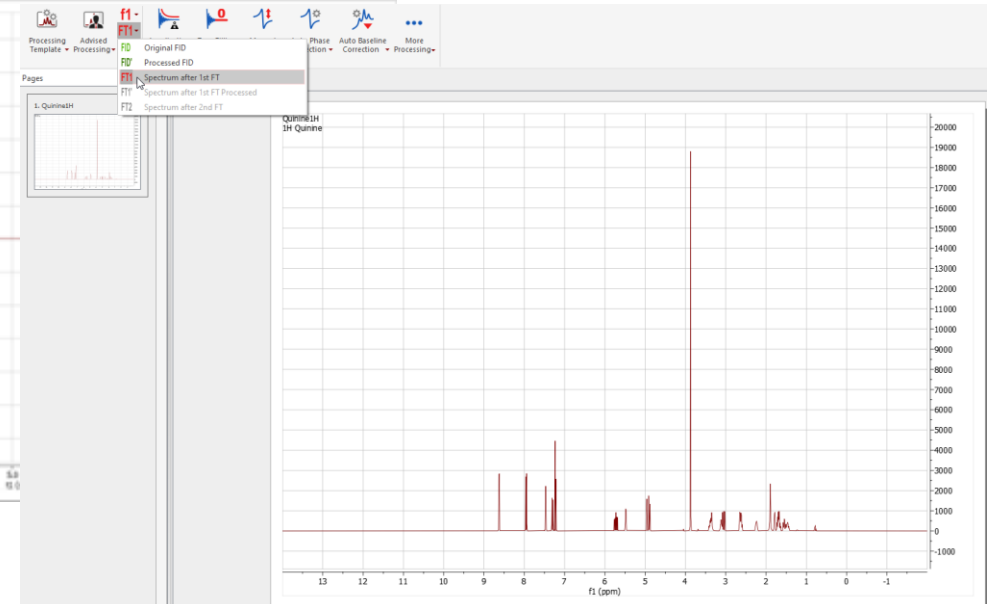
- Users may visualize either the FID or FT data



Raw FID (from instrument)



FID with processing parameters
(ZF, LP, apodization. ...)



FT spectrum

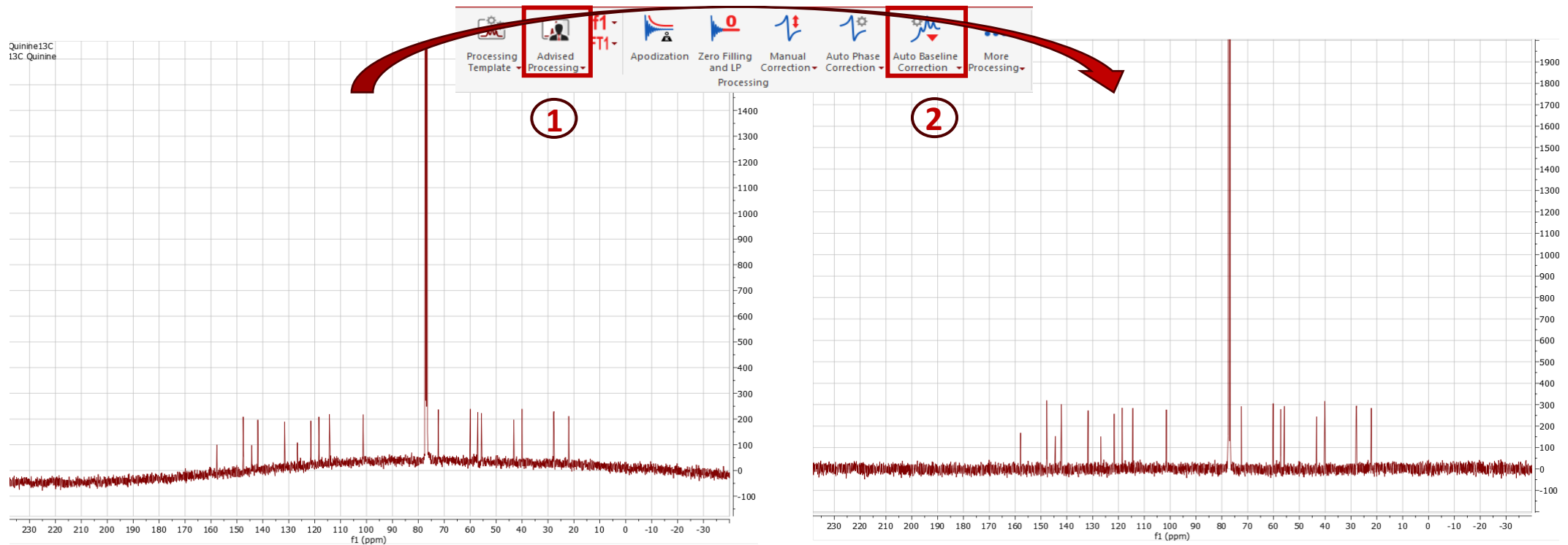


PROCESSING NMR DATA

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❑ ADVISED PROCESSING & AUTO BASELINE CORRECTION

- Most 1D and 2D NMR data can be efficiently processed via the “Advised Processing” and “Auto Baseline Correction”

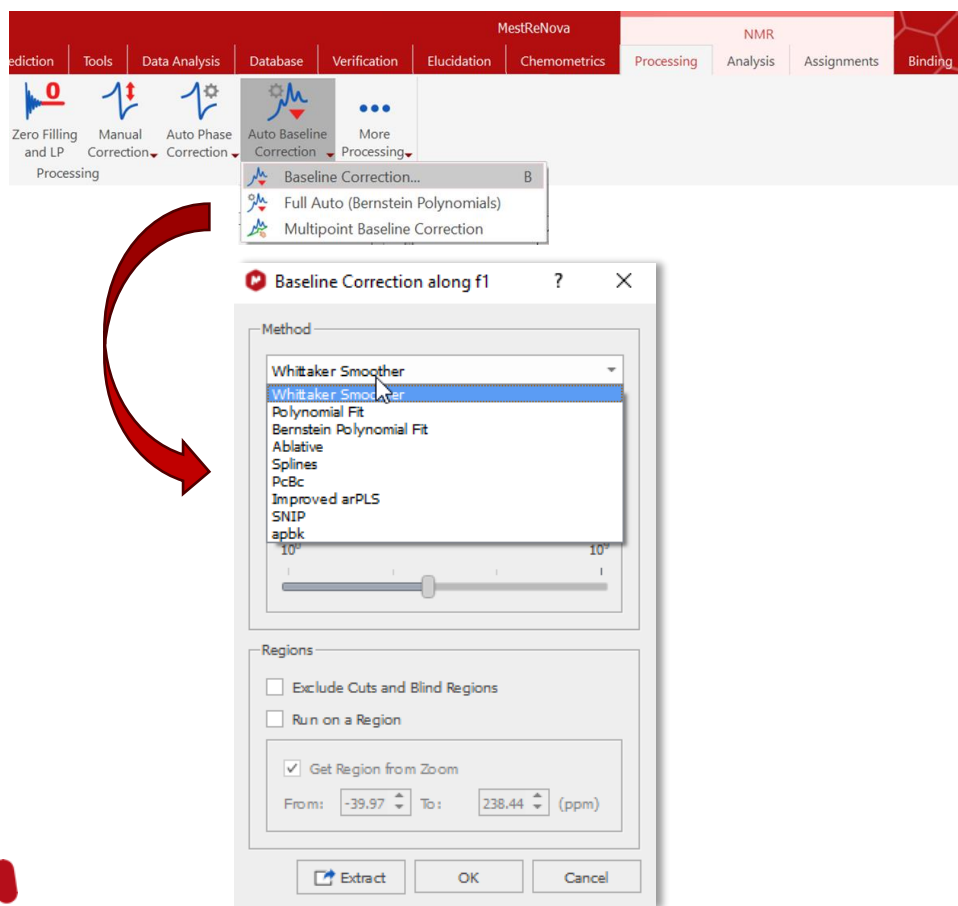


PROCESSING NMR DATA



❏ BASELINE CORRECTION METHODS

- The different baseline correction methods available in Mnova are the following:



Whittaker smoother: 1. Automatic baseline recognition (signal-free regions) based on a Continuous Wavelet Derivative transform (CWT) followed by iterative threshold detection in the Power mode domain. 2. A baseline modelling procedure based on the Whittaker smoother algorithm.

Polynomial fit: Sometimes offers benefit in corner smoothing

$$Y = a_1 + a_2x + a_3x^2 + a_4x^3 + \dots + a_Nx^{N-1}$$

Bernstein Polynomial fit: Modified polynomial fit

$$Y = a_1(1-x)^{N-1} + a_2x(1-x)^{N-2} + a_3x^2(1-x)^{N-3} + \dots + a_Nx^{N-1}(1-x)^1$$

Ablative baseline correction: Powerful for 1D spectra without negative peaks, but cuts off ends of spectra

Splines: Uses smooth curves to link the points

Improved arPLS: Inspired by Raman spectroscopy, this method is based on improved asymmetrically reweighted penalized least squares

SNIP: Sensitive Nonlinear Iterative Peak baseline correction algorithm (see [reference](#))

Apbk: algorithm only applicable on 1H Bruker NMR datasets.

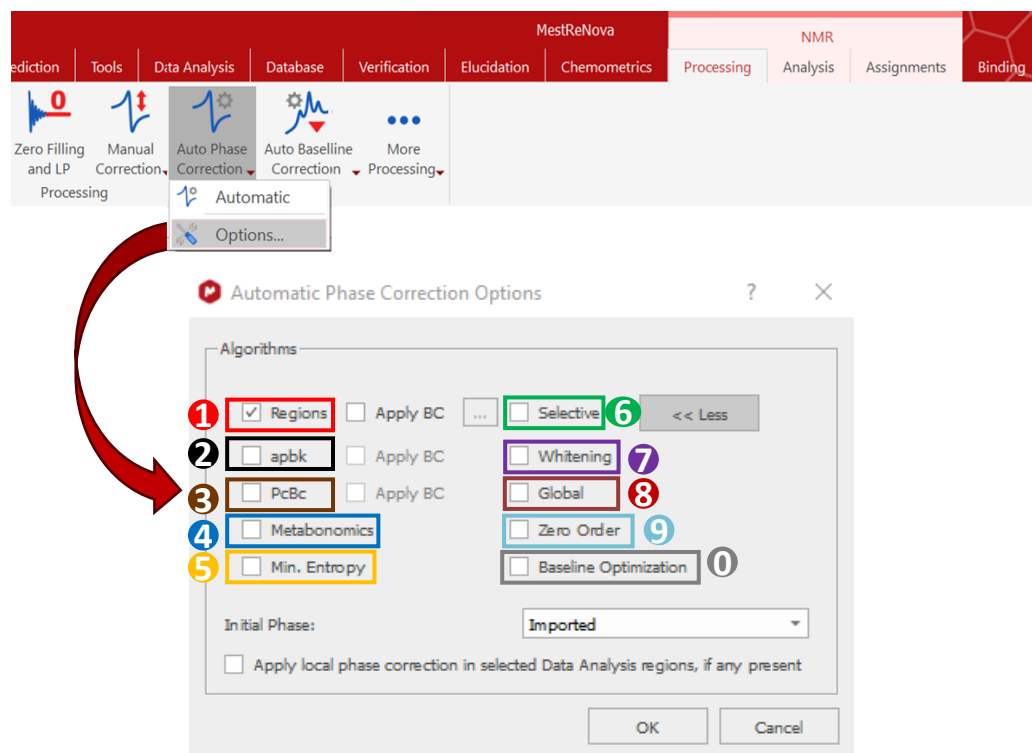


PROCESSING NMR DATA

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☐ PHASE CORRECTION METHODS

- The different phase correction methods available are



1. An autophasing routine which uses complex fit with phase on the peak regions.
2. algorithm for 1H Bruker NMR datasets, with the capability to apply a baseline correction. It requires to have a Java virtual machine installed.

3. Only available for 1D, it will allow users to apply both a phase and baseline correction

4. Especially good for spectra where the signals are concentrated in the centre of the spectral width and there may be a dispersive peak in the centre of the spectrum (usually a biofluid)

5. An algorithm for automatic phase correction of NMR spectra based on entropy minimization. ([reference](#))

6. This automatic method is intended for spectra containing negative and positive peaks (e.g. DEPT, APT, etc) or in the presence of baseline distortions. Mnova creates a list of the highest peaks in the spectrum and then uses symmetrisation criteria to obtain the optimal phasing parameters (α and β).

7. A method for fully automated phasing of Fourier transform NMR spectra based on a combination of the whitening and the metabonomics method. First, the whitening method is applied in order to get good starting phase correction parameters even in spectra that have both positive and negative peaks. Then the most negative peaks are removed, and a simple baseline correction is applied. Finally, the metabonomics method is applied.

8. This method automatically finds phasing parameters (α and β or PH0 and PH1) using an iterative process in which the intensity of the lowest point in the spectrum is optimized. **Not good for low S/N or spectra with bad baseline and many negative peaks.**

9. A method that allows to make an automatic phase correction in PH1 with a zero value




10. A method for fully automated phasing of Fourier transform NMR spectra based on a baseline optimization technique. ([reference](#))



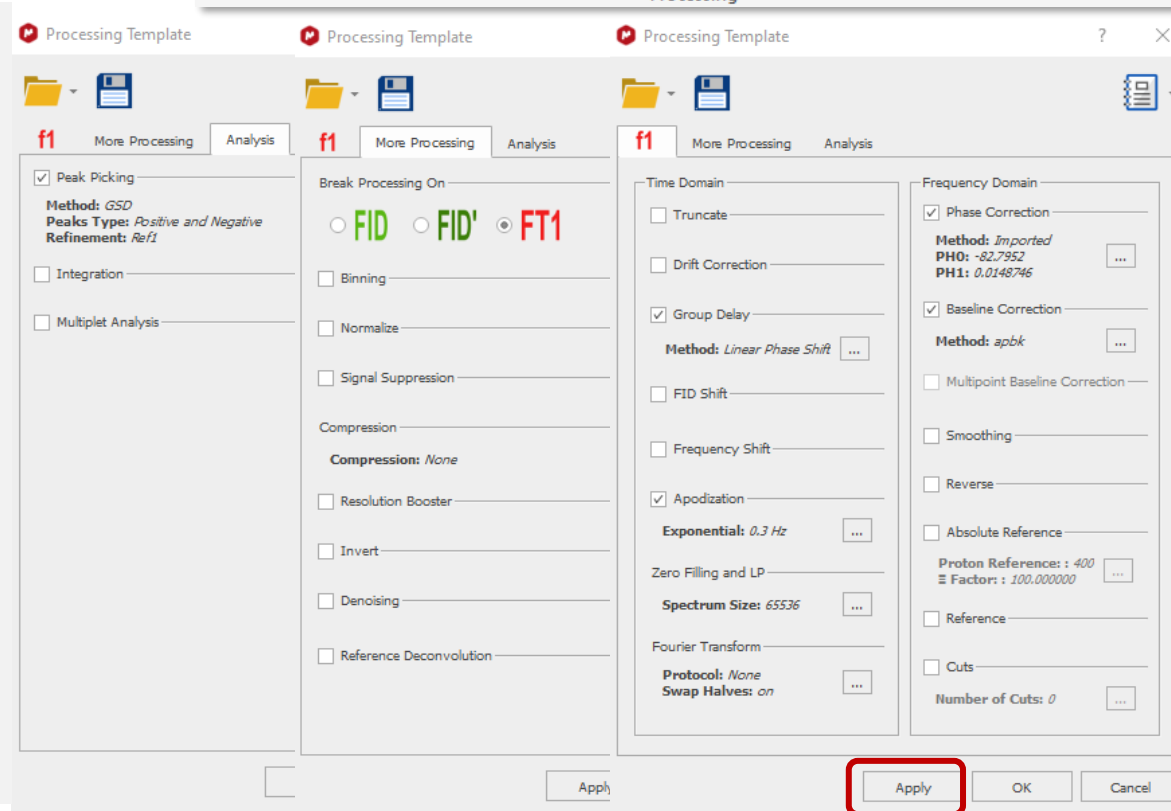
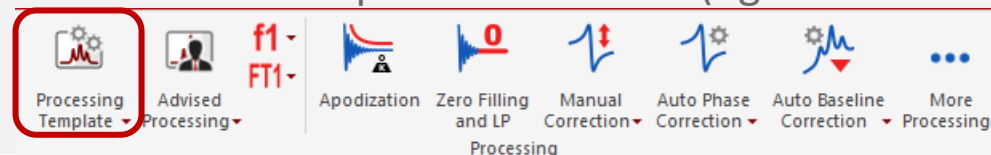
PROCESSING NMR DATA

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❑ PROCESSING TEMPLATE

- Users can create and save processing templates for further use on specific NMR data (eg: processing template for 1D TOCSY, 2D NOESY, ...).
- Click “Processing Template”
- Set-up your specific Time & Frequency domain parameters (F1 panel)*
- Set-up additional processing (more processing panel)
- Set-up additional analysis (Analysis panel)
- Save your template by clicking on 
- Recall your template by clicking c... 
- Apply your template by clicking on “Apply” 

* For 2D NMR data, a F2 panel will also need to be set-up

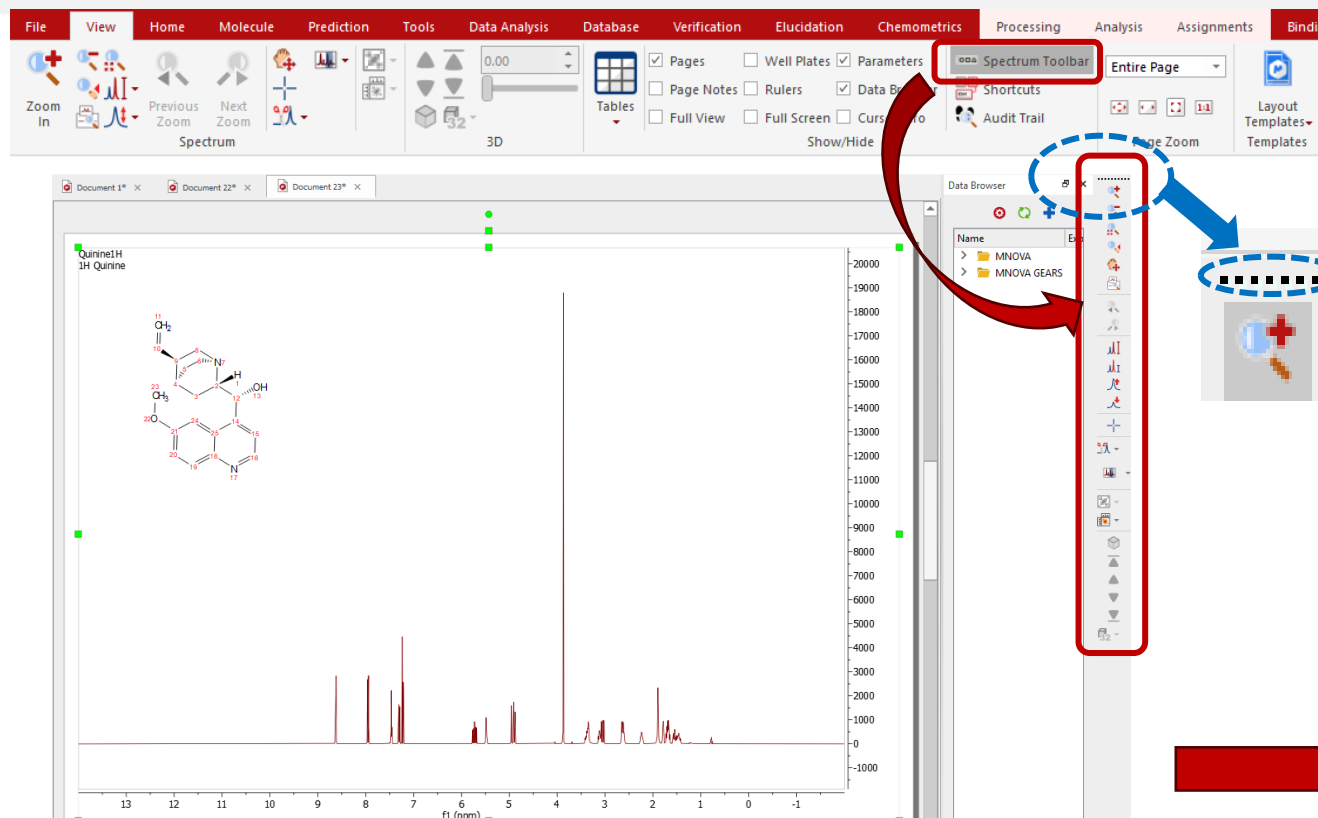


NMR GRAPHIC TOOLBAR & KEYBOARD SHORTCUTS

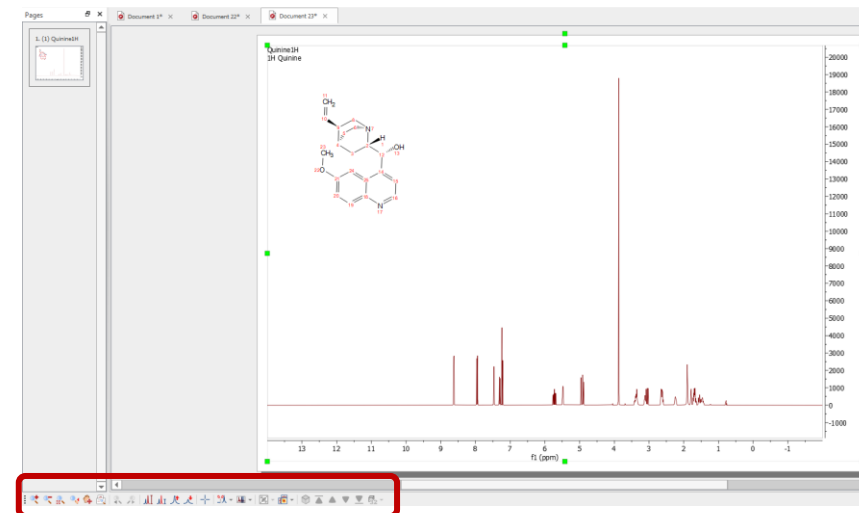
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□ NMR DISPLAY AND GRAPHICAL TOOLBAR

- A series of toolbar are available in the NMR toolbar for all elementary operations (zooming, panning, expanding, scaling, ...). The toolbar can be activated from the View menu by clicking the “Spectrum toolbar” icon as indicated below.



Left click on the dotted line and drag and drop the toolbar as you wish in the interface (second monitor, left, right, up or down the graphic interface)



NMR GRAPHIC TOOLBAR & KEYBOARD SHORTCUTS



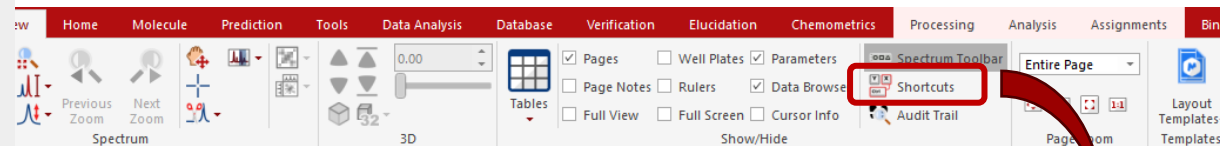
GRAPHICAL TOOLBAR & KEYBOARD SHORTCUTS

- The different tools of the toolbar can also be activated using keyboard shortcuts listed below



- 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)
- Previous Zoom level
- Next Zoom level
- 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
- Edit Blind regions

- The full list of keyboard shortcuts, which are not limited to the NMR graphical toolbar, can be accessed via the View menu as indicated below



Shortcuts		
	Command	Shortcut
42	View > Full Screen	F11
43	View > Intensity > Decrease	-
44	View > Intensity > Fit to Highest Intensity	H
45	View > Intensity > Increase	+
46	View > Pages	Ctrl+F2
47	View > Pan	P
48	View > Zoom > Full Spectrum	F
49	View > Zoom > Manual Zoom	M
50	View > Zoom > Next Zoom	Shift+Right
51	View > Zoom > Previous Zoom	Shift+Left
52	View > Zoom > Zoom In	Z
53	View > Zoom > Zoom Out	Shift+Z

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

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



ANALYZING NMR DATA

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☐ REFERENCING 1D AND 2D NMRs

- 3 way to reference 1D NMR spectra: reference/graphic reference/Reference by solvent

The screenshot displays the software's ribbon interface with tabs for File, View, Home, Molecule, Prediction, Tools, Data Analysis, Database, Verification, Elucidation, Chemometrics, Processing, Analysis, and Assignments. The 'Analysis' tab is active, showing sub-tabs for Multiplets, Integrals, and Fitting. The 'Reference' button in the Multiplets group is highlighted, and its dropdown menu is open. The menu includes options for Reference (L), Graphic Reference (R), Reference By Solvent, Absolute Reference..., Auto Absolute Reference, Correct Xi value..., Xi Values..., Apply Saved Reference, Save Reference..., and Edit Saved References...

Group	Tool	Checkboxes
Multiplets	Auto Multiplet Analysis	<input checked="" type="checkbox"/> Labels <input type="checkbox"/> pCurves
		<input checked="" type="checkbox"/> Multiplet Labels <input checked="" type="checkbox"/> Multiplet Boundaries <input checked="" type="checkbox"/> Multiplet Curves
Integrals	Auto Integration	<input checked="" type="checkbox"/> Integral Labels <input checked="" type="checkbox"/> Integral Boundaries <input checked="" type="checkbox"/> Integral Curves
Fitting	Auto Line Fitting	<input checked="" type="checkbox"/> Peak <input checked="" type="checkbox"/> Sum <input checked="" type="checkbox"/> Residual

- Click **Reference** then click on the peak to reference and set-up the reference value(s)
- Click **Graphic Reference** then click on the peak to reference. Click again the in the spectrum at the chemical shift to use as reference value
- Click **Reference by Solvent** and the solvent peak will be automatically picked as reference.
- Absolute referencing for X- nuclei experiments: see manual §8.1.1, pp226-229

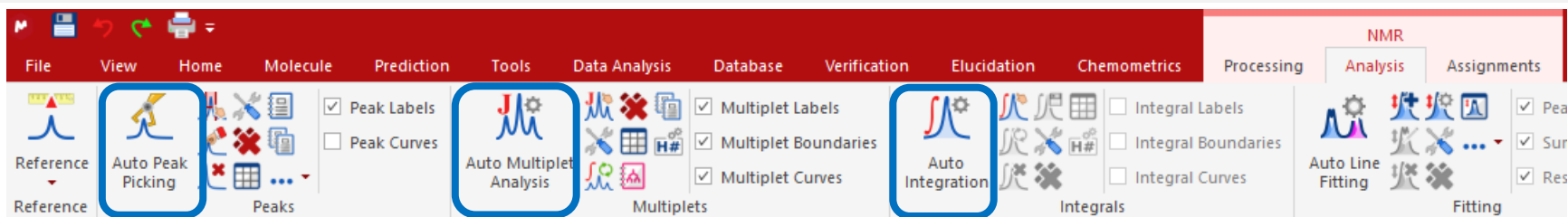



ANALYZING NMR DATA

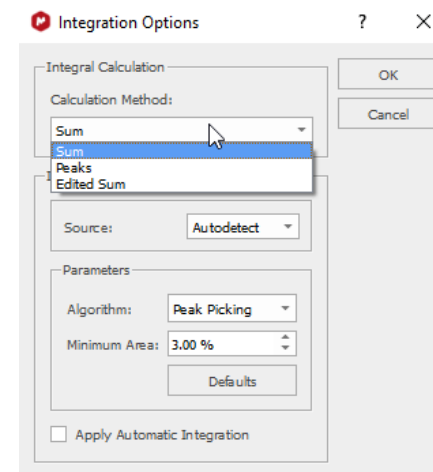
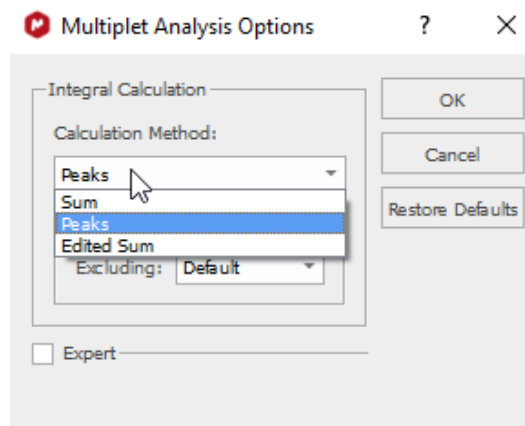
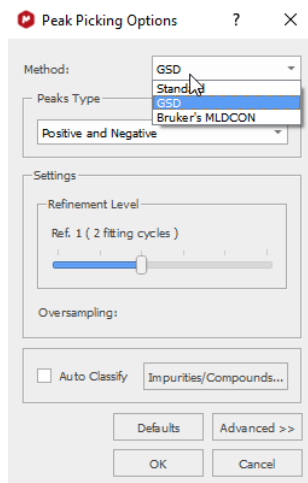
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❑ AUTOMATIC PEAK PICKING, MULTIPLIET ANALYSIS AND INTEGRATION

- 1D NMR & 2D NMR spectra can be conveniently auto peak picked, multiplet analyzed and integrated using the tabs indicated below



- The peak picking, multiplet analysis and integration options can be modified clicking on the respective tool icon 

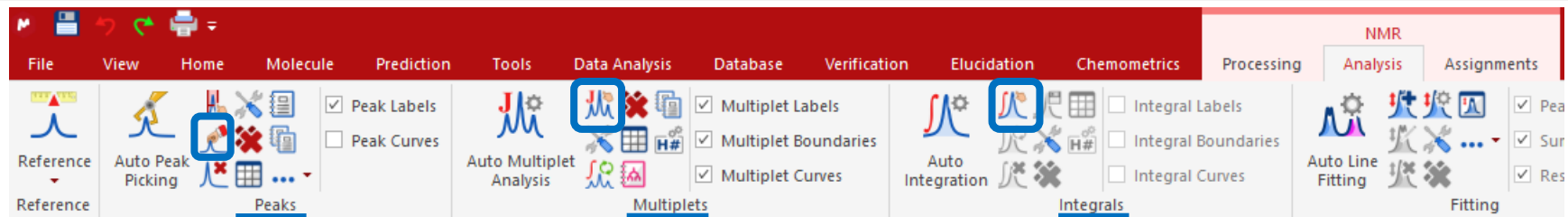


ANALYZING NMR DATA

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☐ MANUAL PEAK PICKING, MULTIPLY ANALYSIS AND INTEGRATION

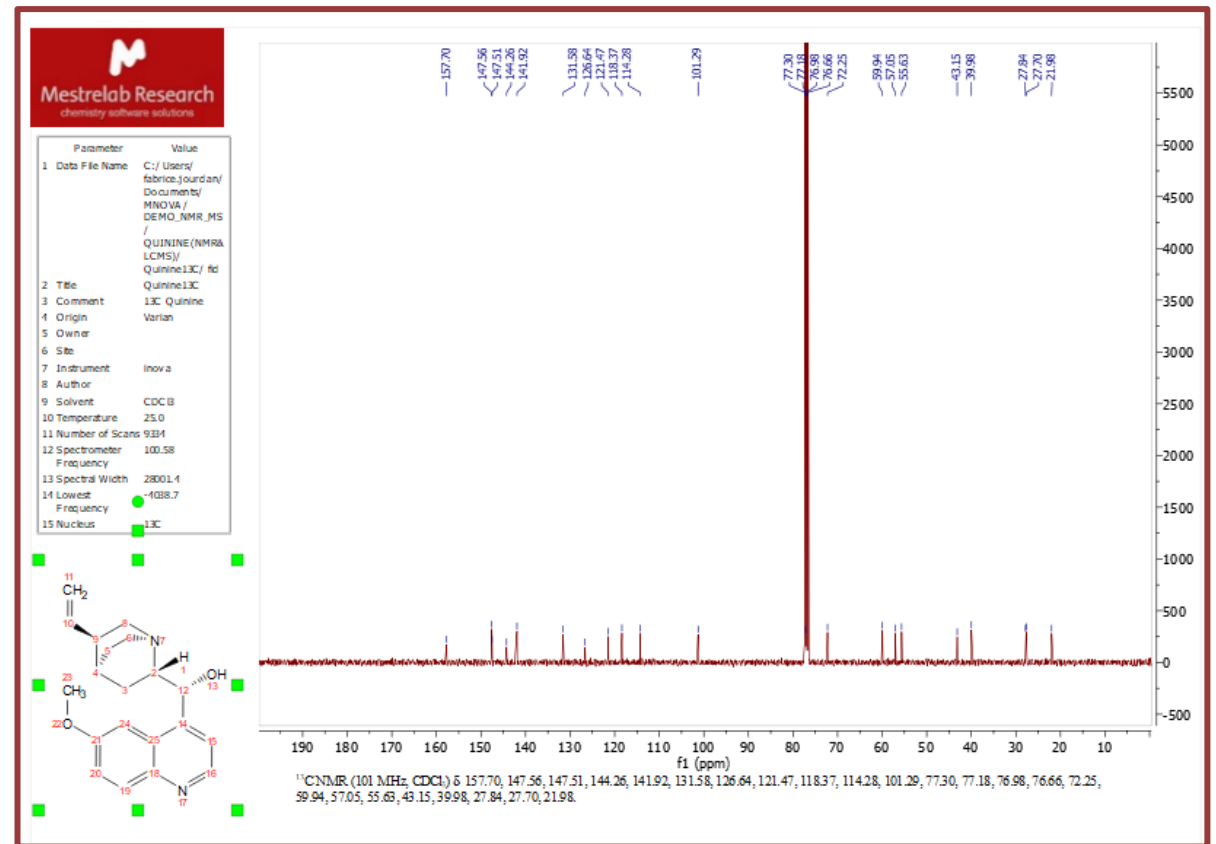
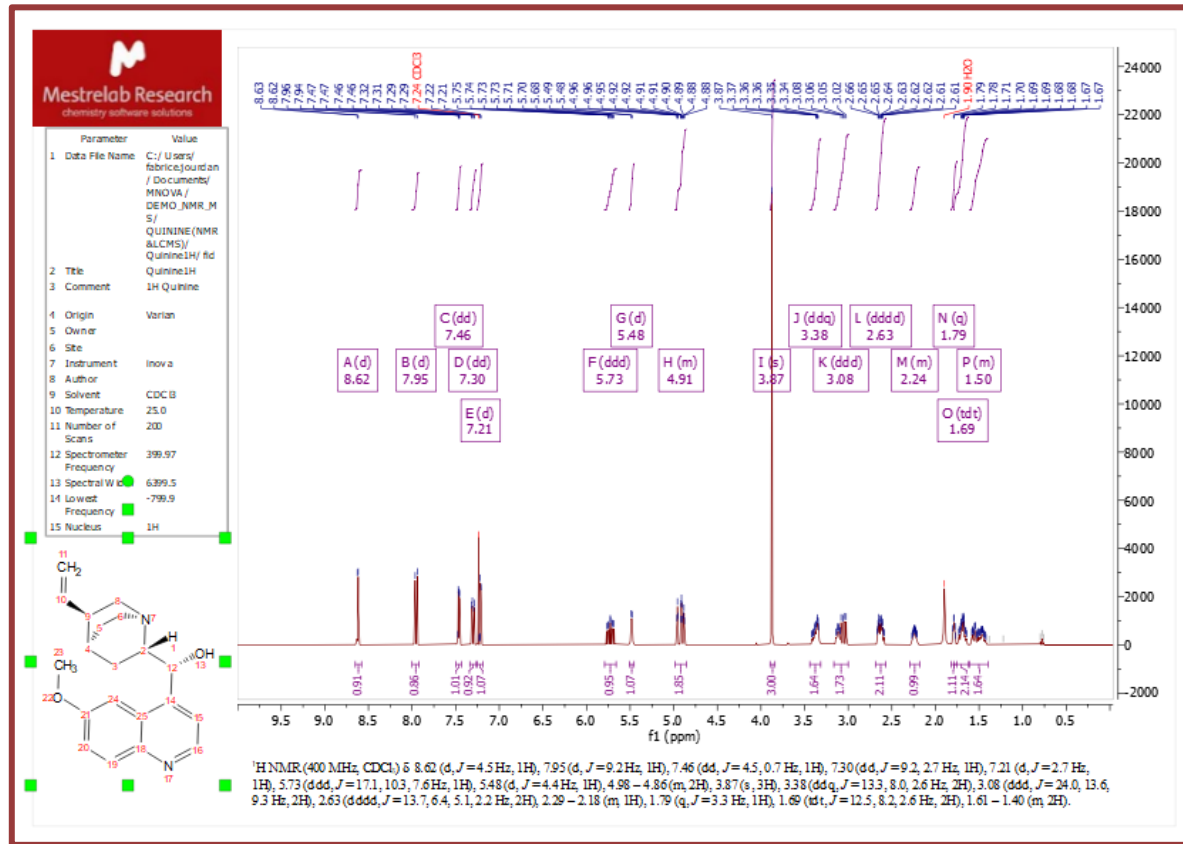
- Users can manually peak pick, analyse and integrate the multiplets by clicking the respective **blue labelled icons** below.



- The peak picking can also be done semi-automatically by manually setting the threshold using
- Peaks, multiplets and integration can be fully cleared with
- Peaks and integration can be individually cleared with, respectively, and
- A multiplet report can be printed on the spectrum with and a peak list with
- Typical reports may look like the ones in the following pages.
- Peak, Multiplet and Integration tables can be accessed from the respective sub-menus using the table icon . Some information in these tables can be modified from these tables (eg: peak/multiplet types). Peak/multiplet/integral list or tables can be copied (and pasted in any type of documents) or reported directly on the spectrum page (see reporting section).

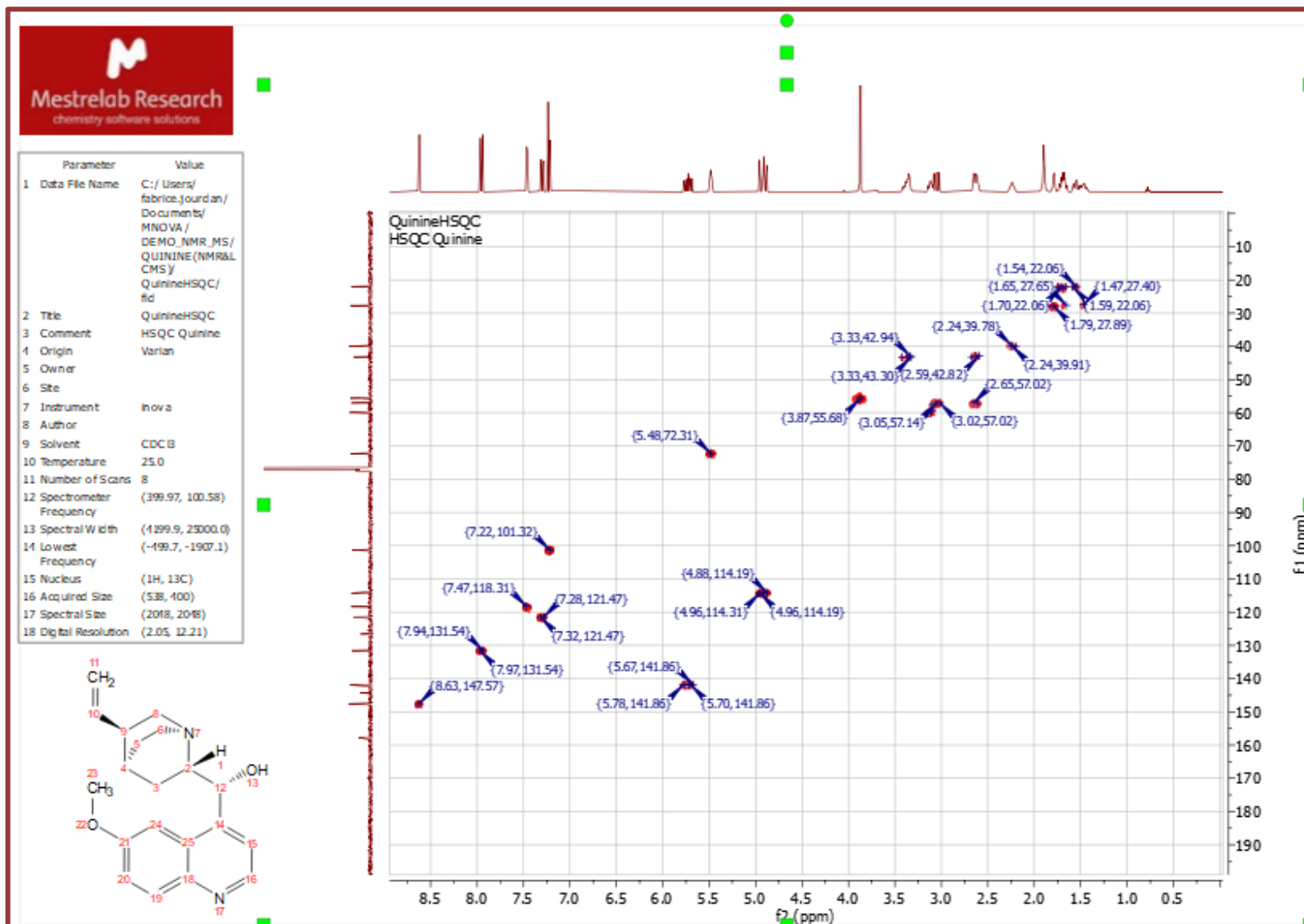


ANALYZING NMR DATA



ANALYZING NMR DATA

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NMR PEAK ASSIGNMENT

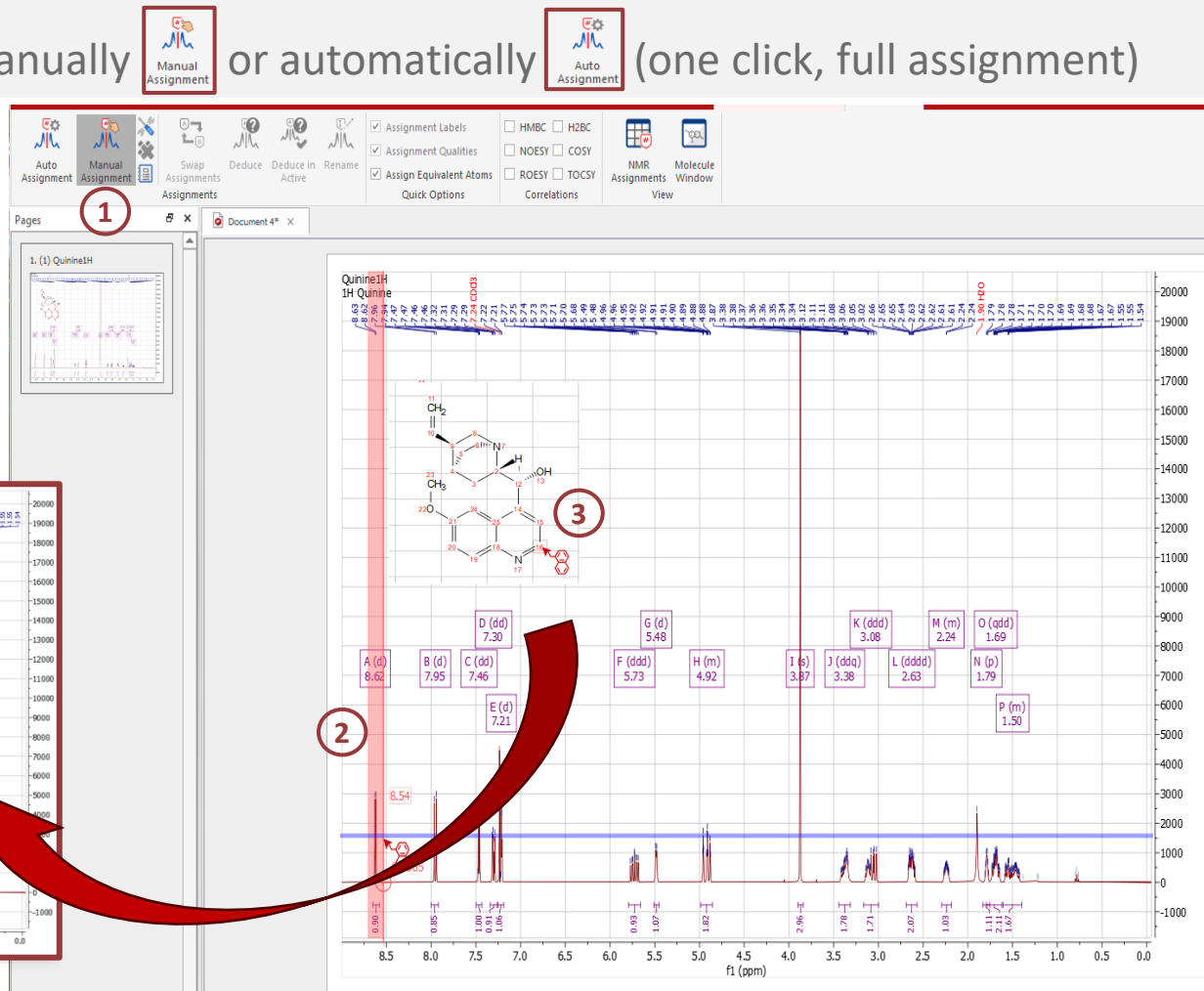
❑ 1D PEAK ASSIGNMENT

- The NMR assignment can be done manually  or automatically  (one click, full assignment)

❑ MANUAL ASSIGNMENT

- Select manual assignment
- Select multiplet (select a peak or drag over multiplet/multiplet box)*
- Click on nucleus to be assigned*

*Steps 2 & 3 can be swapped

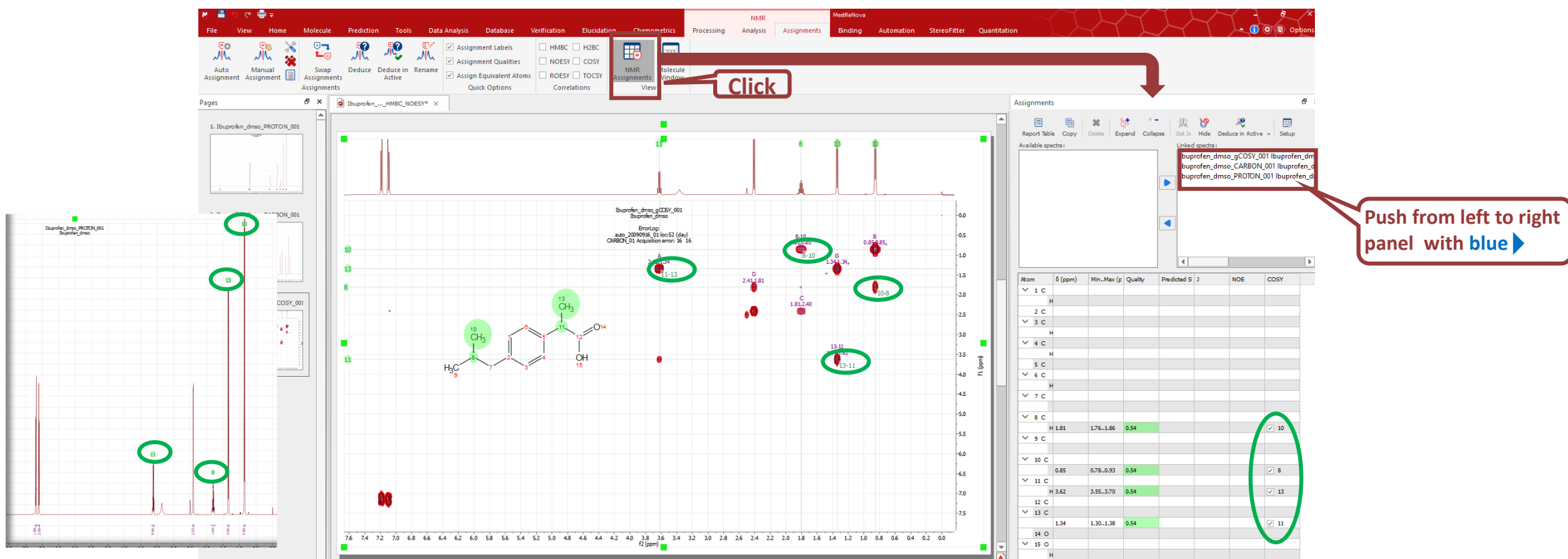


NMR PEAK ASSIGNMENT

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2D PEAK ASSIGNMENT

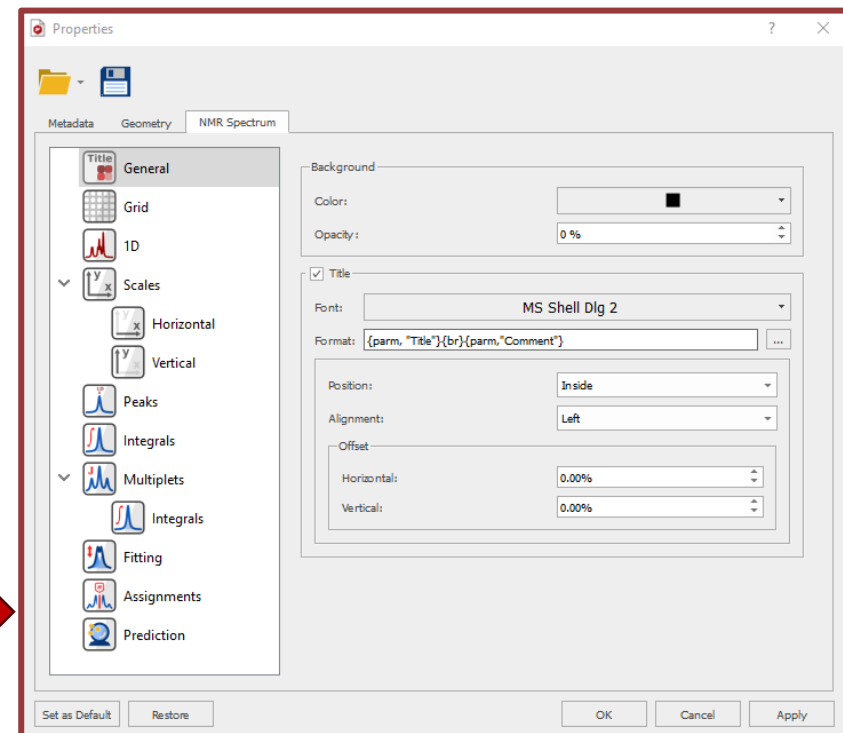
- Select the 2D NMR spectrum to assign and open the NMR Assignment table as indicated below
- Select a cross peak
- Successively click on the nucleus involved in the cross peak (H for COSY, H&C for HMBC/HMQC, ...)



NMR SPECTRUM PROPERTIES

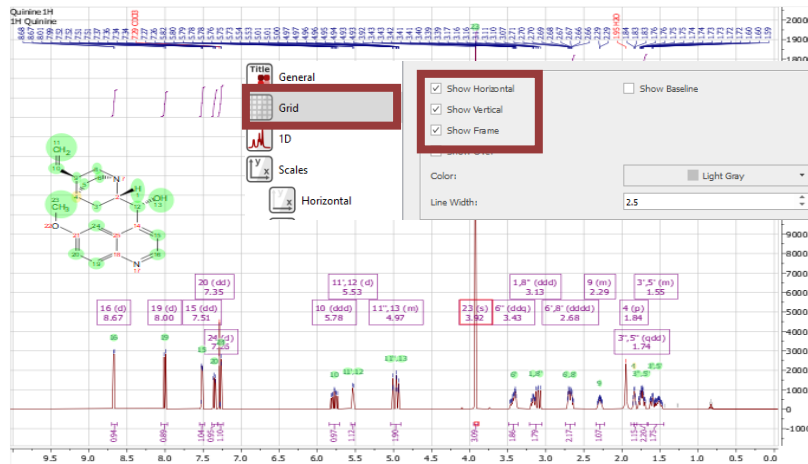
□ ACCESS TO THE PROPERTIES

- The NMR graphic properties can be modified following right mouse clicking over the spectrum and choosing the “properties” option (see below, left). This allows users to modify settings in the sections indicated below (right)

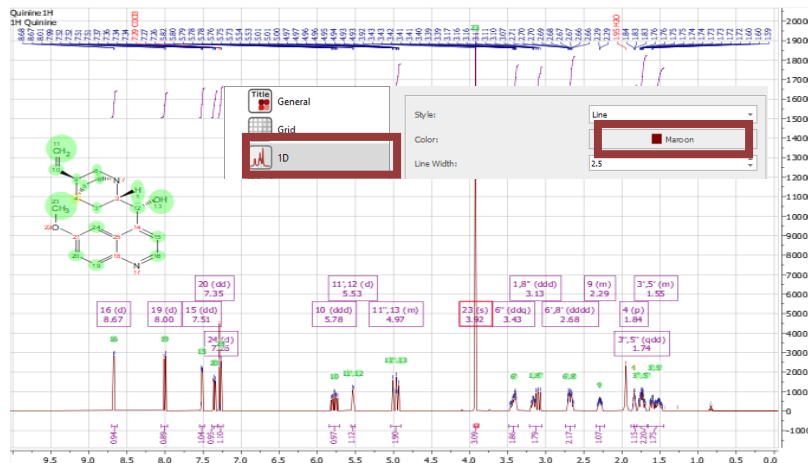


NMR SPECTRUM PROPERTIES

EXAMPLE: GRID AND 1D PROPERTIES



Apply & OK

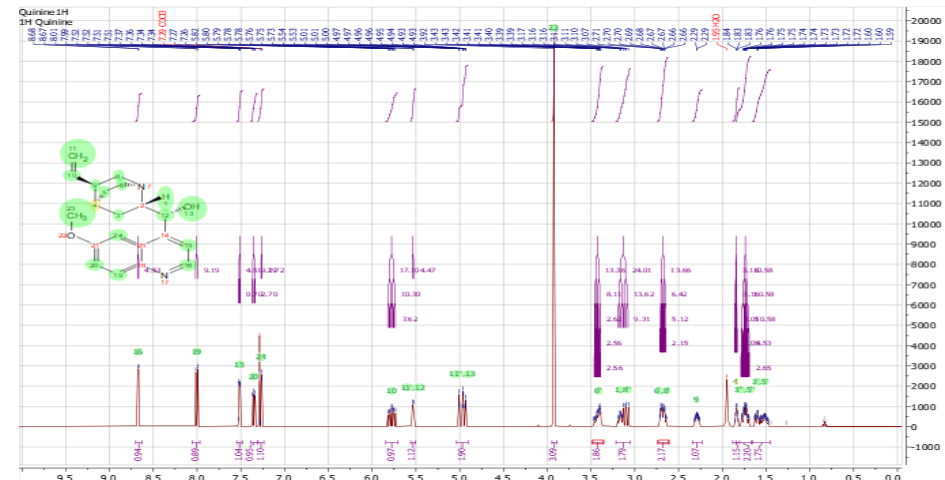


Apply & OK



NMR SPECTRUM PROPERTIES

EXAMPLE: MUTIPLETS



General

☒ Follow Peak Visibility Rules

Opacity Factor: 40.0%

☒ Multiplet Labels

Font: MS Shell Dlg 2

Background Color: White

Label: Name (Category) / Shift

Line Width: 2.5 Position: 30 %

Shift Decimals: 2 Js Decimals: 2

☒ Show Box

☐ J's Tree

Font: MS Shell Dlg 2

Position: 10 % ☒ Show Label

General

☒ Follow Peak Visibility Rules

Opacity Factor: 40.0%

☐ Multiplet Labels

Font: MS Shell Dlg 2

Background Color: White

Label: Name (Category) / Shift

Line Width: 2.5 Position: 30 %

Shift Decimals: 2 Js Decimals: 2

☒ Show Box

☒ J's Tree

Font: MS Shell Dlg 2

Position: 50 % ☒ Show Label





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Mnova MSChrom

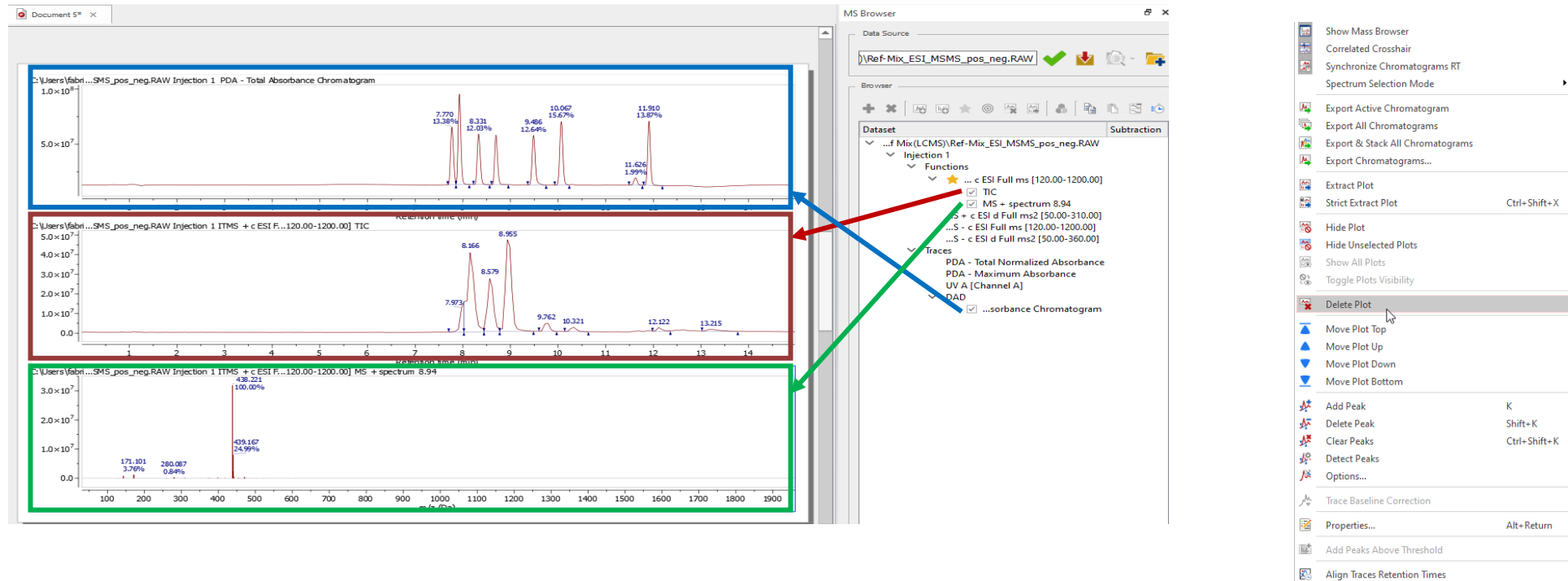


ANALYSING LC-MS DATA

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OVERVIEW

- Upon opening a LCMS (or GC-MS) file, a MS Browser window shall appear allowing users to manage the chromatograms (UV, ELSD, MS, MS-MS, ...) displayed.
- The traces can be called by double clicking on them. A trace can be removed from the central page display by selecting it and right-clicking on the central page to remove it (see image on the right)

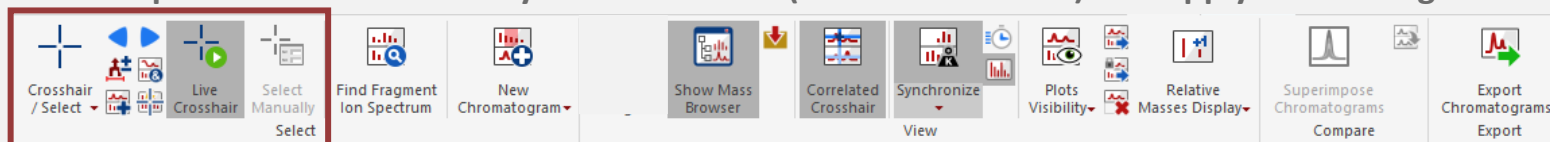





ANALYSING LC-MS DATA



☐ TOOLS MENU

- Note that the Spectrum Toolbar and keyboard shortcuts (see slides 13 & 14) also apply when using LC-MS data



- Crosshair/Select:** This feature allows users to add MS spectra to the document. It also to generate 'CoAdds' and subtractions (see manual section 14.2.2.1, pp622-627). Note that the Live Crosshair switch allows to toggle from live update of the MS display (by simple scrolling over the TIC or UV trace) to update on clicking over a peak.
- The **BLUE ARROWS** allow users to scroll forward/backward MS chromatograms scan by scan
- When activated, the **APPEND** function () allows user to add extra MS spectra to the main window just clicking with the crosshair on the corresponding signal of the TIC. If the 'Append' option is not selected, the current MS spectrum will update each time users click over a peak on the TIC.
- The **MS to UV/MS SWITCH** function () allows users to either display only the MS chromatogram or both MS and UV chromatograms for a specific selected TIC peak
- The **SET MERGE TOLERANCE** tool () allows to select the tolerance (in Da or ppm) of the co-added mass spectra

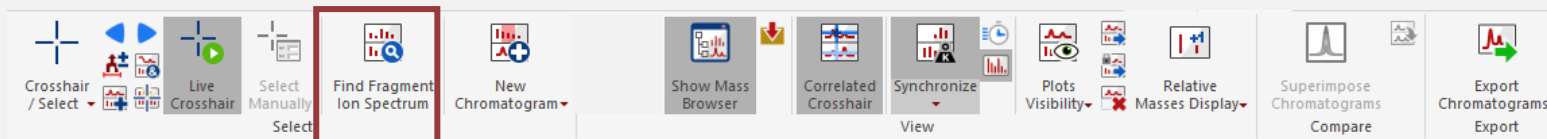
Merged tolerance is a m/z tolerance used any time mass spectra are summed or subtracted. The tolerance is applied to m/z values. Thus a merge tolerance of 0.1 Da means that if two spectra being summed contain, respectively, m/z 100.100 and m/z 100.150, the two mass peaks will be logically summed, since they're within 0.1 Da. The resultant intensity is the simple sum; the resultant m/z value will be the intensity-weighted average of 100.100 and 100.150.



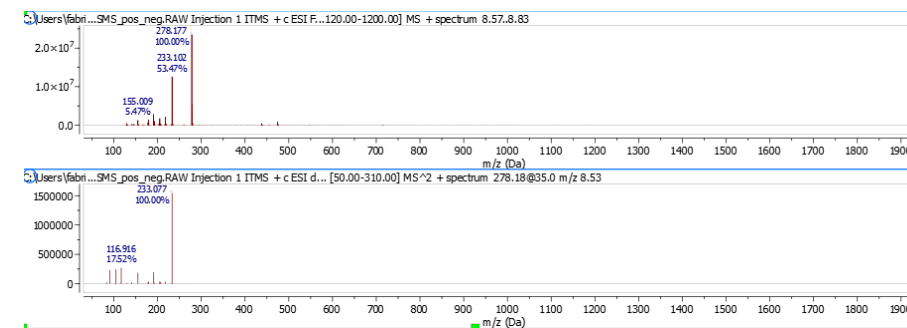
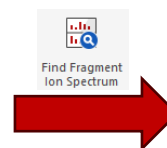
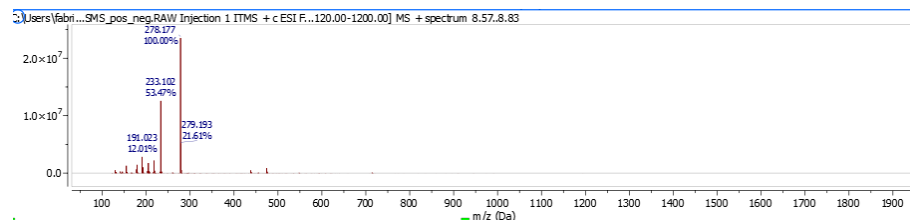
ANALYSING LC-MS DATA

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☐ TOOLS MENU: Find Fragment Ion Spectrum (see manual section 14.2.2.1, pp629-630)

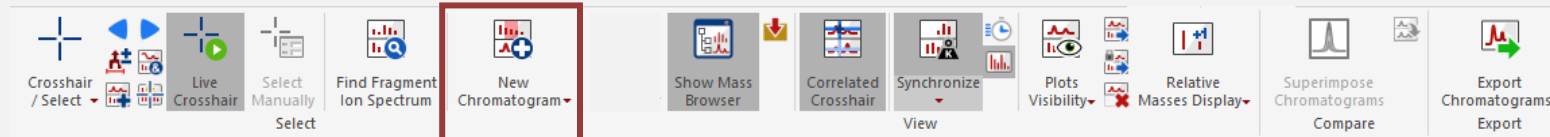


- This Find Fragment Ion Spectrum feature allows to display the applicable MS/MS spectrum from a MS dataset of the precursor, by matching the highest mass peak at around the same RT value.

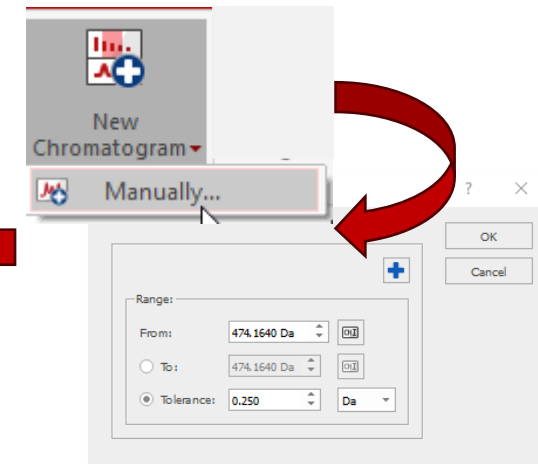
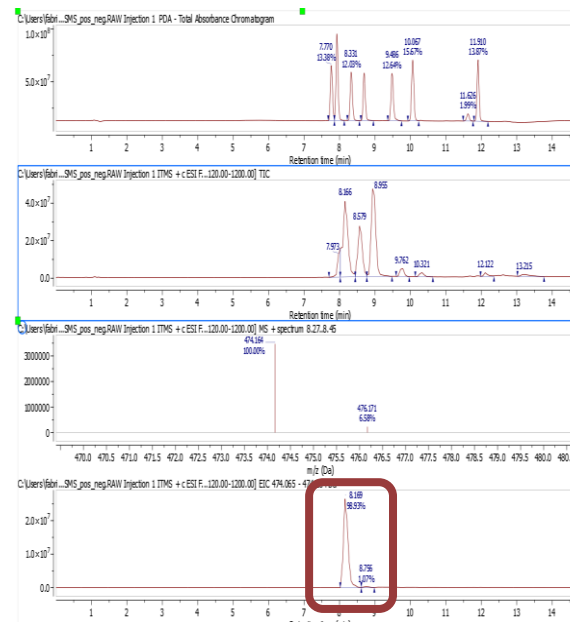
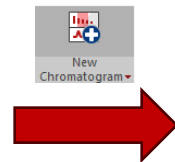
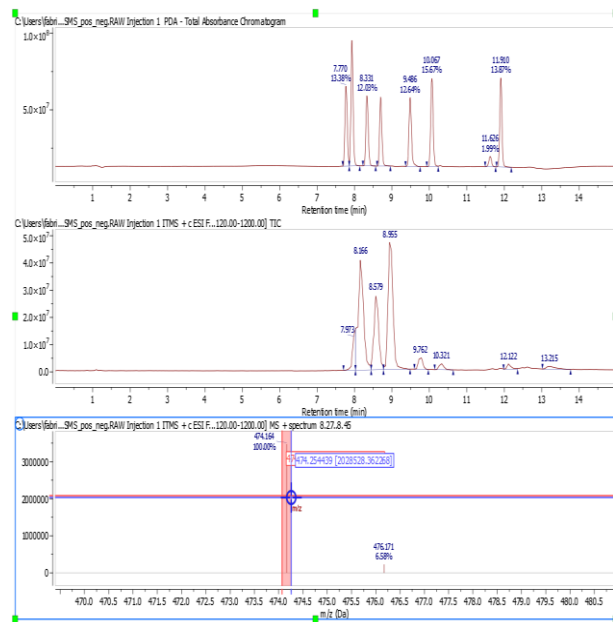


ANALYSING LC-MS DATA

☐ TOOLS MENU: New Chromatogram (see manual section 14.2.2.2, pp630-631):



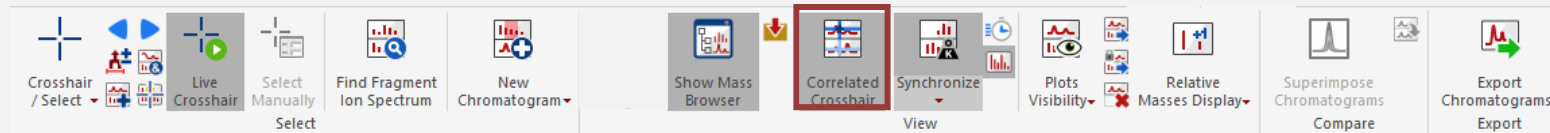
- This New Chromatogram tool is used to extract an EIC from a graphically or manually given m/z value.



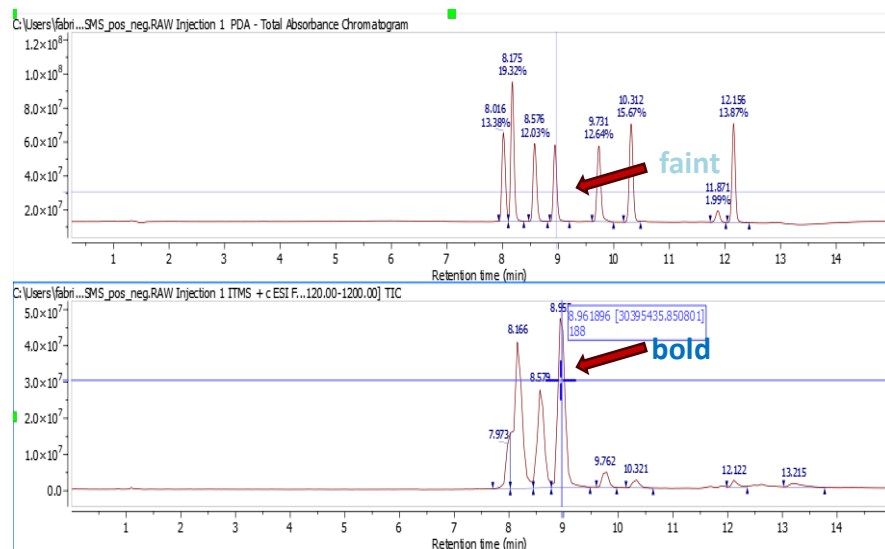
ANALYSING LC-MS DATA

— ..

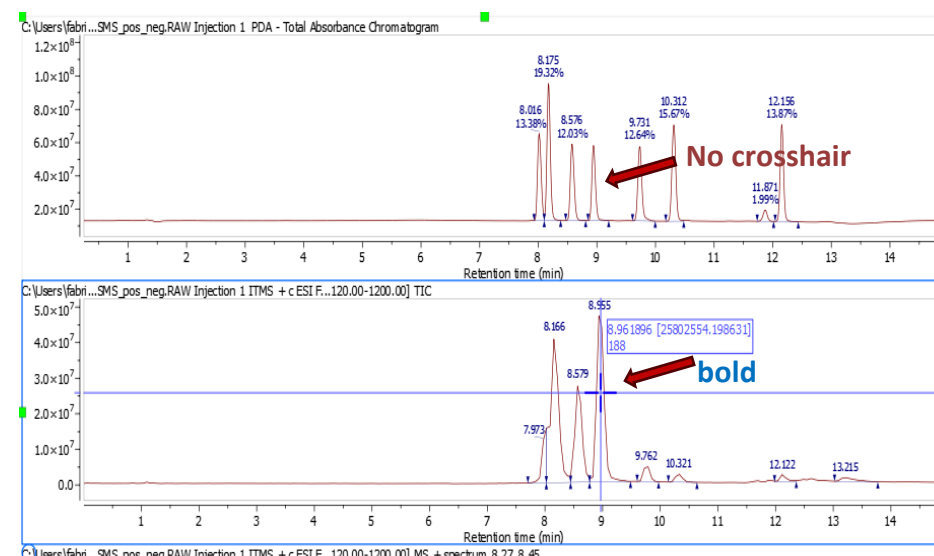
☐ TOOLS MENU: Correlated Crosshair (see manual section 14.2.2.1, pp628-629):



- By default, the Correlated Crosshair mode will display the crosshair as usual in the active plot and as a semi-transparent crosshair in the none-active plots of the same type (chromatograms, TIC, UV spectra). If toggled, the crosshair will only appear in the active chromatogram.



Correlated Crosshair Mode ACTIVE



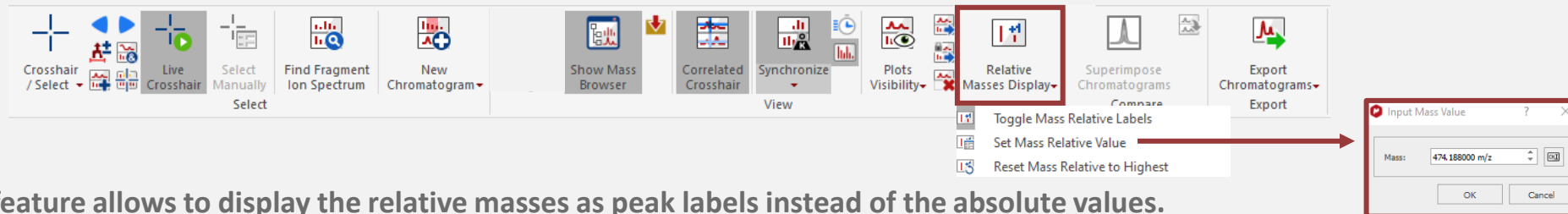
Correlated Crosshair Mode INACTIVE



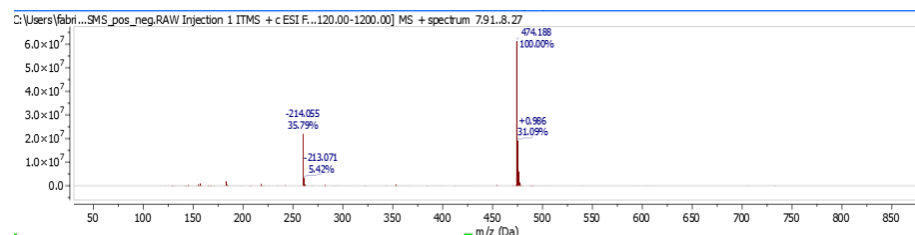
ANALYSING LC-MS DATA

— ..

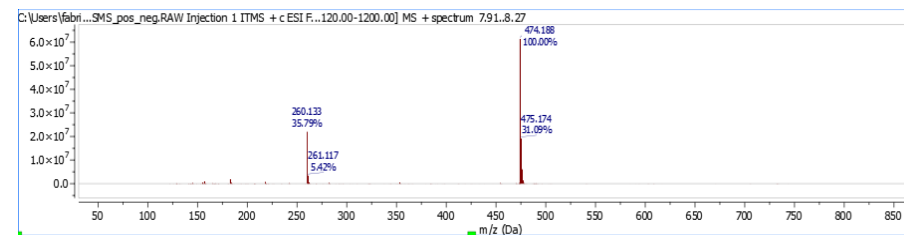
❑ **TOOLS MENU: Relative Masses Display** (see manual section 14.2.2.6, pp653-654):



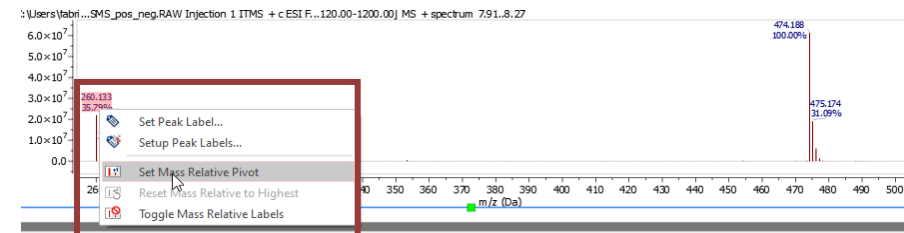
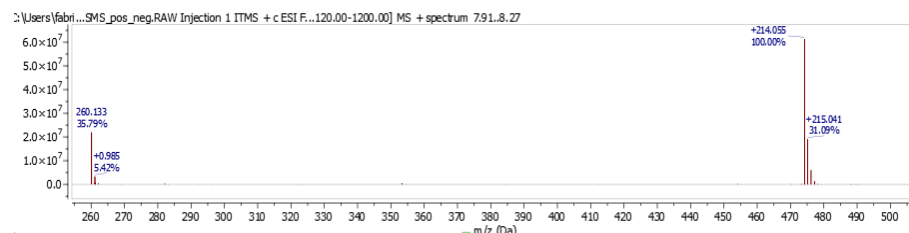
- This feature allows to display the relative masses as peak labels instead of the absolute values.
- The masses values will be relative to the position of the highest peak in the current view. It is however also possible to select any other peak by right clicking on the desired peak label and selecting "Set Mass Relative Pivot" from the context menu (or from the Mass Peaks Table)



RELATIVE MASSES Mode ACTIVE



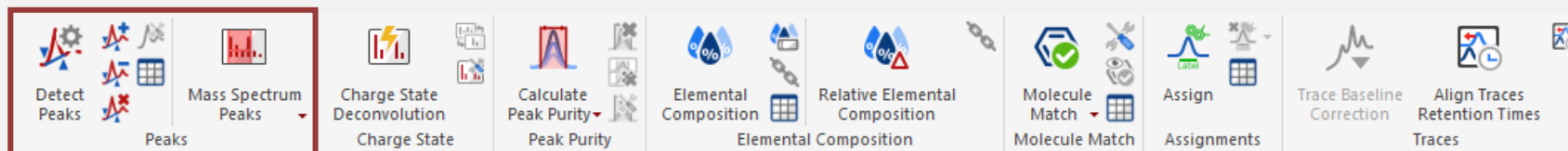
RELATIVE MASSES Mode INACTIVE



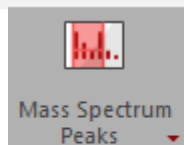
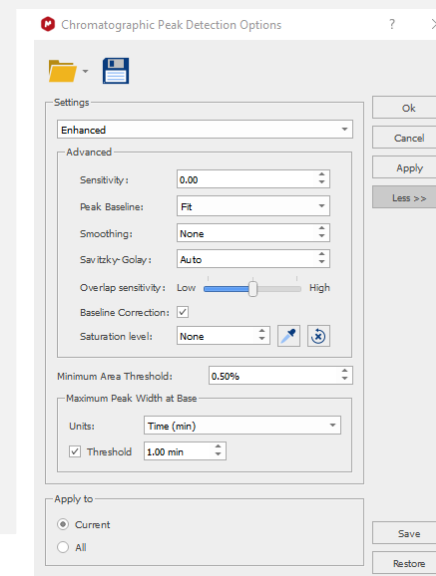
ANALYSING LC-MS DATA

— ..

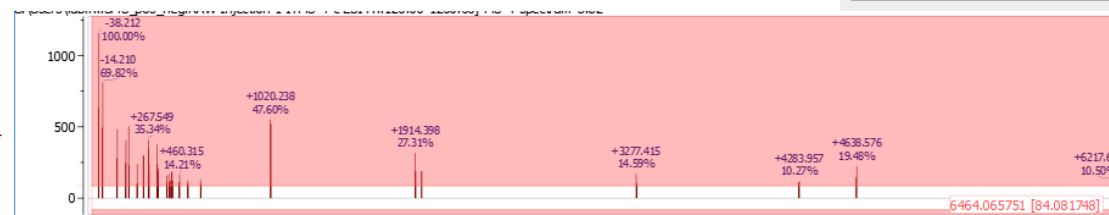
☐ ANALYSIS MENU: Peaks Detection Menu (see manual section 14.2.3, pp659-664):



- The different features of this section allow user to:
 - Auto detect/integrate peaks
 - Manually detect/integrate peaks
 - Clear all peaks
 - Manually delete peaks
- A series of options are available for peak detection (sensitivity, baseline correction, minimum area threshold, ...)
- The Mass Spectrum Peaks feature allows users to add or delete peaks by manually adjusting the threshold in the MS chromatogram (see below).



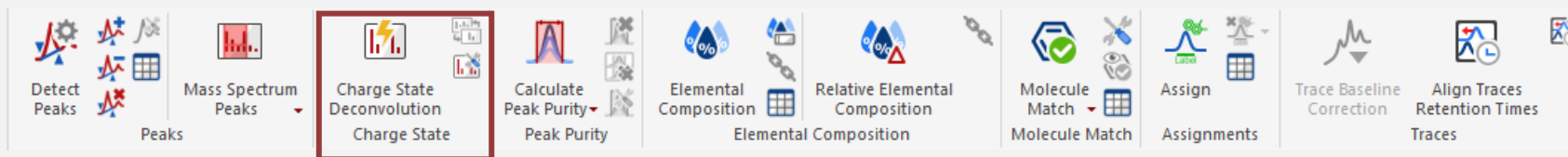
Threshold
adjustment →



ANALYSING LC-MS DATA

— ..

❑ ANALYSIS MENU: Charge State Deconvolution (see manual section 14.2.3.2, pp671-672):



- MS spectrum may be deconvoluted by pressing the button "Charge State Deconvolution". If the Append button is selected, the deconvoluted MS spectrum will be added to a new plot. Otherwise, it will substitute the original MS spectrum.
- The settings for the deconvolution calculations can be modified via the Charge State Deconvolution Settings button
- The default settings are as below:

Charge State Deconvolution Settings

Tolerance: 5 ppm

Abundance Threshold: 1.000%

Charge State Range:

From: 1 To: 10

m/z Range:

From: 0.00 Da To: 1000000.00 Da

Deconvoluted Mass Range:

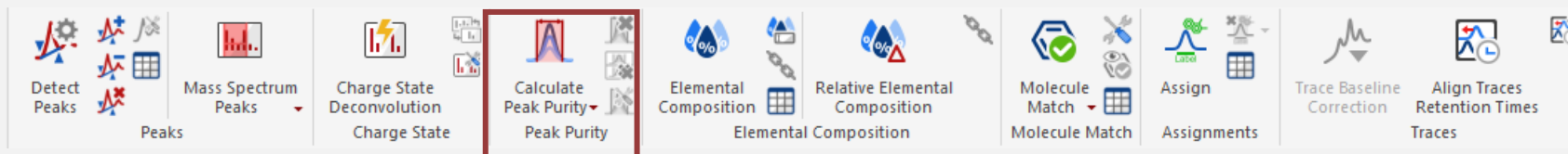
From: 1.00 Da To: 1000000.00 Da

OK Cancel

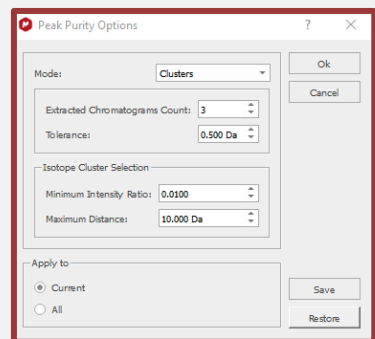
ANALYSING LC-MS DATA

— ..

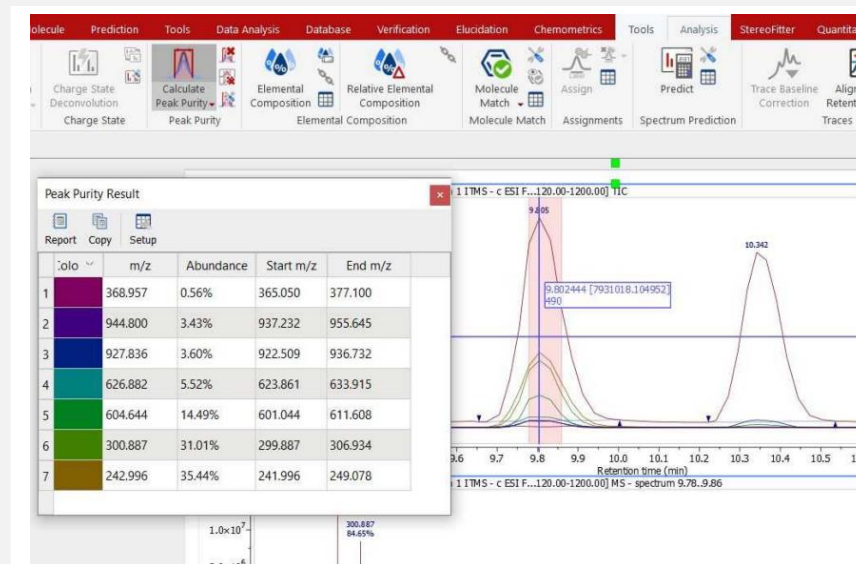
□ ANALYSIS MENU: Peak Purity (see manual section 14.2.3.3, pp672-674):



- This feature will calculate the chromatogram peak (or region) purity associated to the most abundant mass peaks which are displayed under the selected peak.
- The default settings for peak purity are as below:



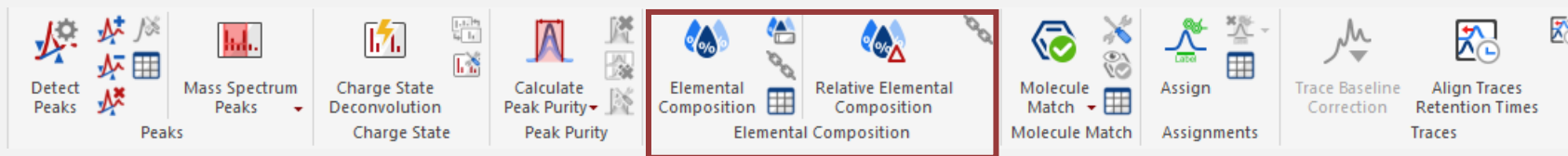
- There are three different modes:
 - Peaks: will use the single chromatogram peak.
 - Cluster: will use isotope clusters instead of single peaks (with the option to select the minimum intensity ratio & the maximum distance)
 - Predefined: will use the mass values/mass ranges provided by the user




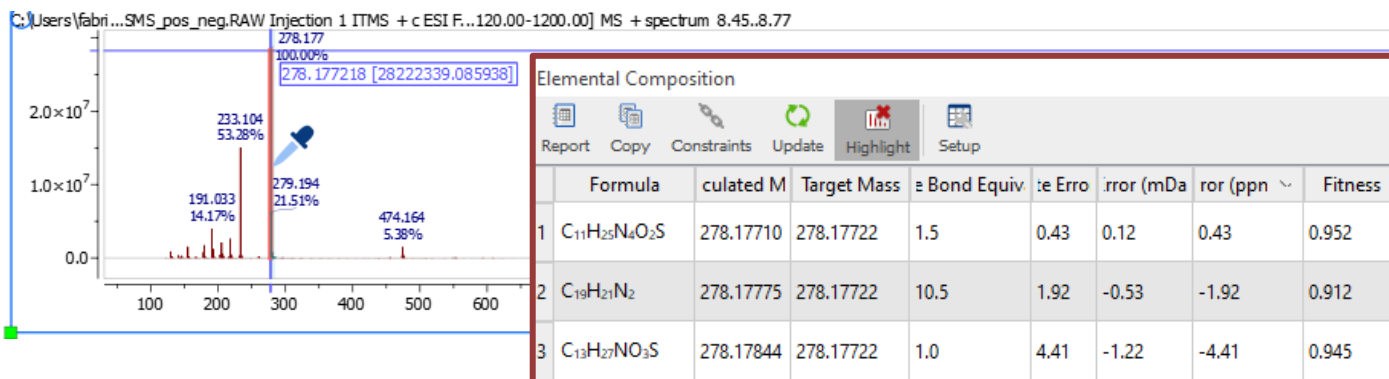
ANALYSING LC-MS DATA

— ..

□ ANALYSIS MENU: Elemental Composition (see manual section 14.2.3.4, pp674-679):



- This feature calculate the elemental composition of one or more mass peaks of a spectrum, if the m/z values are of high accuracy, typically ≤ 5 ppm mass accuracy.
- It is first necessary to establish the constraints of the calculation, just by clicking on the applicable option of the menu  which will display the dialog box below



The screenshot shows the 'Elemental Composition Constraints' dialog box. It contains several sections for setting constraints and tolerances.

Element Constraints:

Element	Minimum	Maximum
1 C	0	100
2 H	0	200
3 N	0	10
4 O	0	10
5 S	0	5

Double Bond Equivalences:

Minimum: -0.50
Maximum: 20.00

Tolerances:

Units: ppm
Value: 5.00

☐ Maximum Result Counts:

Maximum: 1

Other Constraints:

Electron Mode: Both
☒ Adduct: H+
☐ Loss
☐ Charge State: 1
Fitness Threshold: 0.00

Buttons: OK, Save, Restore, Update, Cancel

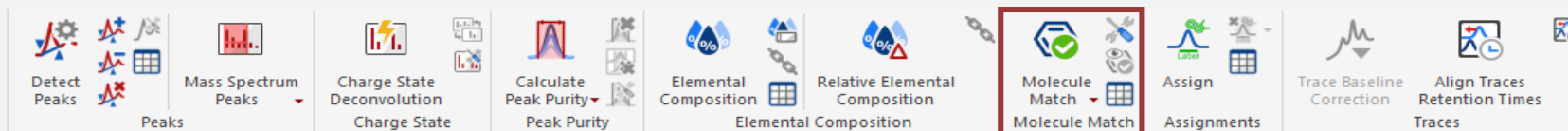
- Note that the Relative Elemental Composition feature works in the same way using a relative mass value



ANALYSING LC-MS DATA



❑ ANALYSIS MENU: MOLECULAR MATCH (see manual section 14.2.3.5, pp679-686):



- The Molecule match analysis determines the possible presence of a given structure or structures within a mass spectral data set. The molecular ion cluster of each structure is computed and compared to each spectrum in the data set. If one or more spectra contain the computed isotope cluster within reasonable matching constraints, the most intense spectrum within the most closely matched chromatographic peak is returned as a positive result. Structures not matched are assigned a “not found” result. The constraints dialog (see below) allows the user to select one or more adducts, specify ion polarity, and other parameters. The algorithm makes use of fast isotope cluster calculations and a sophisticated spectral matching technique.
- Requirement:
 - a LCMS dataset
 - one (or more) molecular structure(s)
 - (see example next slide)

Tolerance

Units:

For MS:

For MS/MS:

Thresholds

Score Thresholds:

Matches per Molecule:

Positive Polarization

Adducts/Losses:

	Adduct	Loss
1		-
2	H+	
3	Na+	
4	K+	
5	NH4+	

Max Positive Charge:

Negative Polarization

Adducts/Losses:

	Adduct	Loss
1	-	
2		H+
3	Cl-	
4	Na+	2H+
5	K+	2H+

Max Negative Charge:

More Settings

☐ Dimers

Spectra Average Count:

MS/MS Settings

☐ Ignore Precursors

Search For:

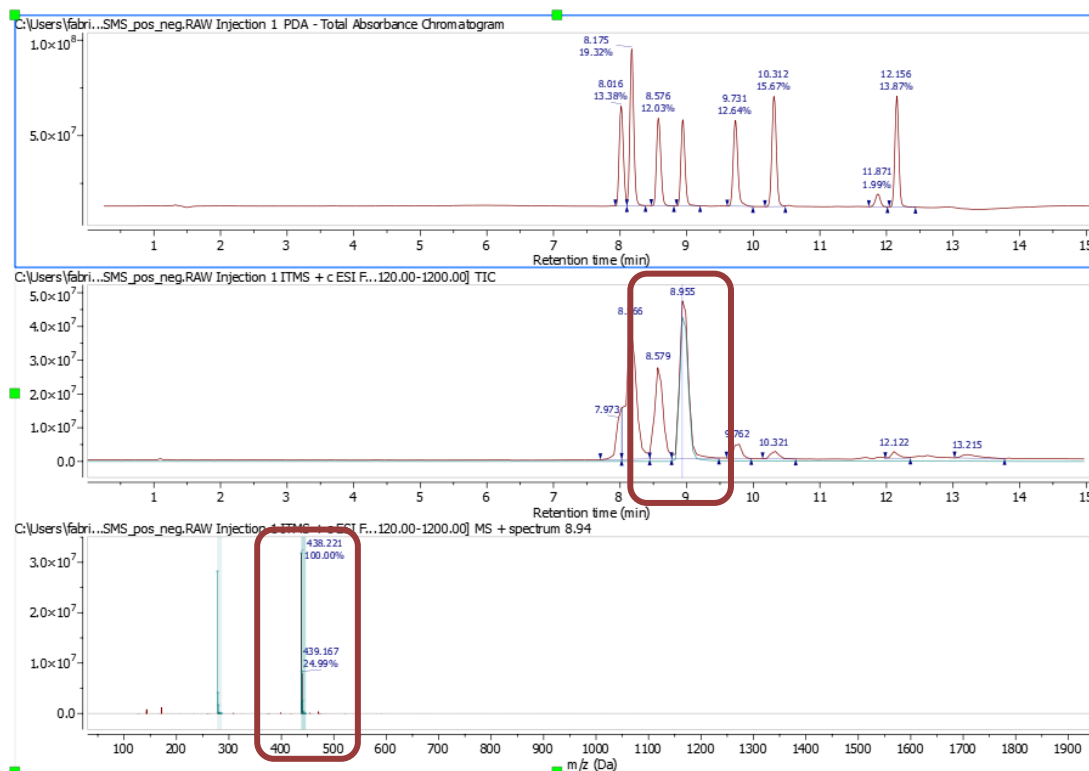
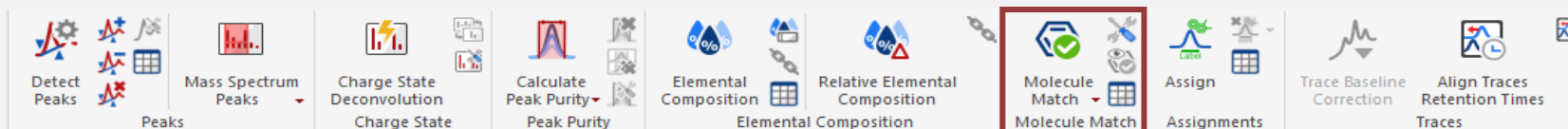
Buttons: OK, Save, Restore, Cancel



ANALYSING LC-MS DATA

— ..

❑ ANALYSIS MENU: MOLECULAR MATCH (see manual section 14.2.3.5, pp679-686):



Molecule Match

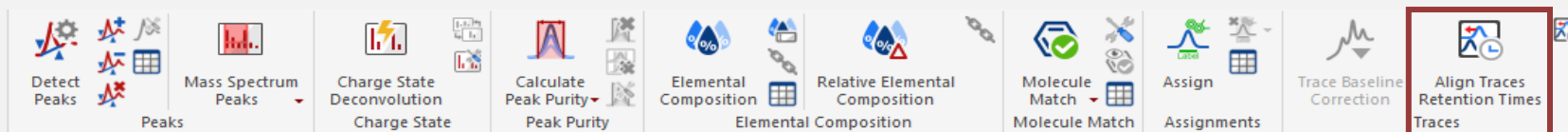
	Molecule	Match	Match Score	MS Purity	RT	Purity	MS Match S	Adduct/Los	Error (ppm)	redicted m
4		✓	1.000	0.897	8.94	43.84%	—	H+ / —	87.997	438.1821
5		✓	0.999	0.229	12.11	0.45%	—	H+ / —	87.997	438.1821
6		✓	0.996	0.049	10.33	0.12%	—	2Na+ / H+	81.785	339.9878
7		✓	0.993	0.245	9.79	0.87%	—	H+ / —	-178.919	303.0185
8		✗	—	—	—	—	—	—	—	—



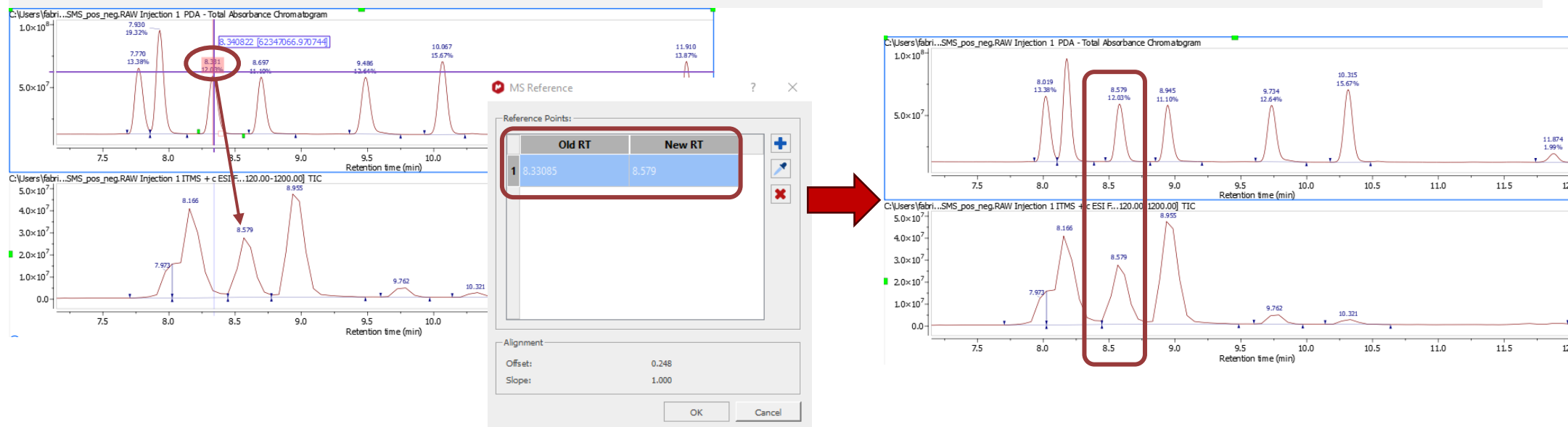
ANALYSING LC-MS DATA

— ..

ANALYSIS MENU: Align traces RT (see manual section 14.2.3.9, pp694-695):



- For some technical reasons, the TIC peaks can be delayed compared to the UV peaks. The “Align traces retention times” feature will re-calibrate the chromatograms so that the peaks match across them. You will only need to click on a peak in the selected chromatogram and enter the new value(s) to change the X scale (time)

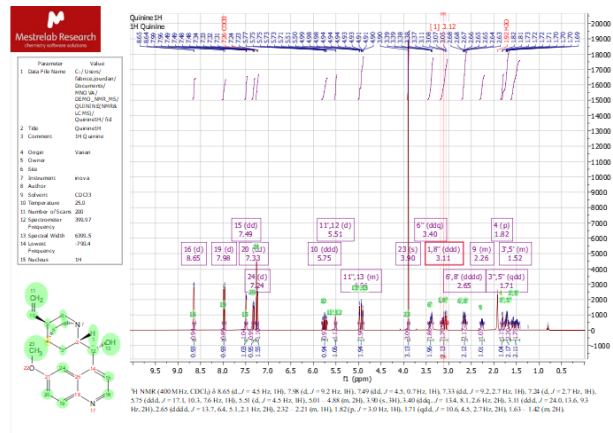
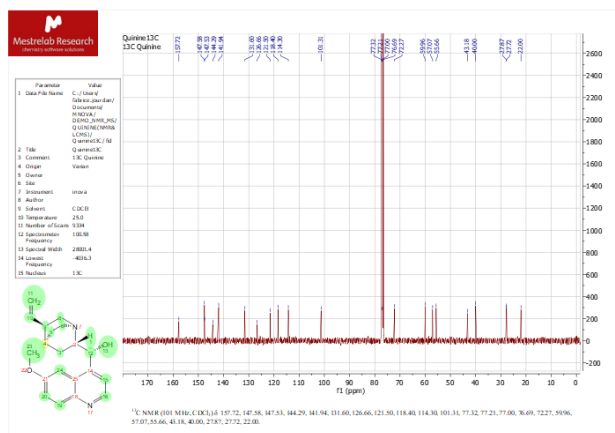


REPORTING – LAYOUT TEMPLATES

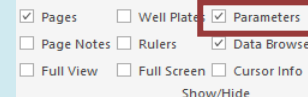
OVERVIEW

Mnova allows users to create layout templates for systematic data reporting. Each layout template can contain one or more pages of any kind of data (NMR, LC-MS, IR, ...). The steps to follow are:

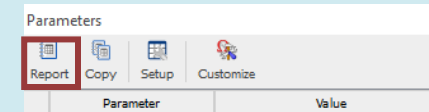
1. Process and analyse your data
2. Design each page with the required information (structure, parameters, logo, ...)



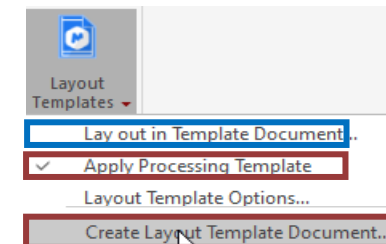
NOTE: The parameter window can be opened from the View sub-menu.



The parameters can then be pasted to the spectrum page by clicking on “Report”



3. Go to View > Layout Templates and create a Layout template document (also applying the processing template used for the NMR data). You will need to save this layout template.
4. When needed on new (unprocessed nor analysed) data, call the template by going to View > Layout Templates and calling a saved Layout template document.





Mestrelab Research
chemistry software solutions

Mnova NMRPredict



MNOVA PREDICT WITHOUT NMR DATA

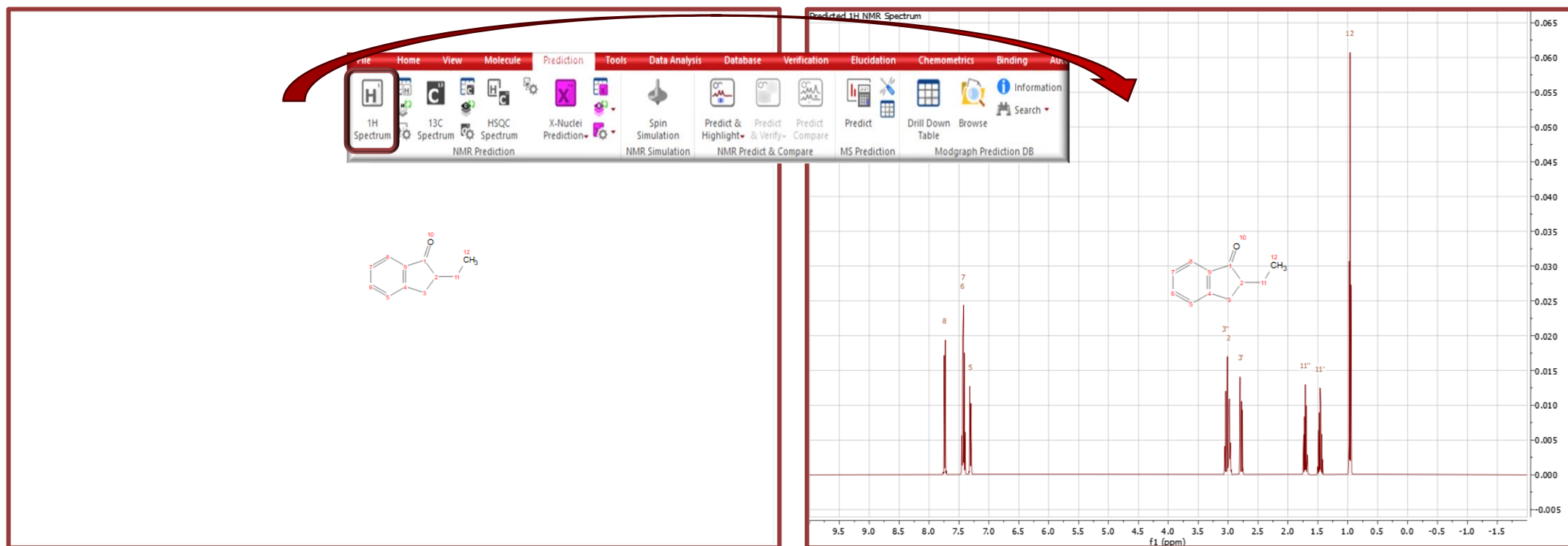
— ...

1. COMPOUND STRUCTURE

- Either open a structure file (.mol, .cdmx) or draw a structure in the active document

2. PREDICT

- Select one of the options available in the Prediction Menu (see example below)



MNOVA PREDICT WITH NMR DATA

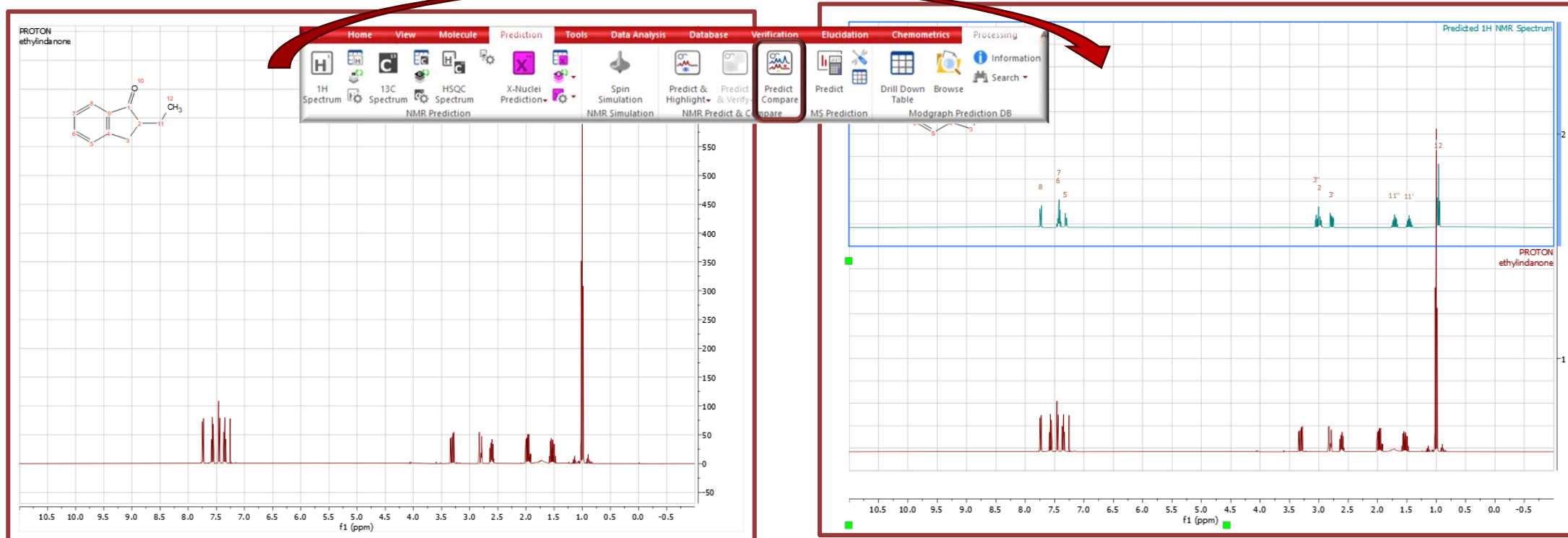
— ...

1. NMR DATA & COMPOUND STRUCTURE

- Open your NMR data and the associated structure file

2. PREDICT

- Select one of the options available* in the Prediction Menu (see example below)

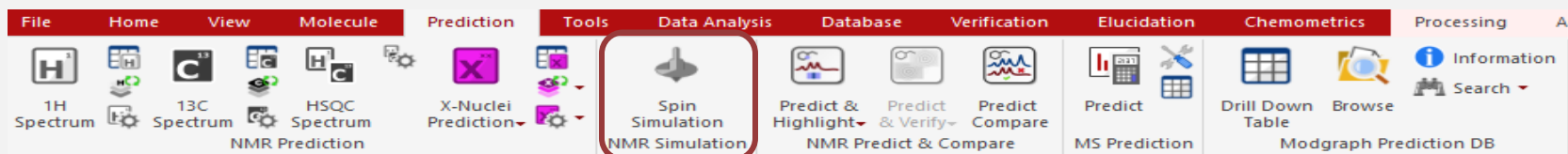


*Note that the prediction tab for a specific nucleus will be active only when the structure contains this specific atom.

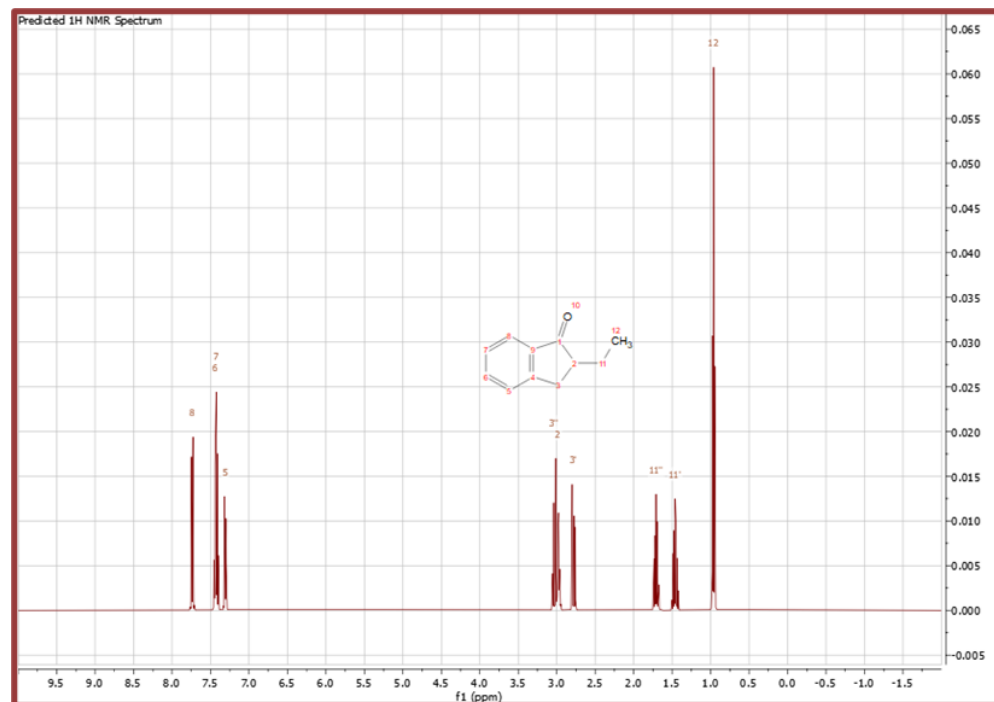
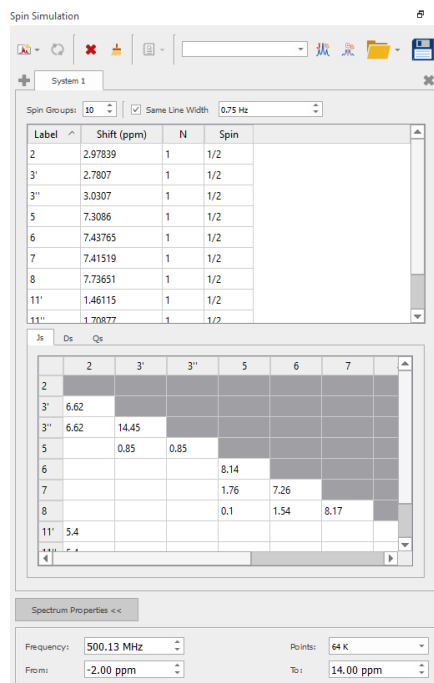
MNOVA PREDICTION OPTIONS

— ..

☐ NMR PREDICTION OPTIONS: SPIN SIMULATION



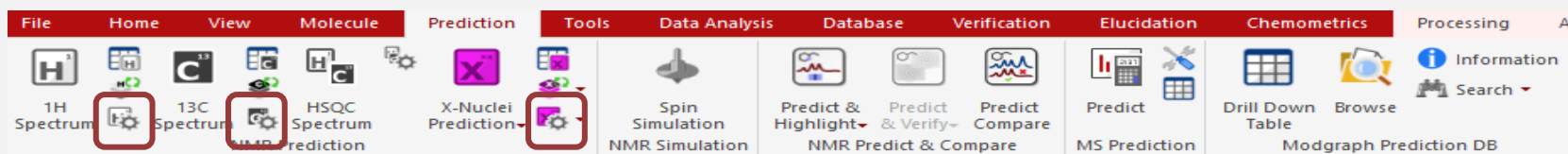
- Spin Simulation: this tool allows users to build an NMR spectrum from a defined system of spin (see manual 13.4, pp588-602).



MNOVA PREDICTION OPTIONS

— ...

□ NMR PREDICTION OPTIONS: ¹H, ¹³C and X-NUCLEI OPTIONS



- These option tabs allow to access the tables below. Users can then define parameters such as ppm range, number of points, field frequency, NMR solvent, ...) (see manual 13.2.1, pp554-555).

1H Prediction Options

Predictors

- ☒ Mestrelab Predictor
- ☒ Modgraph NMRPredict Desktop
- ☐ Modgraph NMRPredict Server

>> Less

From: -2.00 ppm

To: 10.00 ppm

Number of Points: 32 K

Frequency: 500.13 MHz

Line Width: 0.75 Hz

Solvent: Chloroform-d

☐ Exclude Labile Protons

OK Cancel

¹³C Prediction Options

Predictors

- ☒ Mestrelab Predictor
- ☒ Modgraph NMRPredict Desktop
- ☐ Modgraph NMRPredict Server

>> Less

From: -20.00 ppm

To: 230.00 ppm

Number of Points: 128 K

Frequency: 125.03 MHz

Line Width: 1.50 Hz

Solvent: Chloroform-d

☐ DEPT

☐ Protonated Carbons Only

☒ Proton Decoupled

OK Cancel

Spin Simulation

- 15N Options...
- 17O Options...
- 19F Options...
- 29Si Options...
- 31P Options...

17O Prediction Options

Predictors

- ☒ Modgraph NMRPredict Desktop
- ☐ Modgraph NMRPredict Server

>> Less

From: -50.00 ppm

To: 850.00 ppm

Number of Points: 32 K

Frequency: 67.77 MHz

Line Width: 1.50 Hz

Solvent: Chloroform-d

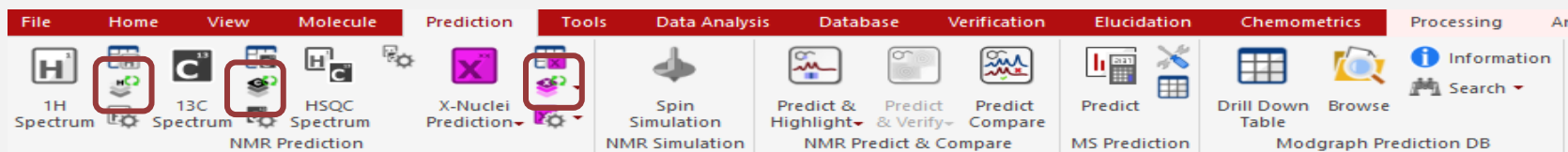
OK Cancel



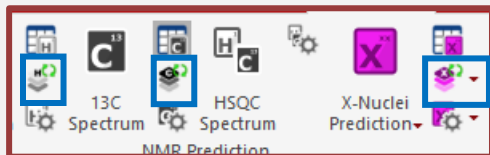
MNOVA PREDICTION OPTIONS



❏ NMR PREDICTION OPTIONS: ^1H , ^{13}C and X-NUCLEI PREDICTION DATABASE



- The Mnova Predict database can be enriched with fully assigned spectra to enhance user's prediction tool. This is done by using the tabs: (see manual 13.2.6, pp572-580 for full details).



Send To 1H DB

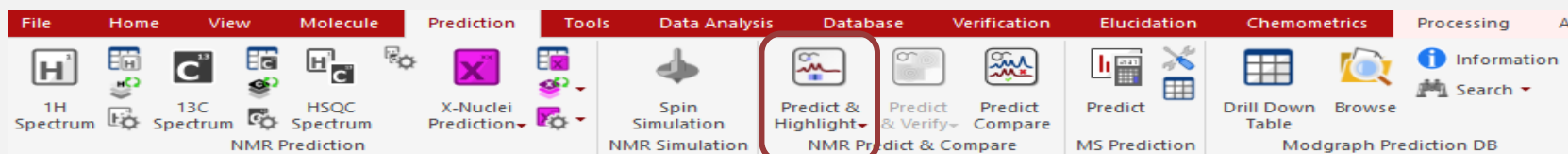
	Atom	Shift
1	1	7.015
2	2	7.275
3	3	7.559
4	5	7.559
5	6	7.275
6	7	9.868
7	9	2.032
8	9	2.032
9	9	2.032

	Tag	Value
1	AUTHOR	
2	CHEMISTID	
3	COMPOUNDNAME	
4	DBLETTER	N
5	FREQUENCY	
6	LITERATURE	
7	SHIFTS	9
8	SOLVENT	dmsd
9	SOURCECODE	1
10	SPECTRUMID	
11	STRUCTUREID	
12	USERNAME	Fabrice Jourdan

OK Cancel

MNOVA PREDICTION OPTIONS

□ NMR PREDICTION OPTIONS: PREDICT & HIGHLIGHT



- This feature calculates in the background a simulation of the spectrum of the structure, highlighting the expected chemical shift(s) when the user hovers the mouse over (a) proton or a carbon. Useful during the assignment process (see manual 13.2.3, pp562-563).
- The table of predicted signals (^1H , ^{13}C , ^nX) can be obtained as a side window by clicking on the corresponding tab

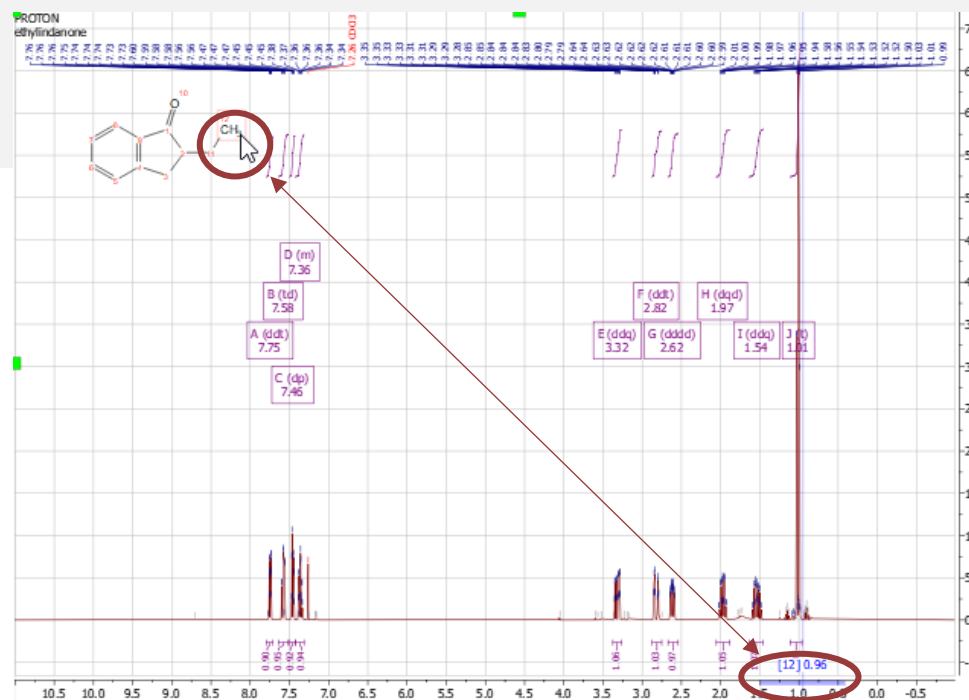


13C Prediction

Report Copy Expand Collapse Setup

Field: 100.619 MHz

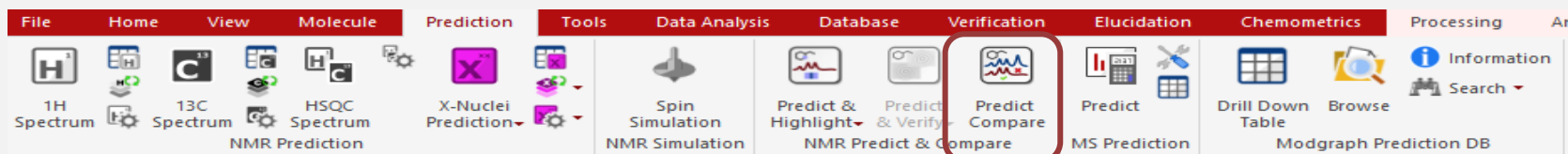
Atom	Value	Error
> 1 C	208.6 pp...	3 ppm
> 2 CH	48.7 ppm	3 ppm
> 3 ...	30.2 ppm	3 ppm
> 4 C	153.5 pp...	3 ppm
> 5 CH	126.8 pp...	3 ppm
> 6 CH	134.3 pp...	3 ppm
> 7 CH	126.3 pp...	3 ppm
> 8 CH	124.0 pp...	3 ppm
> 9 C	136.8 pp...	3 ppm
> 11 ...	24.4 ppm	3 ppm
> 12 ...	11.6 ppm	3 ppm



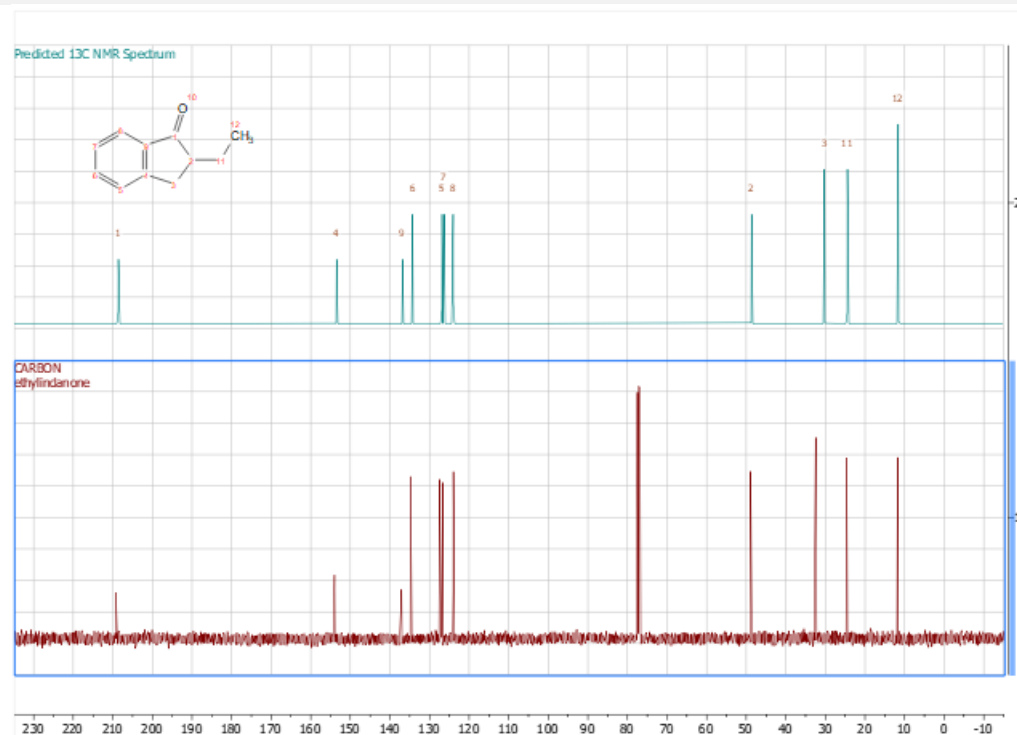
MNOVA PREDICTION OPTIONS

— ..

☐ NMR PREDICTION OPTIONS: PREDICT & COMPARE

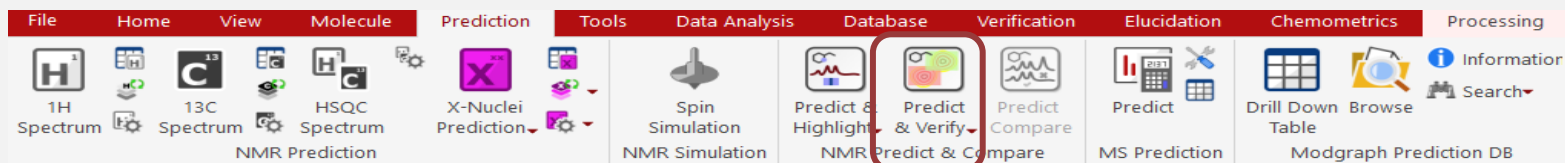


- This feature allows users to compare in a stacked view the predicted spectrum of the proposed structure, with the real NMR spectrum (see manual 13.2.4, pp563-568).

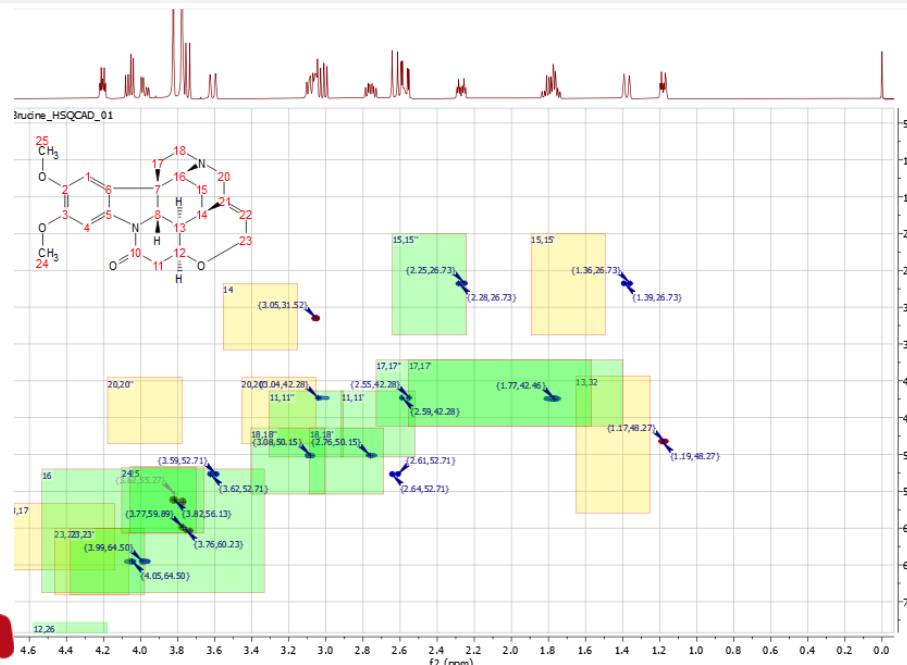
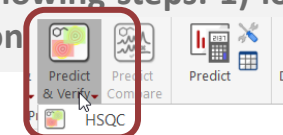


MNOVA PREDICTION OPTIONS

■ NMR PREDICTION OPTIONS: PREDICT & VERIFY



- This new feature is meant to be used with an experimental 2D NMR one-bond correlation spectrum (eg: HMQC, HSQC). (see manual 13.2.5 pp568-572). The procedure to apply a Visual Verification with Mnova is very easy, and requires the following steps: 1) load your HSQC or HMQC spectrum – 2) load the applicable structure and 3) click on the “Predict & verify/HSQC” icon

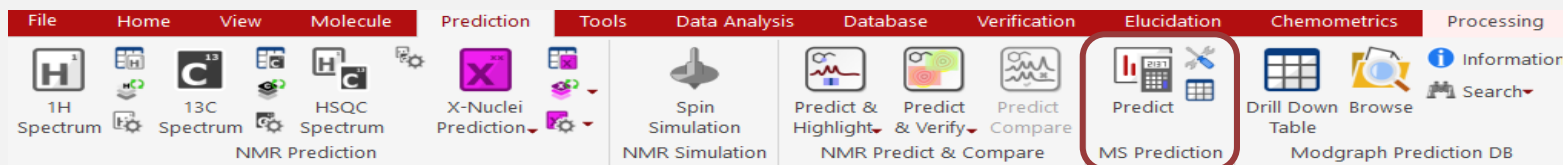


- As seen in the picture (left) green, yellow and red rectangles are produced in the analysis:
 - A green rectangle appears when the predicted value fits with the experimental one (ie the experimental value falls within a rectangular window, drawn around the simulated value, with dimensions of 0.2 ppm along the proton dimension and 2 ppm along the carbon dimension).
 - A yellow rectangle will be displayed when an experimental peak falls within a window which is between 0.2 and 0.4 ppm along the proton dimension and 2 and 4 ppm along the carbon dimension.
 - A red rectangle is displayed when no experimental peak is found within the latter rectangle, with the simulated value at its center and dimensions of 0.4 ppm along the proton dimension and 4 ppm along the carbon dimension



MNOVA MS PREDICTION

MS PREDICTION



- This new feature allows users to simulate the MS spectrum based on a selection of mass adducts or loss (see left table which can be displayed by clicking on the tool icon  This table can be modified (addition/removal of adducts/loss)

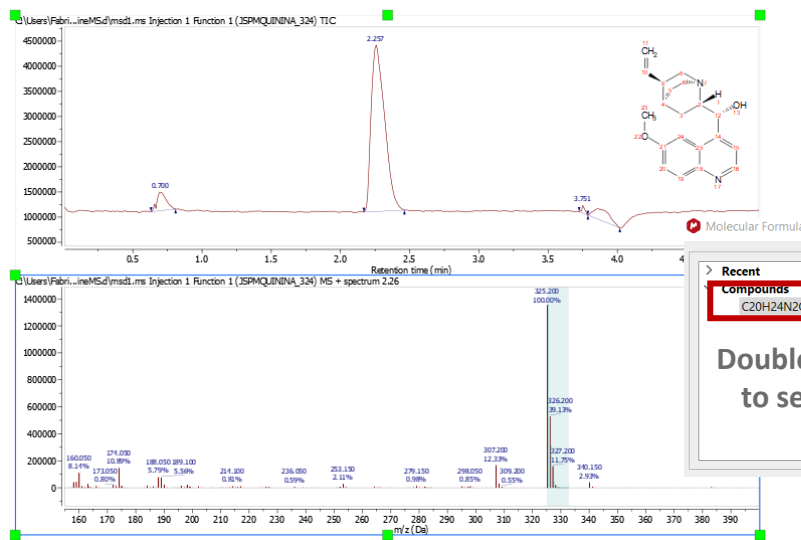
Mass Spectrum Prediction Settings

Resolution: 100.00 ppm

Adducts:

	Adduct	Loss	Charge	Mass	m/z
1	H ⁺		+1	+1.0073	+1.0073
2	Na ⁺		+1	+22.9892	+22.9892
3	K ⁺		+1	+38.9632	+38.9632
4	CH ₃ OH ⁺		+1	+33.0335	+33.0335
5	NH ₄ ⁺		+1	+18.0338	+18.0338
6		H ⁺	-1	-1.0073	-1.0073
7			-1	+34.9694	+34.9694
8		2 (H ₂ O) ⁺	-2	-38.0357	-19.0178
9			-1	+78.9189	+78.9189
10	e		-1	+0.0005	+0.0005
11		e	+1	-0.0005	-0.0005

Buttons: Reset to Default, Make Default, OK, Cancel



Recent Compounds

C₂₀H₂₄N₂O₂








Double click to select

Molecular Formula: C₂₀H₂₄N₂O₂

Formula Weight: 324.1838

Buttons: OK, Cancel, Save, Load

Mass Prediction

						
Report	Copy	Highlight	Export	Delete	Clear	Setup
	Formula	Adduct / Loss	Charge	m/z		
1	C ₂₀ H ₂₄ N ₂ O ₂	H ⁺ / —		325.19105		
2	C ₂₀ H ₂₄ N ₂ O ₂	Na ⁺ / —		347.17300		
3	C ₂₀ H ₂₄ N ₂ O ₂	K ⁺ / —		363.14694		
4	C ₂₀ H ₂₄ N ₂ O ₂	CH ₃ OH ⁺ / —		357.21727		
5	C ₂₀ H ₂₄ N ₂ O ₂	NH ₄ ⁺ / —		342.21760		
6	C ₂₀ H ₂₄ N ₂ O ₂	— / H ⁺		323.17650		
7	C ₂₀ H ₂₄ N ₂ O ₂	Cl ⁻ / —		359.15318		
8	C ₂₀ H ₂₄ N ₂ O ₂	— / 2 (H ₂ O) ⁺		143.07405		
9	C ₂₀ H ₂₄ N ₂ O ₂	Br ⁻ / —		403.10266		
10	C ₂₀ H ₂₄ N ₂ O ₂	e / —		324.18433		
11	C ₂₀ H ₂₄ N ₂ O ₂	— / e		324.18323		





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Mnova Verify

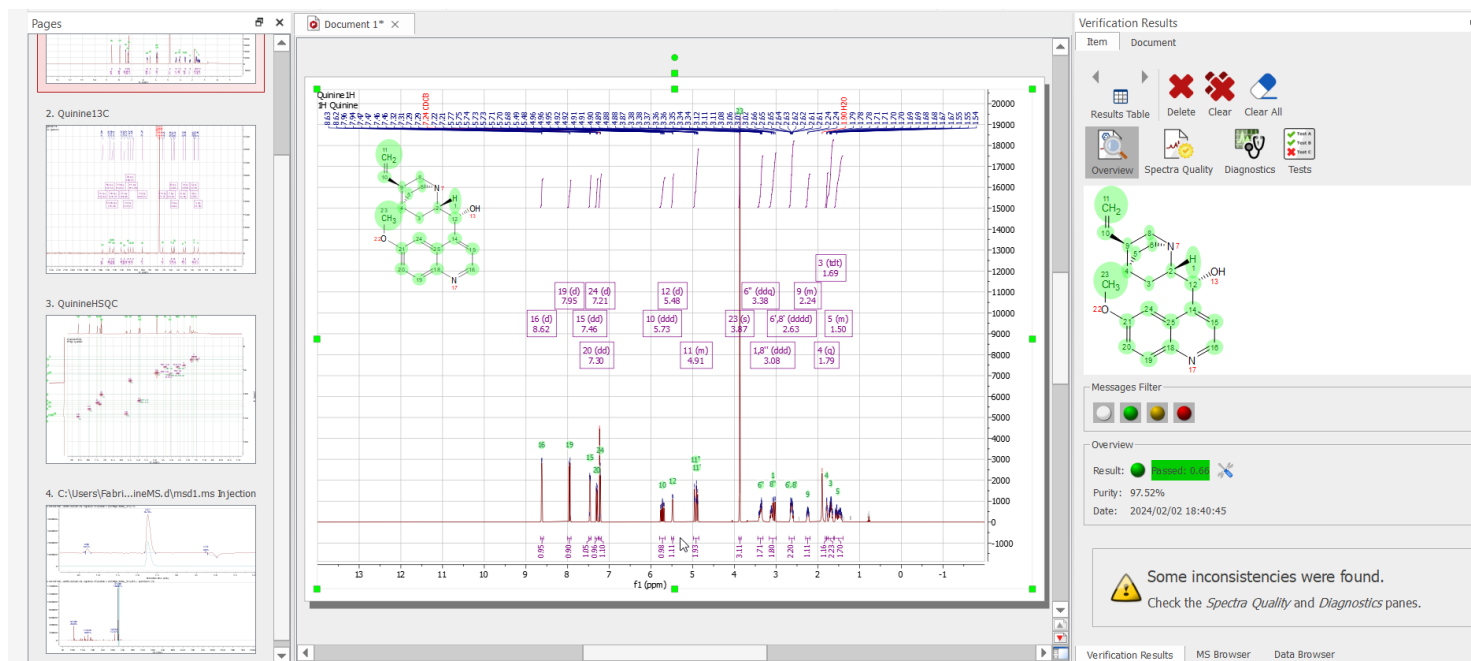


MNOVA VERIFY



INTRODUCTION

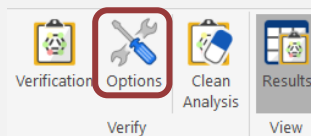
- The goal of Mnova Verify is to help users in their process of validating new structures from the analysis of spectroscopic data, namely NMR and MS data.
- Mnova Verify evaluates a series of elements (GSD, solvent recognition, multiplets and chemical shift predictions) and applies a scoring system to return a Yes/No/I don't know answer. This process may be run either in single or batch mode over large volumes of data.



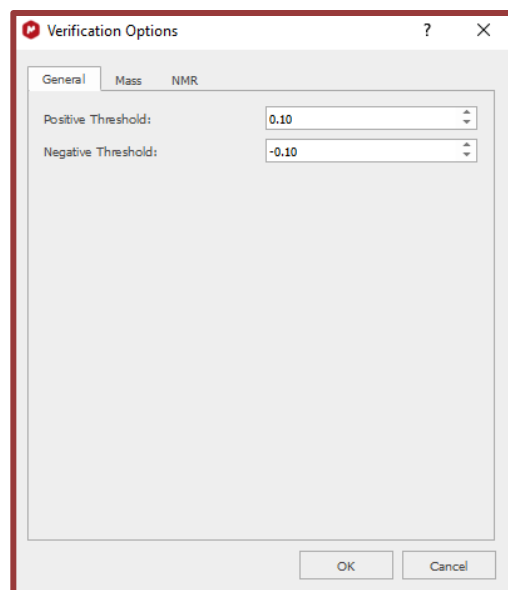
MNOVA VERIFY



MNOVA VERIFY: OPTIONS



- The options available are displayed below and relate to some General settings (the positive and negative threshold for passedg/failed a structure), some Mass Spectroscopy and NMR parameters (see manual 10, pp 474-487).



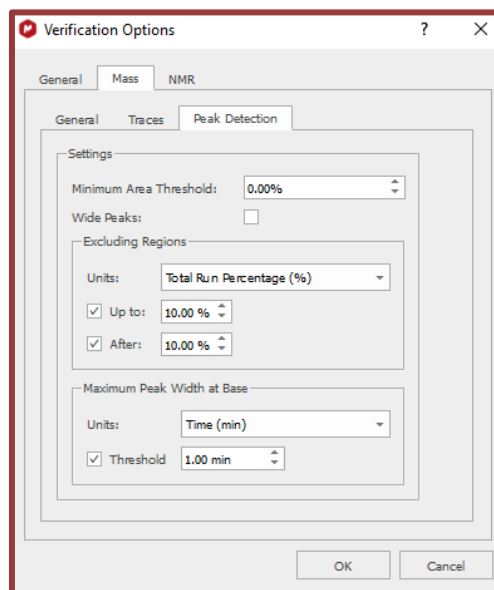
Verification Options

General Mass NMR

Positive Threshold: 0.10

Negative Threshold: -0.10

OK Cancel



Verification Options

General Mass NMR

General Traces Peak Detection

Settings

Minimum Area Threshold: 0.00%

Wide Peaks: ☐

Excluding Regions

Units: Total Run Percentage (%)

☒ Up to: 10.00 %

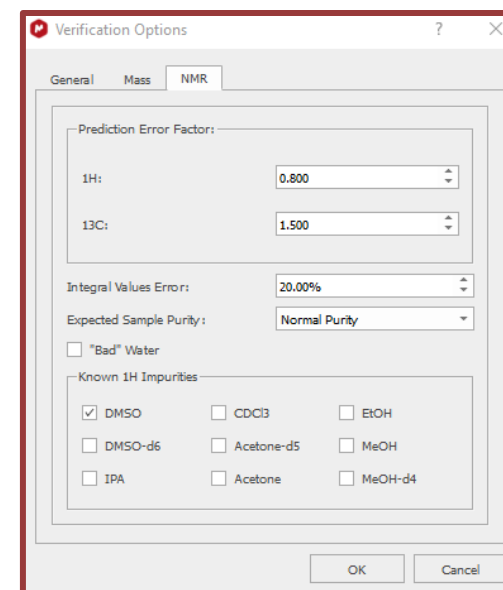
☒ After: 10.00 %

Maximum Peak Width at Base

Units: Time (min)

☒ Threshold 1.00 min

OK Cancel



Verification Options

General Mass NMR

Prediction Error Factor:

1H: 0.800

13C: 1.500

Integral Values Error: 20.00%

Expected Sample Purity: Normal Purity

☐ "Bad" Water

Known 1H Impurities

☒ DMSO ☐ CDCl3 ☐ EtOH

☐ DMSO-d6 ☐ Acetone-d5 ☐ MeOH

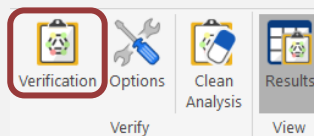
☐ IPA ☐ Acetone ☐ MeOH-d4

OK Cancel

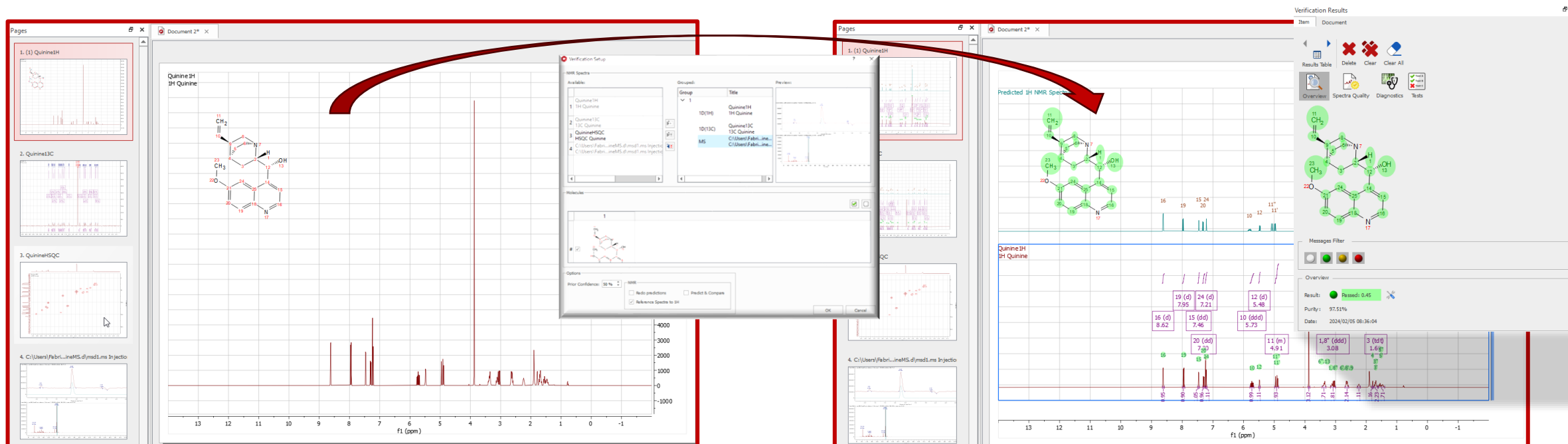


MNOVA VERIFY

MNOVA VERIFY: VERIFICATION



- The Verification Setup window allows users to 1) pick-up the experiments to be used in the Verification and 2) a couple of options (prior confidence, Predict & Compare, ...) (see manual 10.1, pp 475-480).



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— ...

QUESTION TIME!



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*thank
you*