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Mnova Training– Basics

For Mnova v16.0
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Main Topics

- Installation and Activation of Mnova
- Opening and processing 1D ^{1}H NMR
- Multiplet analysis for 1D ^{1}H NMR
- Opening and processing 1D ^{13}C NMR
- Peak picking for 1D ^{13}C NMR
- Opening and analyzing LC-MS
- Reporting and publishing results
- Visualizing IR, UV etc.
- Saving the results

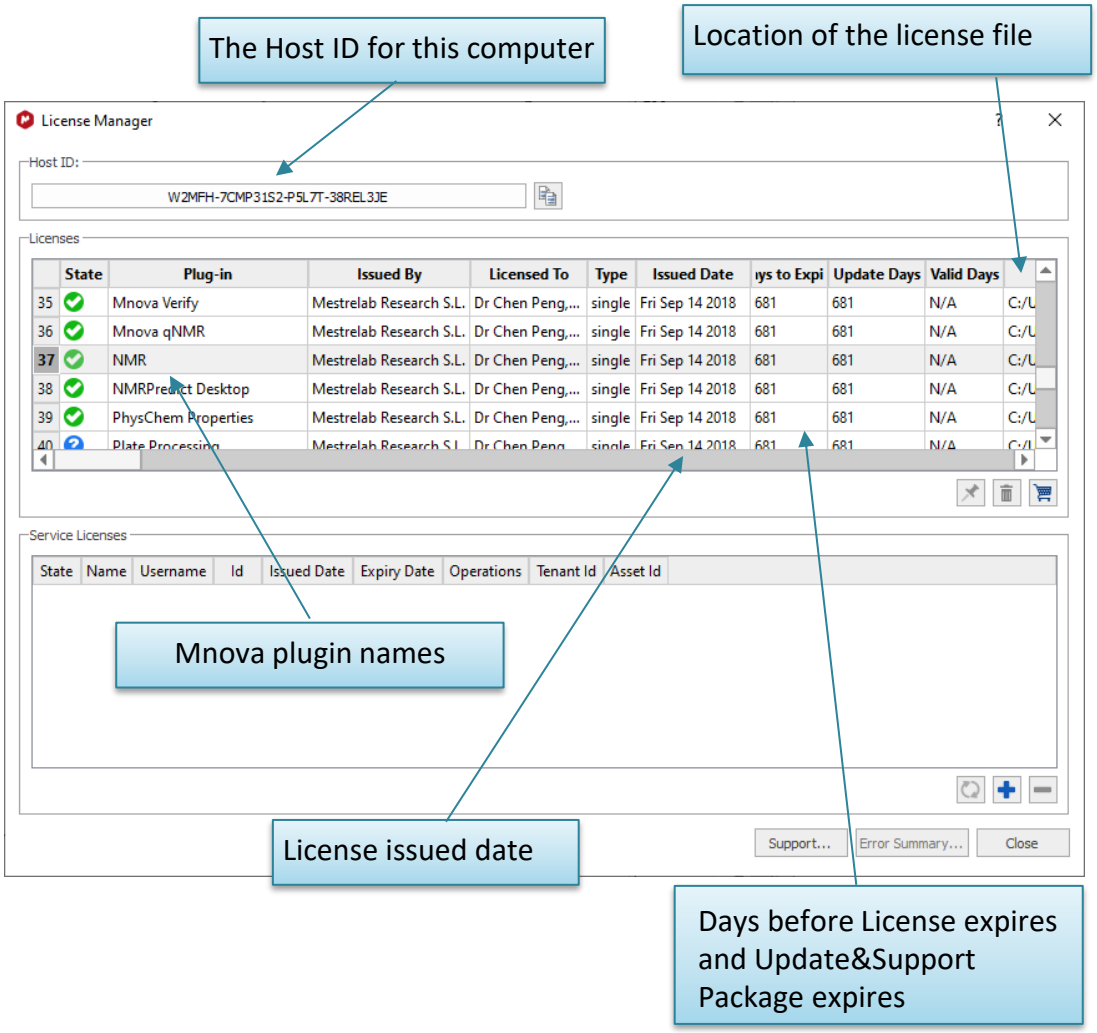
Note: This tutorial covers the NMR, NMRPredict, MSChrom & ElViS plugins of Mnova

Installation and Activation of Mnova, and General Setup*

*You will need to have Mnova Suite (NMR, NMRPredict, MSChrom, and ElViS) licenses for this tutorial.
For the Advanced tutorial, you will also need Mnova qNMR and Reaction Monitoring Licenses.

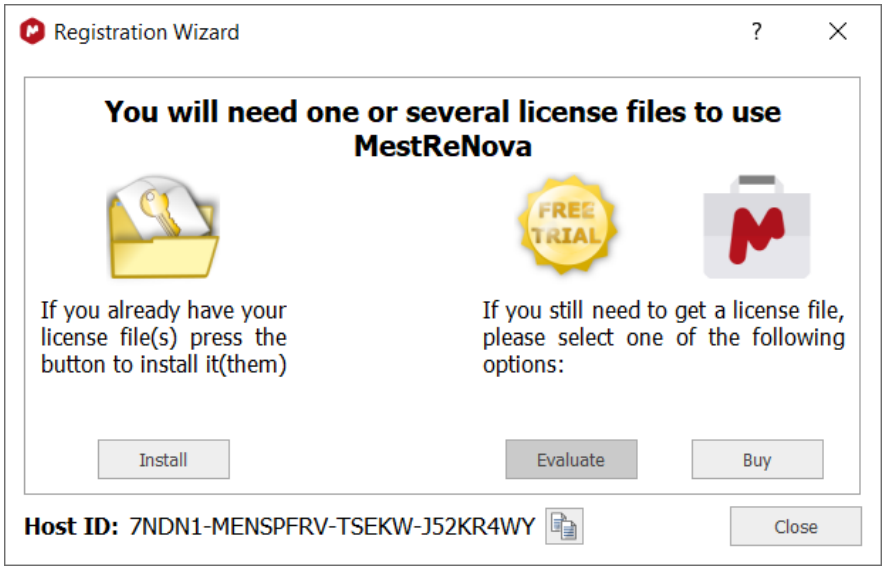
Install and activate Mnova

- Download and install Mnova from www.mestrelab.com/download.
- Choose ***File > Help > License Manager*** to open the License Manager dialog.
- It lists the status of the license activation of the plugins you've installed. You can hover the cursor on the State icon and it will display the status of that plugin.
- To activate the plugins, click the button to open the Registration Wizard (see next page)



Activate Mnova

- If you have a license file (.lic or .zip), click *Install* to open it.
- If you don't have license files, click *Evaluate* to apply for 45-day free trial licenses online; or click Buy to purchase a license.
- For managing campus/site/ concurrent licenses, click here.



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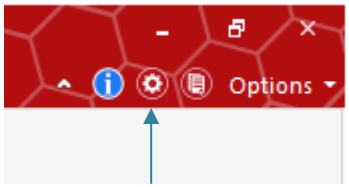
PREFERENCES

Turn on Auto Baseline Correction for 1D NMR

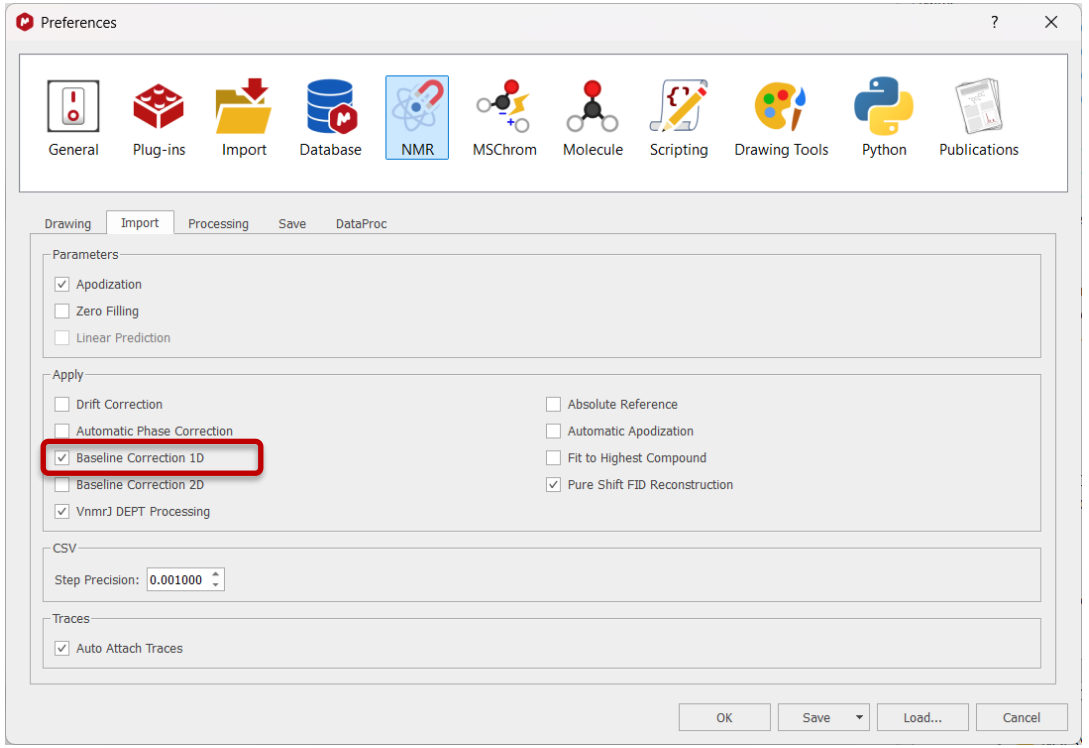
Choose File/Preferences. In the NMR> Import Tab, check Baseline Correction 1D so that baseline correction is automatically done when you open an NMR spectrum.



Shortcut for Preferences

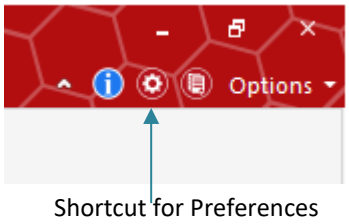
Note: Automatic Baseline Correction use the default algorithm of "Bernstein Polynomial with order of 3", or the one that you used previously. Be aware of the default baseline algorithm it uses.
We don't recommend to check the Baseline Correction for 2D NMR because it may make manual phasing of 2D NMR sluggish. You can apply baseline correction manually after the phase has been corrected.

Tip: There are many other options and settings that you can change in the Preferences Dialog.



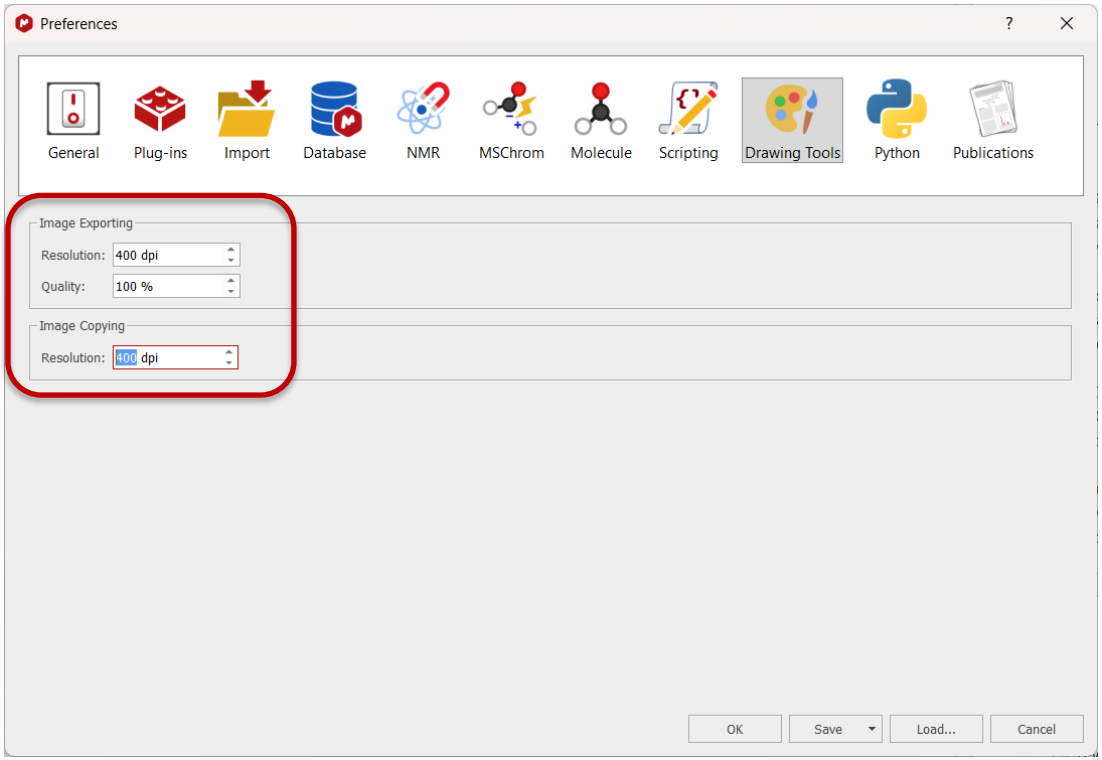
Setup the resolution for publishing spectra

Choose File/Preferences. In the Drawing Tools tab, change the resolutions for Image Exporting and Image Copying to numbers similar to something shown below.



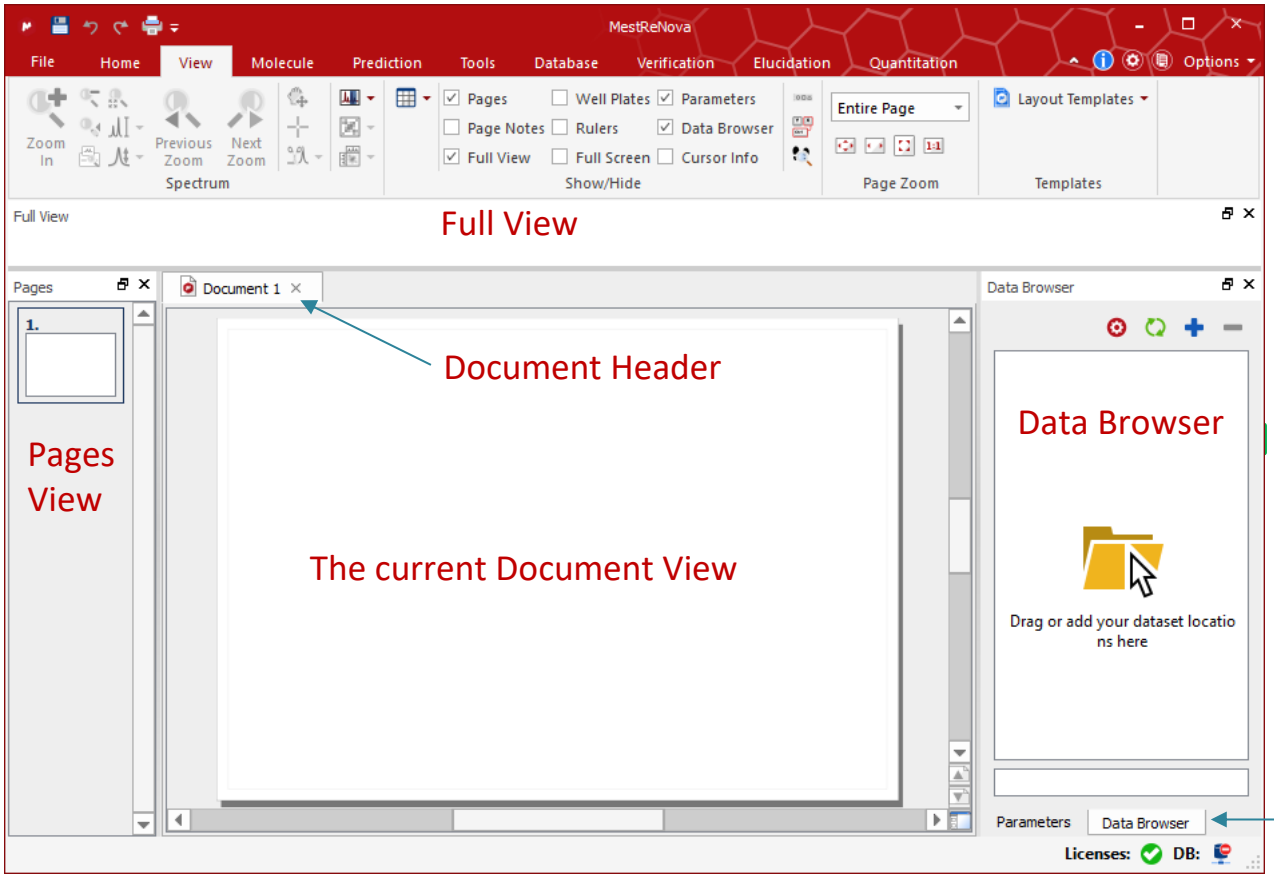
The resolution for Image Exporting is used when you choose File > Save As and save the selected objects in Mnova as a graphical image file.

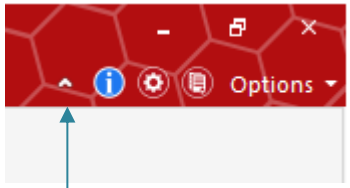
The resolution for Image Copying is used when you copy selected objects in Mnova and paste them to another application.



Setup the Workspace

- In the View Ribbon, check the Pages, Full View, Parameters, and Data Browser Views
- Dock and arrange them as shown below



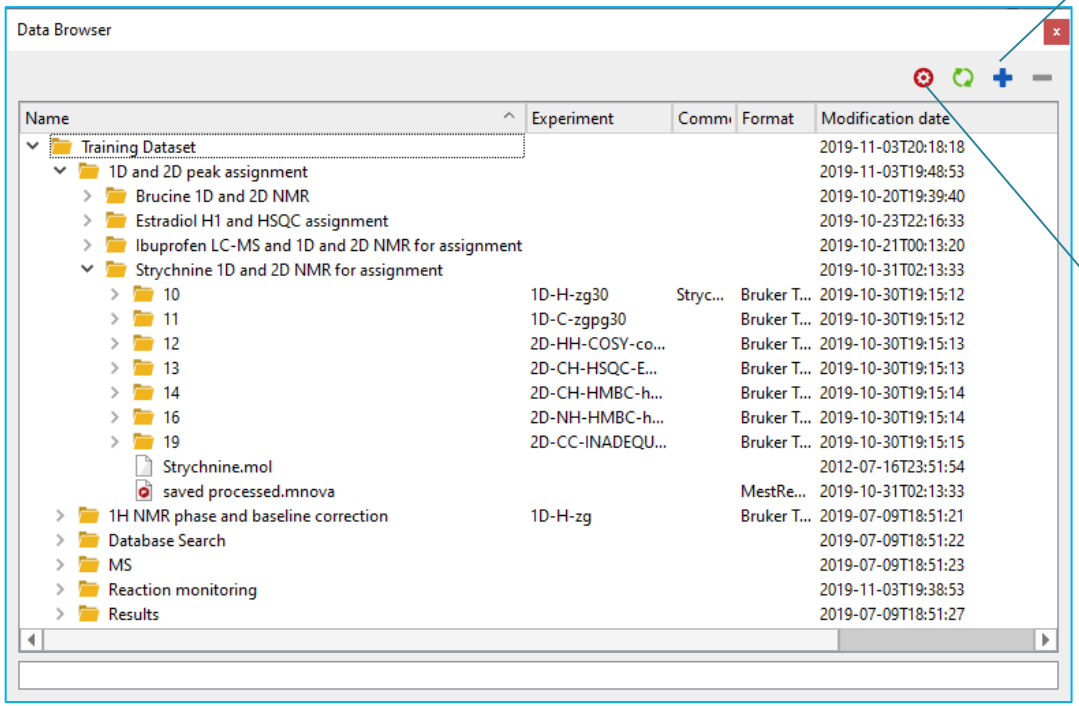


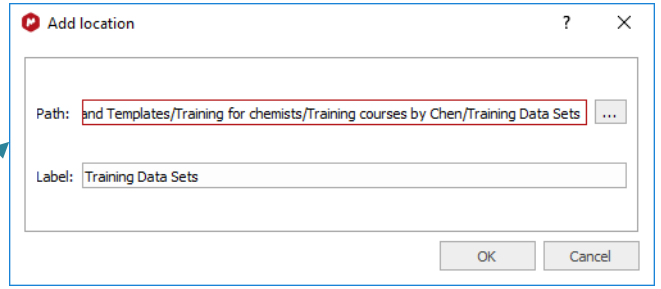
Click here to minimize the ribbon if needed

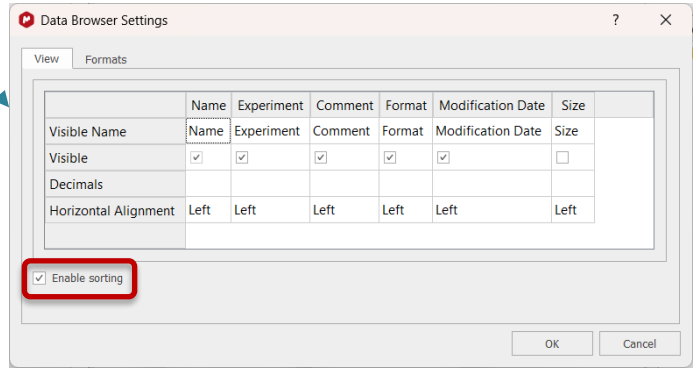
Click here to switch to a panel or table docked together

Setup Data Browser

- Click "+" in the Data Browser, navigate to the directory where the sample NMR data are located and click OK to add it.
- Click the Settings button to turn on the display of the meta data, date and time, and enable sorting
- Make sure you see the data files similar to those shown below

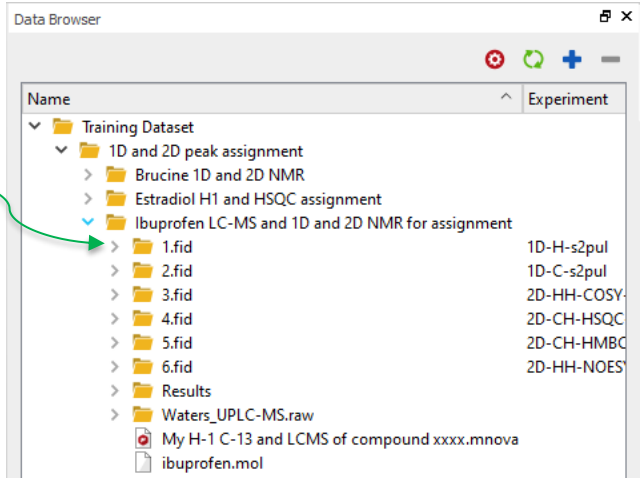






1D ^{1}H NMR Spectrum Processing, Analysis, and Reporting

Sample data



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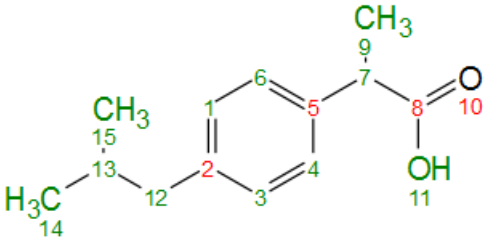
PROCEDURE

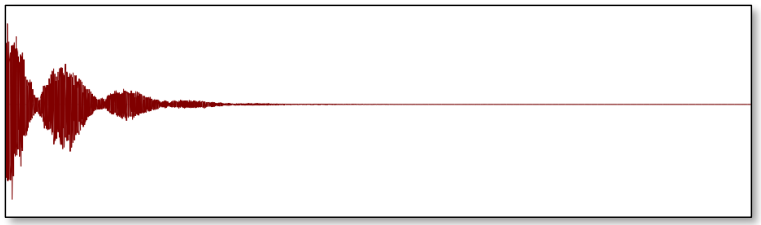
^{1}H processing and analysis: general procedure

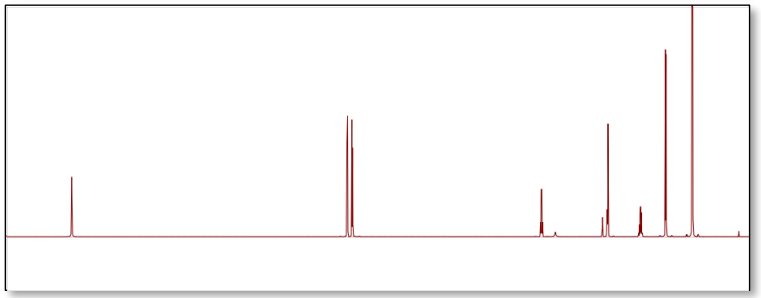
- Open the raw data
- Pre-process the FID: drift correct, apodize, zero fill, linear predict, etc.
- Fourier transform
- Phase correct and baseline correct
- Chemical shift reference
- Peak-pick, integrate, multiplet analysis
- Structure verification and peak assignment
- Report and publish

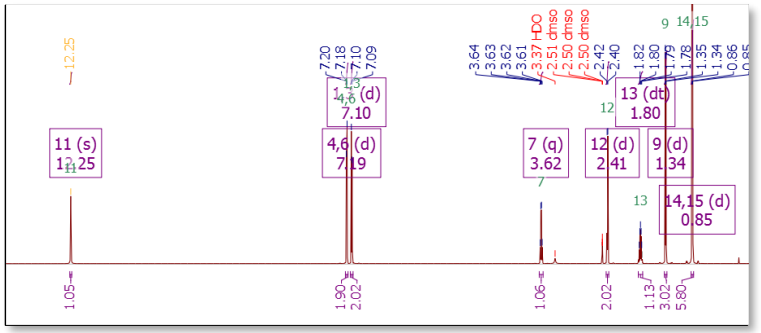


^{1}H NMR (600 MHz, DMSO-d_6) δ 12.25 (s, 1H), 7.19 (d, J = 7.8 Hz, 2H), 7.10 (d, J = 7.9 Hz, 2H), 3.62 (q, J = 7.1 Hz, 1H), 2.41 (d, J = 7.2 Hz, 2H), 1.80 (dt, J = 13.5, 6.8 Hz, 1H), 1.34 (d, J = 7.1 Hz, 3H), 0.85 (d, J = 6.7 Hz, 6H).

Note: Most of these steps are done automatically by Mnova. However, you retain full control at all times

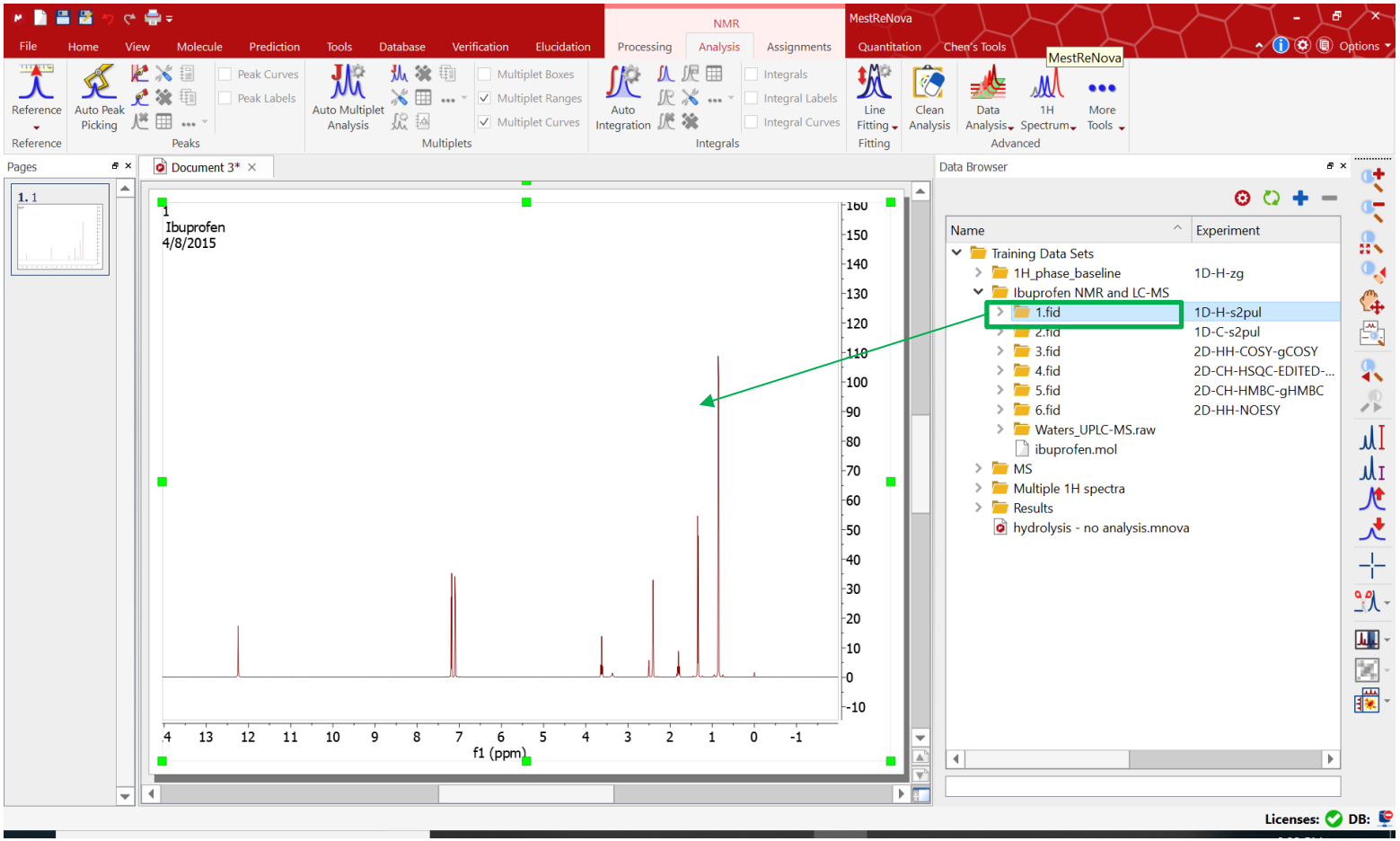






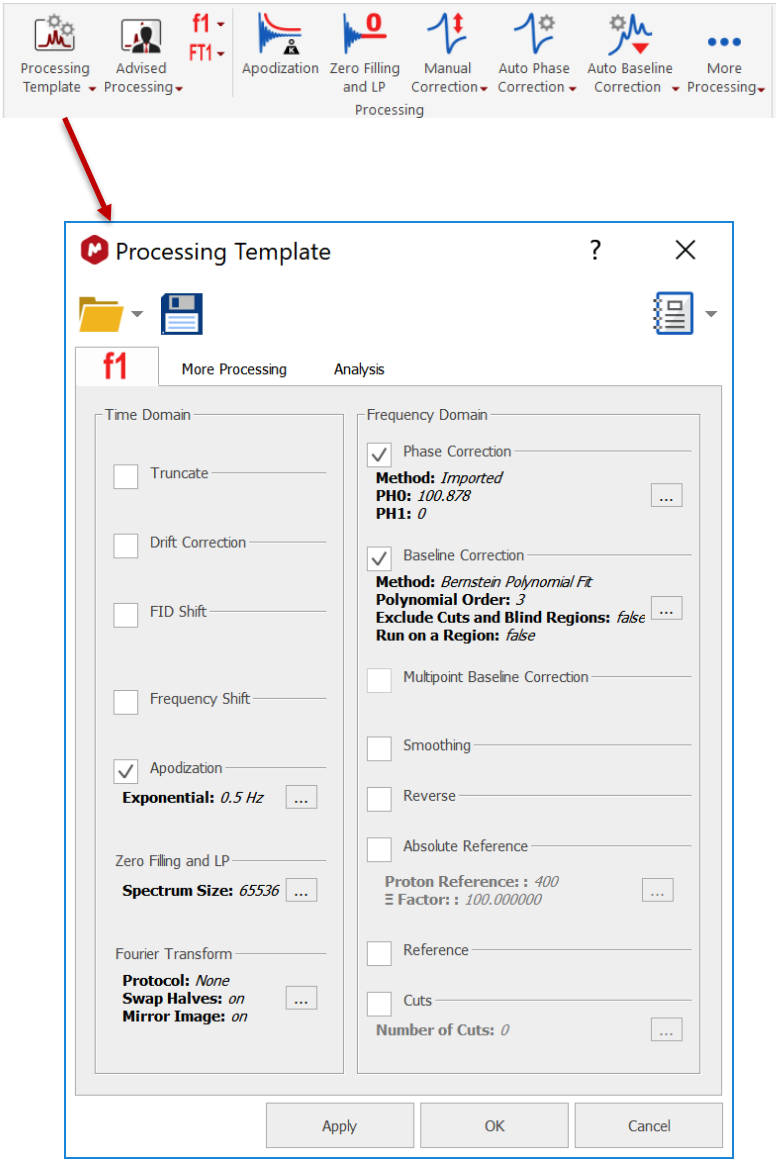
Open a H-1 spectrum

- In Data Browser, expand the folders Training Datasets > Ibuprofen NMR and LC-MS, and drag the “1.fid” folder (1D H-1 spectrum) to the main window.
- Notice the H-1 spectrum is automatically processed and displayed.



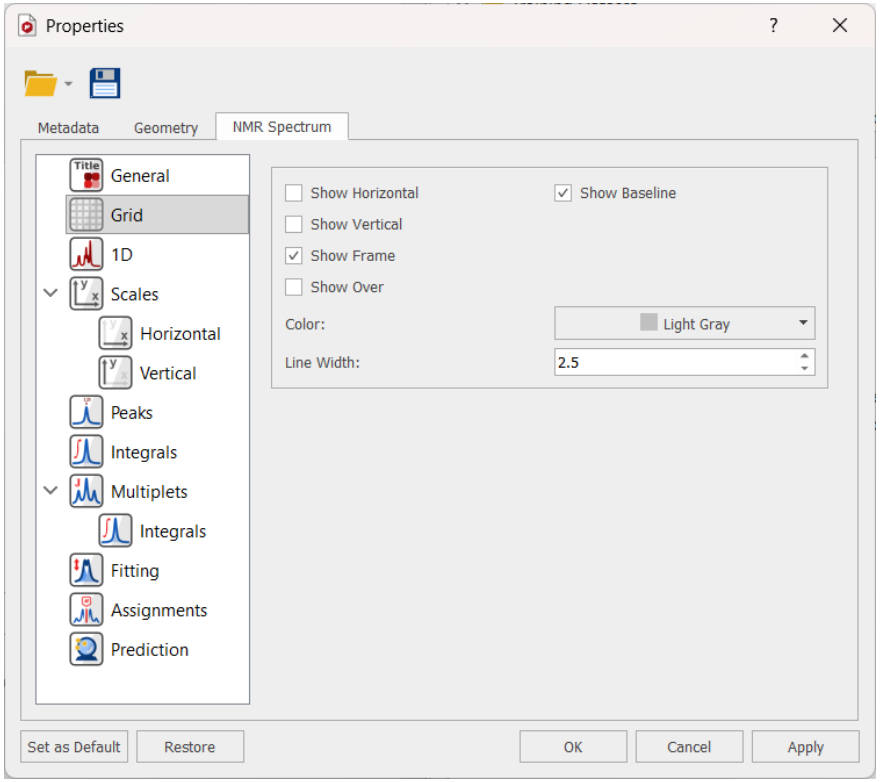
Verify the processing parameters

- In most cases, Mnova processes the spectrum automatically using the parameters from the instrument. The spectrum should be well-processed if the original processing parameters were well set. The Processing Tab is for you to re-process the spectrum when needed.
- Choose Processing > Processing Template to verify the processing parameters. Make sure they look the same as displayed on the right.
- Click OK or Apply to re-process the spectrum.



Change the Display Properties

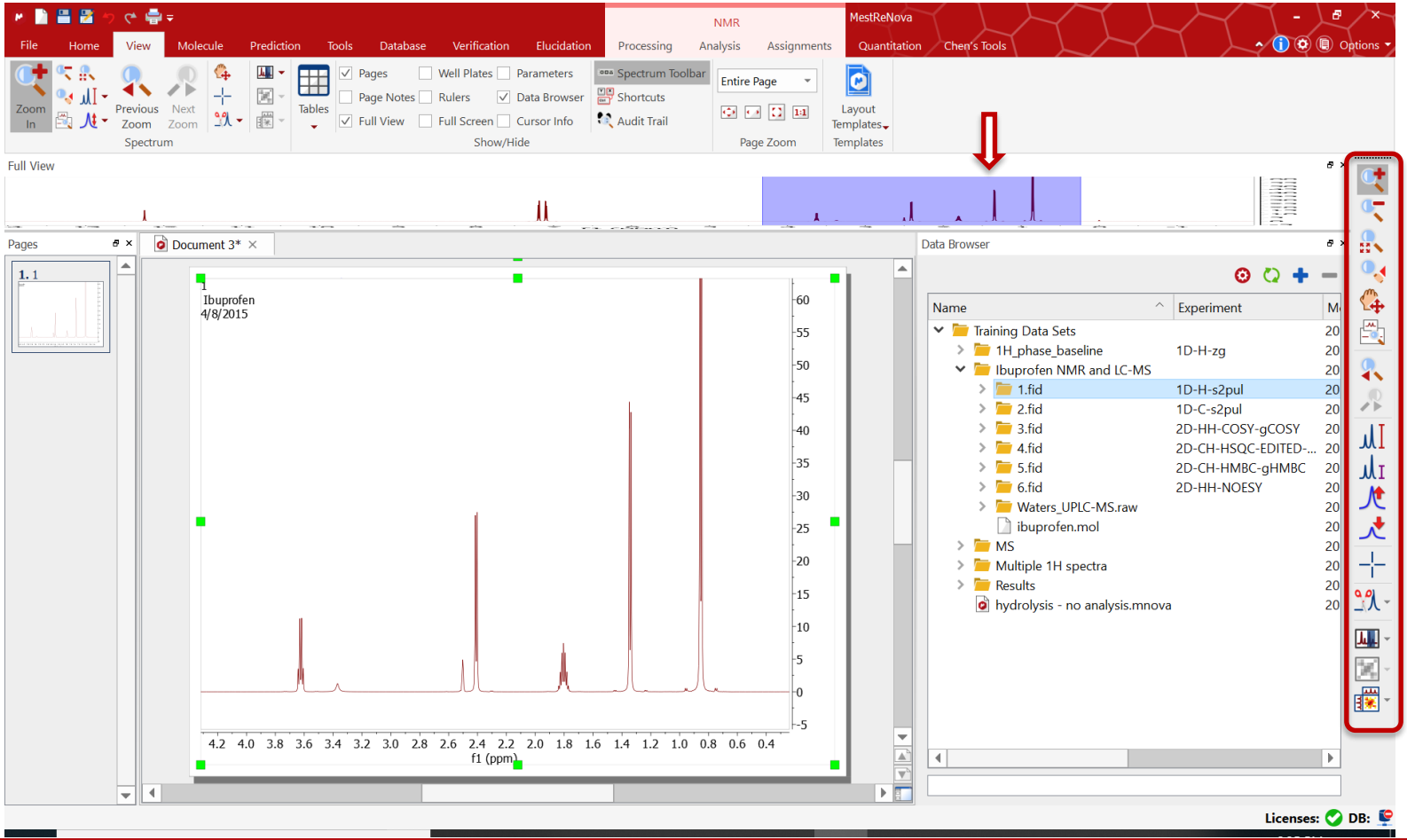
- Right click* on the spectrum and choose Properties to open the Properties Dialog, view the properties that can be changed.
- In the Grid Category, uncheck Show Horizontal, and Show Vertical, check Show Baseline
- Click Apply, and then Set as Default to apply the settings to 1D spectra opened in the future



**Starting from Version 14, double-clicking changes the display to full-spectrum if you are in the default pointer mode.*

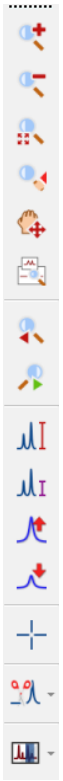
Navigate in the H-1 Spectrum

- Use the Spectrum Toolbar to zoom in/out, pan, and change the Y scale (see next slide for details)
- Use the Full View to move to different zoom in area (click or drag)

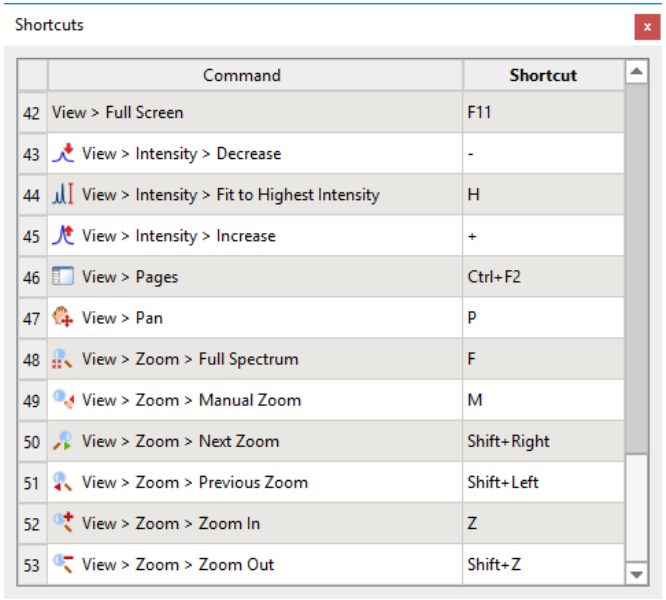


Spectrum visualization tools

- The Spectrum Toolbar is visible only after you open a spectrum.
- Learn some short-cut keys by choosing View > Shortcuts



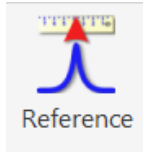
Zoom in/Zoom out (or press Z) *
Zoom out**
Full spectrum (or press F)
Manual Zoom in to defined ppm range
Pan spectrum (or press P) ***
Expansion – click&drag to draw an inset (or press E)
Previous Zoom level
Next Zoom level
Fit to Highest Intensity (or press H)
Fit to highest compound peak
Increase 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



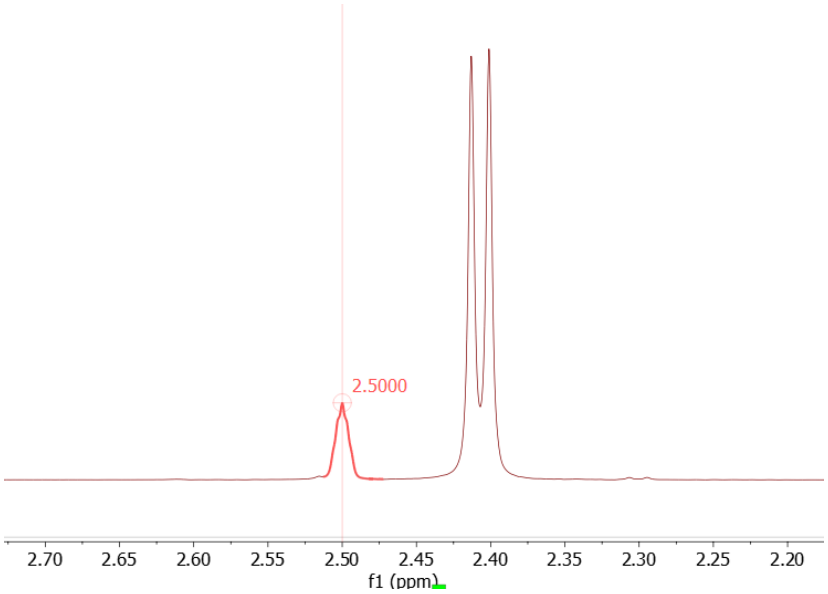
	Command	Shortcut
42	View > Full Screen	F11
43	View > Intensity > Decrease	-
44	View > Intensity > Fit to Highest Intensity	H
45	View > Intensity > Increase	+
46	View > Pages	Ctrl+F2
47	View > Pan	P
48	View > Zoom > Full Spectrum	F
49	View > Zoom > Manual Zoom	M
50	View > Zoom > Next Zoom	Shift+Right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

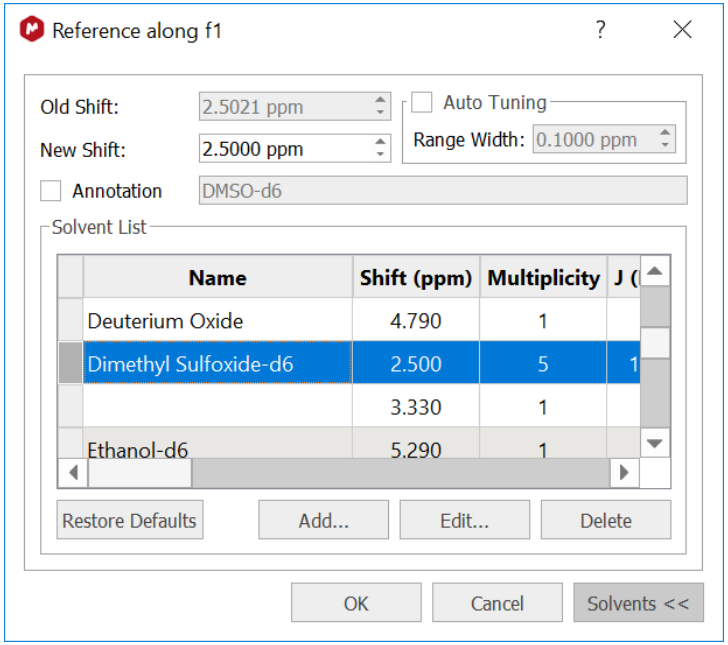
** Press **Z** several times to toggle between horizontal/vertical/box zoom*
*** Press **P** several times to toggle between free/horizontal/vertical panning*

Chemical Shift Referencing



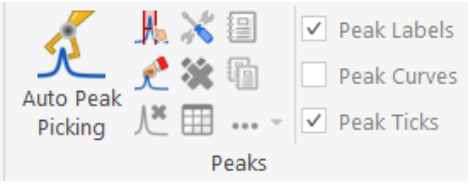
- This spectrum uses DMSO-d6 as the solvent. We can reference the chemical shifts by setting its middle peak to 2.5 ppm.
- Zoom to the DMSO peak at around 2.5 ppm. Choose Analysis > Reference, and click on the top of the middle peak.
- Set it to 2.5 ppm either manually or from the Solvent List.

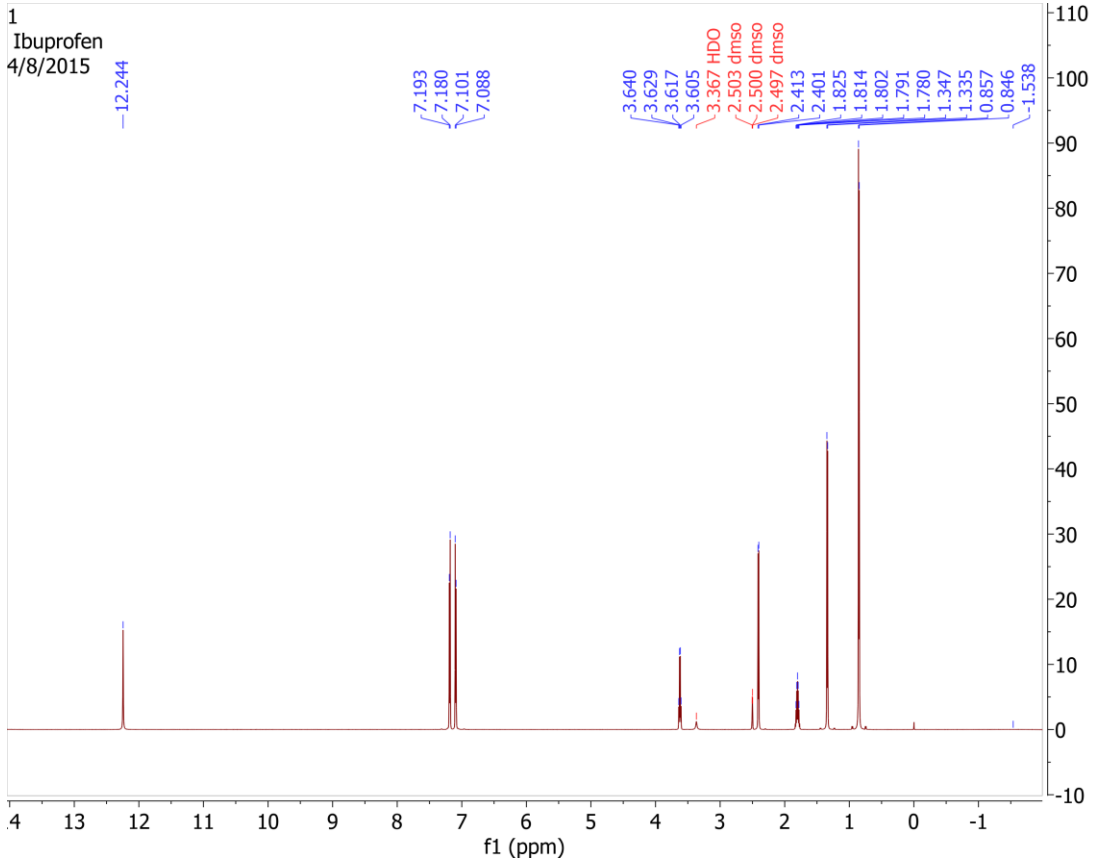


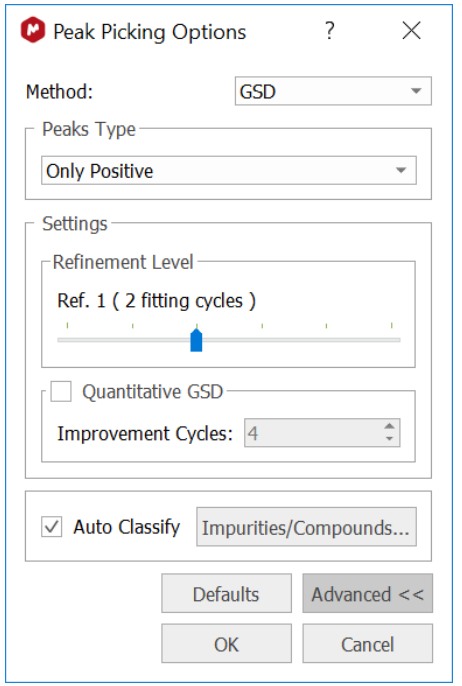


Peak picking

- Click the Peaks > Options  to verify the peak picking options. Default settings are used here as shown to the right.
- Click the Auto Peak Picking tool to pick all the peaks
- Using other peak picking tools to display/delete/add/change peaks as needed.

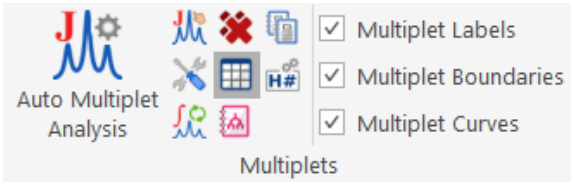


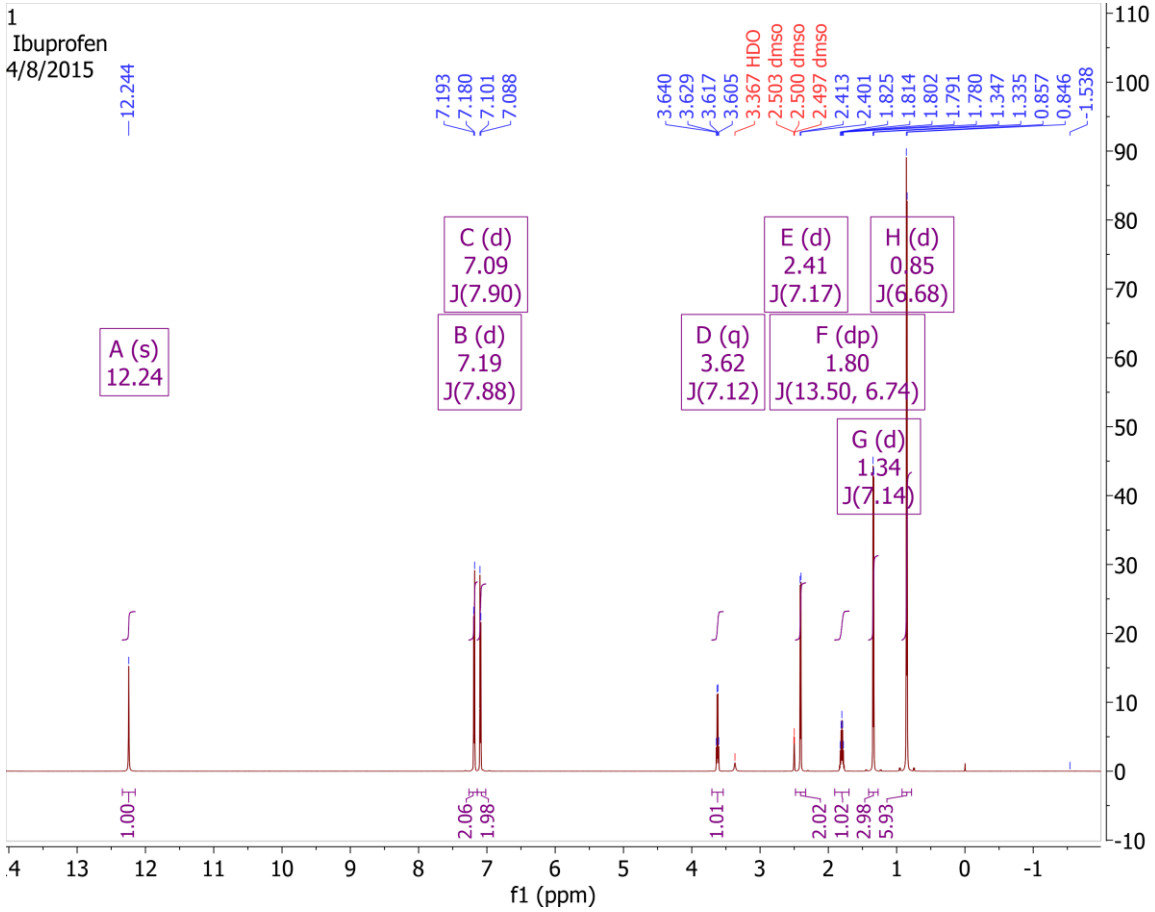


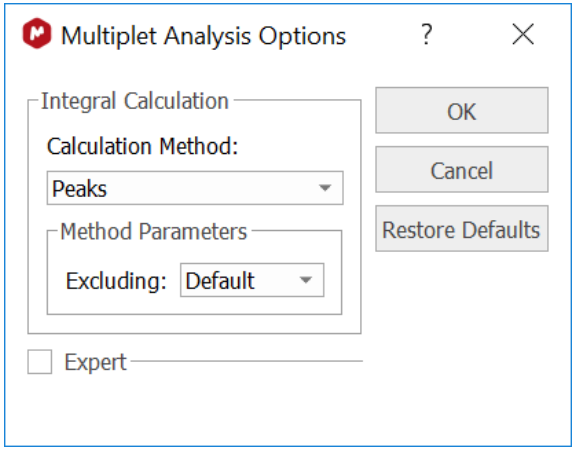


Multiplet analysis

- Click the Multiplets > Options  to verify the multiplet analysis options. Default settings are used here as shown to the right.
- Click the Auto Multiplet Analysis tool to do the multiplet analysis based on the picked peaks

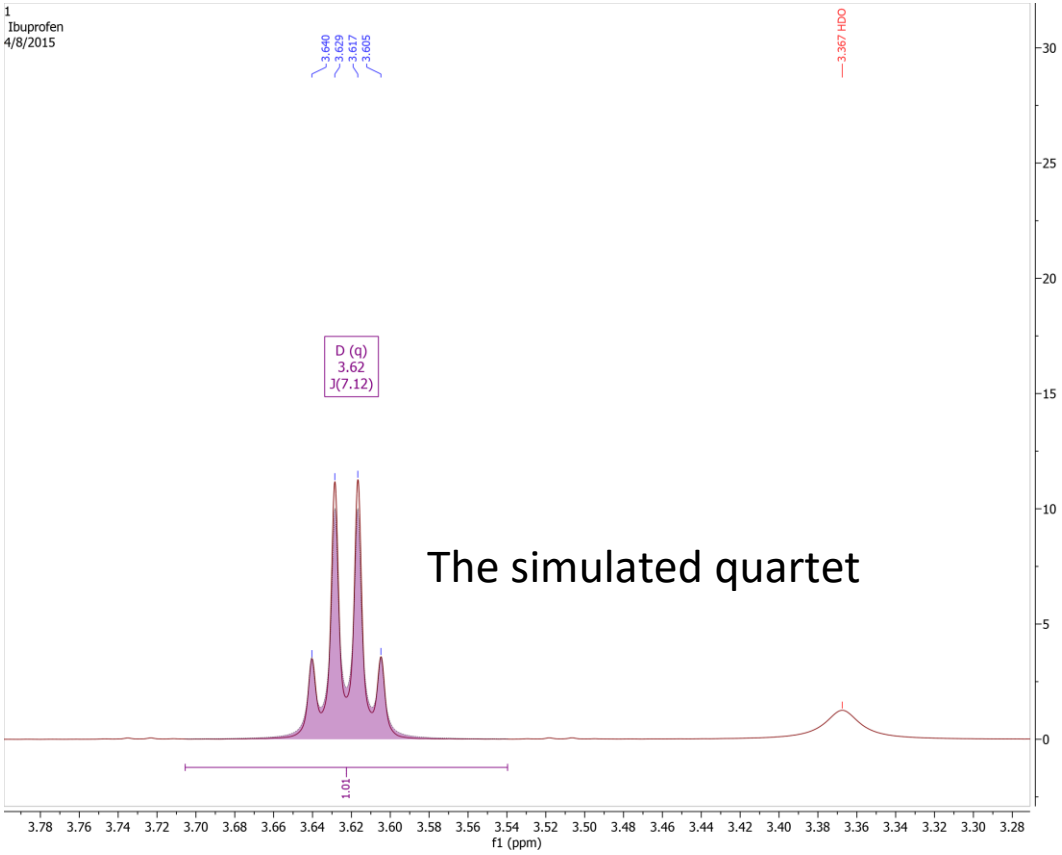


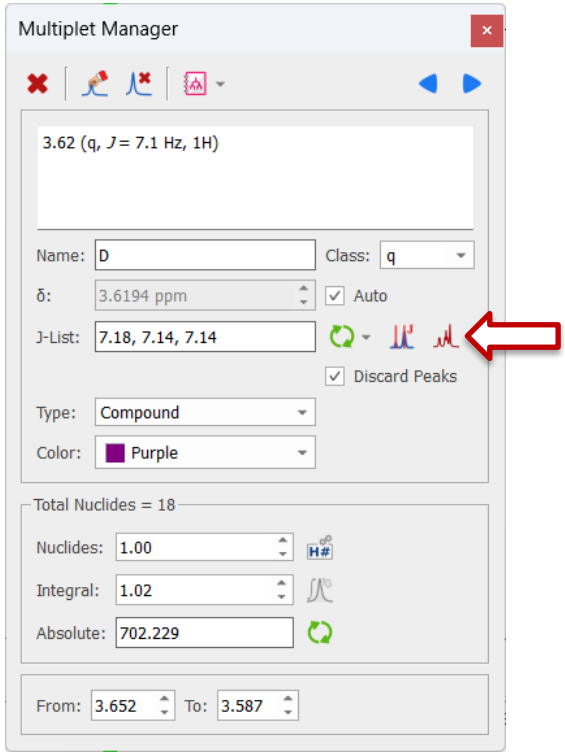




Multiplet Manager

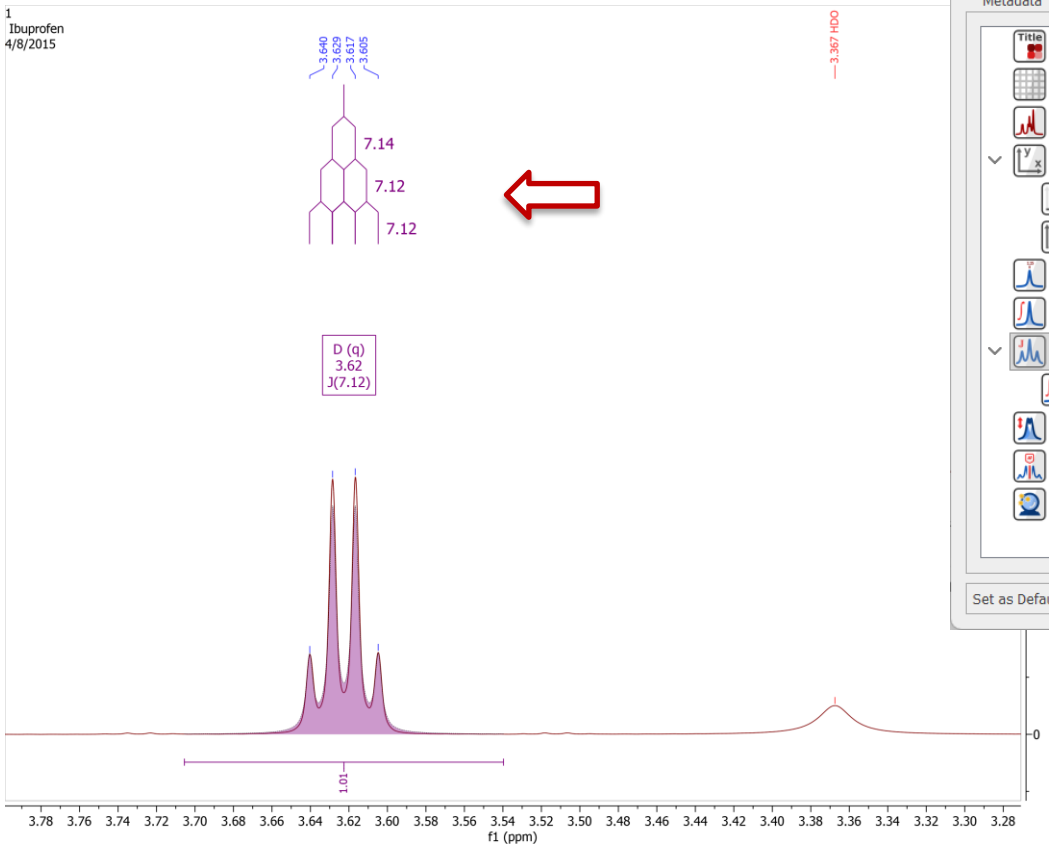
- Double click on a multiplet label to open the Multiplet Manager.
- Use the tools there to verify and change multiplet analysis results if needed.

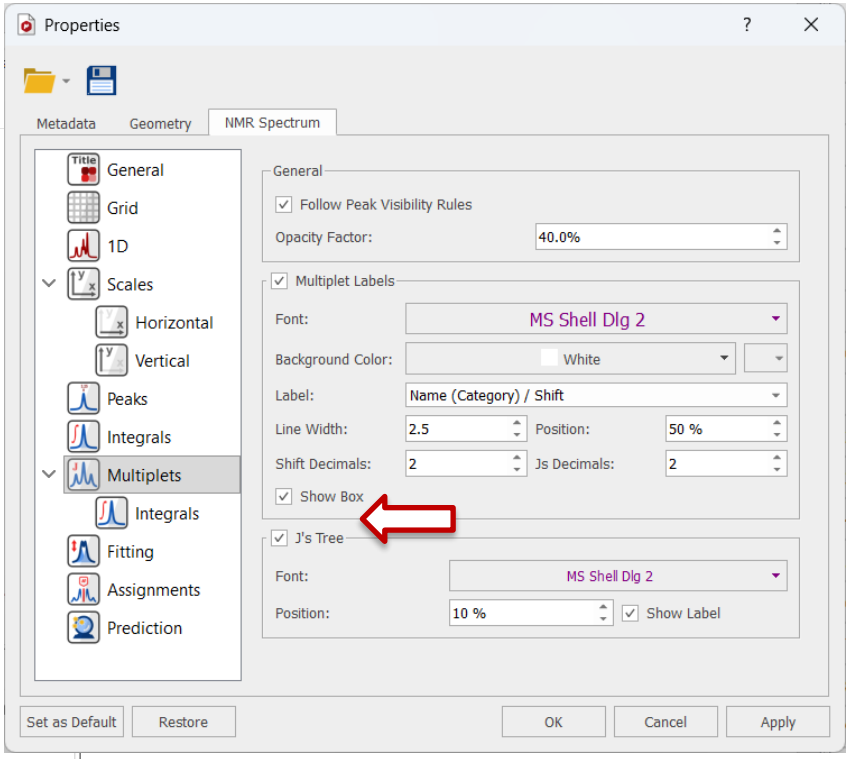




Multiplet Manager

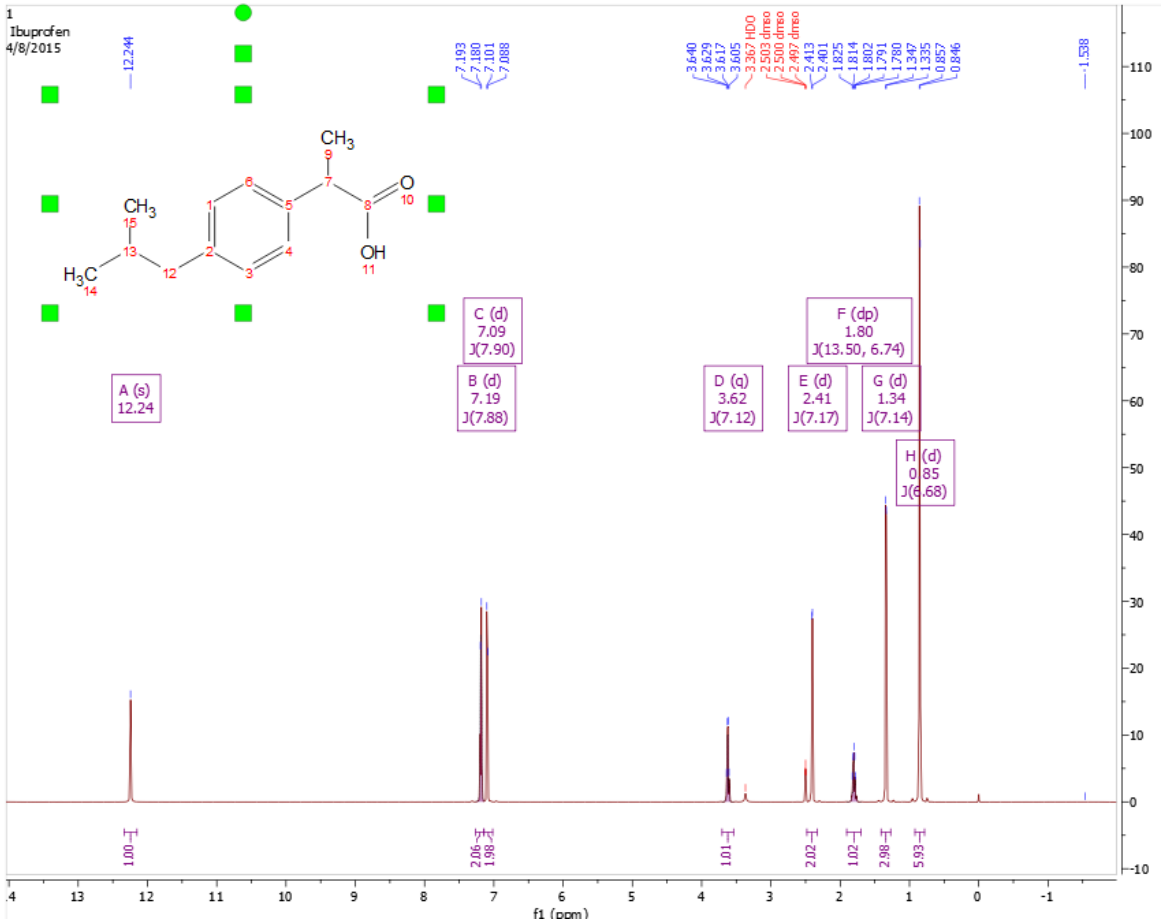
- Double click on the spectrum to open the Properties dialog.
- Choose Multiplets, and check J's Tree to display the J-coupling tree for visual verification of the multiplet analysis results.

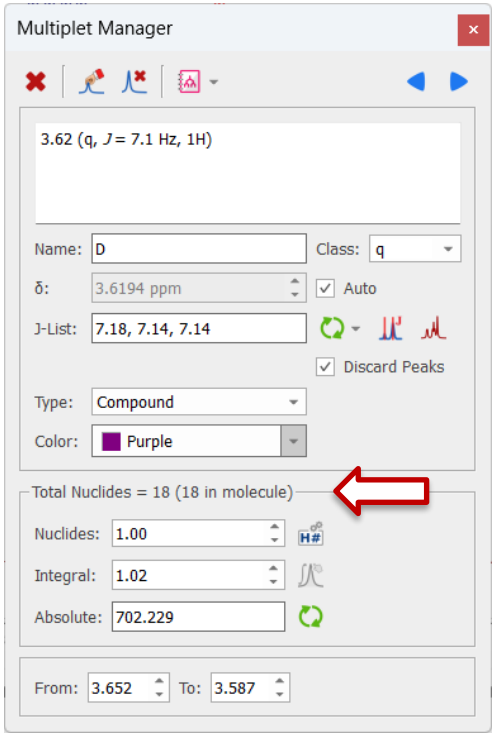




Verify the number of Hs

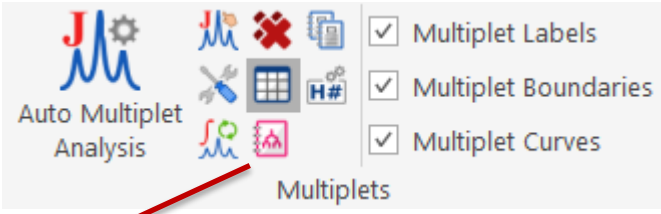
- Open the Ibuprofen.mol file from the Data Browser.
- Note the number of protons from multiplet analysis vs. that from the structure

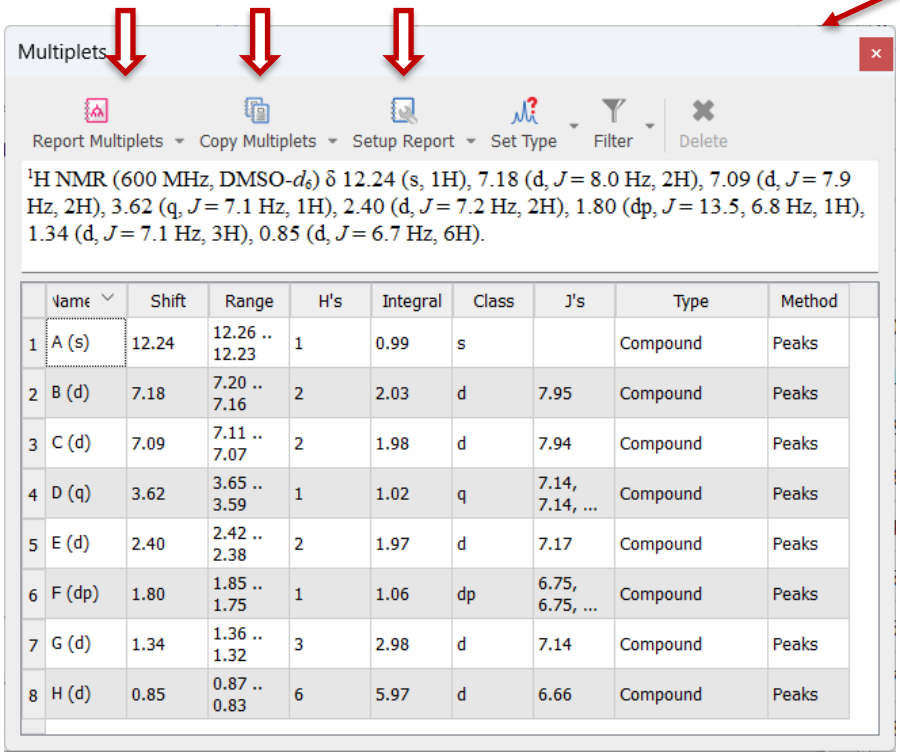




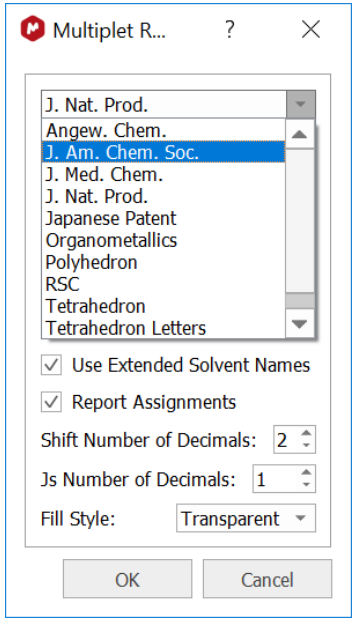
Report the multiplets

- Use the Multiplet Table tool to display the Multiplets Table.
- Click Setup Report to change the reporting format
- Click Report to report the multiplets texts





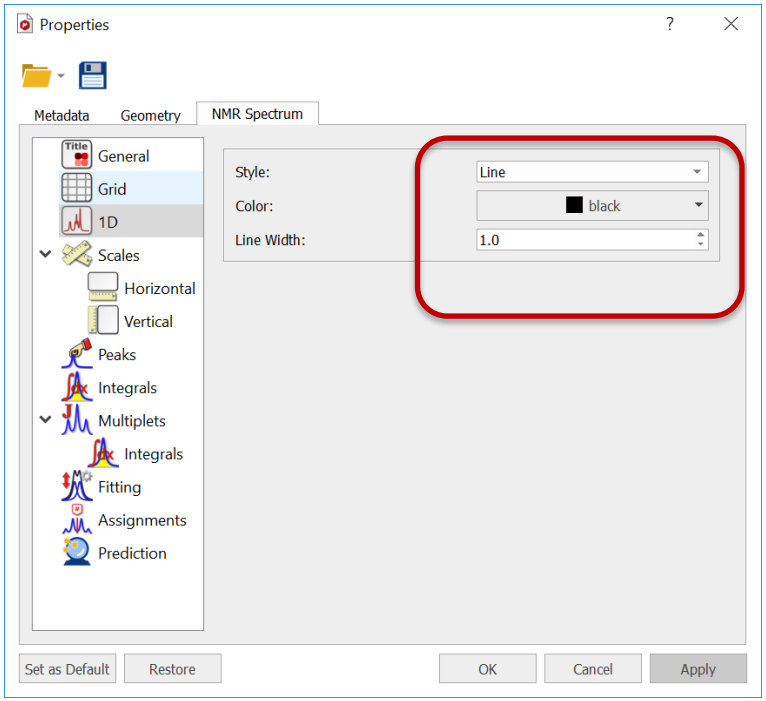
	Name	Shift	Range	H's	Integral	Class	J's	Type	Method
1	A (s)	12.24	12.26 .. 12.23	1	0.99	s		Compound	Peaks
2	B (d)	7.18	7.20 .. 7.16	2	2.03	d	7.95	Compound	Peaks
3	C (d)	7.09	7.11 .. 7.07	2	1.98	d	7.94	Compound	Peaks
4	D (q)	3.62	3.65 .. 3.59	1	1.02	q	7.14, 7.14, ...	Compound	Peaks
5	E (d)	2.40	2.42 .. 2.38	2	1.97	d	7.17	Compound	Peaks
6	F (dp)	1.80	1.85 .. 1.75	1	1.06	dp	6.75, 6.75, ...	Compound	Peaks
7	G (d)	1.34	1.36 .. 1.32	3	2.98	d	7.14	Compound	Peaks
8	H (d)	0.85	0.87 .. 0.83	6	5.97	d	6.66	Compound	Peaks



¹H NMR (DMSO-d_6, 600 MHz) δ 12.24 (1H, s), 7.19 (2H, d, J=7.9 Hz), 7.09 (2H, d, J=7.9 Hz), 3.62 (1H, q, J=7.1 Hz), 2.41 (2H, d, J=7.2 Hz), 1.80 (1H, dp, J=13.5, 6.7 Hz), 1.34 (3H, d, J=7.1 Hz), 0.85 (6H, d, J=6.7 Hz)

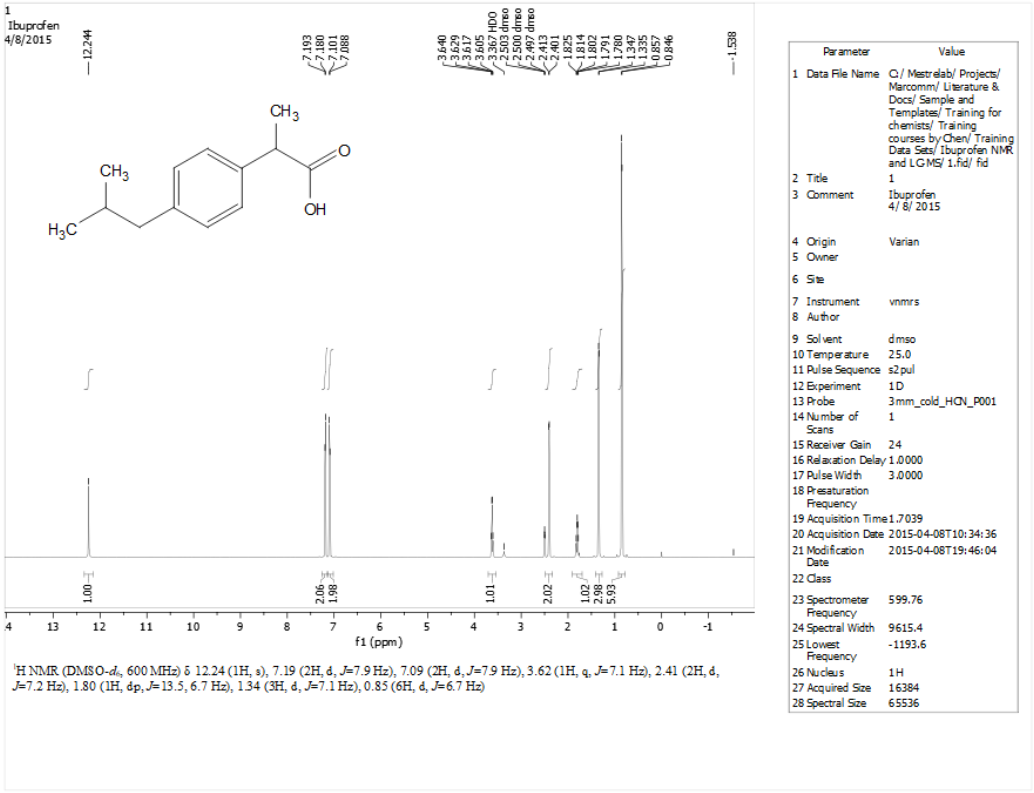
Publishing a spectrum

- To publish the spectrum on a black and white journal, double click the spectrum to open the Properties Dialog, and set the 1D properties to as shown on the right.
- Choose other properties to display, such as the peak labels, multiplet labels, integrals, etc.
- Copy the spectrum and structure objects and paste them to other documents, such as MicroSoft Word or PPT.



Display the parameters

- Check View > Parameters Table to display the Parameters Table, and report the parameters on the spectrum. Manually resize the text box to similar to as shown below.
- Report the multiplets and resize the box to as shown below.



	Parameter	Value
1	Data File Name	C:/ Mestrelab/ Projects/ Marcomm/ Literature & Docs/ Sample and Templates/ Training for chemists/ Training courses by Chen/ Training Data Sets/ Ibuprofen NMR and LCMS/ 1.fid/ fid
2	Title	1
3	Comment	Ibuprofen 4/ 8/ 2015
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	vnmrs
8	Author	
9	Solvent	dmso
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	3mm_cold_HCN_P001
14	Number of Scans	1
15	Receiver Gain	24
16	Relaxation Delay	1.0000
17	Pulse Width	3.0000
18	Presaturation Frequency	
19	Acquisition Time	1.7039
20	Acquisition Date	2015-04-08T10:34:36
21	Modification Date	2015-04-08T19:46:04
22	Class	
23	Spectrometer Frequency	599.76
24	Spectral Width	9615.4
25	Lowest Frequency	-1193.6
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	65536

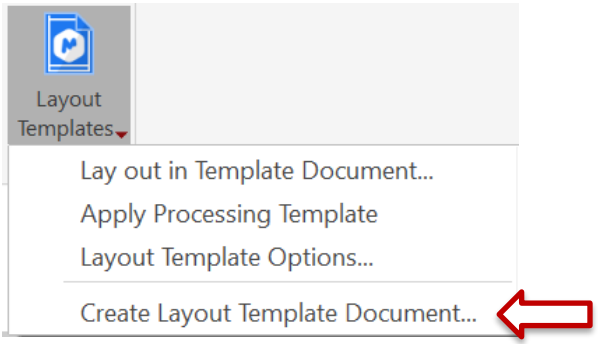
Parameters

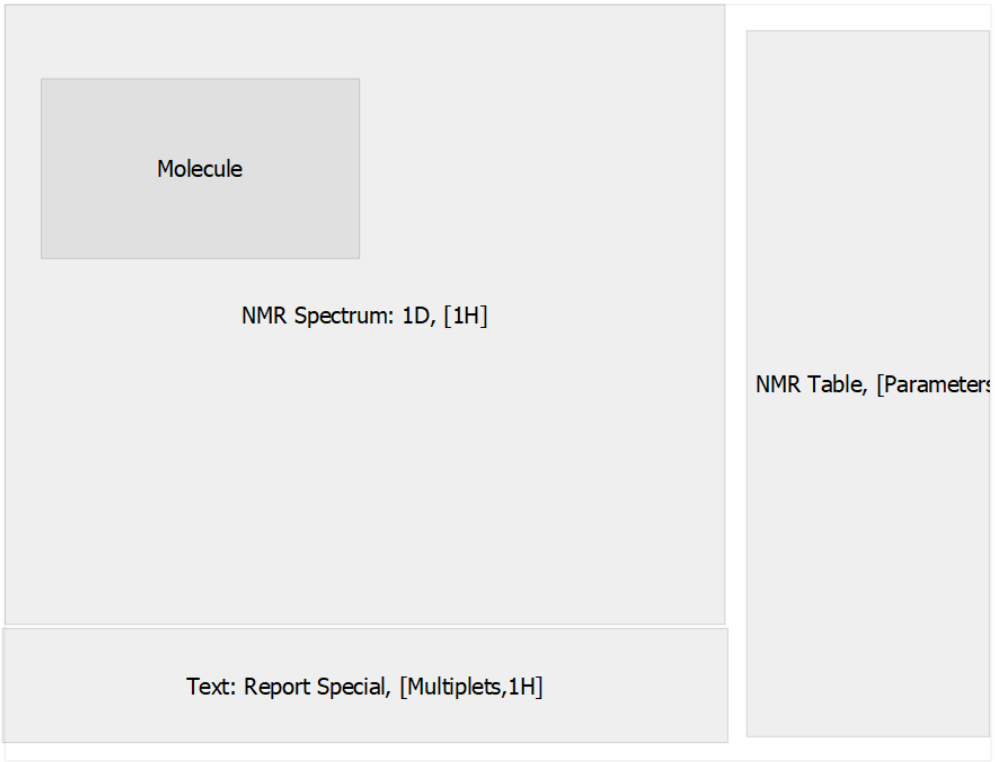
Report Copy Setup Customize

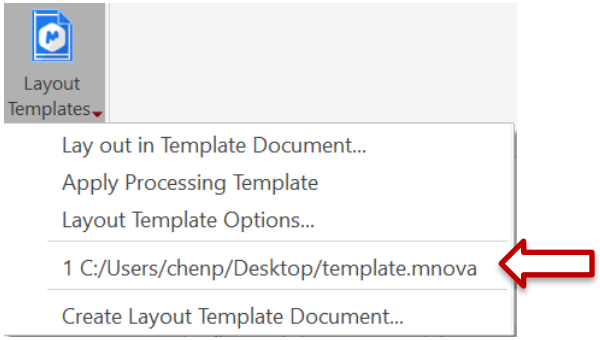
	Parameter	Value
1	Data File Name	C:/Mestrelab/Projects/Marcomm/Liter...
2	Title	1
3	Comment	Ibuprofen 4/8/2015
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	vnmrs
8	Author	
9	Solvent	dmso
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	3mm_cold_HCN_P001
14	Number of Scans	1
15	Receiver Gain	24
16	Relaxation Delay	1.0000
17	Pulse Width	3.0000

Create a layout template

- Click on View > Layout Template and choose Create Layout Template to save a layout template. You can edit it.
- Choose File > New and open the H-1 spectrum again, and choose View > Layout Template > [*Saved Template Name*] to apply it.



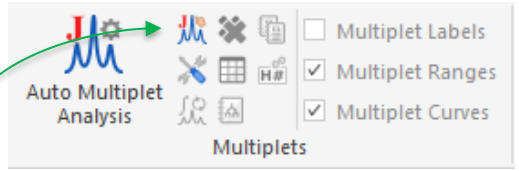


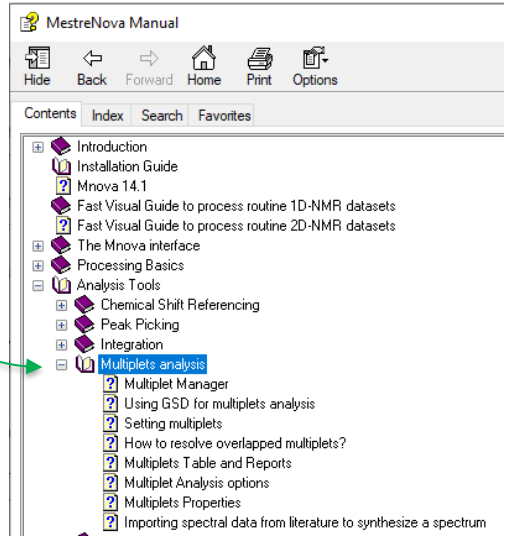


Tip: Mnova uses all pages in the document to create the layout template. So if you have multiple pages, make sure you delete the unwanted ones before creating the layout template.

More about H-1 processing

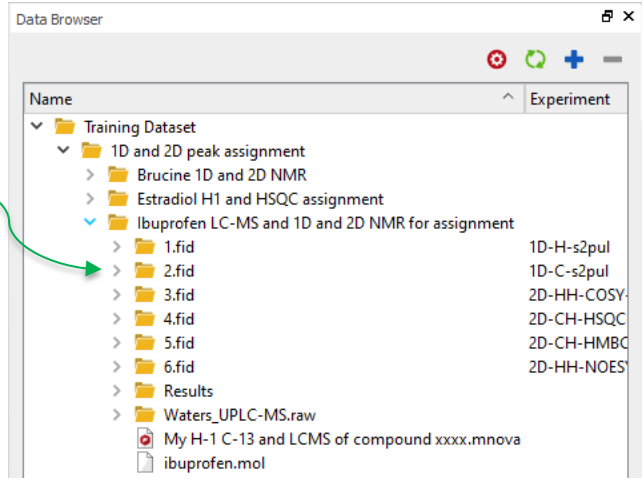
- There are several other 1D H-1 NMR spectra in the tutorial datasets that you can use for practice.
- When the spectrum is more crowded and has more artefacts or impurity peaks, you can also use the manual multiplet analysis tools to have more control.
- There are many other ways to correct the multiplet analysis results, such as splitting and assigning individual lines to different mulitplets. See File > Help > Contents > Analysis Tools > Multiplet analysis for more details.
- If you start the auto multiplet analysis without any peaks, it will do a peak picking automatically
- Integration is always done automatically during multiplet analysis. If you do manual integration before multiplet analysis, the integration regions will be used for multiplet analysis, and the integration values will be retained as the integrals of the resulting multiplets.





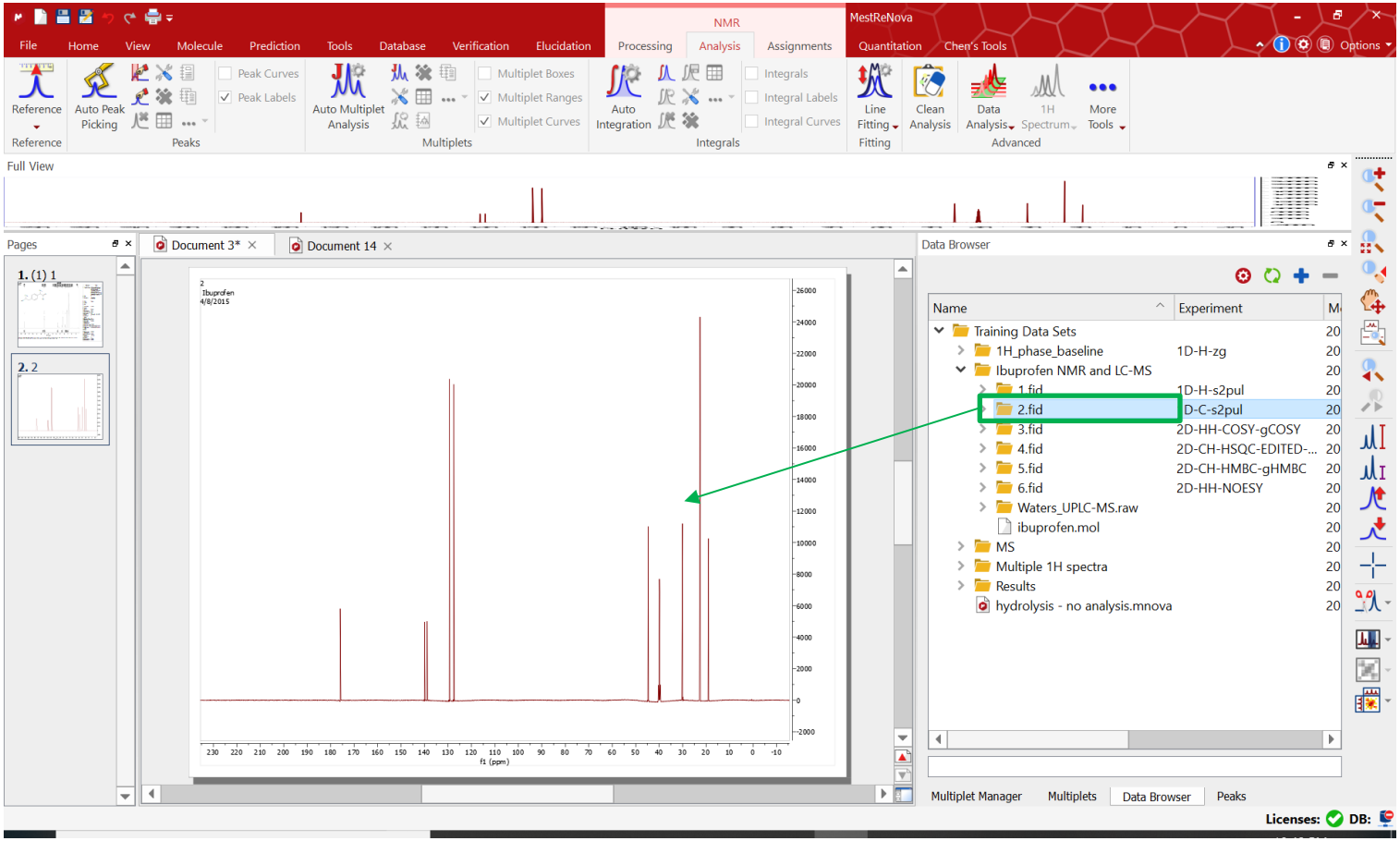
1D ^{13}C NMR Spectrum Processing, Analysis, and Reporting

Sample data



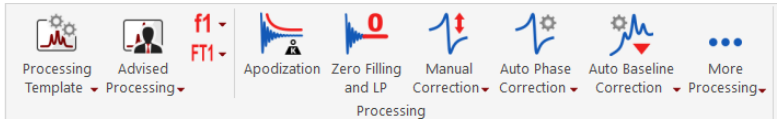
Open a C-13 spectrum

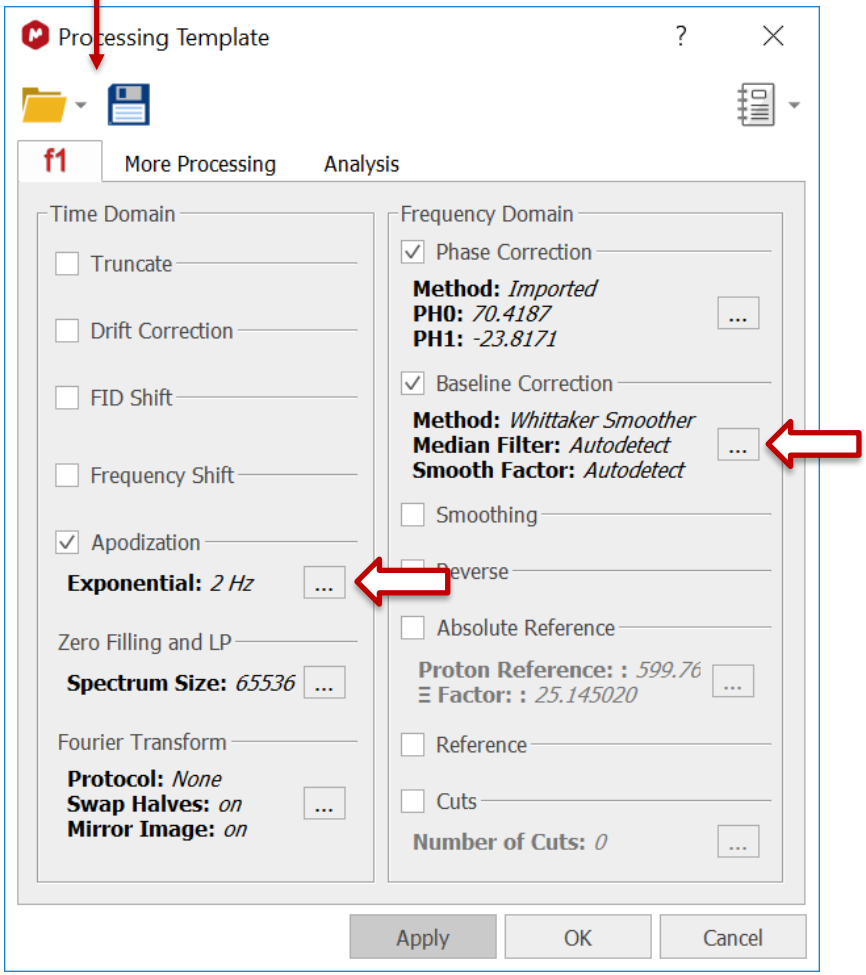
➢ In Data Browser, open the C-13 spectrum of Ibuprofen by dragging the “2.fid” folder to the main area.

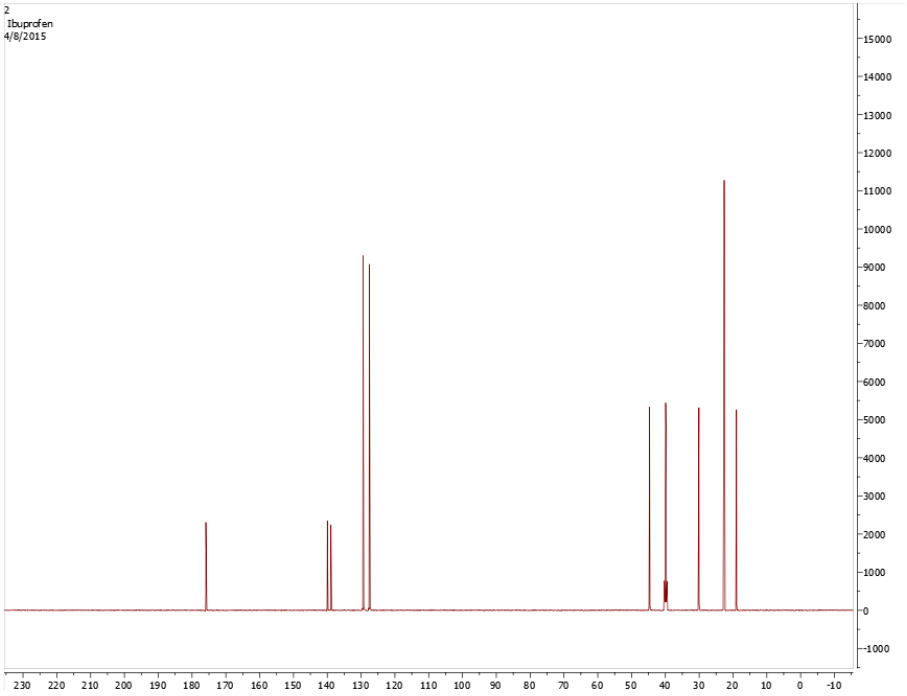


Verify the processing parameters

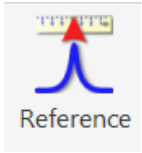
- Choose Processing > Processing Template, and set the parameters similar to the ones shown to the right.
- Click OK or Apply to re-process the spectrum.



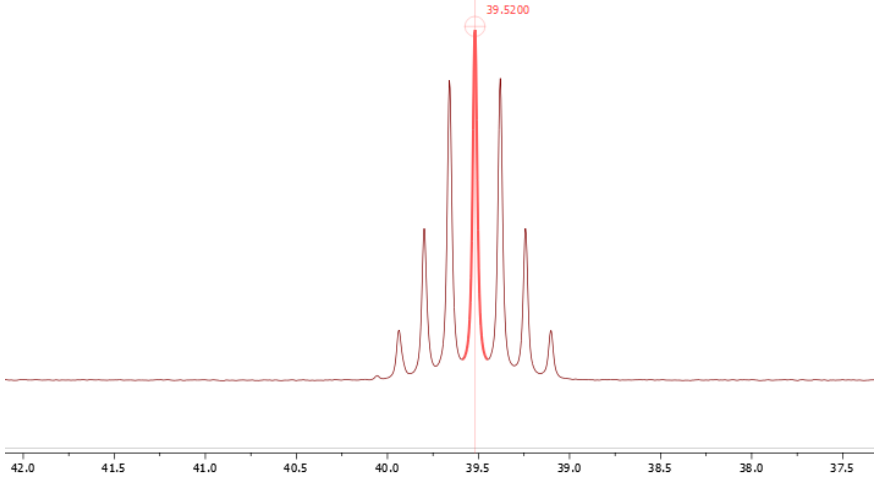


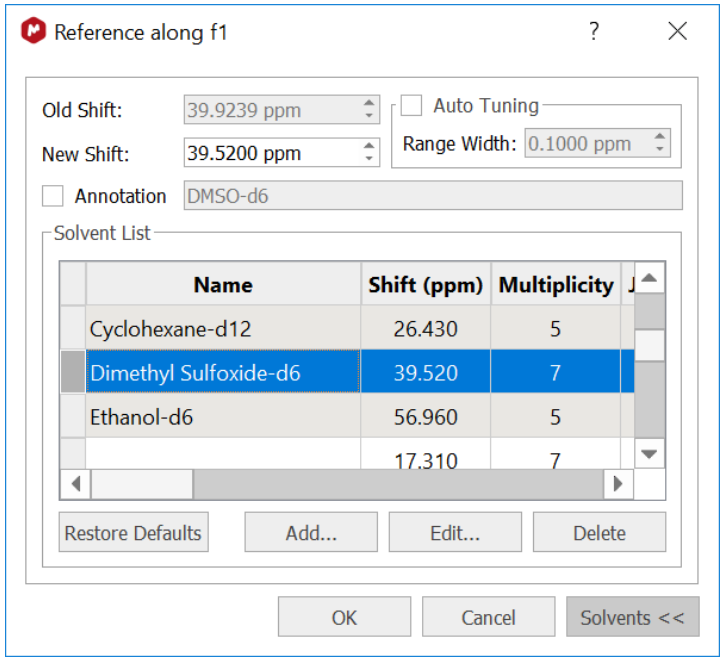


Chemical Shift Referencing



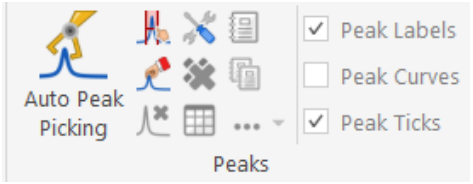
- This spectrum uses DMSO-d6 as the solvent. We can reference the chemical shifts by setting its middle peak to 39.52 ppm.
- Zoom to the DMSO peak at around 39 ppm. Choose Analysis > Reference, and click on the top of the middle peak.
- Set it to 39.52 ppm either manually or from the Solvent List.

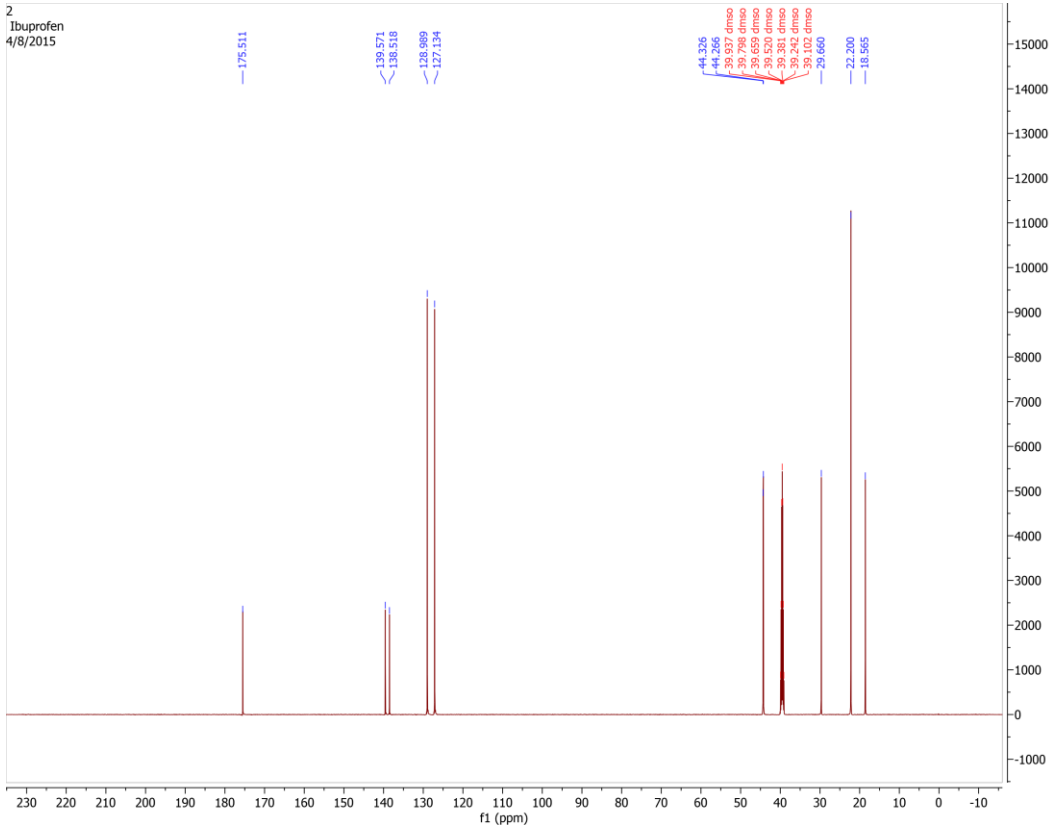


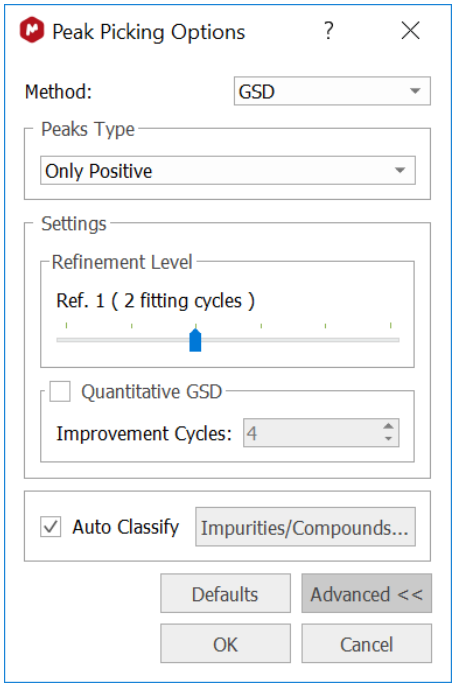


Peak picking

- Click the Peaks > Options  to verify the peak picking options. Default settings are used here as shown to the right.
- Click the Auto Peak Picking tool to pick all the peaks
- Using other peak picking tools to display/delete/add/change peaks as needed.

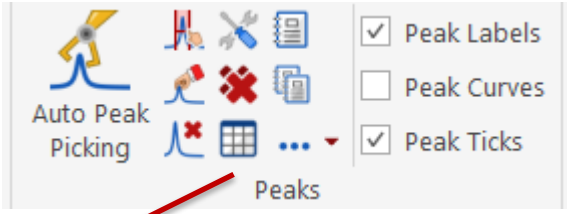


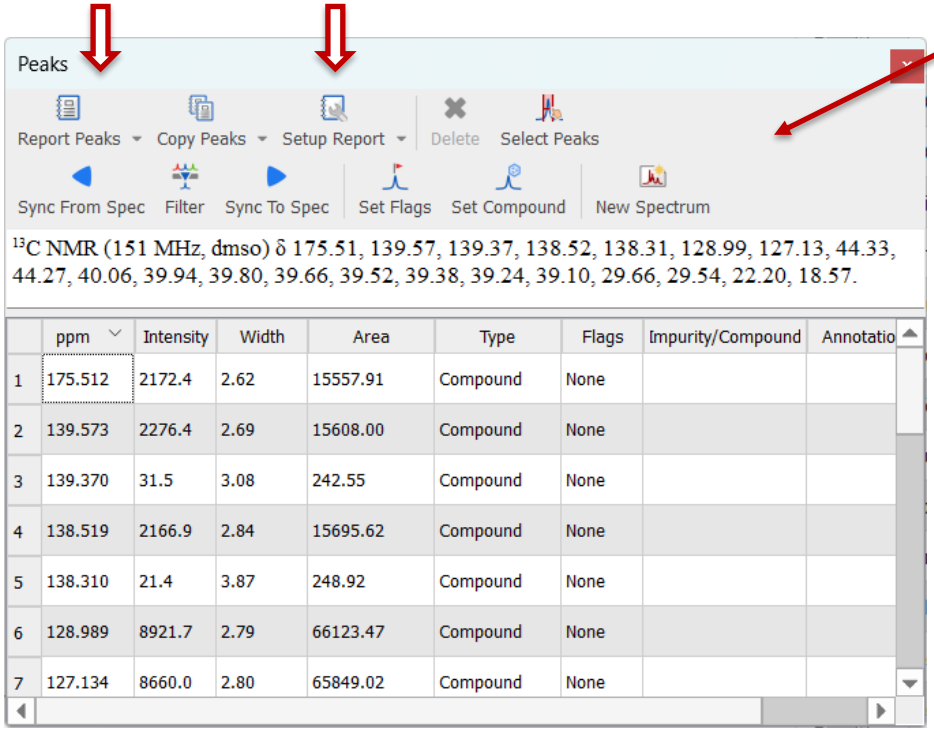




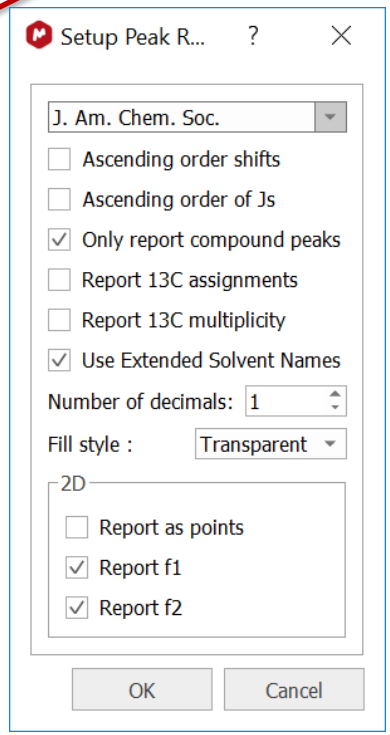
Report the C-13 peaks

- Use the Peak Table tool to display the Peaks Table.
- Click Setup Report to change the reporting format
- Click Report to report the multiplets texts



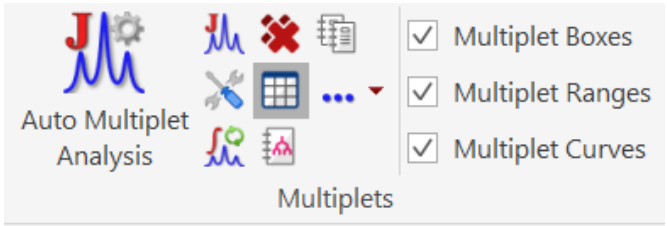


	ppm	Intensity	Width	Area	Type	Flags	Impurity/Compound	Annotatio
1	175.512	2172.4	2.62	15557.91	Compound	None		
2	139.573	2276.4	2.69	15608.00	Compound	None		
3	139.370	31.5	3.08	242.55	Compound	None		
4	138.519	2166.9	2.84	15695.62	Compound	None		
5	138.310	21.4	3.87	248.92	Compound	None		
6	128.989	8921.7	2.79	66123.47	Compound	None		
7	127.134	8660.0	2.80	65849.02	Compound	None		

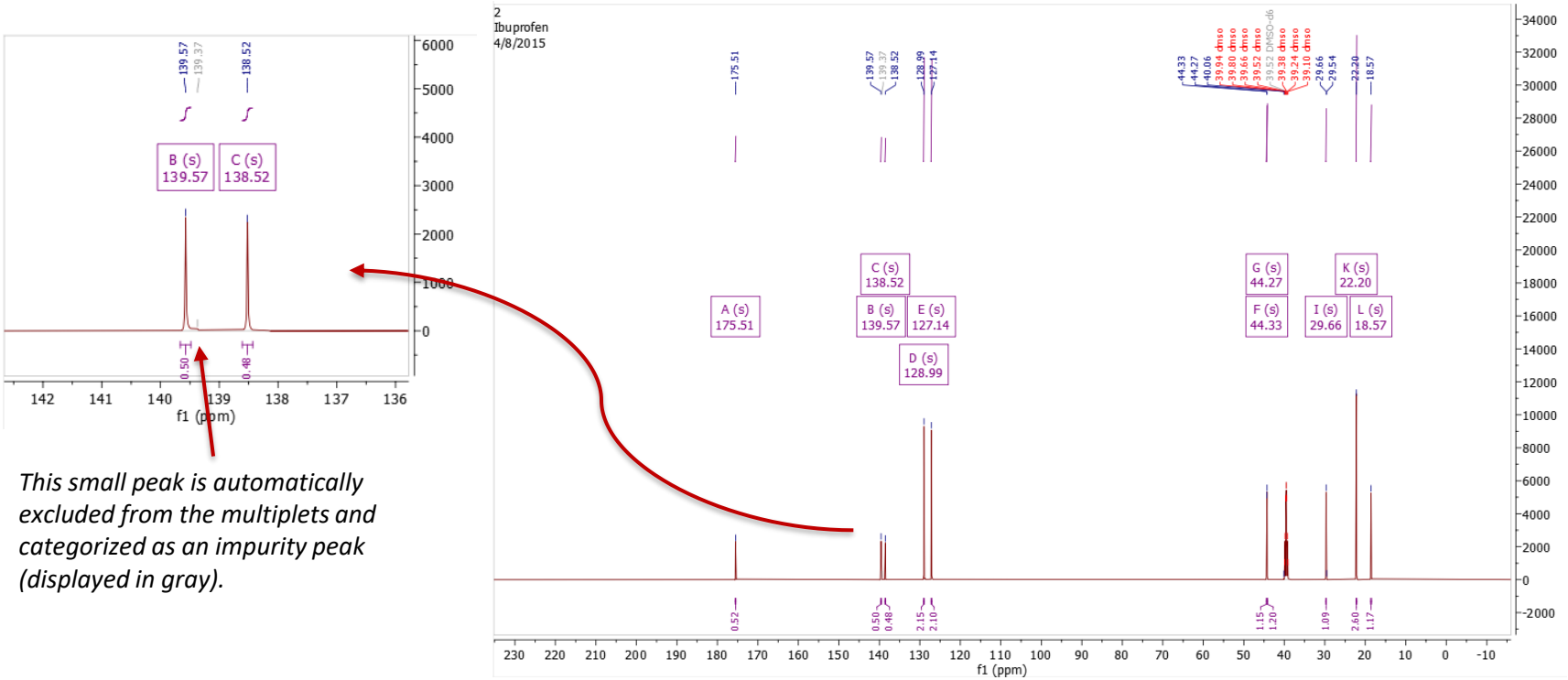


^{13}C NMR (151 MHz, DMSO-d_6) δ 175.5, 139.6, 138.5, 129.0, 127.1, 44.3, 44.3, 29.7, 22.2, 18.6.

Multiplet Analysis



➢ Alternatively, click Auto Multiplet Analysis to group the C-13 peaks as "multiplets"*

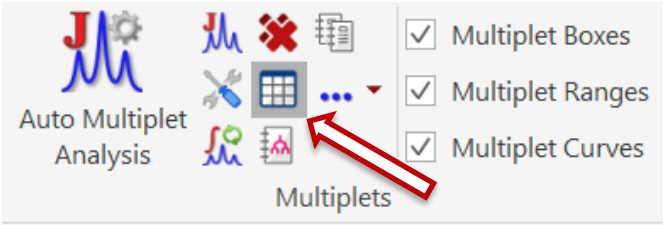


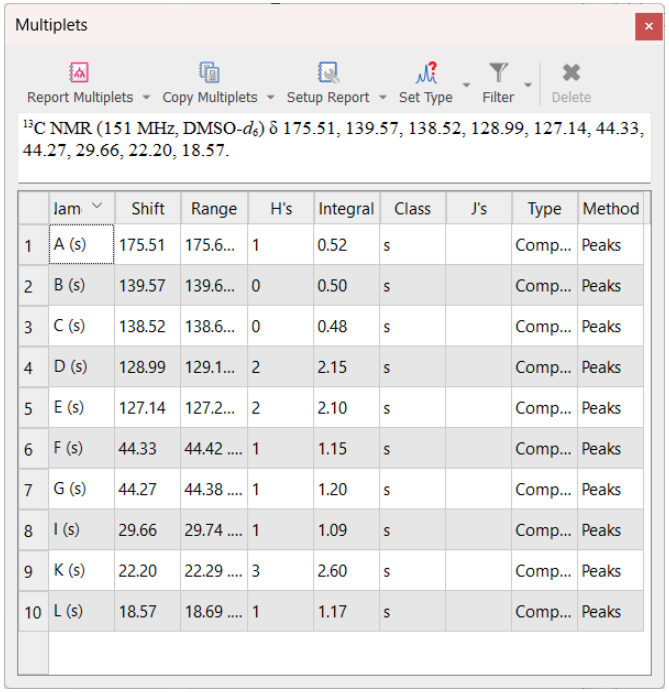
This small peak is automatically excluded from the multiplets and categorized as an impurity peak (displayed in gray).

**This process will ignore very small C-13 peaks typically corresponding to impurities. Although C-13 spectra are often acquired as proton decoupled, and hence the C-13 peaks are singlets, there can be exceptions when, e.g., F atoms are present in the structure.*

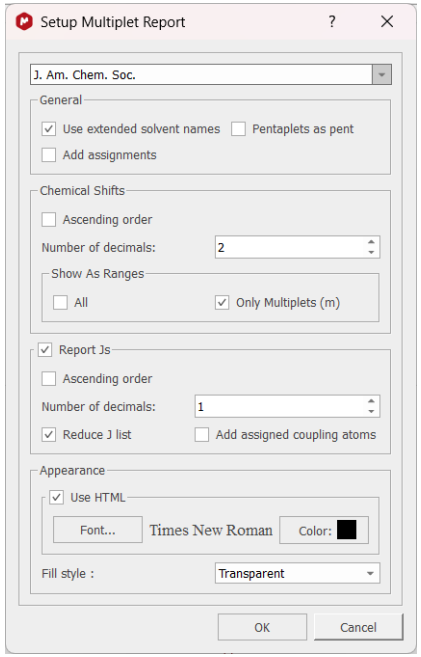
Report C-13 "Multiplets"

- Display the Multiplets Table, set up the format for the reporting
- Use the reporting tools to get the list of multplet information for publication





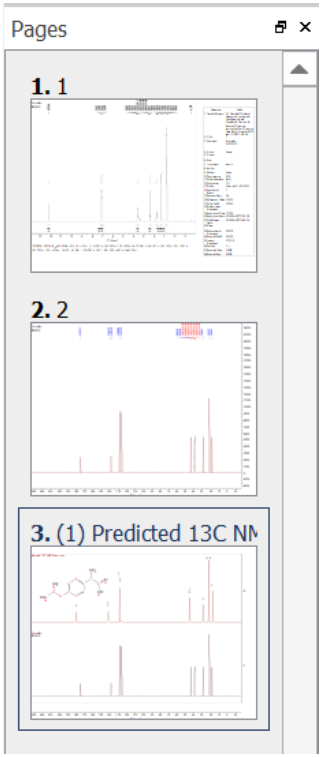
	Iam	Shift	Range	H's	Integral	Class	J's	Type	Method
1	A (s)	175.51	175.6...	1	0.52	s		Comp...	Peaks
2	B (s)	139.57	139.6...	0	0.50	s		Comp...	Peaks
3	C (s)	138.52	138.6...	0	0.48	s		Comp...	Peaks
4	D (s)	128.99	129.1...	2	2.15	s		Comp...	Peaks
5	E (s)	127.14	127.2...	2	2.10	s		Comp...	Peaks
6	F (s)	44.33	44.42	1	1.15	s		Comp...	Peaks
7	G (s)	44.27	44.38	1	1.20	s		Comp...	Peaks
8	I (s)	29.66	29.74	1	1.09	s		Comp...	Peaks
9	K (s)	22.20	22.29	3	2.60	s		Comp...	Peaks
10	L (s)	18.57	18.69	1	1.17	s		Comp...	Peaks

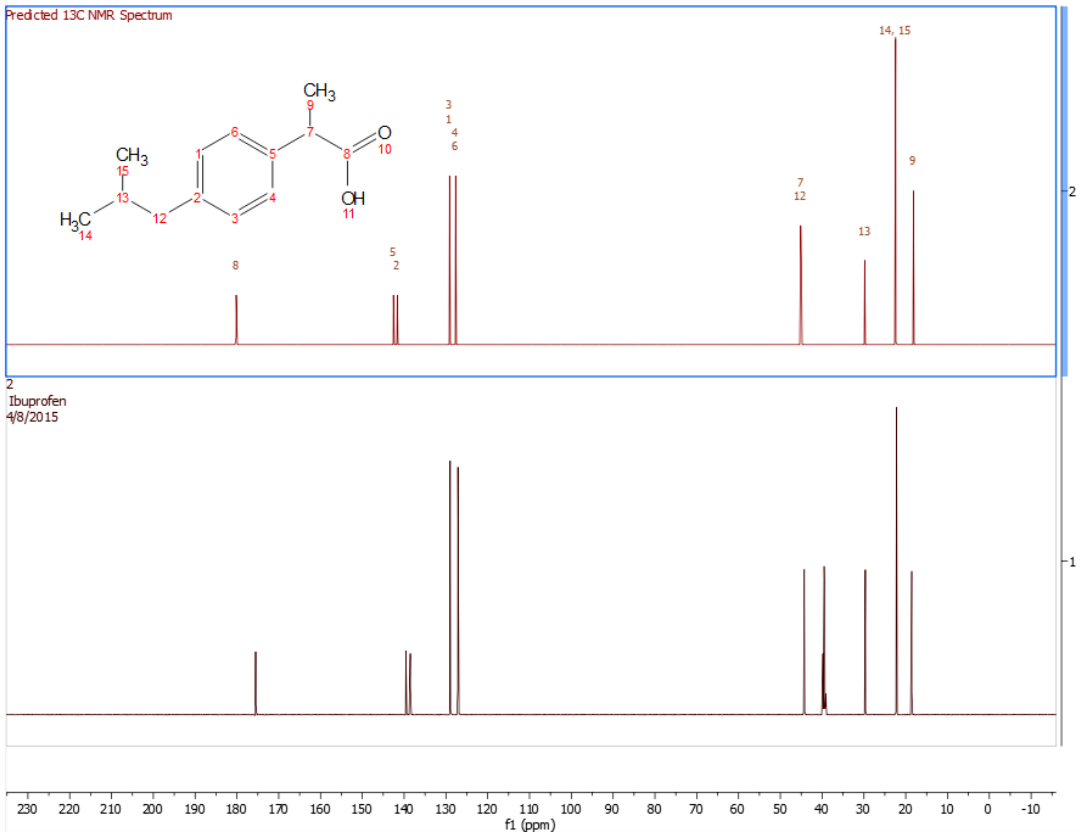


^{13}C NMR (151 MHz, DMSO-d_6) δ 175.51, 139.57, 138.52, 128.99, 127.14, 44.33, 44.27, 29.66, 22.20, 18.57.

Verify the structure by predict and compare

- Make a copy of the C-13 spectrum (Ctrl-C and Ctrl-V in the Pages View).
- Open the Ibuprofen.mol to bring in the structure to the C-13 spectrum.
- Choose Predict > Predict Compare.

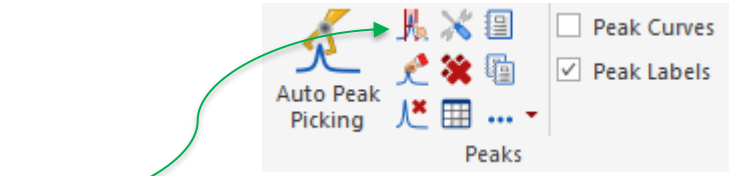




Tip: if you want to delete the predicted C-13 spectrum from the stack, choose Stacked > Stacked Items Table, and use the Delete tool in the Table to delete the predicted C-13 spectrum.

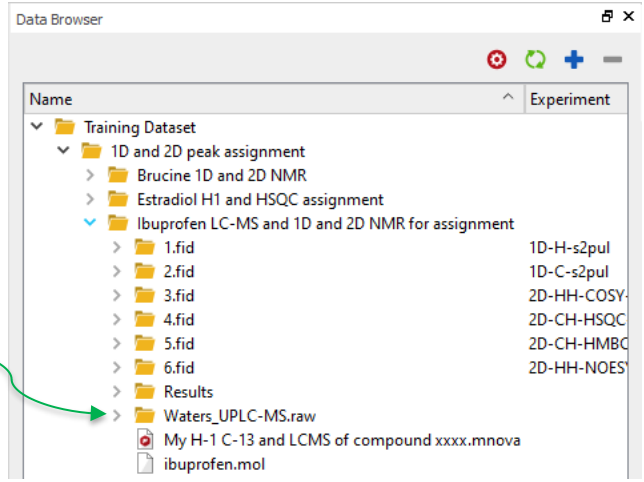
More about C-13 processing and analysis

- There are several other 1D C-13 NMR spectra in the tutorial datasets that you can use for practice.
- When the spectrum is more crowded and has more artefacts or impurity peaks, you can also use the manual peak picking tools to have more control.
- You can also do multiplet analysis for the C-13 peaks, especially when you there are F-C couplings, and report the results from the Multiplet Table.



LC/MS Processing, Analysis, and Reporting

Sample data



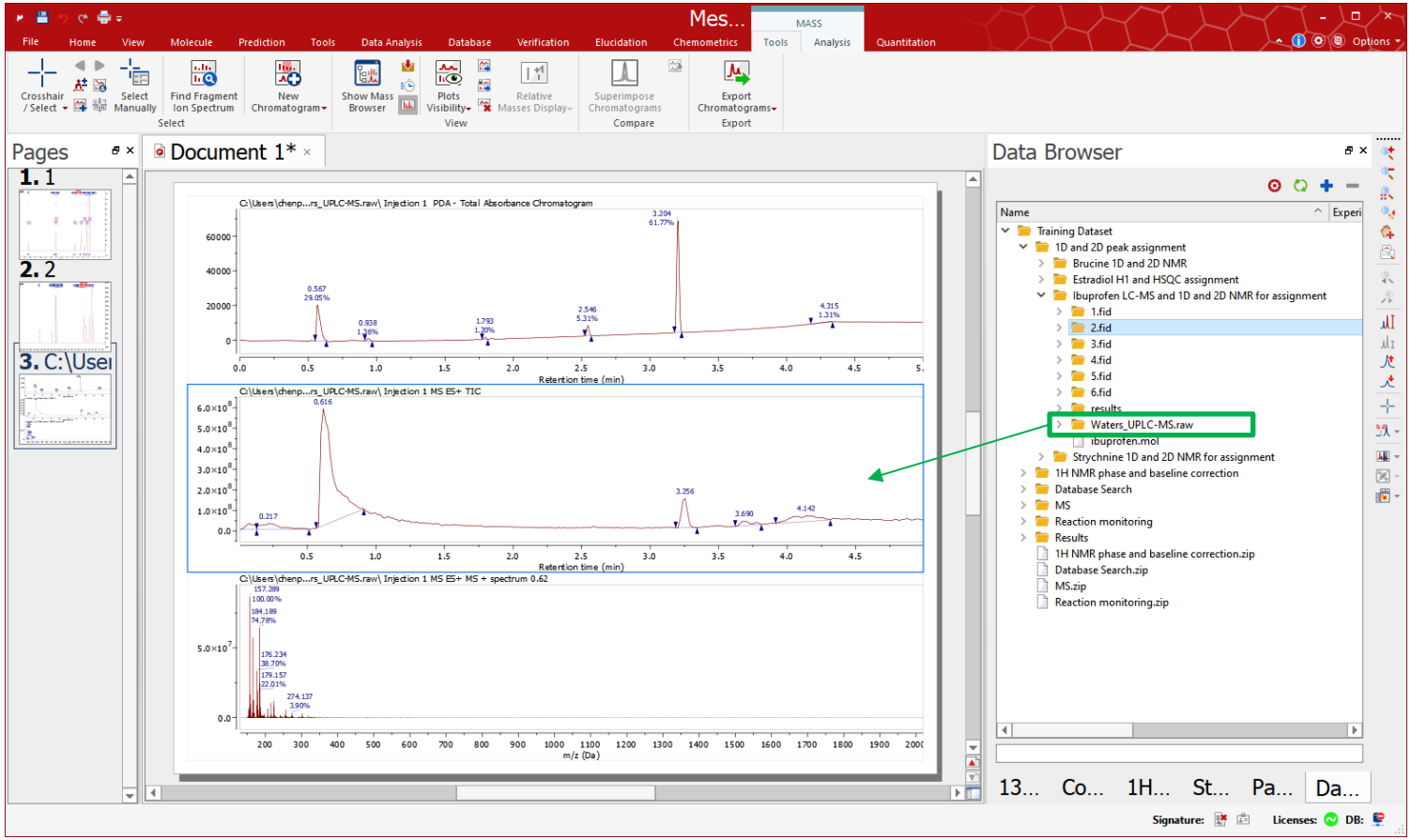
Open the LC-MS data

- In Data Browser, open the LC-MS data Ibuprofen (low resolution data acquired on Waters).
- The PDA, TIC and the mass spec at the highest TIC peak are displayed.

H-1

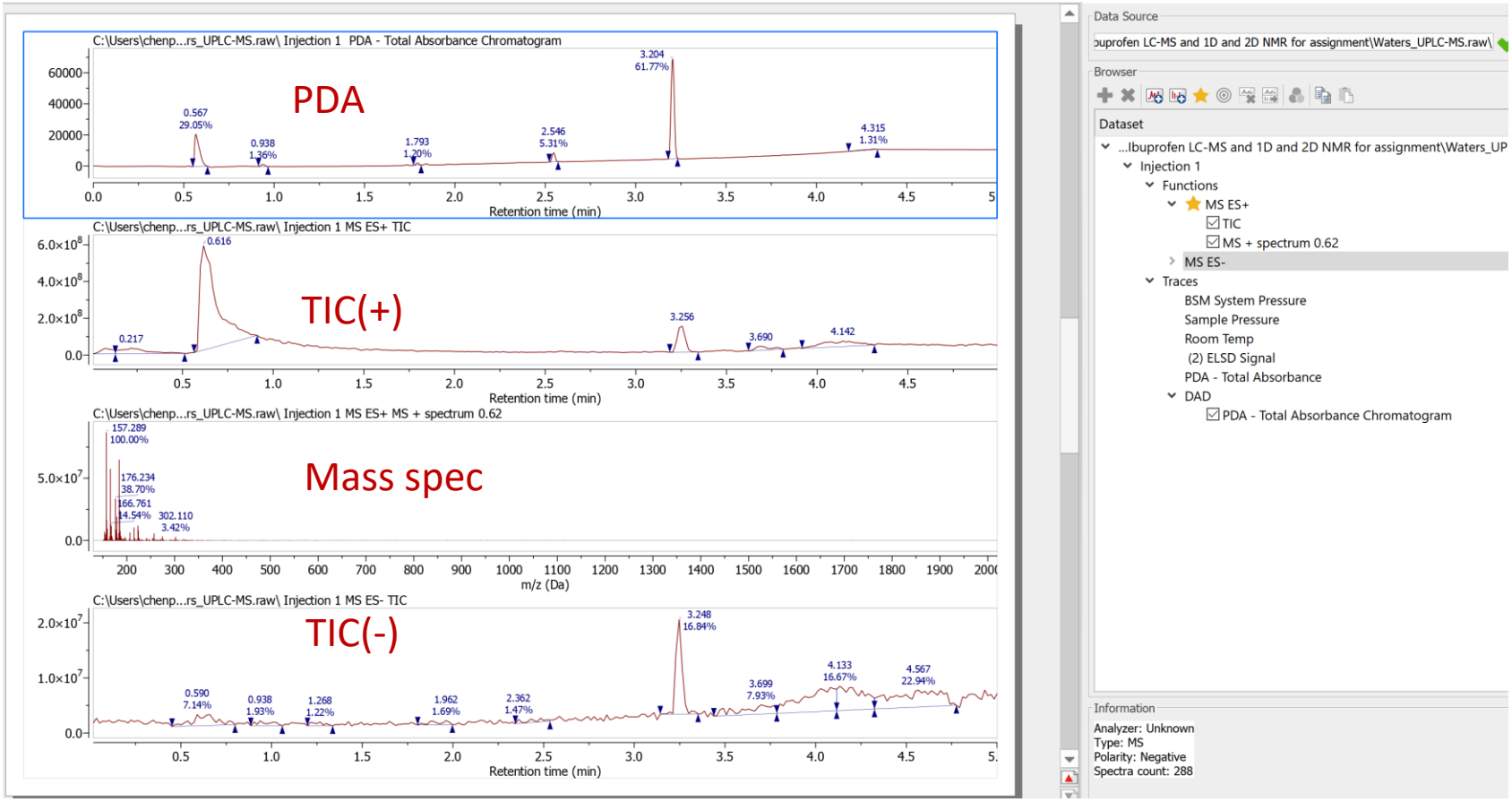
C-13

MS



Display chromatograms

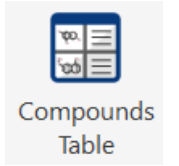
- The Mass Browser is automatically displayed.*
- Open the negative polarization TIC by double clicking on “MS ES-”
- Right on the PDA and choose Hide Plot to hide PDA.

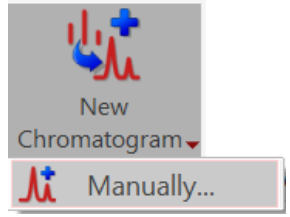


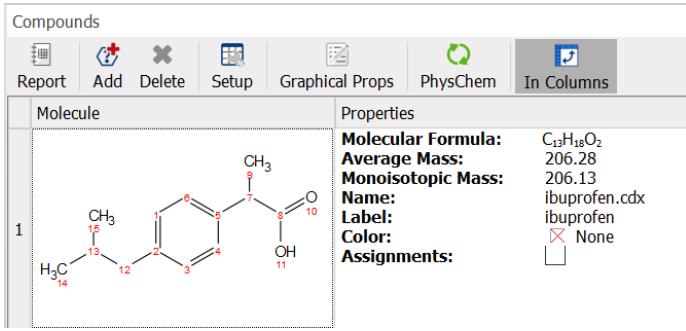
If the Mass Browser is closed, you can open it using the Show Mass Browser tool in the MASS Tools ribbon.

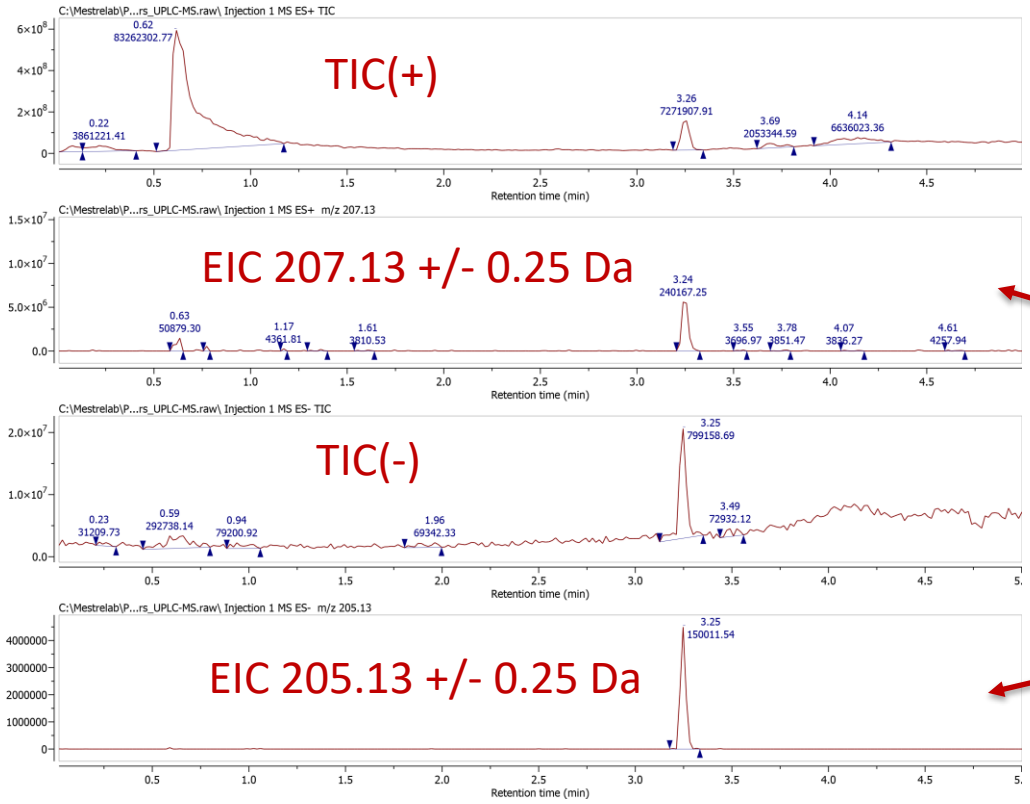
Verify the elemental composition

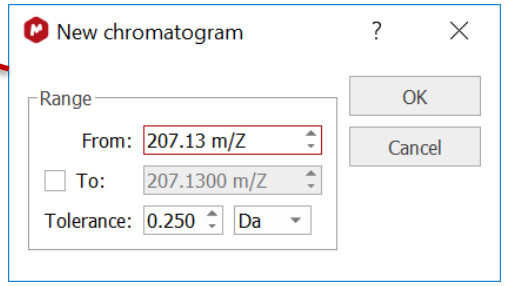
- Open the Ibuprofen.mol file from the Data Browser.
- Choose Molecule > Compound Table to find its monoisotopic mass: 206.13
- Hight the TIC(+), click Mass > New Chromatogram > Manually, and enter a value of 207.13 +/- 0.25 Da to display the new chromatogram (also called Extracted Icon Chrom., EIC)

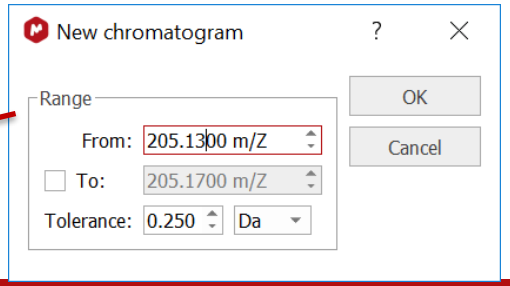






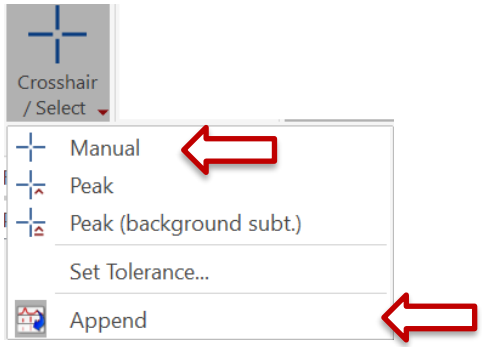


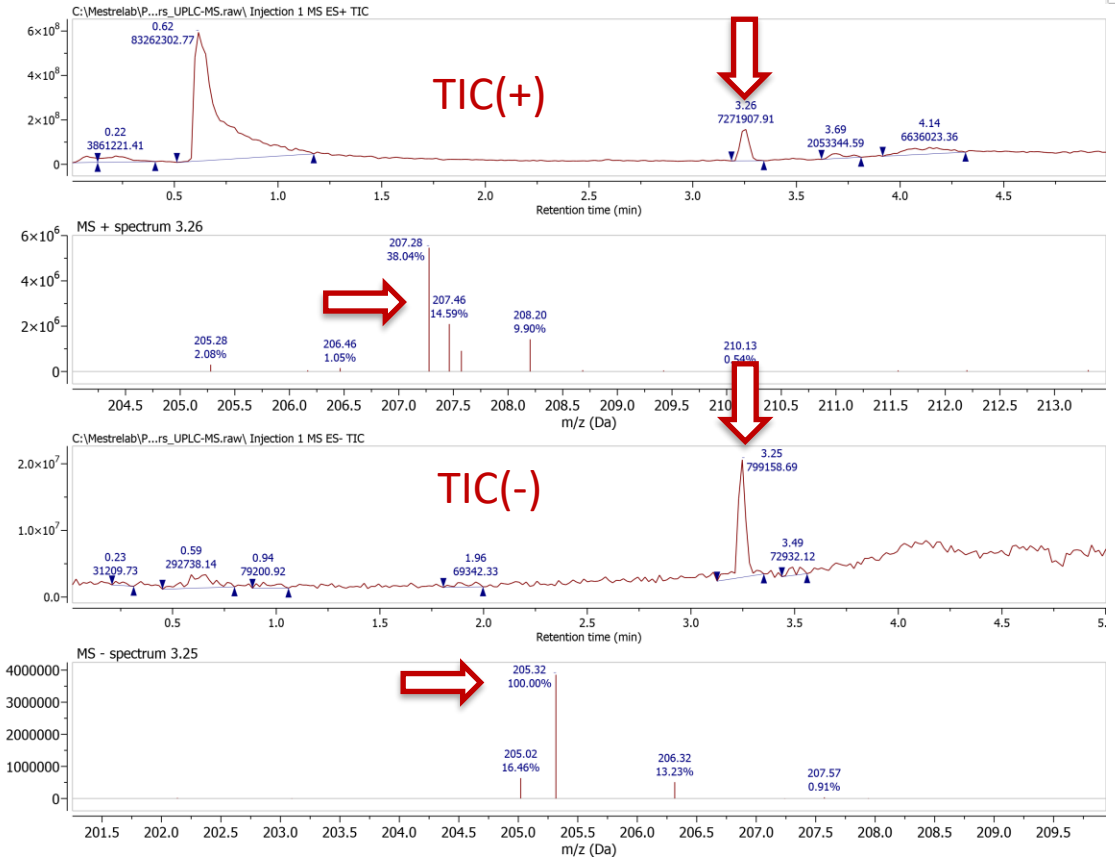




Find the molecule ion peaks

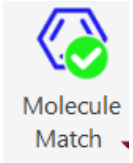
- Click the Crosshair tool, and click on the peak around 3.25 min in both TIC(+) and TIC(-)
- Zoom into the mass spec to find the mol. Ion peaks at around 207.13 and 205.13 Da, respectively.



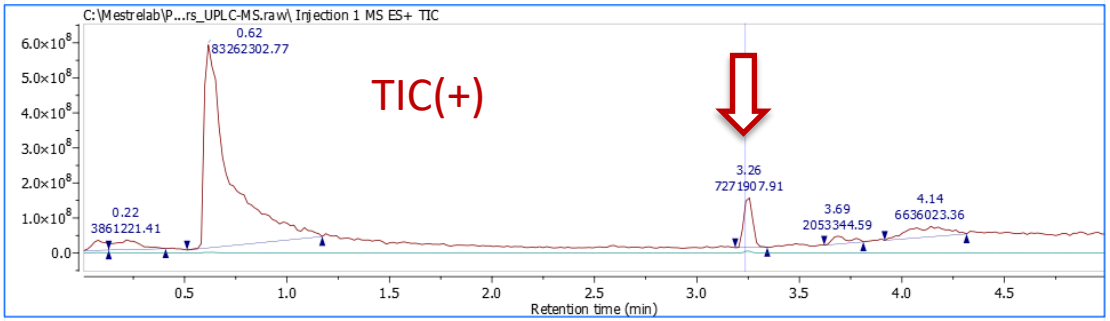


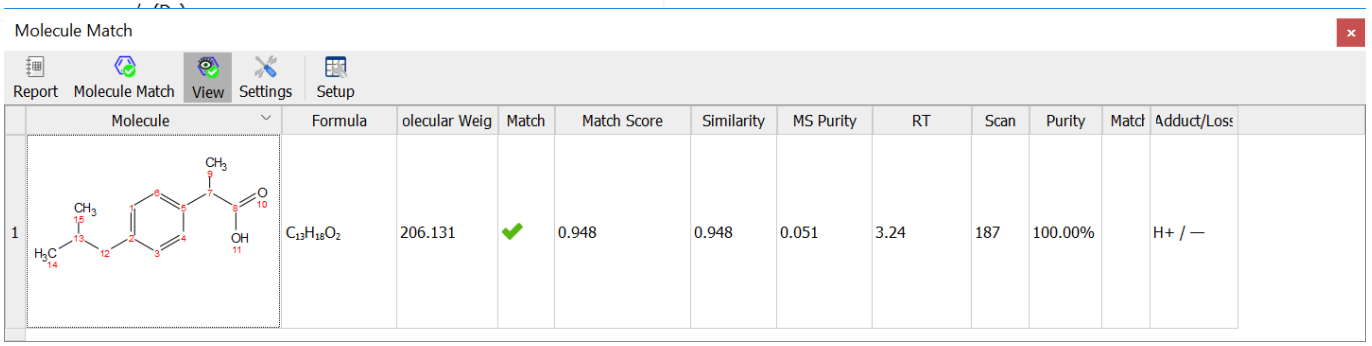
Tip: Use the Mass Browser to hide or delete unwanted plots. Right-click on a plot and choose Move up/Move Down etc. to re-order of the plots

Use Mol Match to verify the elemental composition

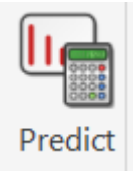


- Open the Ibuprofen.mol. Click Molecule Match.
- The Molecule Match Table shows the matching results.
- Click on the structure in the table to display the mol match results on the spectrum

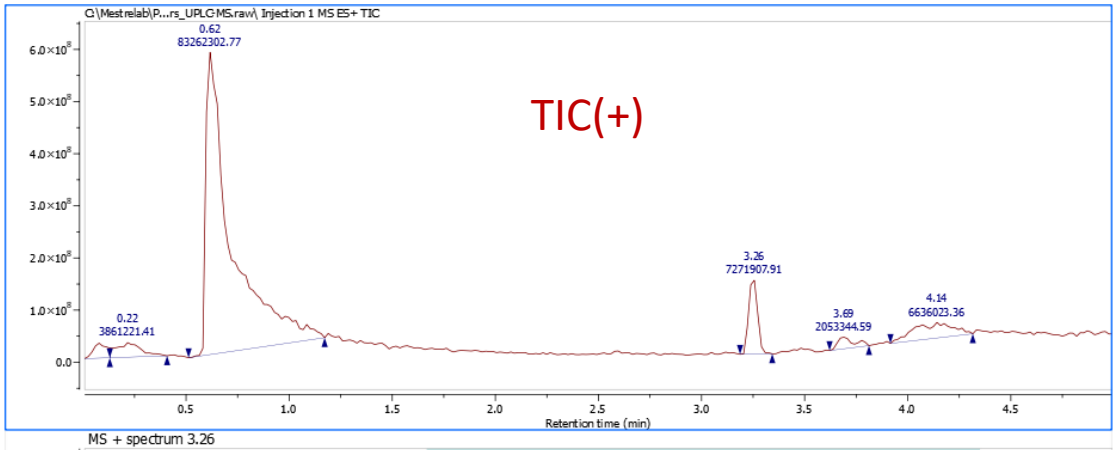


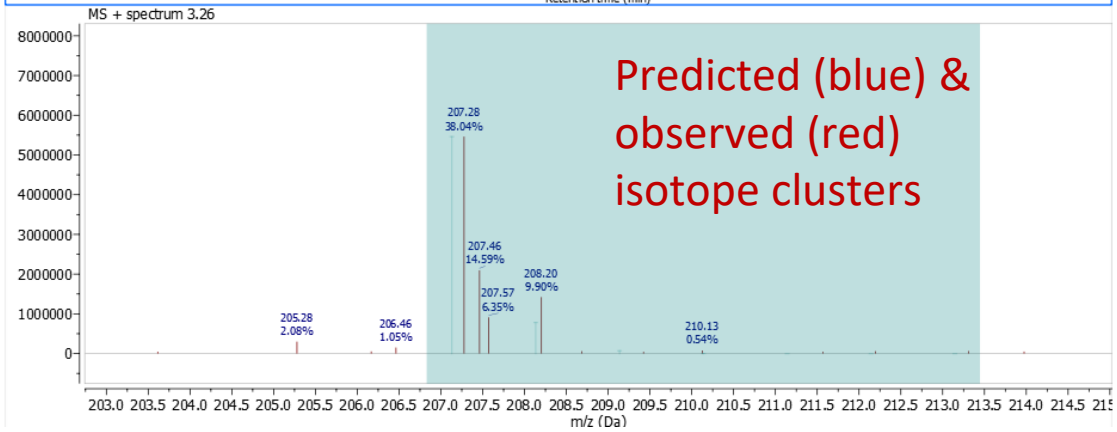


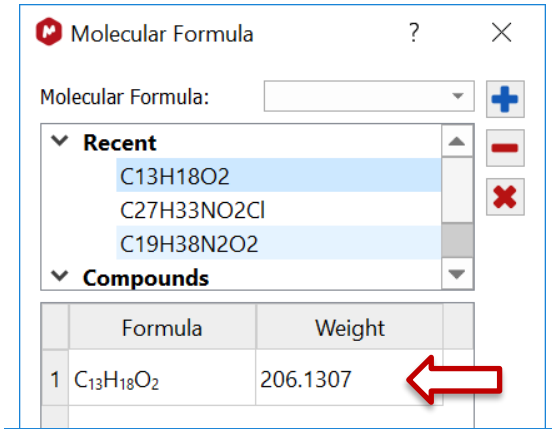
Predict and verify the molecule ion peaks

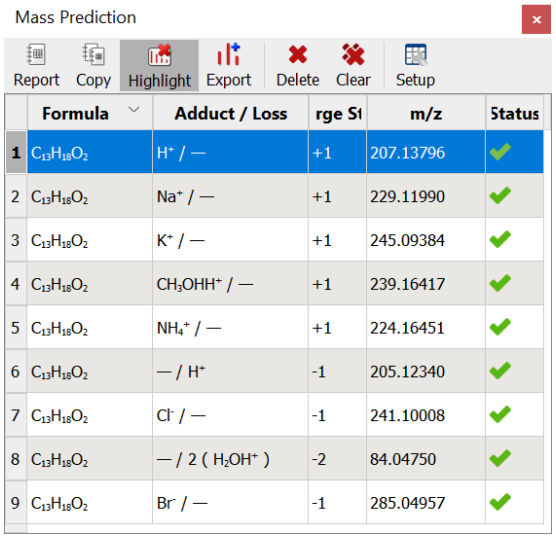


- Click the Predict tool, and choose the MF C13H18O2 and press “+” to use it for prediction
- In the Mass Prediction List, highlight the first row. The predicted molecule ion and isotope peaks are displayed on top of the experiment peak for comparison.





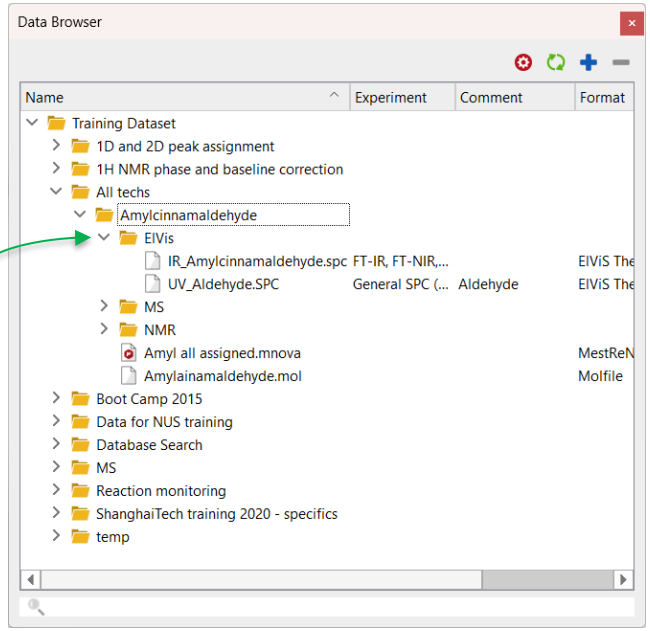




	Formula	Adduct / Loss	rge St	m/z	Status
1	$C_{13}H_{18}O_2$	H^+ / —	+1	207.13796	✓
2	$C_{13}H_{18}O_2$	Na^+ / —	+1	229.11990	✓
3	$C_{13}H_{18}O_2$	K^+ / —	+1	245.09384	✓
4	$C_{13}H_{18}O_2$	CH_3OHH^+ / —	+1	239.16417	✓
5	$C_{13}H_{18}O_2$	NH_4^+ / —	+1	224.16451	✓
6	$C_{13}H_{18}O_2$	— / H^+	-1	205.12340	✓
7	$C_{13}H_{18}O_2$	Cl^- / —	-1	241.10008	✓
8	$C_{13}H_{18}O_2$	— / 2 (H_2OH^+)	-2	84.04750	✓
9	$C_{13}H_{18}O_2$	Br^- / —	-1	285.04957	✓

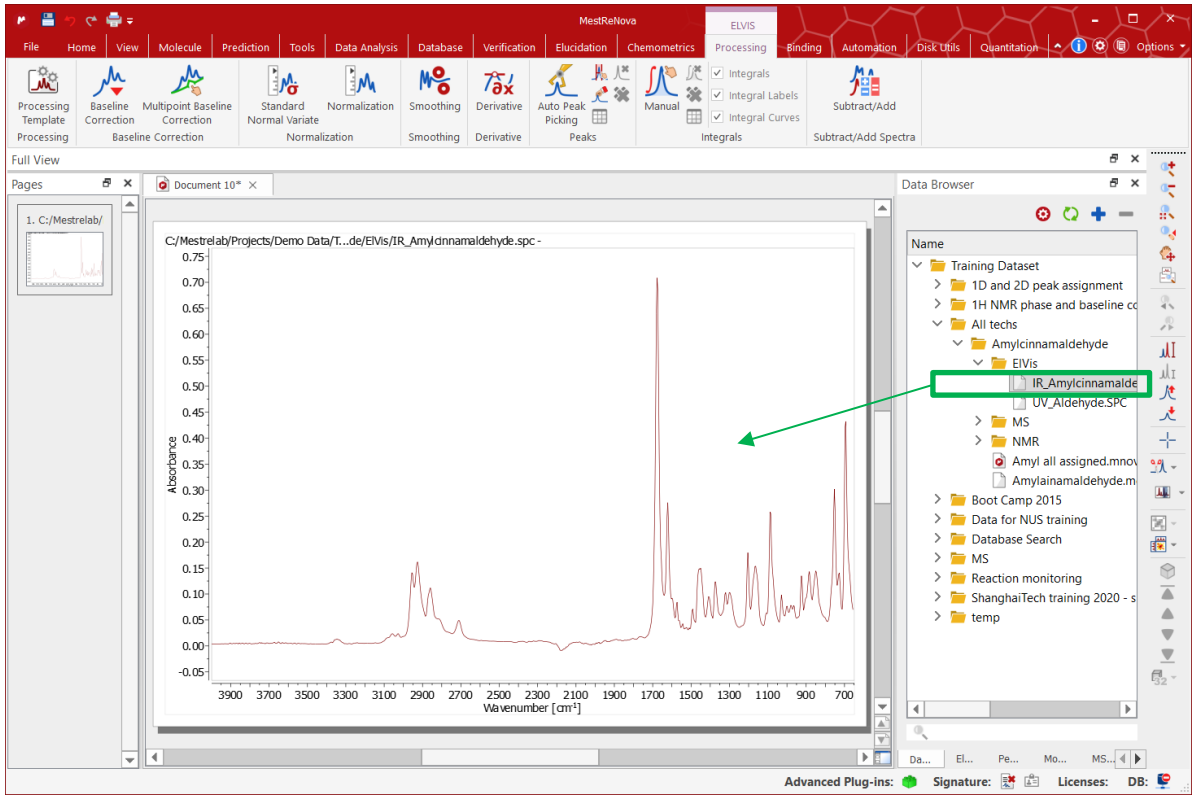
Visualization of IR and UV Spectra, etc.

Sample data



Open the IR data

- In Data Browser, open the IR data of Amylainamaldehyde.
- By default, the spectrum is displayed as shown below.

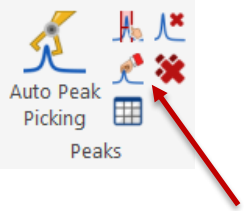


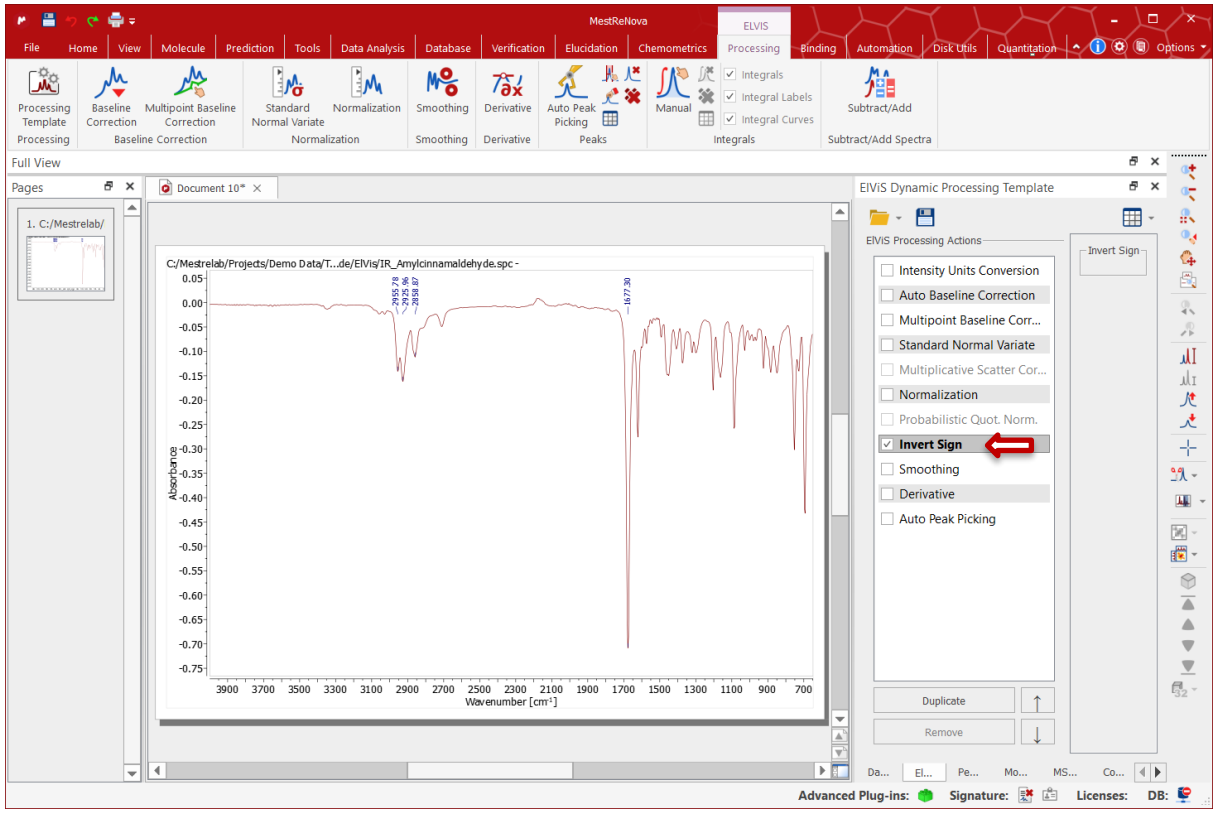
The main formats supported by Mnova ElViS:

- JCAMP-DX (.jcamp, .dx, .jdx, .jcm)
- OPUS (.0, .1,...)
- Thermo Nicolet Omnic (.spa)
- Thermo Galactic GRAMS (.spc)
- ASCII (.txt, .csv).

Open the IR data

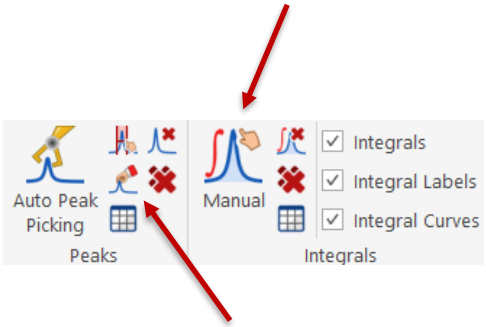
- Click ELVIS Processing > Processing Template to display the ElViS Dynamic Processing Template.
- Check Invert Sign to display the spectrum in the conventional way.
- Use the Peak by Peak tool to pick peaks manually.

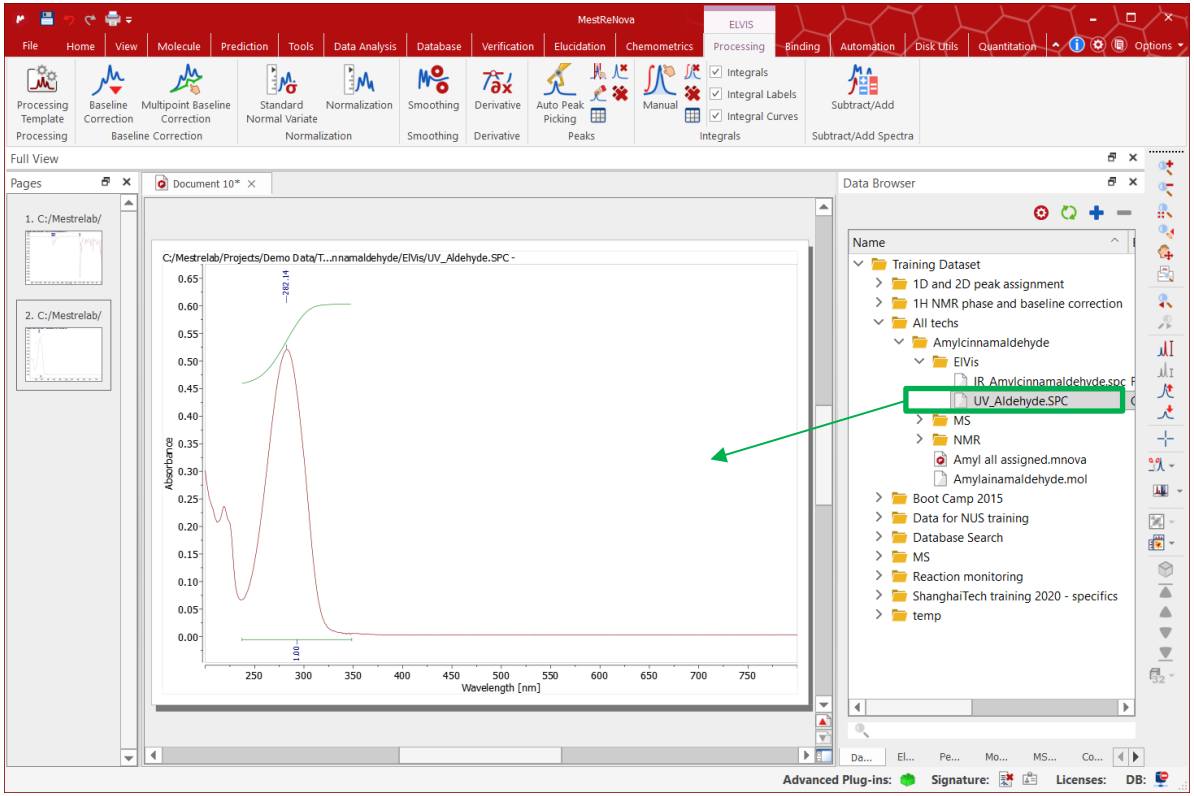




Open the UV data

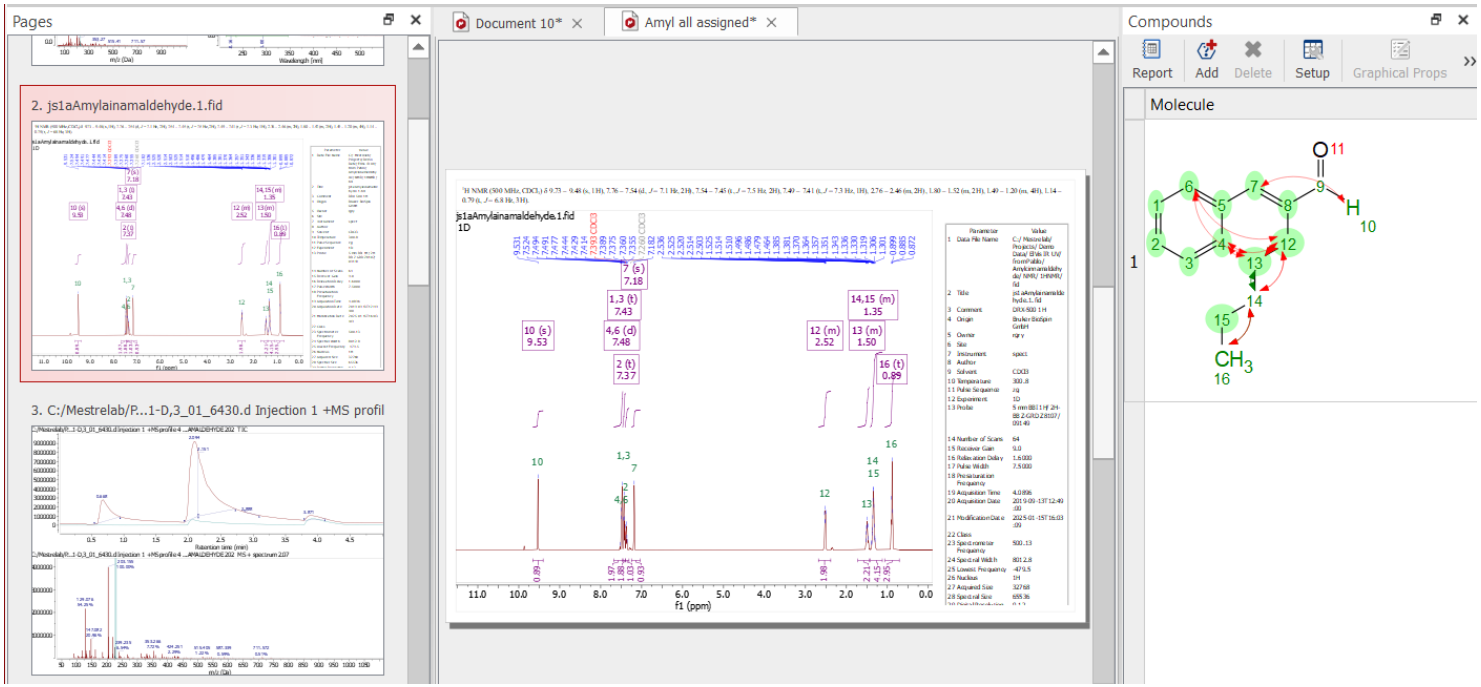
- In Data Browser, open the UV data of Amylainamaldehyde.
- Use the Peak by Peak tool to pick peaks.
- Use the Manual Integration tool to integrate peak.





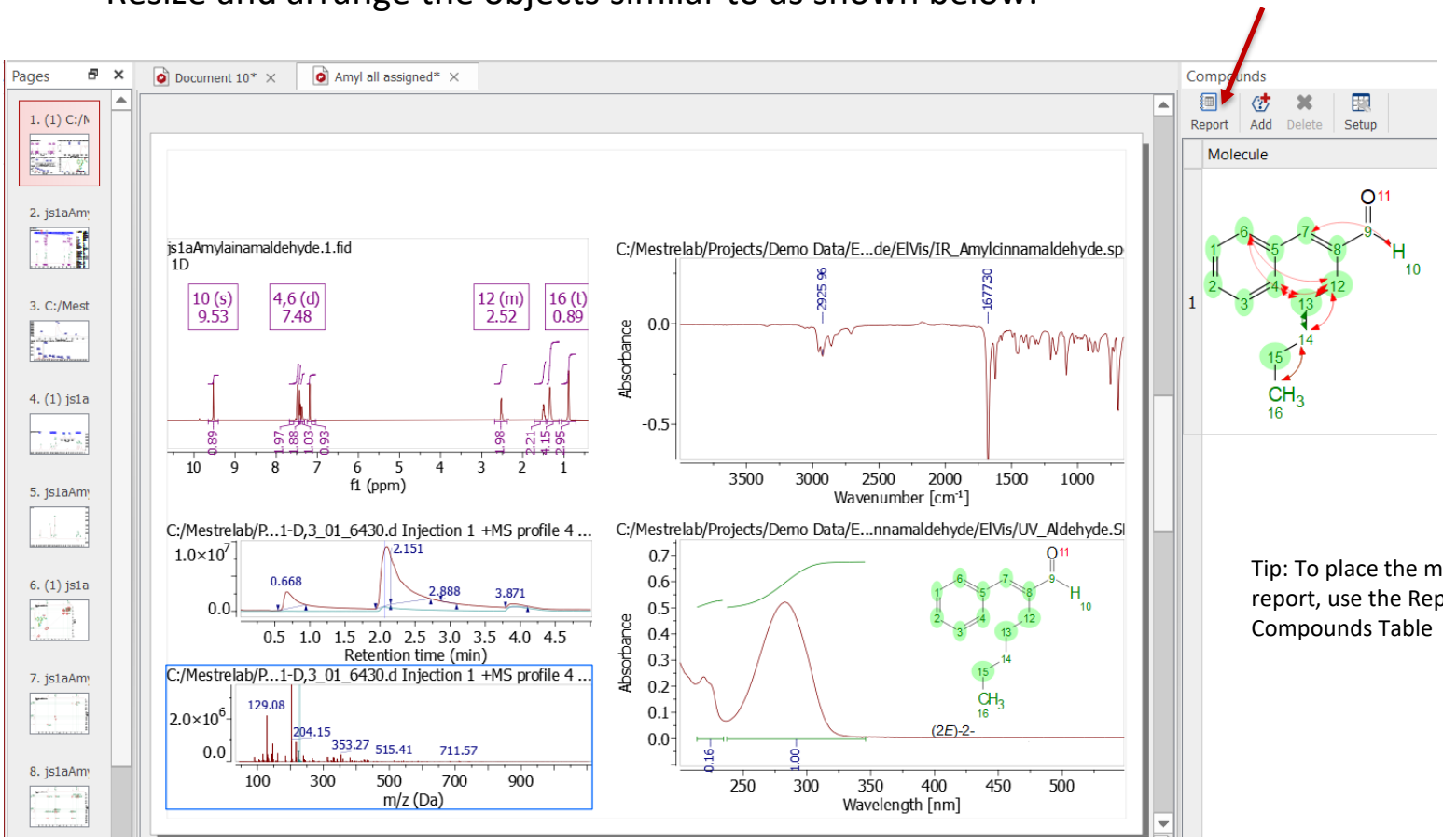
Open the HNMR and LC-MS data

- In Data Browser, open 1H NMR and LCMS data of Amylainamaldehyde.
- Open the mol file of Amylainamaldehyde.
- Do the routine analysis of them, such as multiplet analysis, mol match, peak assignment etc.



Display all IR, UV, NMR and LCMS on the Same Page

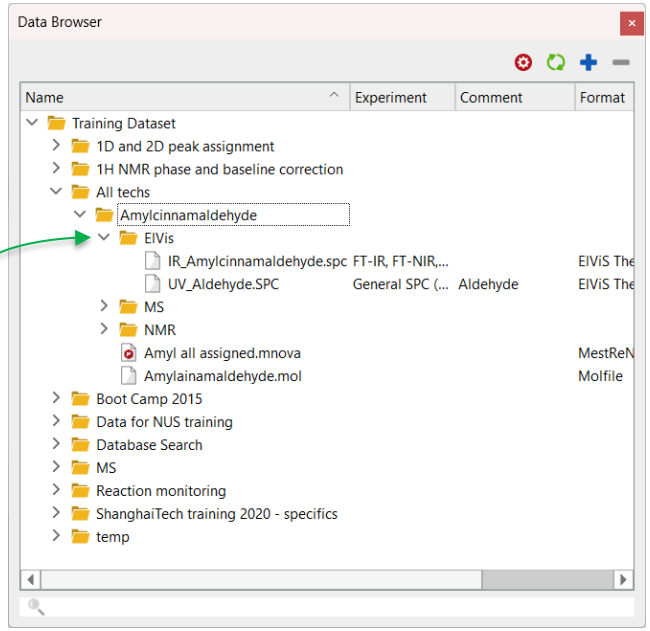
- Choose Home > New Page to open a new page.
- Copy and paste the IR, UV, 1H NMR, and LC-MS to the new page one by one.
- Resize and arrange the objects similar to as shown below:



Tip: To place the molecule to the report, use the Report tool in the Compounds Table

Saving the Results

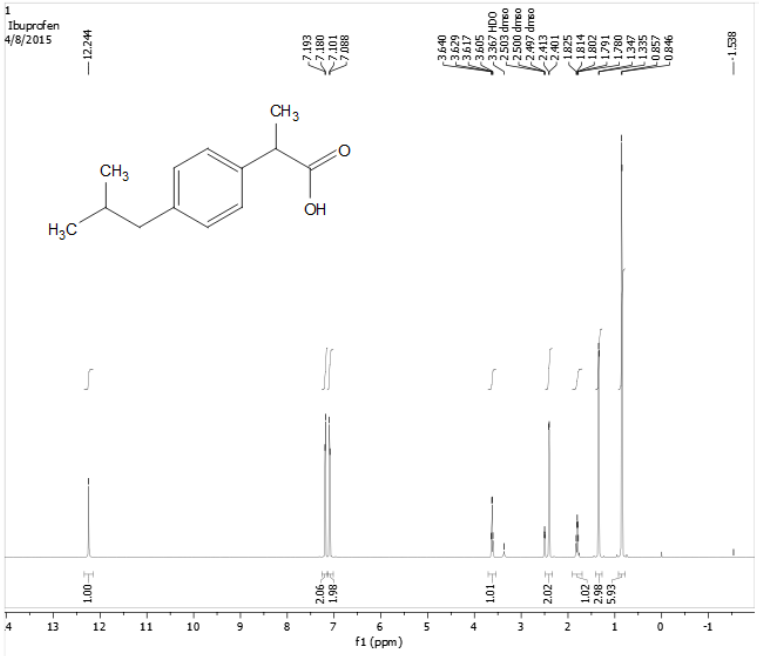
Sample data



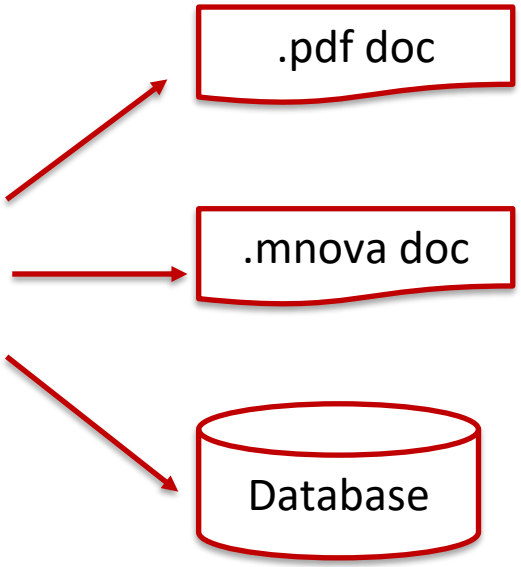
SAVING RESULTS

Save the results

- Choose File > Export to PDF to save a PDF report of the page.
- Chose File > Save as to save all the results to a .mnova file.
- In the Advanced Tutorial we will learn to save the results to a database (if you have Mnova DB licenses)
- Now you can close the document.



	Parameter	Value
1	Data File Name	C:/ Mestrelab/ Projects/ Marcomm/ Literature & Docs/ Sample and Templates/ Training for chemists/ Training courses by Chen/ Training Data Sets/ Ibuprofen NMR and LCMS/ 1.fid/ fid
2	Title	1
3	Comment	Ibuprofen 4/ 8/ 2015
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	vnmrs
8	Author	
9	Solvent	dmso
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	3mm_cold_HCN_P001
14	Number of Scans	1
15	Receiver Gain	24
16	Relaxation Delay	1.0000
17	Pulse Width	3.0000
18	Presaturation Frequency	
19	Acquisition Time	1.7039
20	Acquisition Date	2015-04-08T10:34:36
21	Modification Date	2015-04-08T19:46:04
22	Class	
23	Spectrometer Frequency	599.76
24	Spectral Width	9615.4
25	Lowest Frequency	-1193.6
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	65536



Help information

More help information

- Use the Help Facility of Mnova: Help > Contents
- Visit www.mestrelab.com for manuals, tutorials, videos and publications
- Email support@mestrelab.com for technical questions