



Mestrelab Research

chemistry software solutions

Mnova Training– Basics

For Mnova v16.0

Updated Oct. 2025

Chen Peng, PhD,

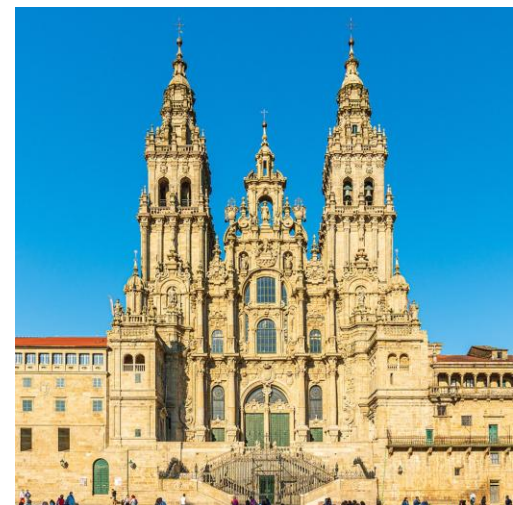
VP of Business Development, North America & Asia

Mestrelab Research SL

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Main Topics

- Installation and Activation of Mnova
- Opening and processing 1D ^1H NMR
- Multiplet analysis for 1D ^1H 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



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.*

INSTALLATION

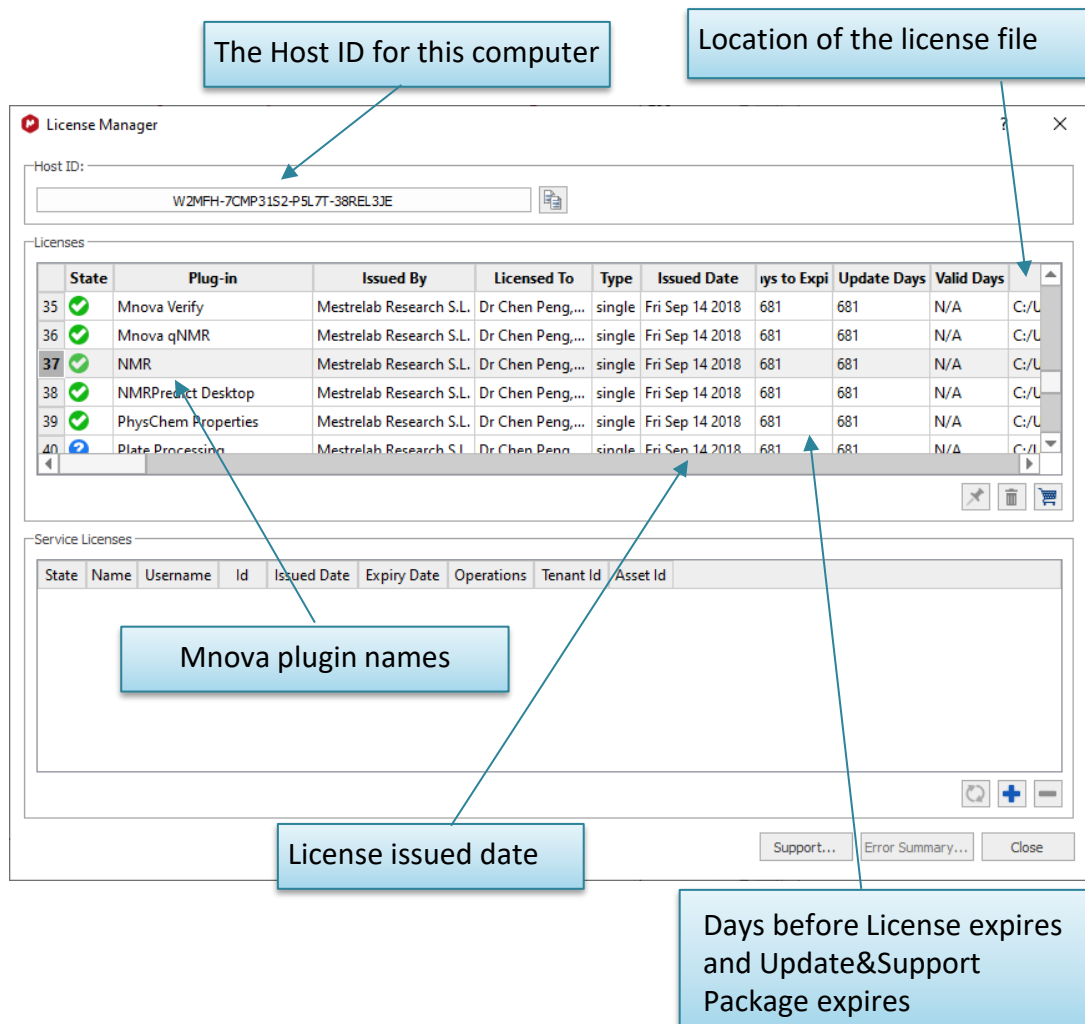
- Download and install Mnova from www.mestrelab.com/download.

- 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)

Install and activate Mnova



The Host ID for this computer

Location of the license file

License Manager

Host ID: W2MFH-7CMP3152-PSL7T-38REL3JE

Licenses

	State	Plug-in	Issued By	Licensed To	Type	Issued Date	Days to Expi	Update Days	Valid Days	
35	✓	Mnova Verify	Mestrelab Research S.L.	Dr Chen Peng,...	single	Fri Sep 14 2018	681	681	N/A	C:/U
36	✓	Mnova qNMR	Mestrelab Research S.L.	Dr Chen Peng,...	single	Fri Sep 14 2018	681	681	N/A	C:/U
37	✓	NMR	Mestrelab Research S.L.	Dr Chen Peng,...	single	Fri Sep 14 2018	681	681	N/A	C:/U
38	✓	NMRPredict Desktop	Mestrelab Research S.L.	Dr Chen Peng,...	single	Fri Sep 14 2018	681	681	N/A	C:/U
39	✓	PhysChem Properties	Mestrelab Research S.L.	Dr Chen Peng,...	single	Fri Sep 14 2018	681	681	N/A	C:/U
40	⚙	Plate Processing	Mestrelab Research S.L.	Dr Chen Peng,...	single	Fri Sep 14 2018	681	681	N/A	C:/U

Mnova plugin names

License issued date

Days before License expires and Update&Support Package expires

Service Licenses

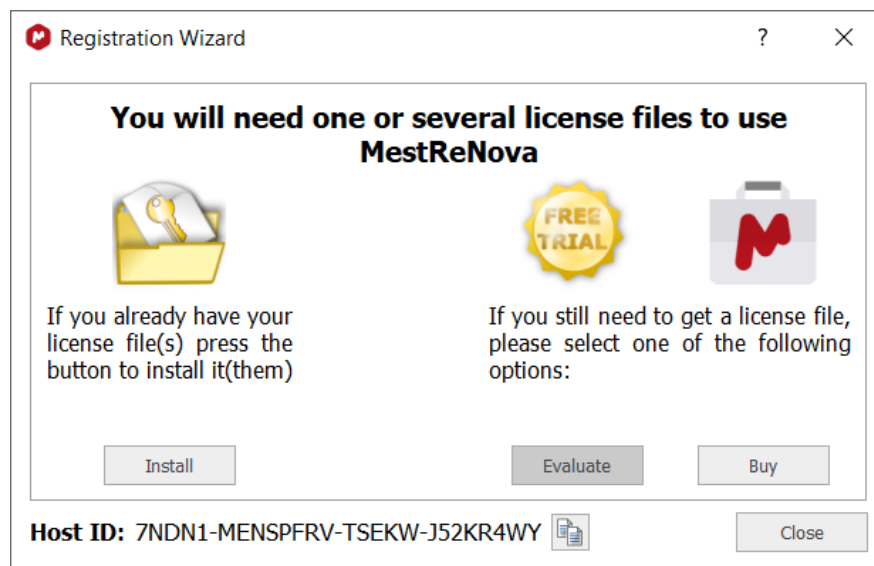
State	Name	Username	Id	Issued Date	Expiry Date	Operations	Tenant Id	Asset Id

Support... Error Summary... Close

INSTALLATION

- 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](#).

Activate Mnova



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.

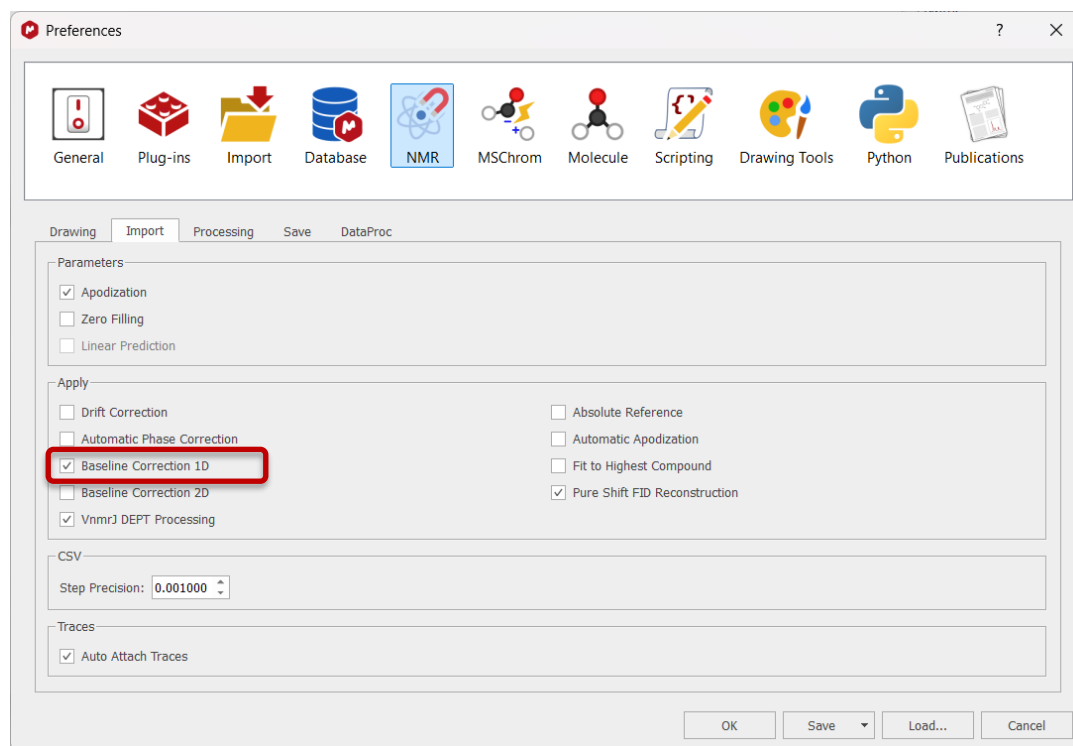


Shortcut for Preferences

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.

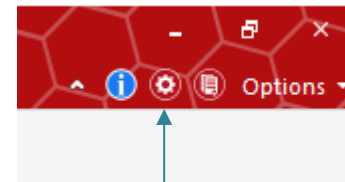
Tip: There are many other options and settings that you can change in the Preferences Dialog.



PREFERENCES

Setup the resolution for publishing spectra

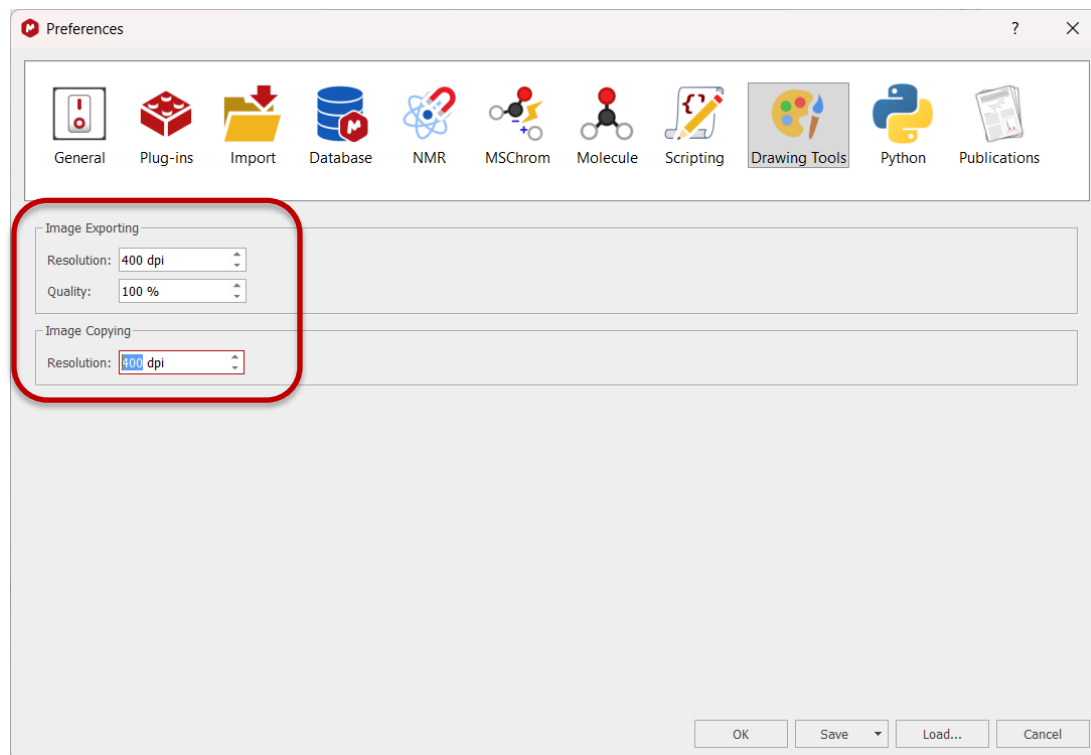
Choose File/Preferences. In the Drawing Tools tab, change the resolutions for Image Exporting and Image Copying to numbers similar to something shown below.



Shortcut for Preferences

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.

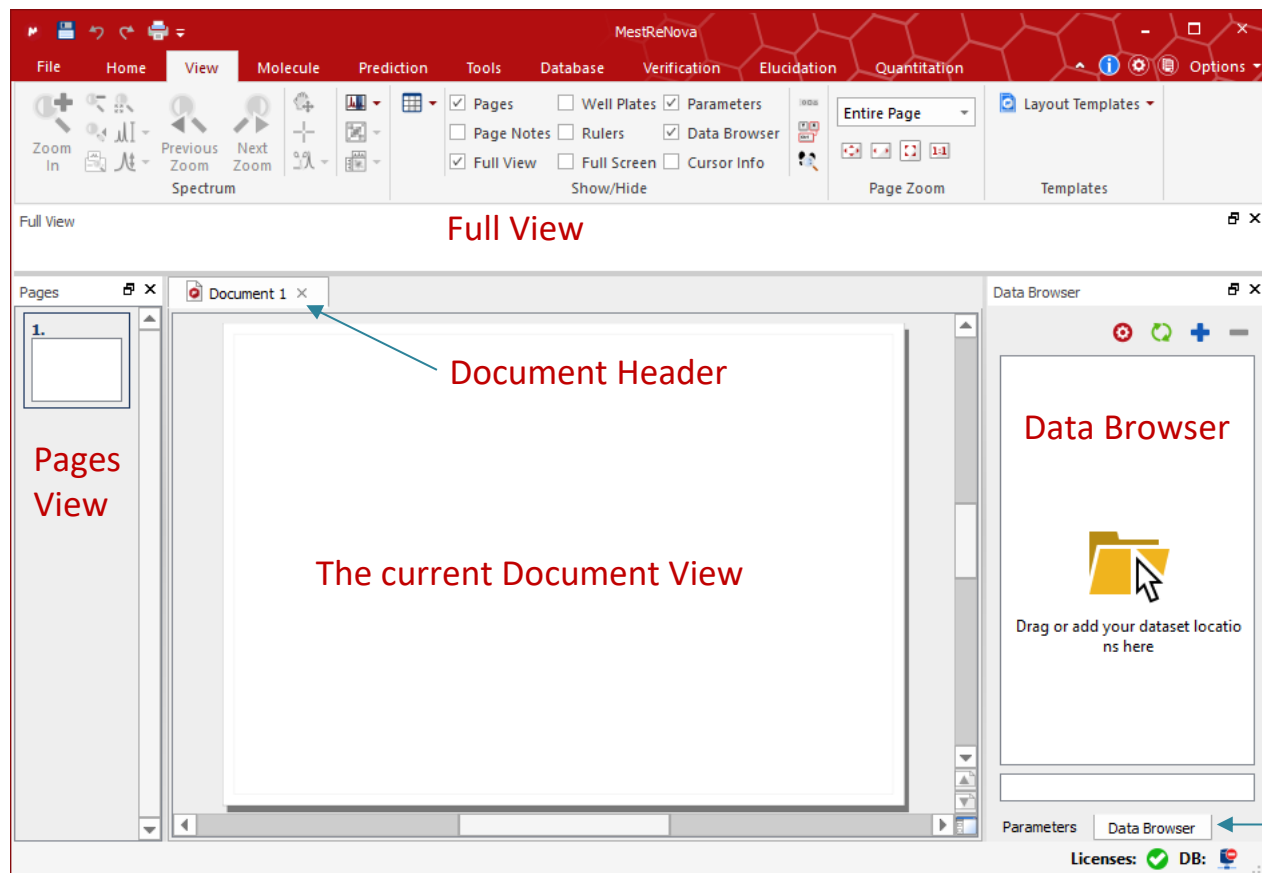
The resolution for Image Copying is used when you copy selected objects in Mnova and paste them to another application.



SETUP

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

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

Data Browser

Name	Experiment	Comm	Format	Modification date
Training Dataset				2019-11-03T20:18:18
1D and 2D peak assignment				2019-11-03T19:48:53
Brucine 1D and 2D NMR				2019-10-20T19:39:40
Estradiol H1 and HSQC assignment				2019-10-23T22:16:33
Ibuprofen LC-MS and 1D and 2D NMR for assignment				2019-10-21T00:13:20
Strychnine 1D and 2D NMR for assignment				2019-10-31T02:13:33
10	1D-H-zg30	Stryc...	Bruker T...	2019-10-30T19:15:12
11	1D-C-zpgp30	Bruker T...	Bruker T...	2019-10-30T19:15:12
12	2D-HH-COSY-co...	Bruker T...	Bruker T...	2019-10-30T19:15:13
13	2D-CH-HSQC-E...	Bruker T...	Bruker T...	2019-10-30T19:15:13
14	2D-CH-HMBC-h...	Bruker T...	Bruker T...	2019-10-30T19:15:14
16	2D-NH-HMBC-h...	Bruker T...	Bruker T...	2019-10-30T19:15:14
19	2D-CC-INADEQU...	Bruker T...	Bruker T...	2019-10-30T19:15:15
Strychnine.mol				2012-07-16T23:51:54
saved processed.mnova				2019-10-31T02:13:33
1H NMR phase and baseline correction	1D-H-zg		MestRe...	2019-07-09T18:51:21
Database Search				2019-07-09T18:51:22
MS				2019-07-09T18:51:23
Reaction monitoring				2019-11-03T19:38:53
Results				2019-07-09T18:51:27

Add location

Path: and Templates/Training for chemists/Training courses by Chen/Training Data Sets

Label: Training Data Sets

OK Cancel

Data Browser Settings

View Formats

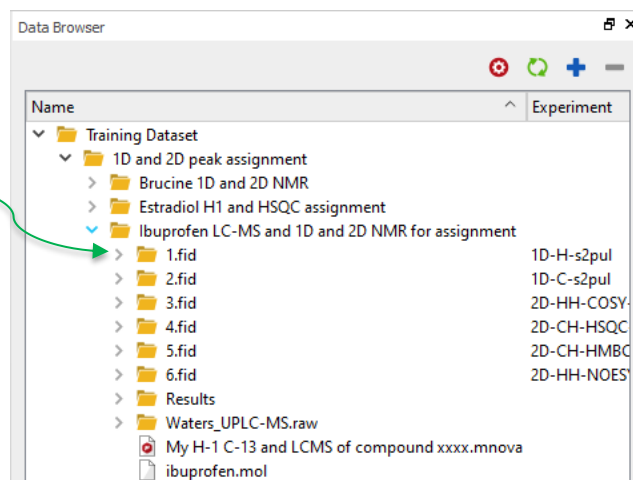
	Name	Experiment	Comment	Format	Modification Date	Size
Visible Name	Name	Experiment	Comment	Format	Modification Date	Size
Visible	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Decimals						
Horizontal Alignment	Left	Left	Left	Left	Left	Left

☒ Enable sorting

OK Cancel

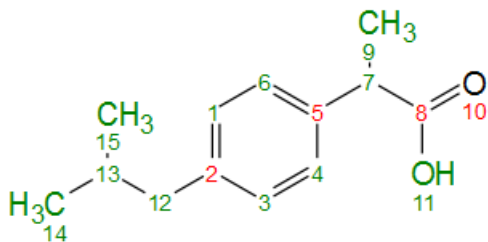
1D ^1H NMR Spectrum Processing, Analysis, and Reporting

Sample data



PROCEDURE

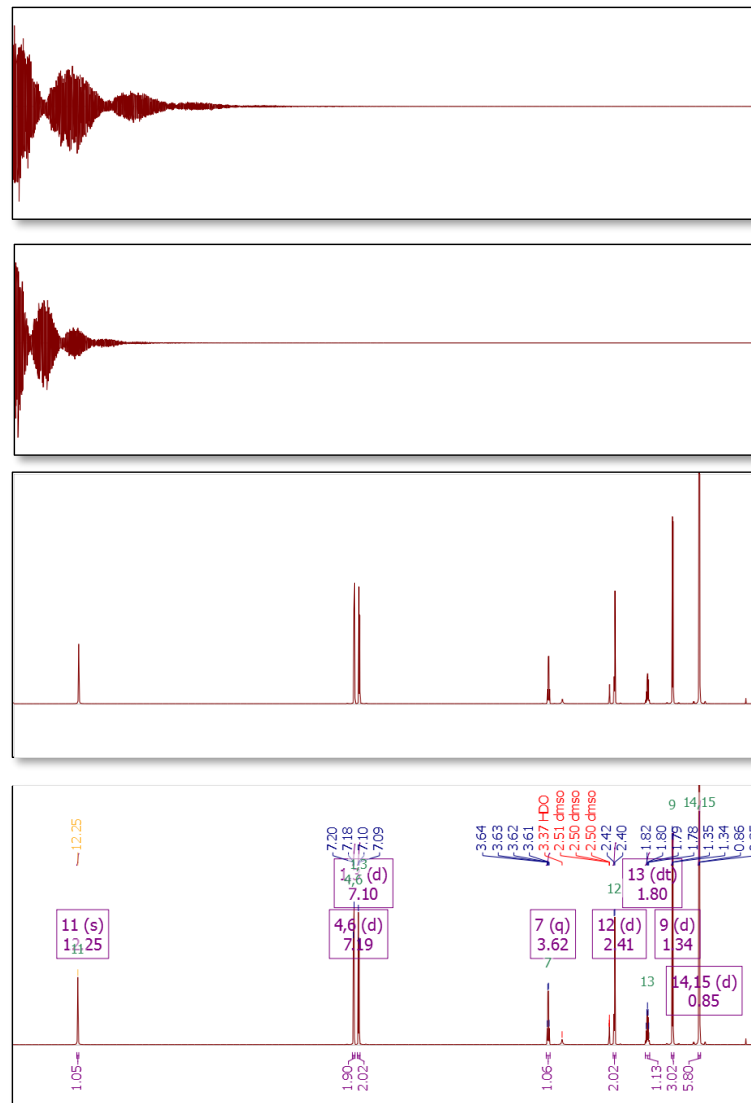
- Open the raw data
- Pre-process the FID: drift correct, apodize, zero fill, linear predict, etc.
- Fourier transform
- Phase correct and baseline correct
- Chemical shift reference
- Peak-pick, integrate, multiplet analysis
- Structure verification and peak assignment
- Report and publish



^1H 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

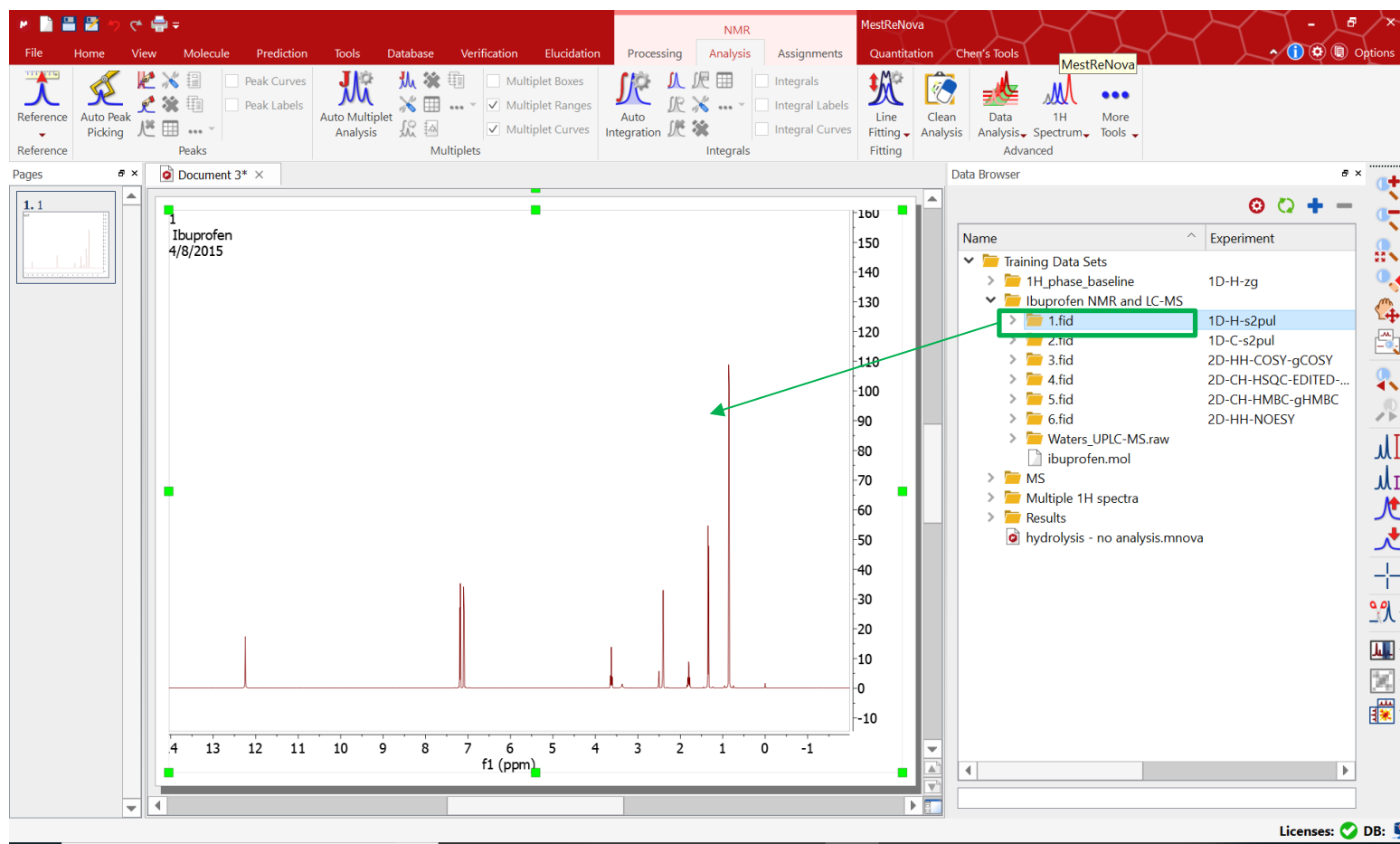
^1H processing and analysis: general procedure



PROCESSING

Open a H-1 spectrum

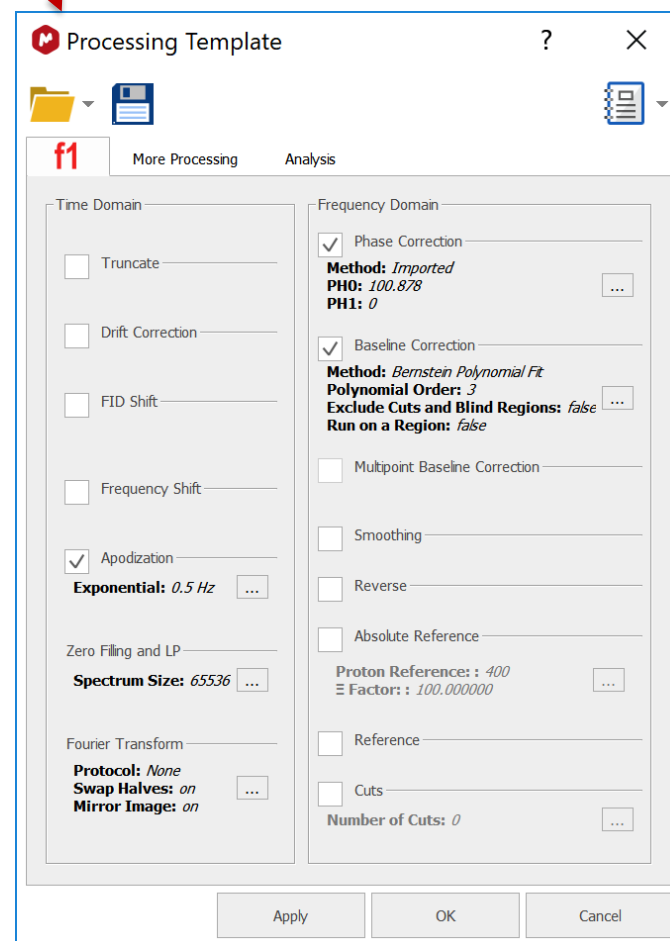
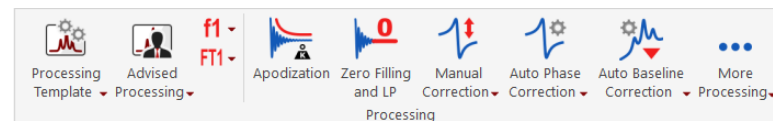
- In Data Browser, expand the folders Training Datasets > Ibuprofen NMR and LC-MS, and drag the “1.fid” folder (1D H-1 spectrum) to the main window.
- Notice the H-1 spectrum is automatically processed and displayed.



PROCESSING

- 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.

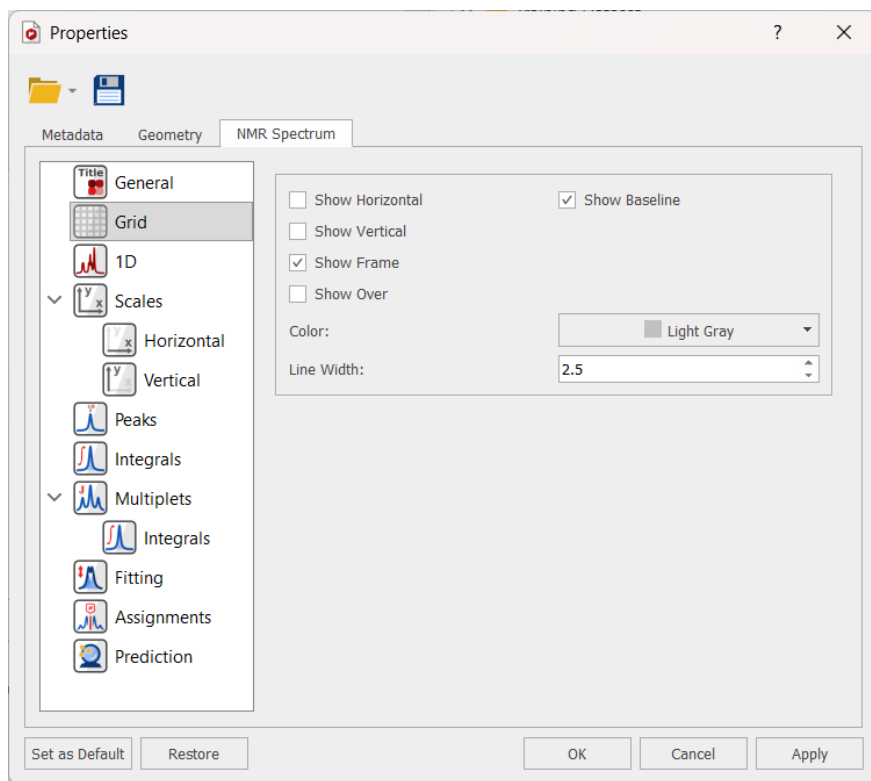
Verify the processing parameters



DISPLAY

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

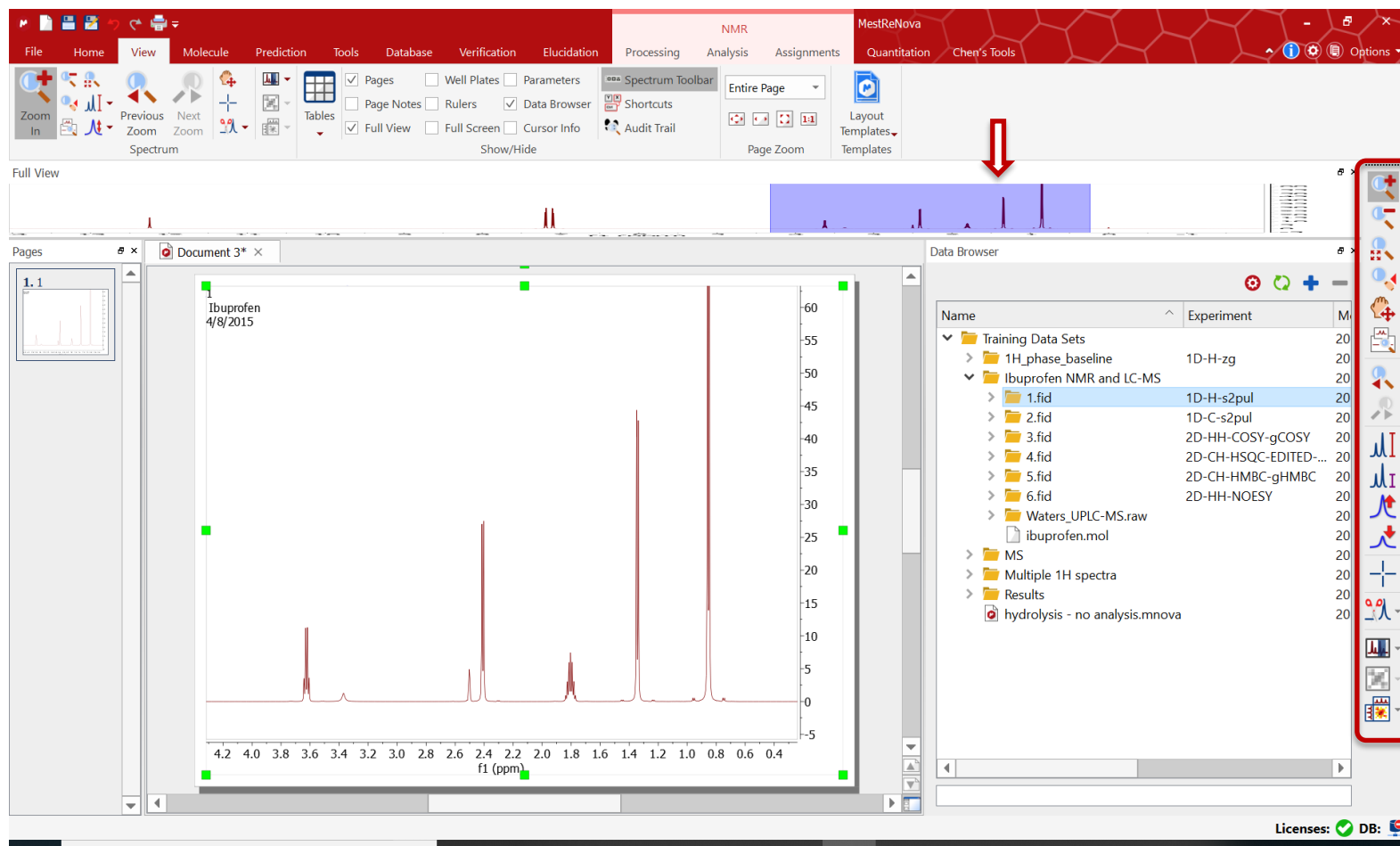


**Starting from Version 14, double-clicking changes the display to full-spectrum if you are in the default pointer mode.*

VISUALIZATION

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 <i>J</i> -couplings
	Cut (or press X) to hide parts of the spectrum
	Edit Blind regions

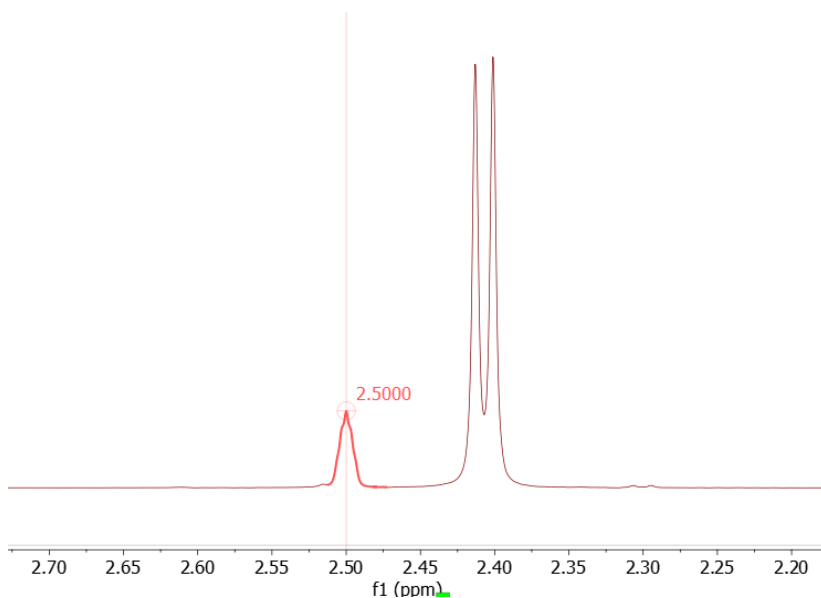
Shortcuts		
	Command	Shortcut
42	View > Full Screen	F11
43	View > Intensity > Decrease	-
44	View > Intensity > Fit to Highest Intensity	H
45	View > Intensity > Increase	+
46	View > Pages	Ctrl+F2
47	View > Pan	P
48	View > Zoom > Full Spectrum	F
49	View > Zoom > Manual Zoom	M
50	View > Zoom > Next Zoom	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

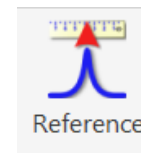
** Press **P** several times to toggle between free/horizontal/vertical panning

ANALYSIS

- 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.



Chemical Shift Referencing



Reference along f1

Old Shift: 2.5021 ppm

New Shift: 2.5000 ppm

Range Width: 0.1000 ppm

☐ Annotation: DMSO-d6


Solvent List

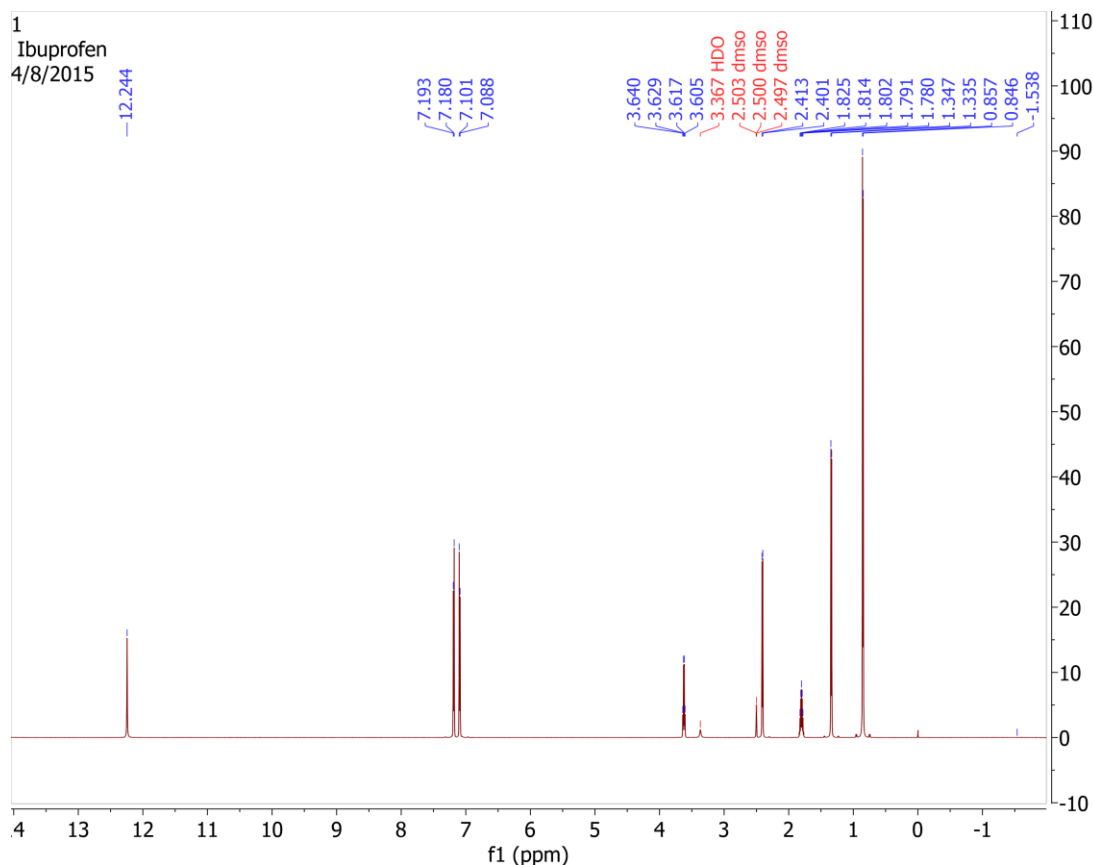
Name	Shift (ppm)	Multiplicity	J (Hz)
Deuterium Oxide	4.790	1	
Dimethyl Sulfoxide-d6	2.500	5	1
	3.330	1	
Ethanol-d6	5.290	1	

Restore Defaults Add... Edit... Delete

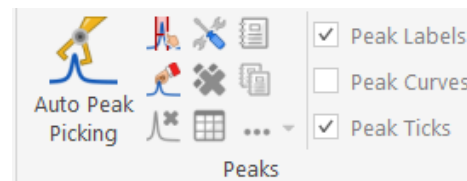
OK Cancel Solvents <<

ANALYSIS

- 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.



Peak picking



Peak Picking Options

Method: GSD

Peaks Type: Only Positive

Settings

Refinement Level: Ref. 1 (2 fitting cycles)

☐ Quantitative GSD


Improvement Cycles: 4

☒ Auto Classify Impurities/Compounds...

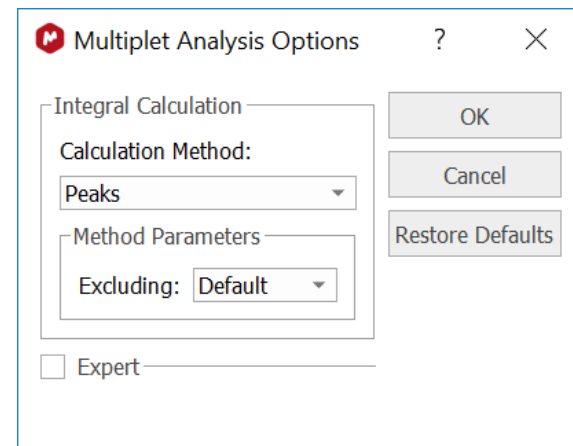
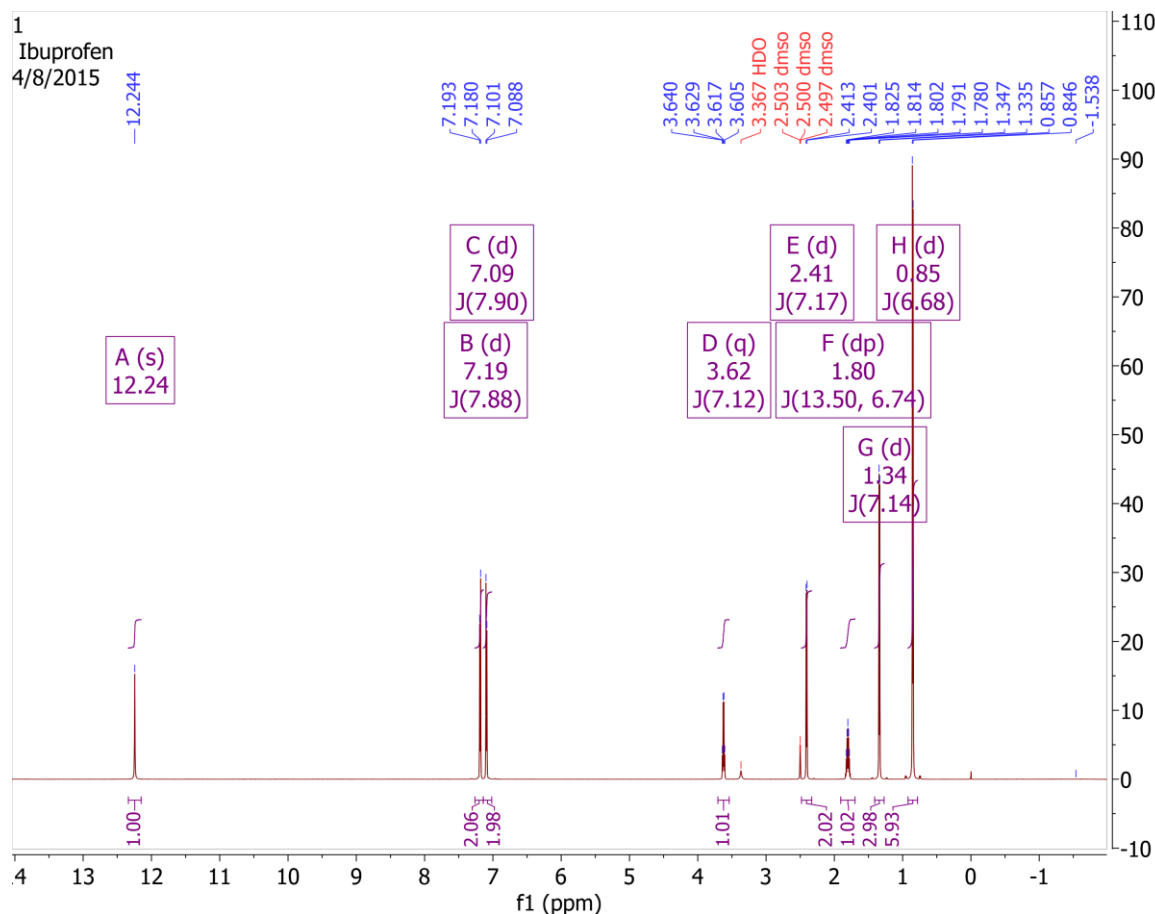
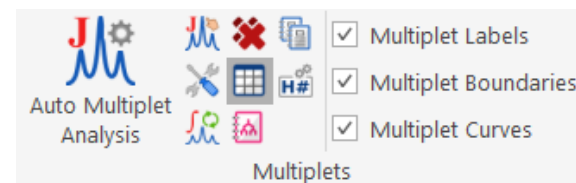
Defaults Advanced <<

OK Cancel

ANALYSIS

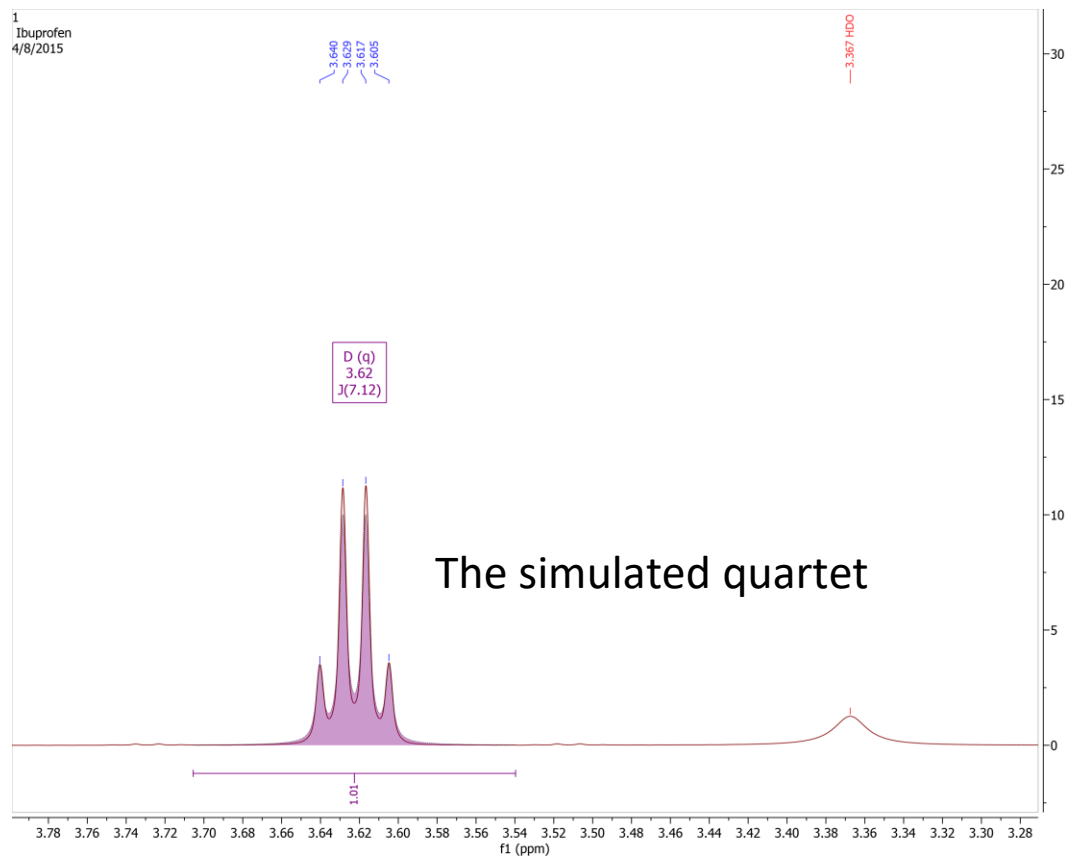
- Click the Multiplets > Options  to verify the multiplet analysis options. Default settings are used here as shown to the right.
- Click the Auto Multiplet Analysis tool to do the multiplet analysis based on the picked peaks

Multiplet analysis



ANALYSIS

- 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

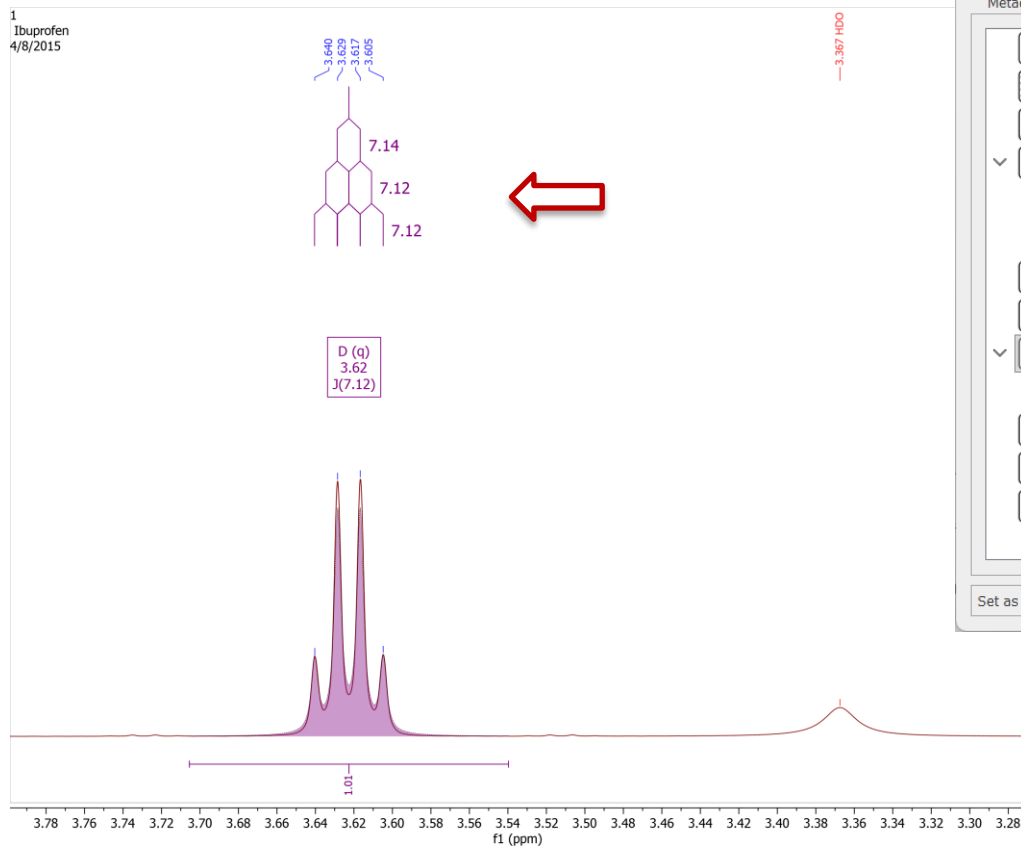
The screenshot shows the 'Multiplet Manager' dialog box. It contains the following fields and controls:

- Name:** D
- Class:** q
- δ:** 3.6194 ppm
- J-List:** 7.18, 7.14, 7.14
- Type:** Compound
- Color:** Purple
- Total Nuclides = 18**
- Nuclides:** 1.00
- Integral:** 1.02
- Absolute:** 702.229
- From:** 3.652
- To:** 3.587

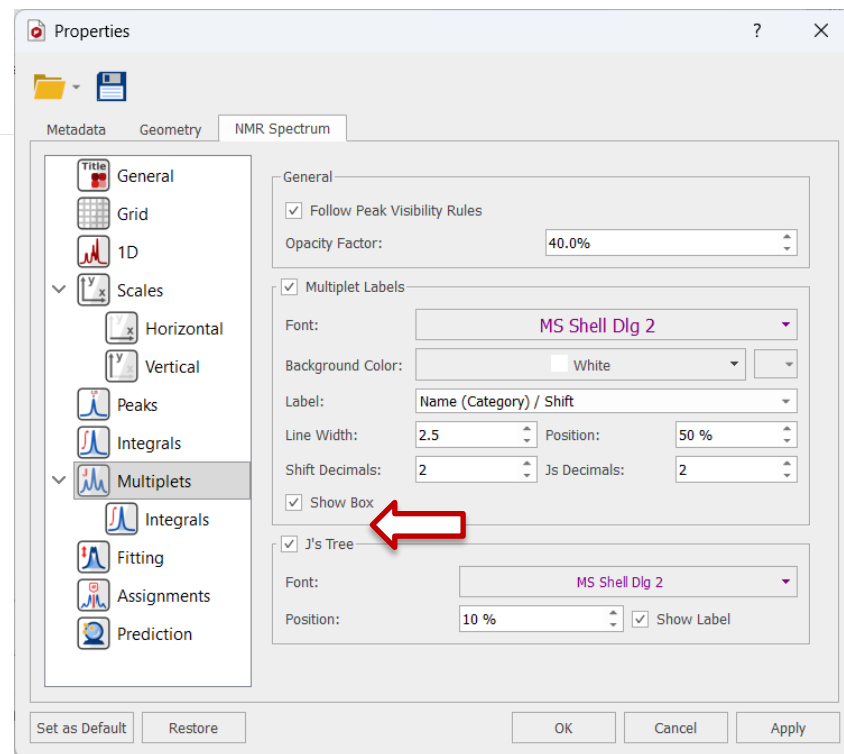
A red arrow points to the 'J-List' field, indicating the coupling constants.

ANALYSIS

- 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.



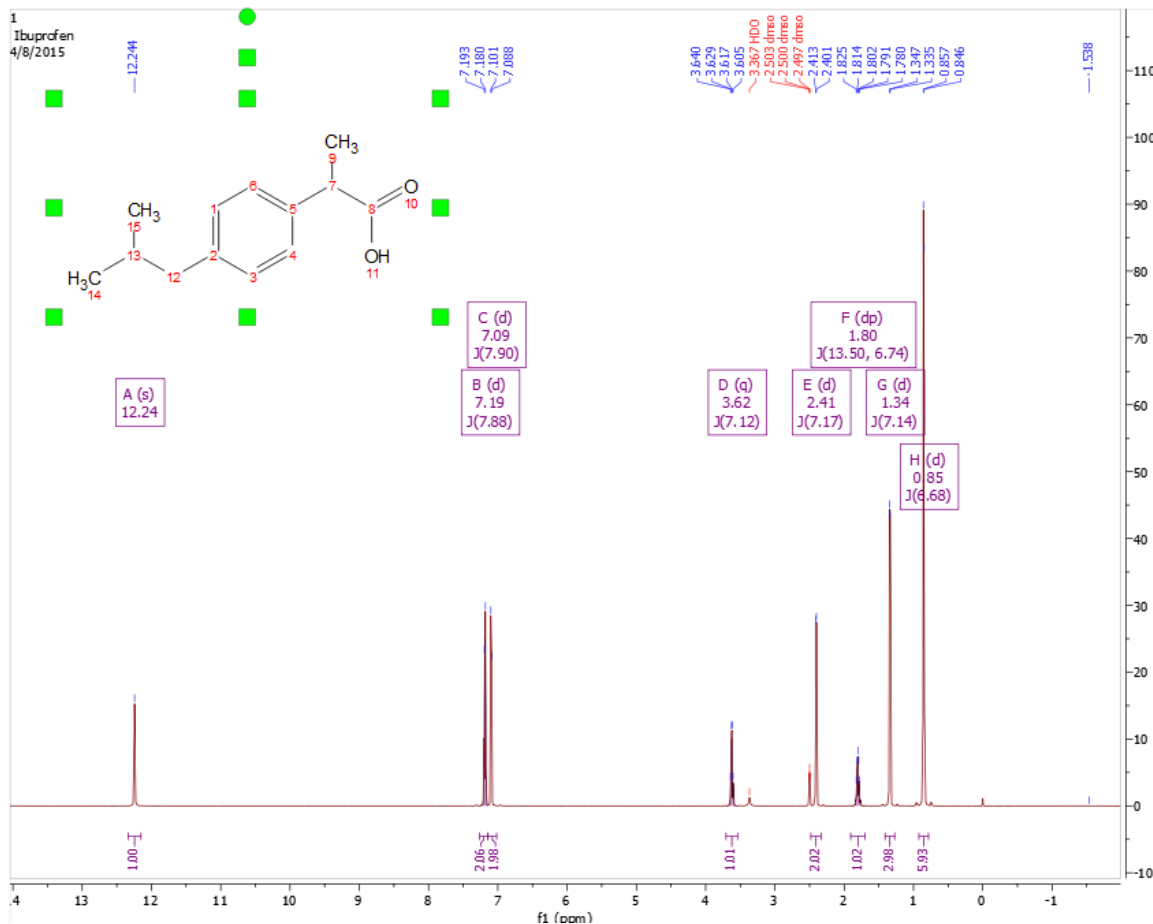
Multiplet Manager



ANALYSIS

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

Verify the number of Hs



Multiplet Manager

3.62 (q, J = 7.1 Hz, 1H)

Name: D Class: q

δ: 3.6194 ppm Auto

J-List: 7.18, 7.14, 7.14

Type: Compound

Color: Purple

Total Nuclides = 18 (18 in molecule)

Nuclides: 1.00 H#

Integral: 1.02

Absolute: 702.229

From: 3.652 To: 3.587

PUBLISHING

- 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

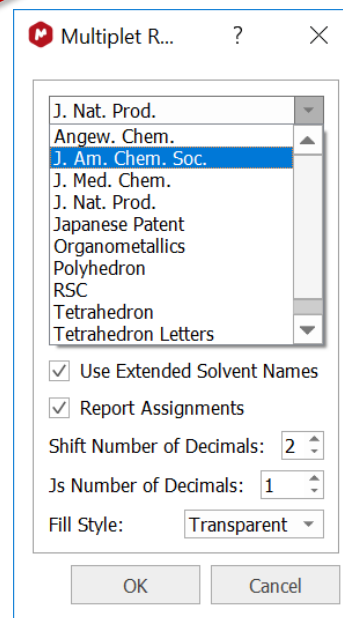
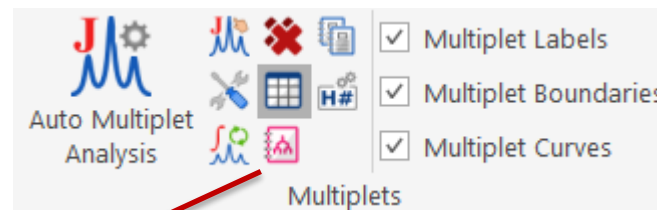
Multiplets

Report Multiplets Copy Multiplets Setup Report Set Type Filter Delete

¹H NMR (600 MHz, DMSO-*d*₆) δ 12.24 (s, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 3.62 (q, *J* = 7.1 Hz, 1H), 2.40 (d, *J* = 7.2 Hz, 2H), 1.80 (dp, *J* = 13.5, 6.8 Hz, 1H), 1.34 (d, *J* = 7.1 Hz, 3H), 0.85 (d, *J* = 6.7 Hz, 6H).

	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

Report the multiplets

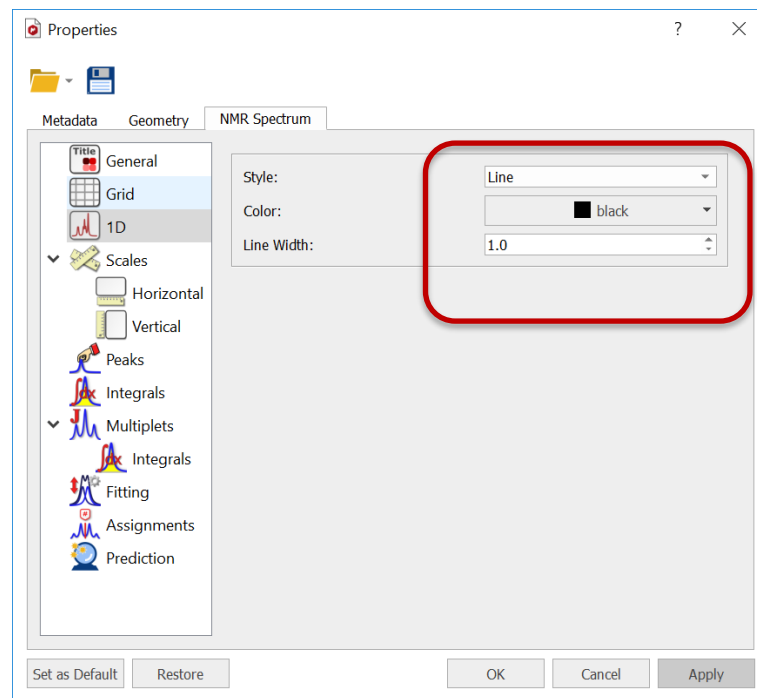
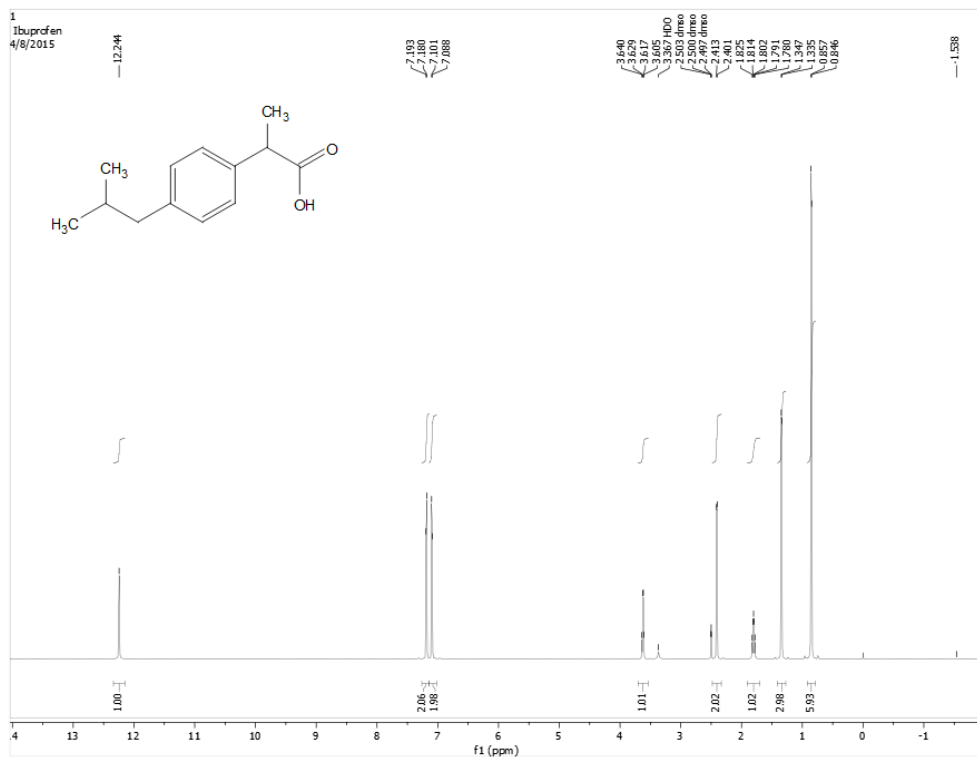


¹H NMR (DMSO-*d*₆, 600 MHz) δ 12.24 (1H, s), 7.19 (2H, d, *J*=7.9 Hz), 7.09 (2H, d, *J*=7.9 Hz), 3.62 (1H, q, *J*=7.1 Hz), 2.41 (2H, d, *J*=7.2 Hz), 1.80 (1H, dp, *J*=13.5, 6.7 Hz), 1.34 (3H, d, *J*=7.1 Hz), 0.85 (6H, d, *J*=6.7 Hz)

PUBLISHING

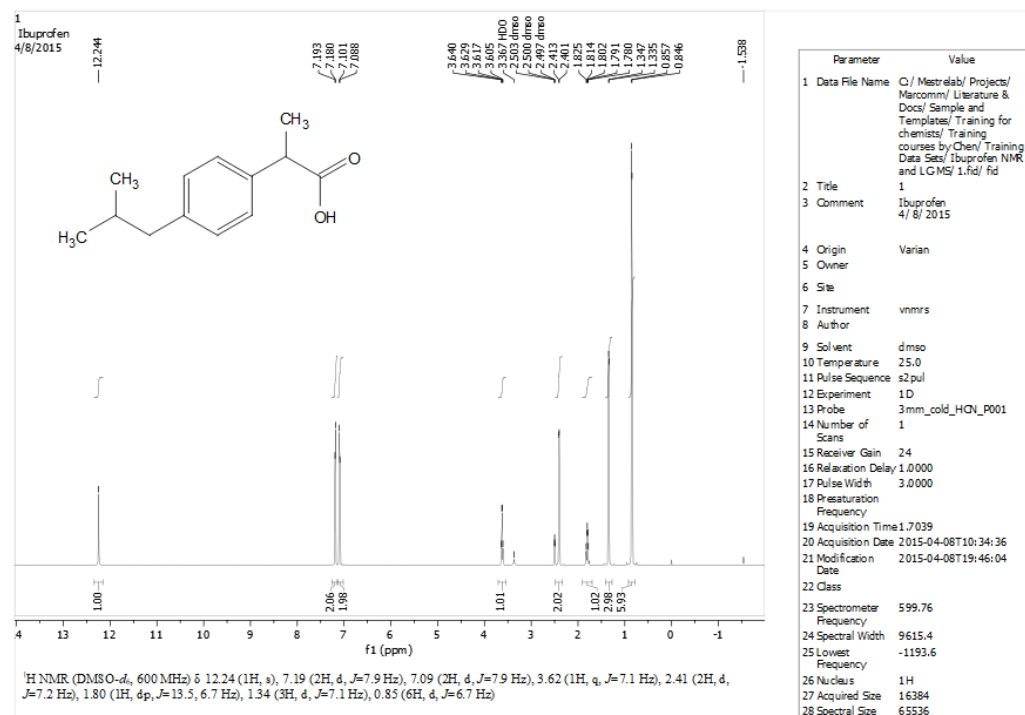
- To publish the spectrum on a black and white journal, double click the spectrum to open the Properties Dialog, and set the 1D properties to as shown on the right.
- Choose other properties to display, such as the peak labels, multiplet labels, integrals, etc.
- Copy the spectrum and structure objects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

Publishing a spectrum



Display the parameters

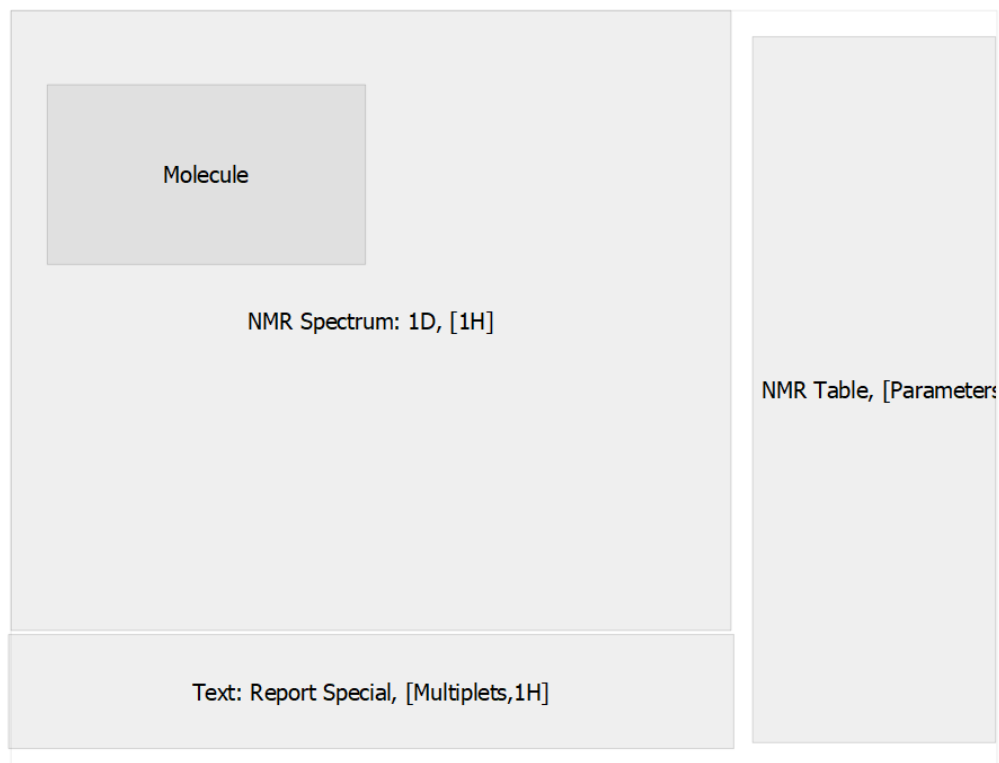
- Check View > Parameters Table to display the Parameters Table, and report the parameters on the spectrum. Manually resize the text box to similar to as shown below.
- Report the multiplets and resize the box to as shown below.



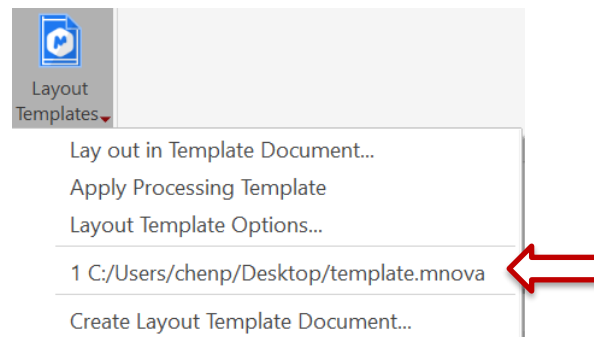
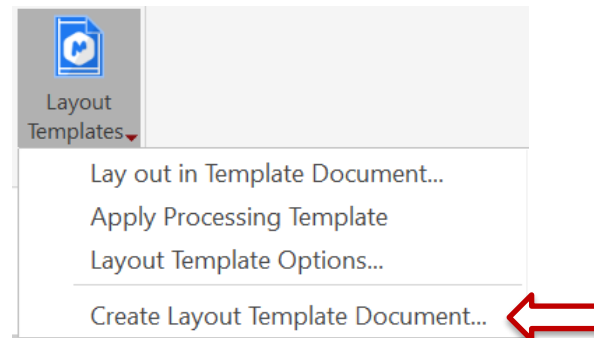
Parameters		
<div> <div>Report</div> <div>Copy</div> <div>Setup</div> <div>Customize</div> </div>		
	Parameter	Value
1	Data File Name	C:/Mestrelab/Projects/Marcomm/Liter...
2	Title	1
3	Comment	Ibuprofen 4/8/2015
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	vnmr5
8	Author	
9	Solvent	dmso
10	Temperature	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

PUBLISHING

- 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.



Create a layout template

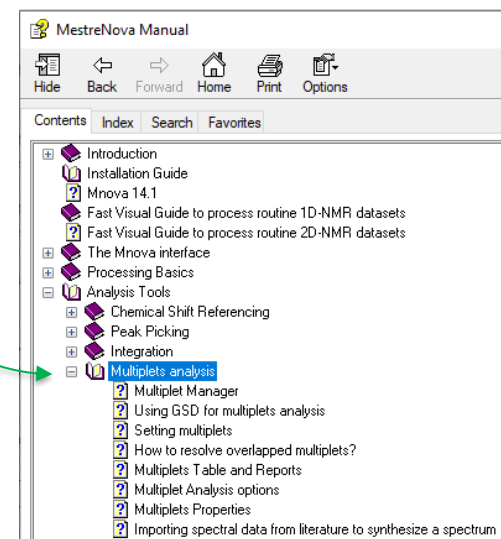
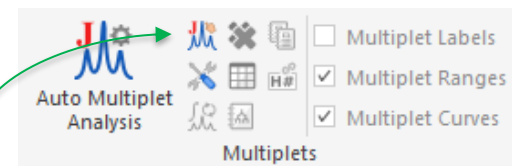


Tip: Mnova uses all pages in the document to create the layout template. So if you have multiple pages, make sure you delete the unwanted ones before creating the layout template.

PROCESSING

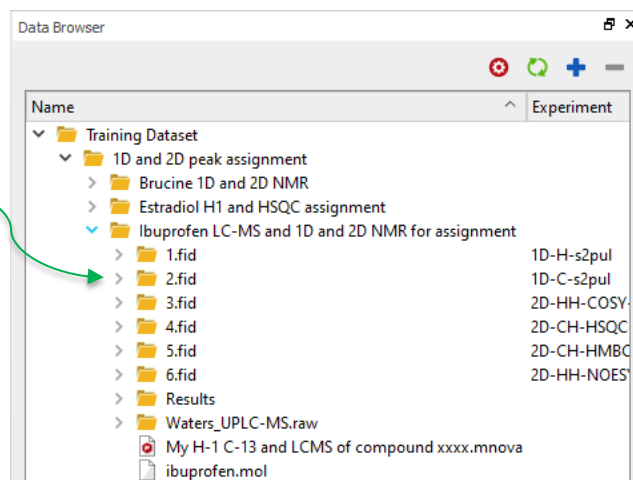
More about H-1 processing

- 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 multiplets. 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



PROCESSING

Open a C-13 spectrum

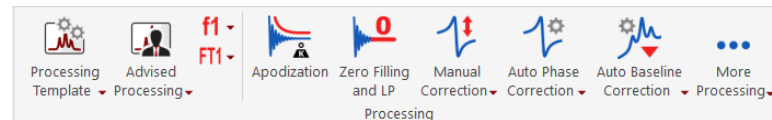
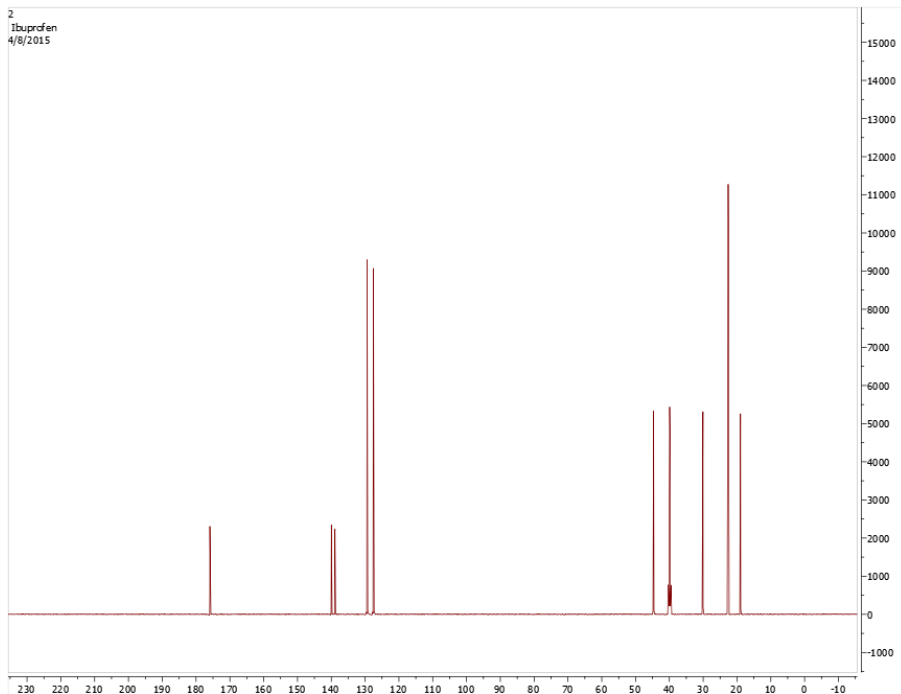
- In Data Browser, open the C-13 spectrum of Ibuprofen by dragging the “2.fid” folder to the main area.

The screenshot displays the MestReNova software interface. The top menu bar includes File, Home, View, Molecule, Prediction, Tools, Database, Verification, Elucidation, Processing, Analysis, Assignments, Quantitation, and Chen's Tools. The main toolbar contains various icons for peak picking, integration, and analysis. The central plot area shows a 1D ¹³C NMR spectrum of Ibuprofen, with peaks labeled from 1 to 14. The x-axis represents chemical shift in ppm, ranging from 230 to -10. The y-axis represents intensity, ranging from -2000 to 26000. The Data Browser panel on the right lists the contents of the 'Ibuprofen NMR and LC-MS' folder, including '1.fid', '2.fid', '3.fid', '4.fid', '5.fid', '6.fid', 'Waters_UPLC-MS.raw', 'ibuprofen.mol', 'MS', 'Multiple 1H spectra', 'Results', and 'hydrolysis - no analysis.mnova'. The '2.fid' folder is highlighted with a green box, and a green arrow points from it to the main spectrum plot area.

PROCESSING

- 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.

Verify the processing parameters



Processing Template

f1 More Processing Analysis

Time Domain

☐ Truncate

☐ Drift Correction

☐ FID Shift

☐ Frequency Shift

☒ Apodization
Exponential: 2 Hz

Zero Filling and LP
Spectrum Size: 65536

Fourier Transform
Protocol: None
Swap Halves: on
Mirror Image: on

Frequency Domain

☒ Phase Correction
Method: Imported
PH0: 70.4187
PH1: -23.8171

☒ Baseline Correction
Method: Whittaker Smoother
Median Filter: Autodetect
Smooth Factor: Autodetect

☐ Smoothing

☐ Reverse

☐ Absolute Reference
Proton Reference: : 599.76
Factor: : 25.145020

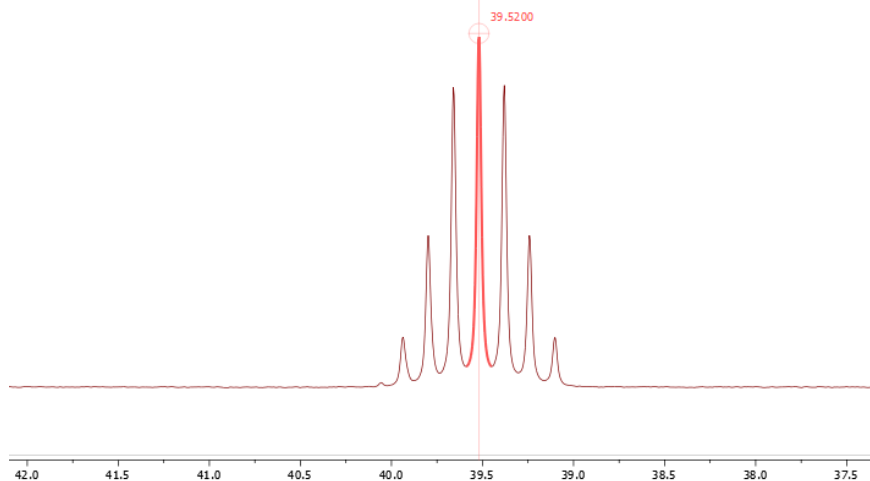
☐ Reference

☐ Cuts
Number of Cuts: 0

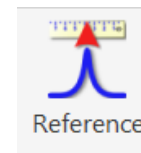
Apply OK Cancel

ANALYSIS

- 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.



Chemical Shift Referencing



Reference along f1

Old Shift: 39.9239 ppm

New Shift: 39.5200 ppm

☐ Auto Tuning

Range Width: 0.1000 ppm

☐ Annotation DMSO-d6


Solvent List

Name	Shift (ppm)	Multiplicity
Cyclohexane-d12	26.430	5
Dimethyl Sulfoxide-d6	39.520	7
Ethanol-d6	56.960	5
	17.310	7

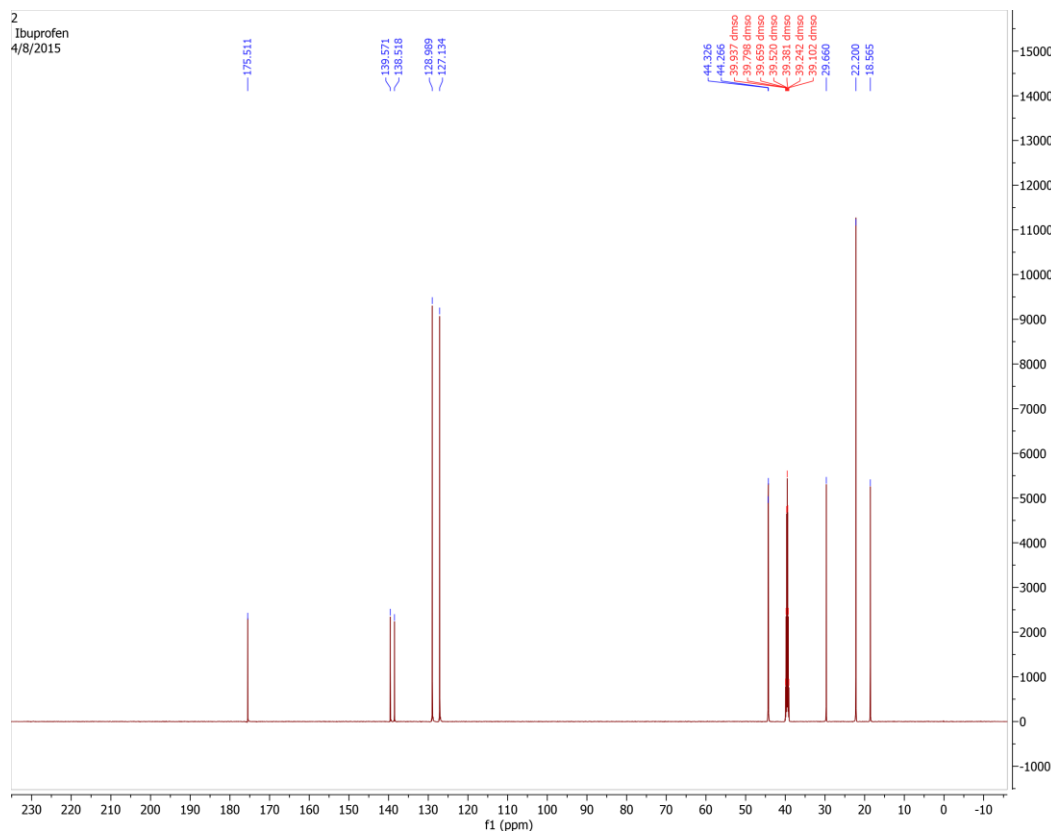
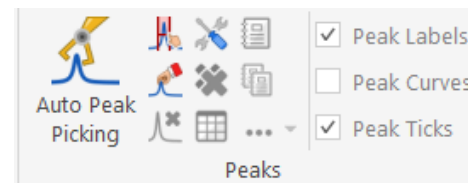
Restore Defaults Add... Edit... Delete

OK Cancel Solvents <<

ANALYSIS

- 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.

Peak picking



Peak Picking Options

Method: GSD

Peaks Type: Only Positive

Settings

Refinement Level: Ref. 1 (2 fitting cycles)

☐ Quantitative GSD

Improvement Cycles: 4

☒ Auto Classify Impurities/Compounds...

Defaults Advanced <<

OK Cancel

PUBLISHING

- 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

Report the C-13 peaks

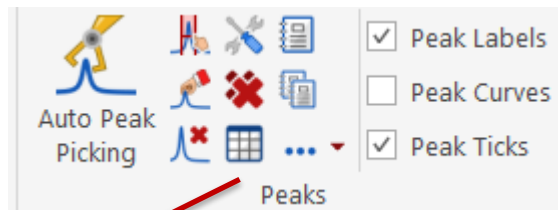
Peaks

Report Peaks ▾ Copy Peaks ▾ Setup Report ▾ Delete Select Peaks

Sync From Spec Filter Sync To Spec Set Flags Set Compound New Spectrum

¹³C NMR (151 MHz, dms_o) δ 175.51, 139.57, 139.37, 138.52, 138.31, 128.99, 127.13, 44.33, 44.27, 40.06, 39.94, 39.80, 39.66, 39.52, 39.38, 39.24, 39.10, 29.66, 29.54, 22.20, 18.57.

	ppm ▾	Intensity	Width	Area	Type	Flags	Impurity/Compound	Annotation
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		



Setup Peak R... ? X

J. Am. Chem. Soc. ▾

☐ Ascending order shifts

☐ Ascending order of Js

☒ Only report compound peaks

☐ Report 13C assignments

☐ Report 13C multiplicity

☒ Use Extended Solvent Names

Number of decimals: 1 ▾

Fill style : Transparent ▾

2D

☐ Report as points

☒ Report f1

☒ Report f2

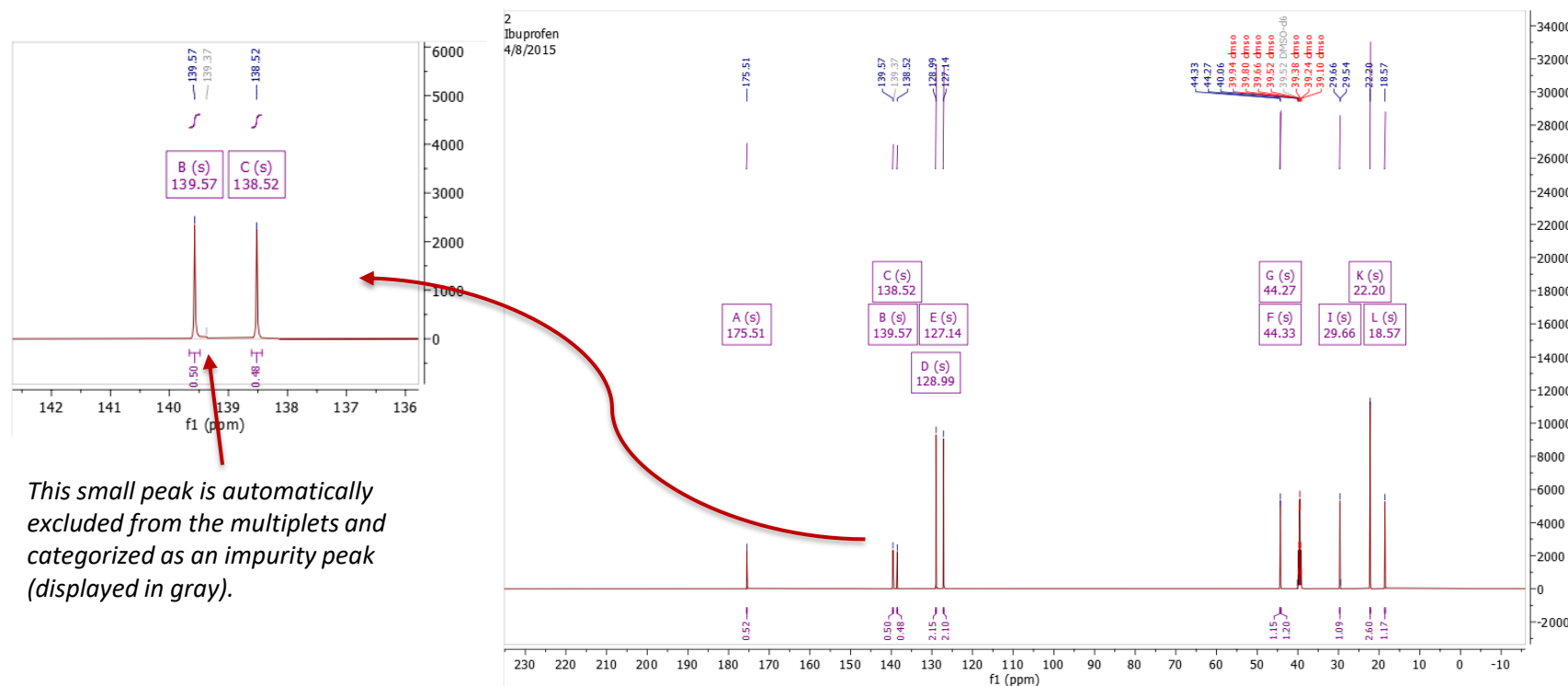
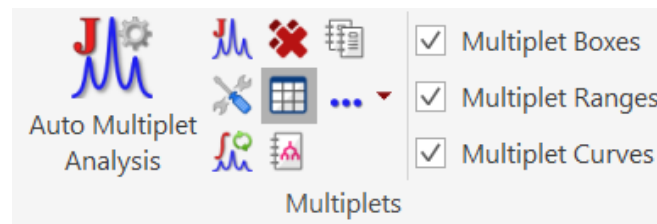
OK Cancel

¹³C 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.

ANALYSIS

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

Multiplet Analysis



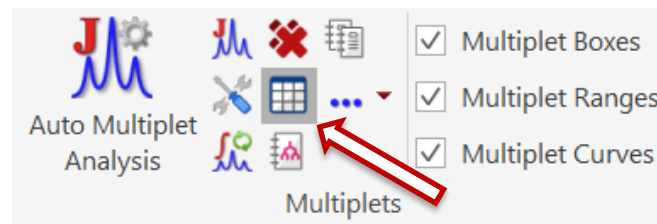
This small peak is automatically excluded from the multiplets and categorized as an impurity peak (displayed in gray).

**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.*

ANALYSIS

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

Report C-13 “Multiplets”



Multiplets

Report Multiplets Copy Multiplets Setup Report Set Type Filter Delete

¹³C 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.

	lam	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

Setup Multiplet Report

J. Am. Chem. Soc.

General

☒ Use extended solvent names ☐ Pentaplets as pent

☐ Add assignments

Chemical Shifts

☐ Ascending order

Number of decimals: 2

Show As Ranges

☐ All ☒ Only Multiplets (m)

☒ Report Js

☐ Ascending order

Number of decimals: 1

☒ Reduce J list ☐ Add assigned coupling atoms

Appearance

☒ Use HTML

Font: Times New Roman Color: [Black]

Fill style: Transparent

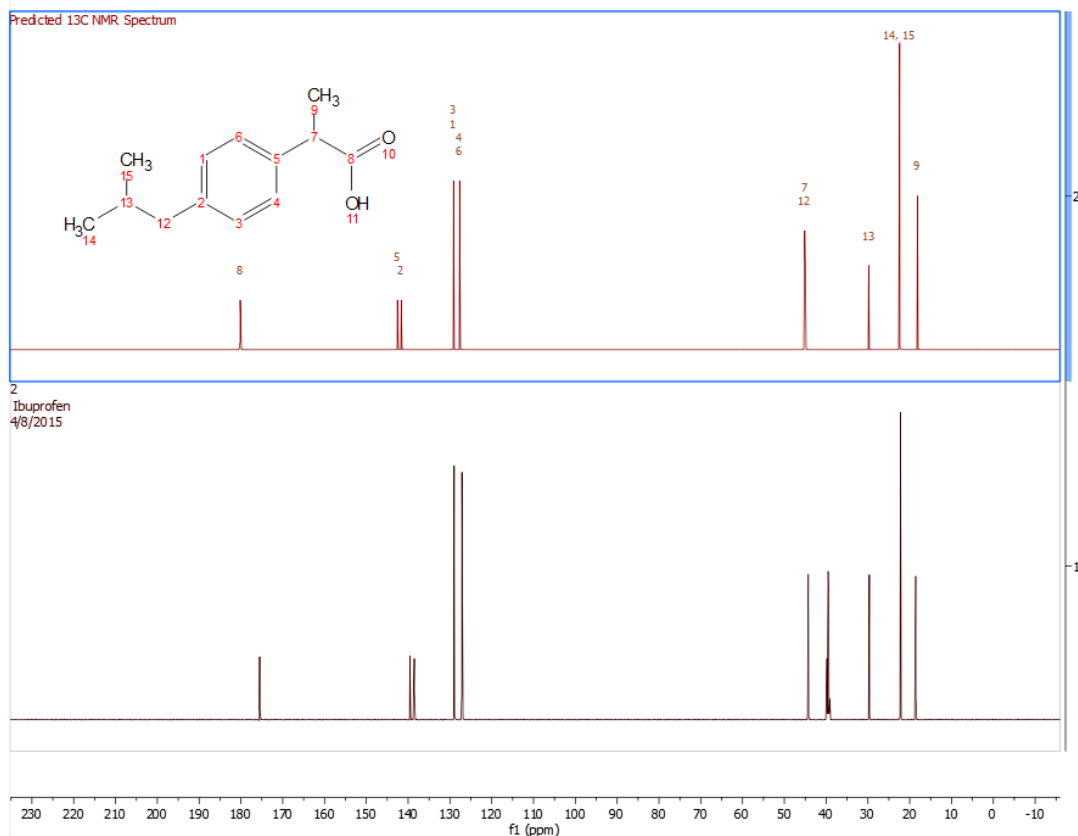
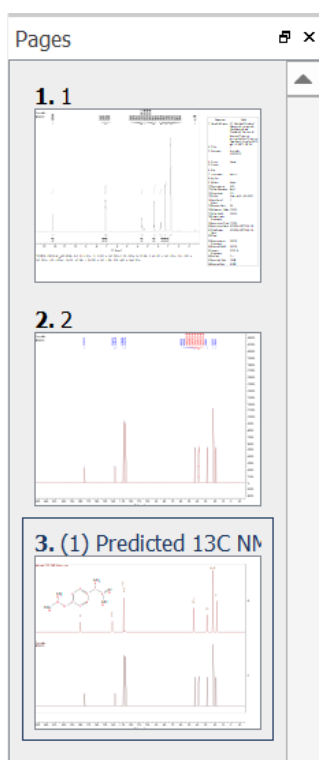
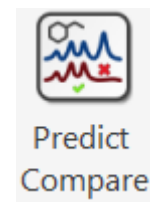
OK Cancel

¹³C 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

PREDICTION

- 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.

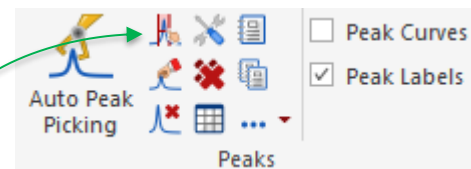


Tip: if you want to delete the predicted C-13 spectrum from the stack, choose Stacked > Stacked Items Table, and use the Delete tool in the Table to delete the predicted C-13 spectrum.

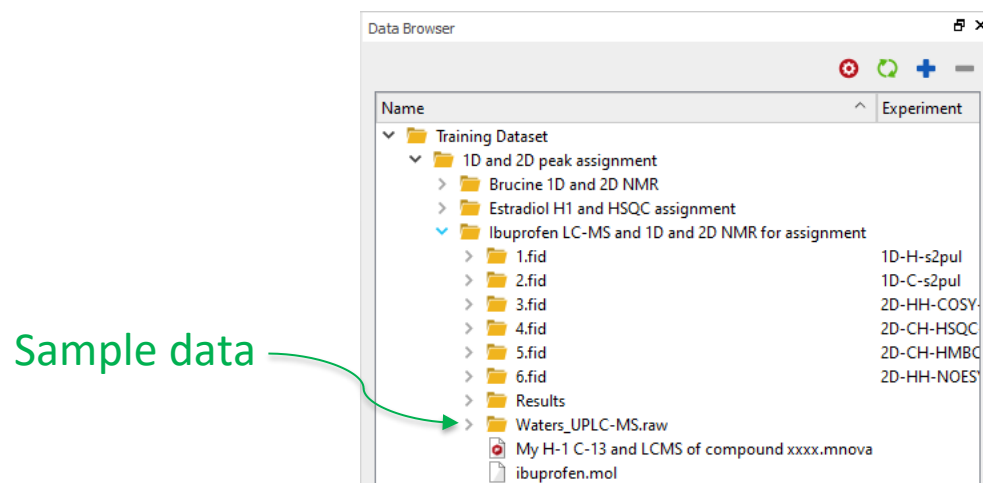
PROCESSING

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 there are F-C couplings, and report the results from the Multiplet Table.



LC/MS Processing, Analysis, and Reporting



Open the LC-MS data

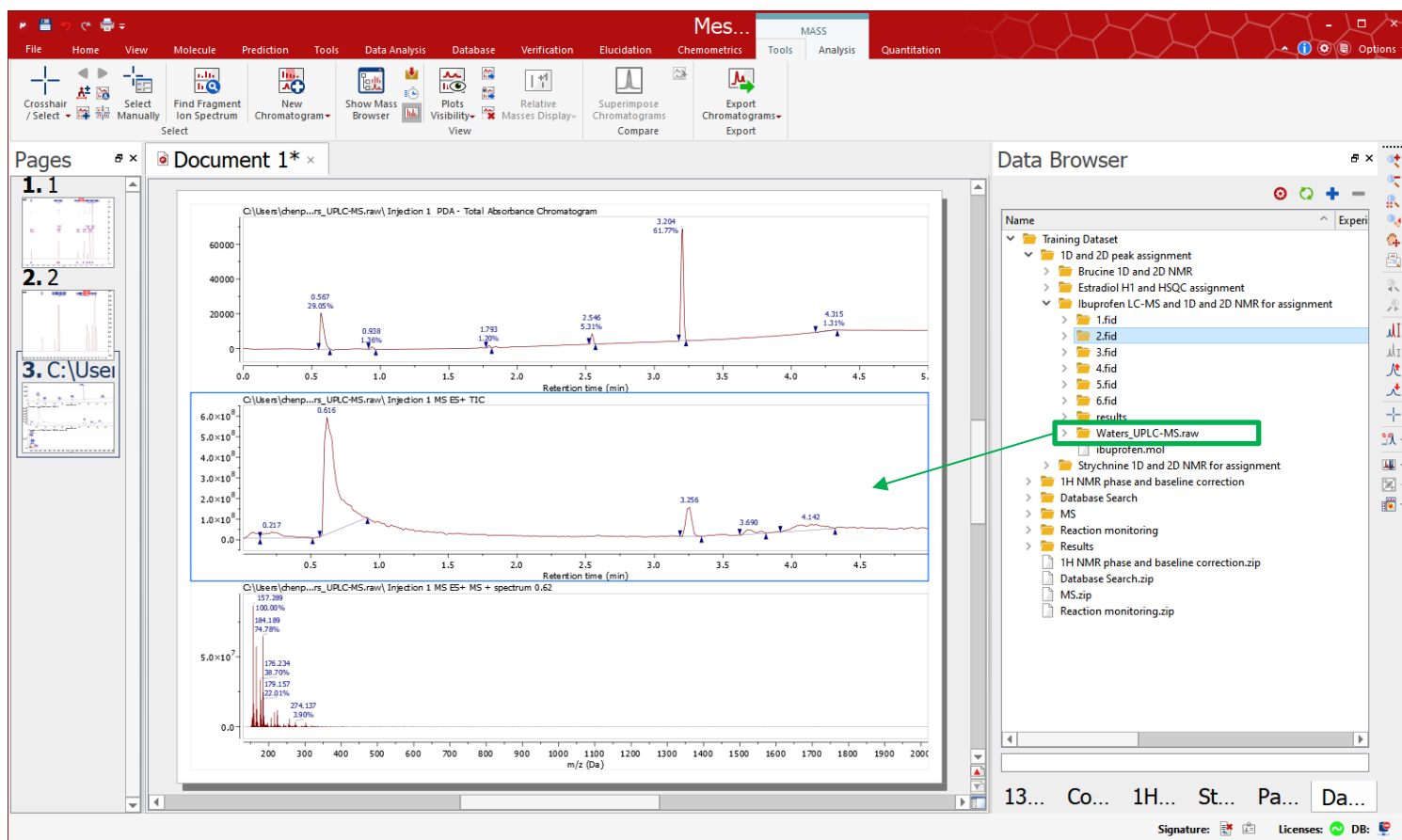
LC-MS

- 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



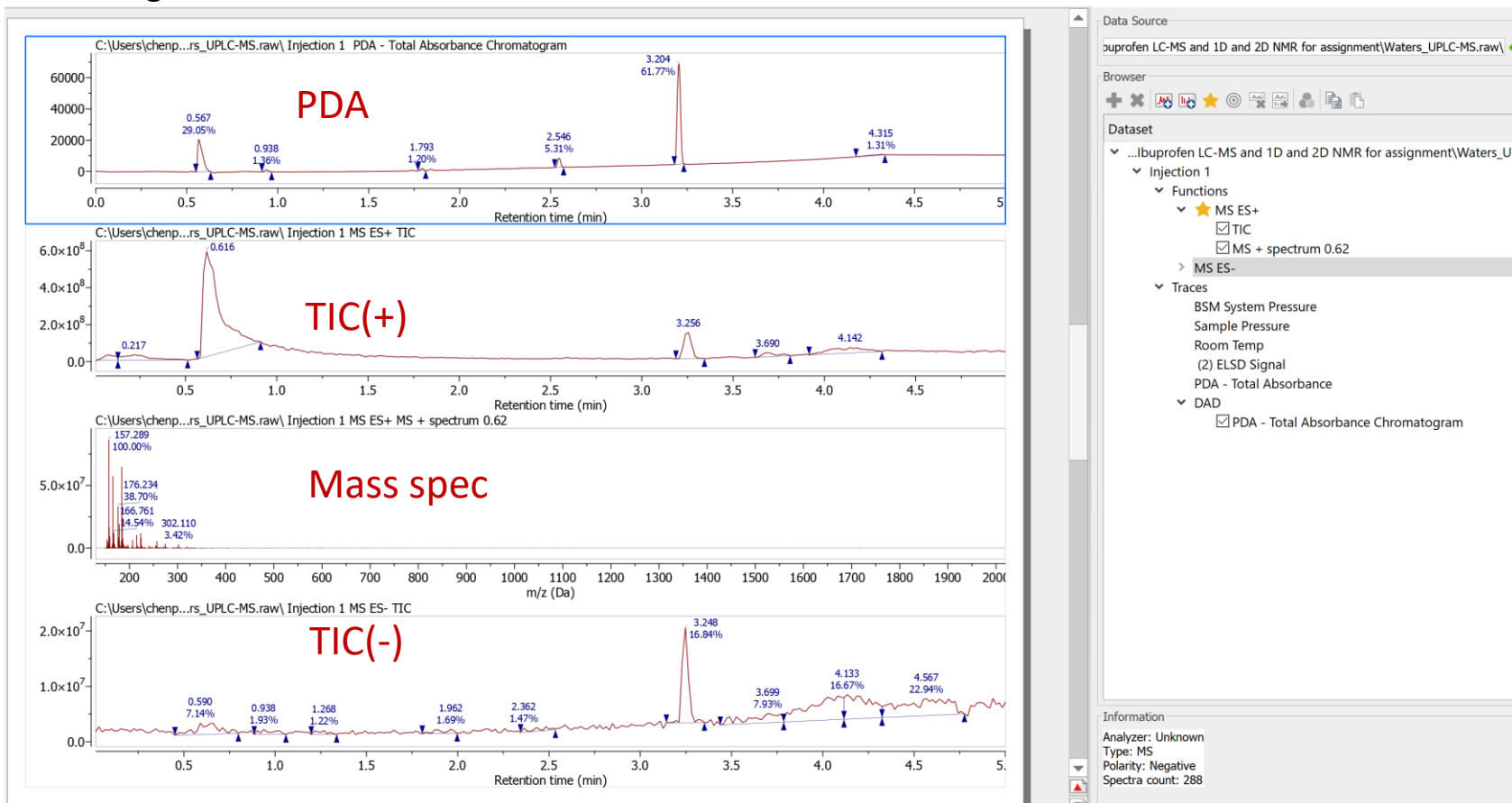
VISUALIZATION

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.



Show Mass
Browser

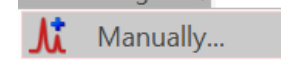
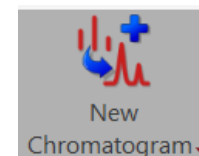
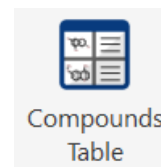
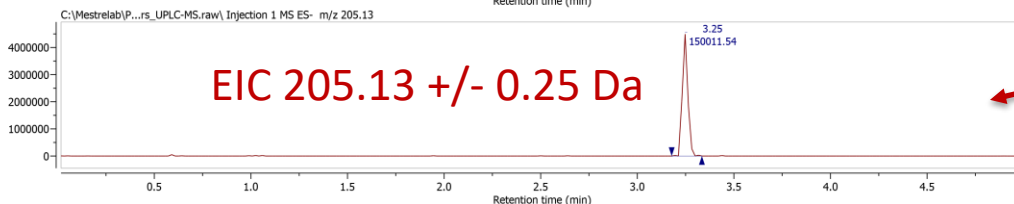
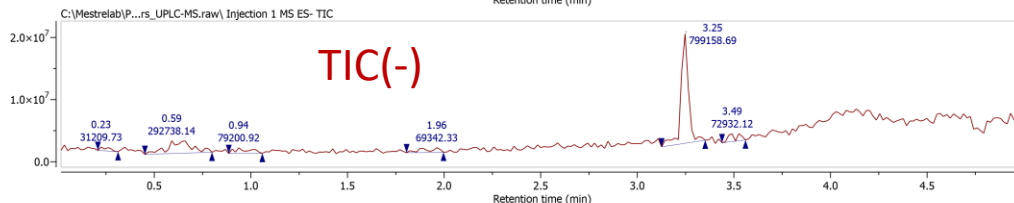
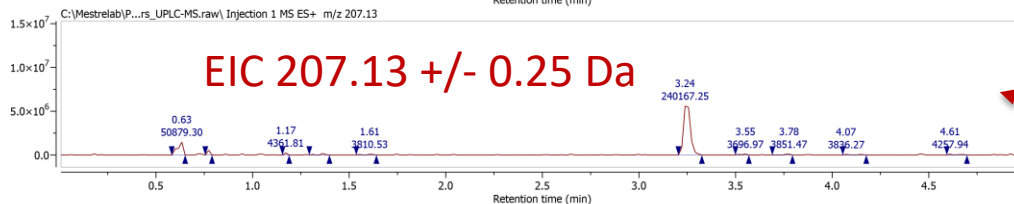
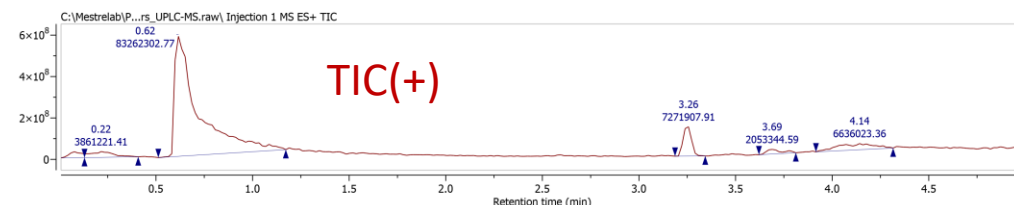


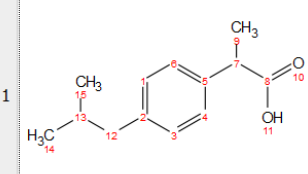
*If the Mass Browser is closed, you can open it using the Show Mass Browser tool in the MASS Tools ribbon.

Verify the elemental composition

ANALYSIS

- Open the Ibuprofen.mol file from the Data Browser.
- Choose Molecule > Compound Table to find its monoisotopic mass: 206.13
- Highlight 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 Ion Chrom., EIC)



Compounds	
Report	Add
Delete	Setup
Graphical Props	PhysChem
In Columns	
Molecule	Properties
	Molecular Formula: C ₁₃ H ₁₈ O ₂
	Average Mass: 206.28
	Monoisotopic Mass: 206.13
	Name: ibuprofen.cdx
	Label: ibuprofen
	Color: <input checked="" type="checkbox"/> None
	Assignments: <input type="checkbox"/>

New chromatogram

Range

From: 207.13 m/z

To: 207.1300 m/z

Tolerance: 0.250 Da

OK Cancel

New chromatogram

Range

From: 205.1300 m/z

To: 205.1700 m/z

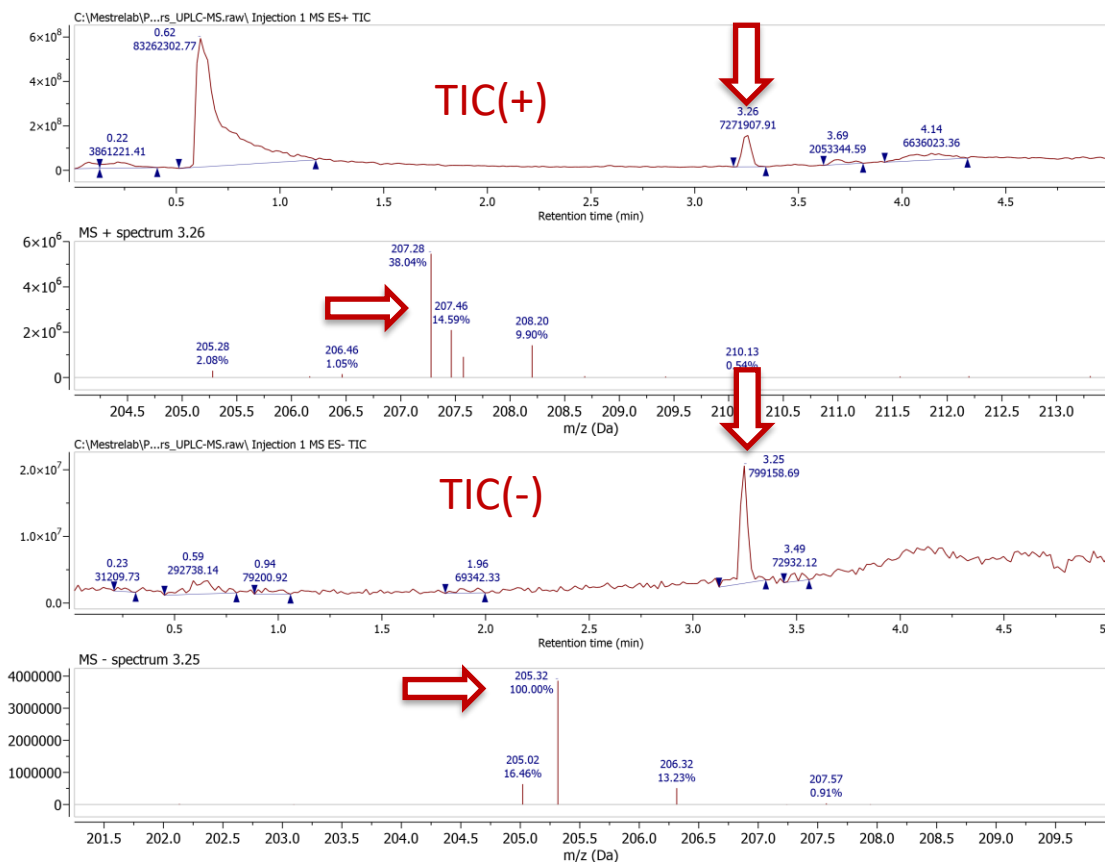
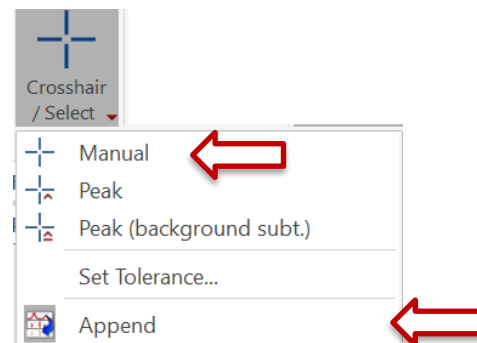
Tolerance: 0.250 Da

OK Cancel

ANALYSIS

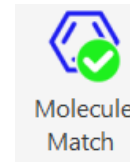
Find the molecule ion peaks

- 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.

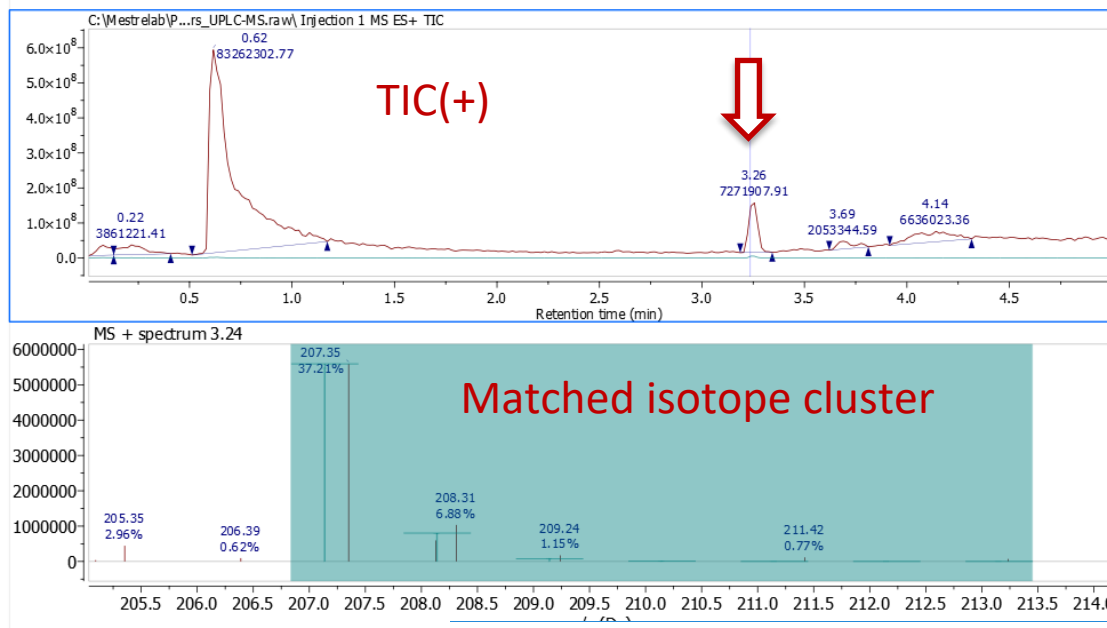


Tip: Use the Mass Browser to hide or delete unwanted plots. Right-click on a plot and choose Move up/Move Down etc. to re-order of the plots

Use Mol Match to verify the elemental composition



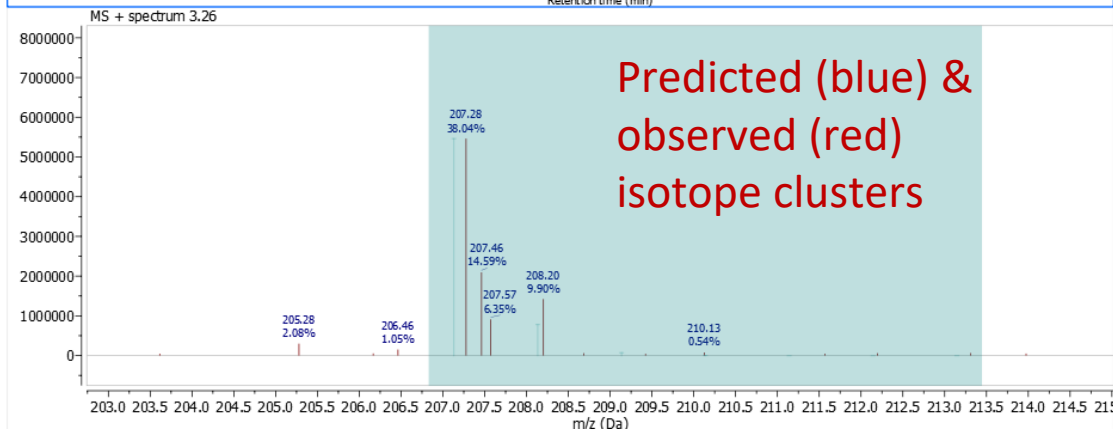
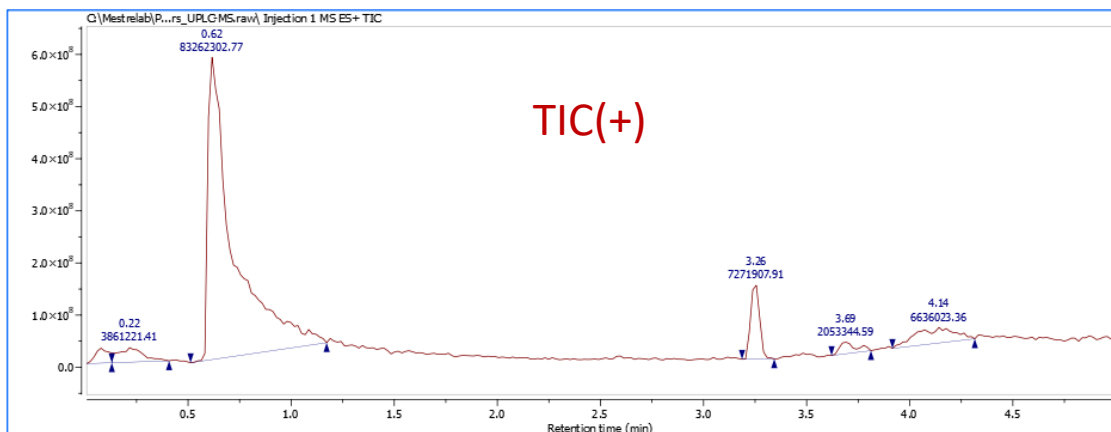
- Open the Ibuprofen.mol. Click Molecule Match.
- The Molecule Match Table shows the matching results.
- Click on the structure in the table to display the mol match results on the spectrum



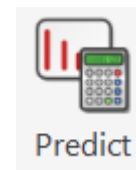
Molecule Match												
Report	Molecule Match	View	Settings	Setup								
	Molecule	Formula	Molecular Weig	Match	Match Score	Similarity	MS Purity	RT	Scan	Purity	Matcd	Adduct/Loss
1		C ₁₃ H ₁₈ O ₂	206.131	✓	0.948	0.948	0.051	3.24	187	100.00%	H+ / —	

ANALYSIS

- 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.



Predict and verify the molecule ion peaks



Molecular Formula ? X

Molecular Formula:

Recent

- C₁₃H₁₈O₂
- C₂₇H₃₃NO₂Cl
- C₁₉H₃₈N₂O₂

Compounds

	Formula	Weight
1	C ₁₃ H ₁₈ O ₂	206.1307

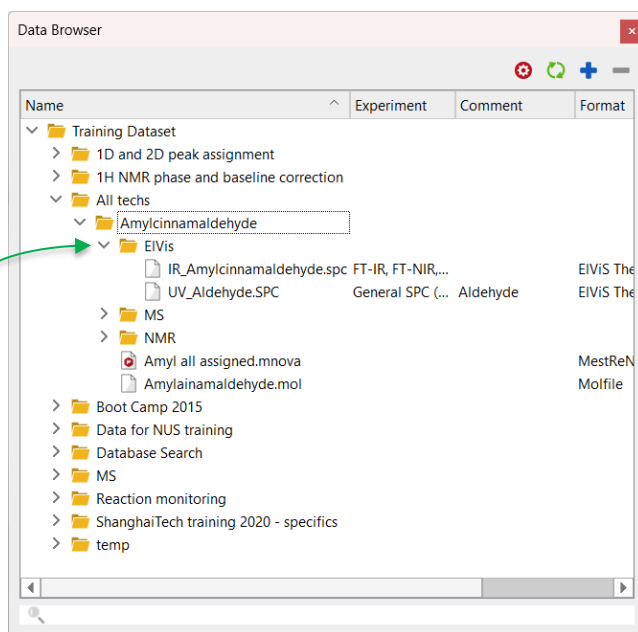
Mass Prediction X

Report Copy Highlight Export Delete Clear Setup

	Formula	Adduct / Loss	rgc SI	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 ₃ OH ⁺ / —	+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 ₂ OH ⁺)	-2	84.04750	✓
9	C ₁₃ H ₁₈ O ₂	Br ⁻ / —	-1	285.04957	✓

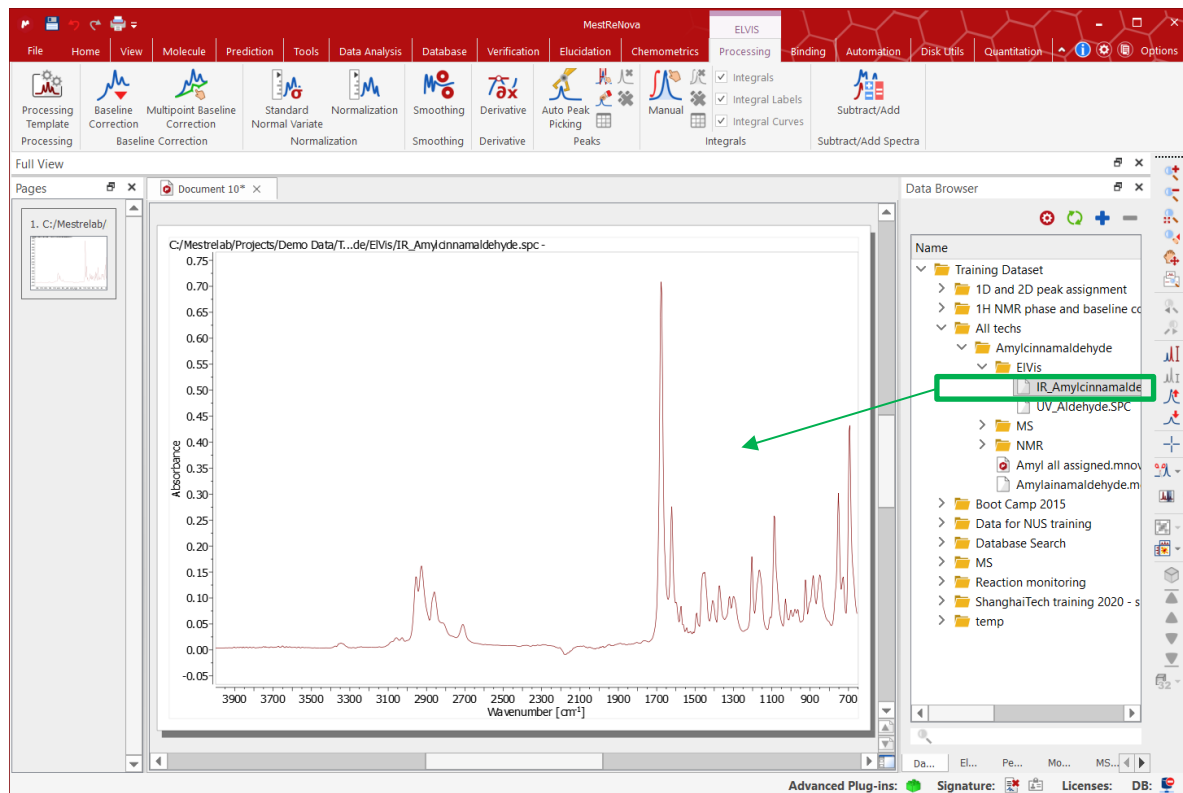
Visualization of IR and UV Spectra, etc.

Sample data



Open the IR data

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



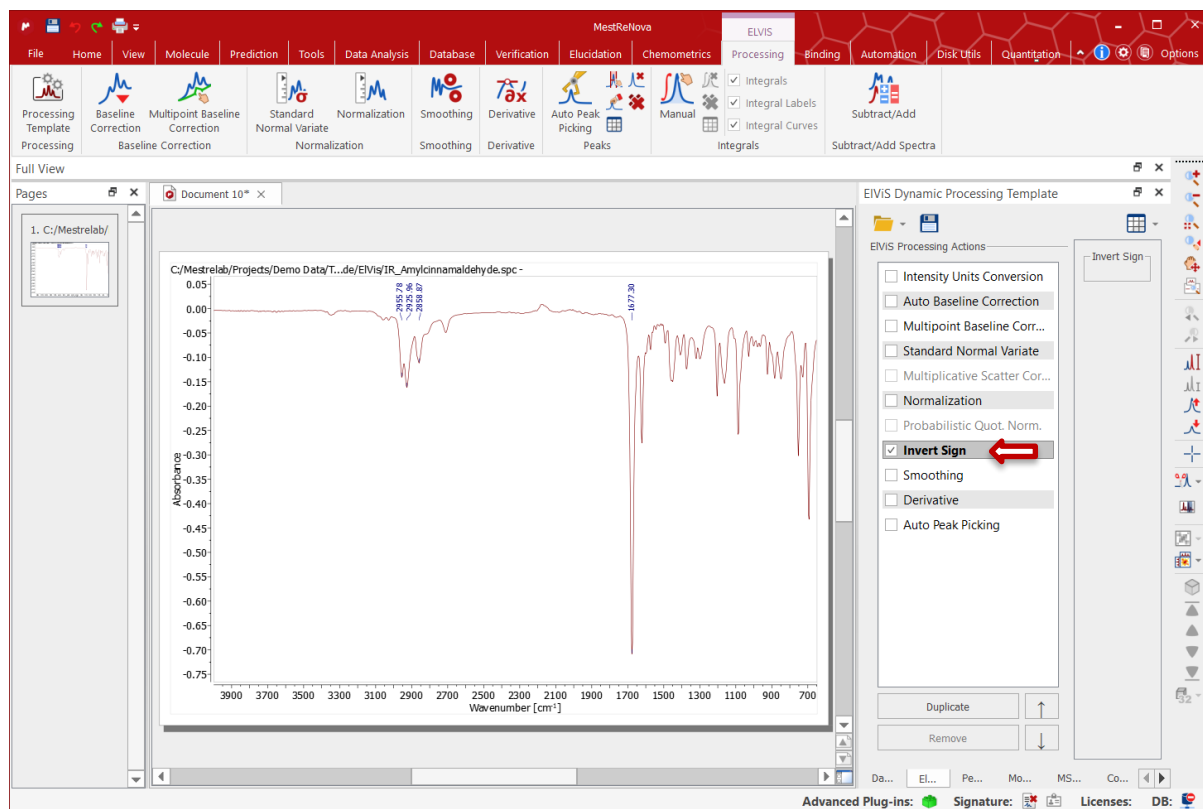
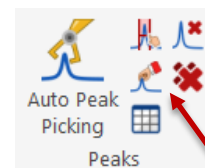
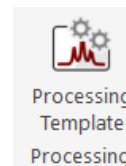
The main formats supported by Mnova
EIVIS:

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

IR

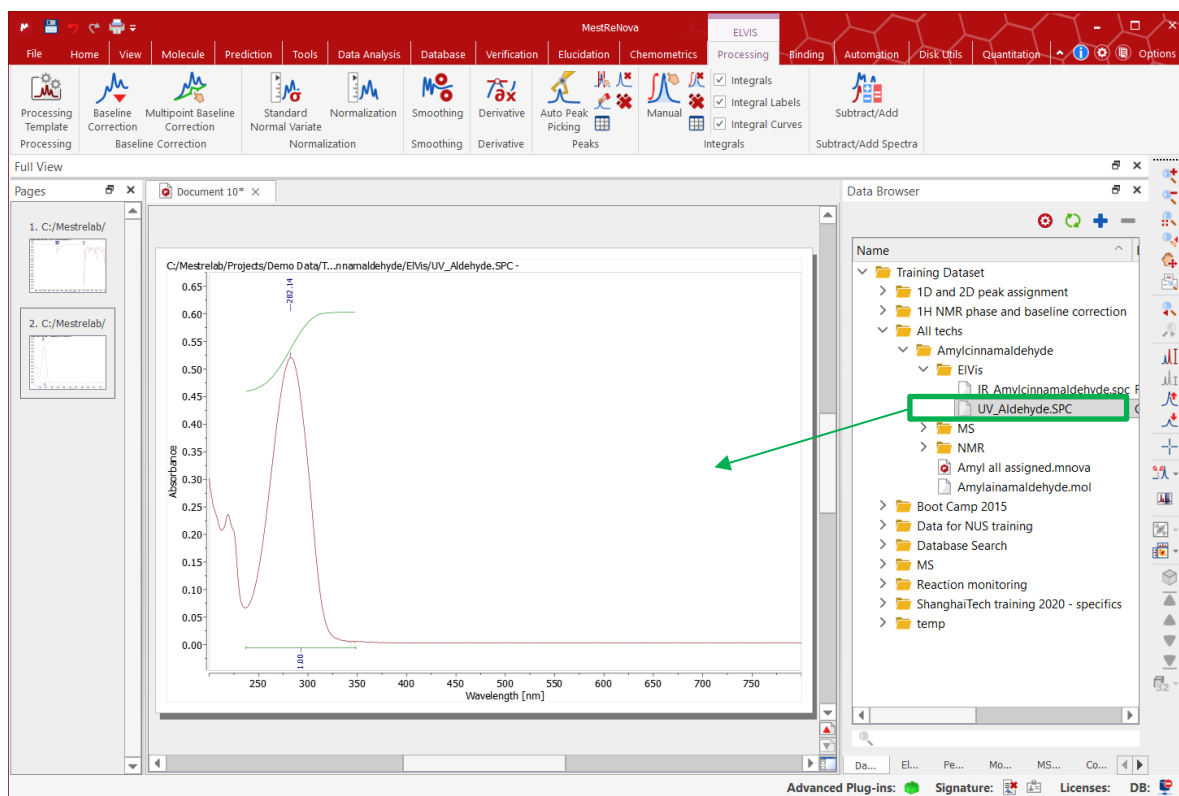
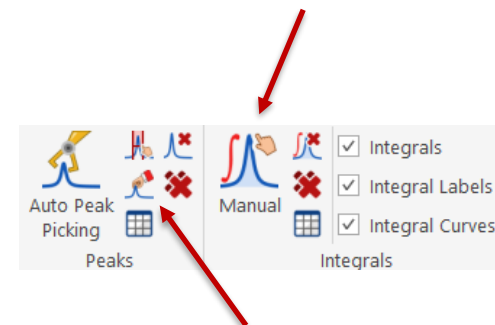
Open the IR data

- 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

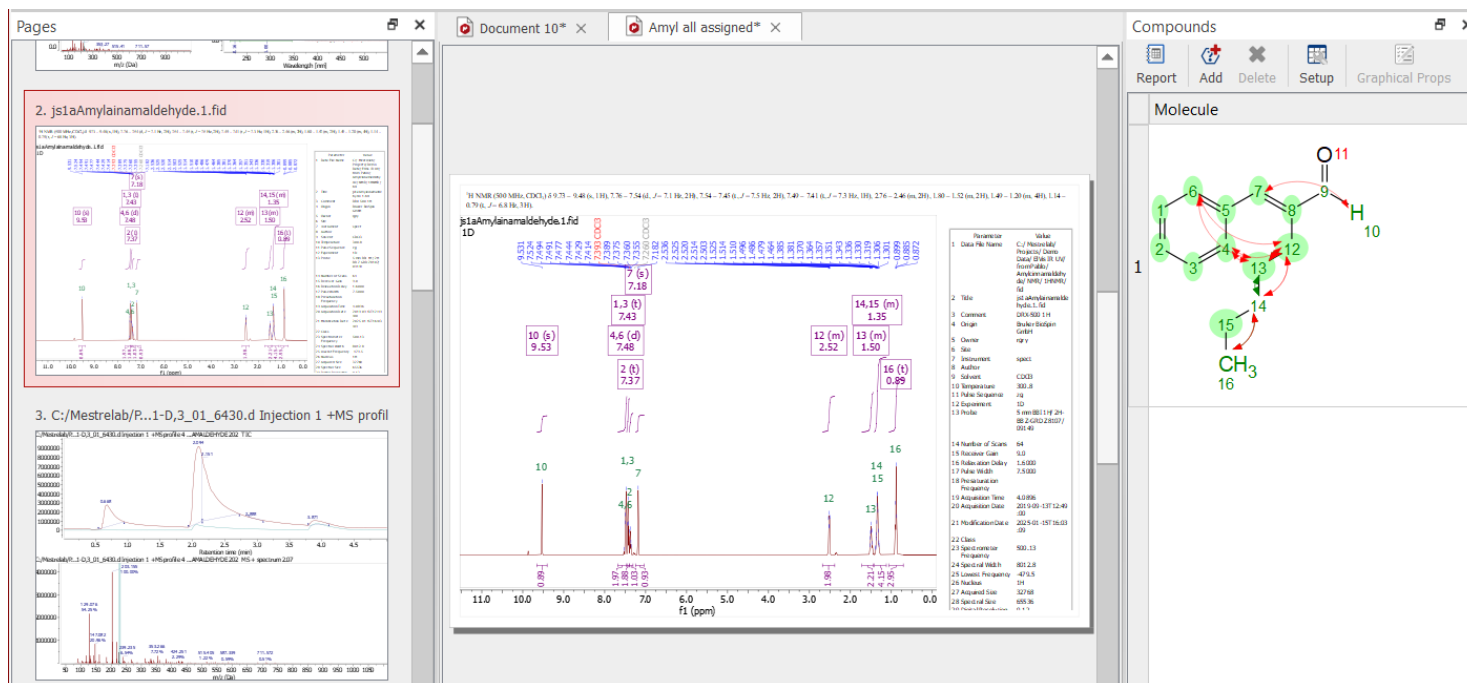
- In Data Browser, open the UV data of Amylinalmaldehyde.
- Use the Peak by Peak tool to pick peaks.
- Use the Manual Integration tool to integrate peak.



Open the HNMR and LC-MS data

NMR and LC-MS

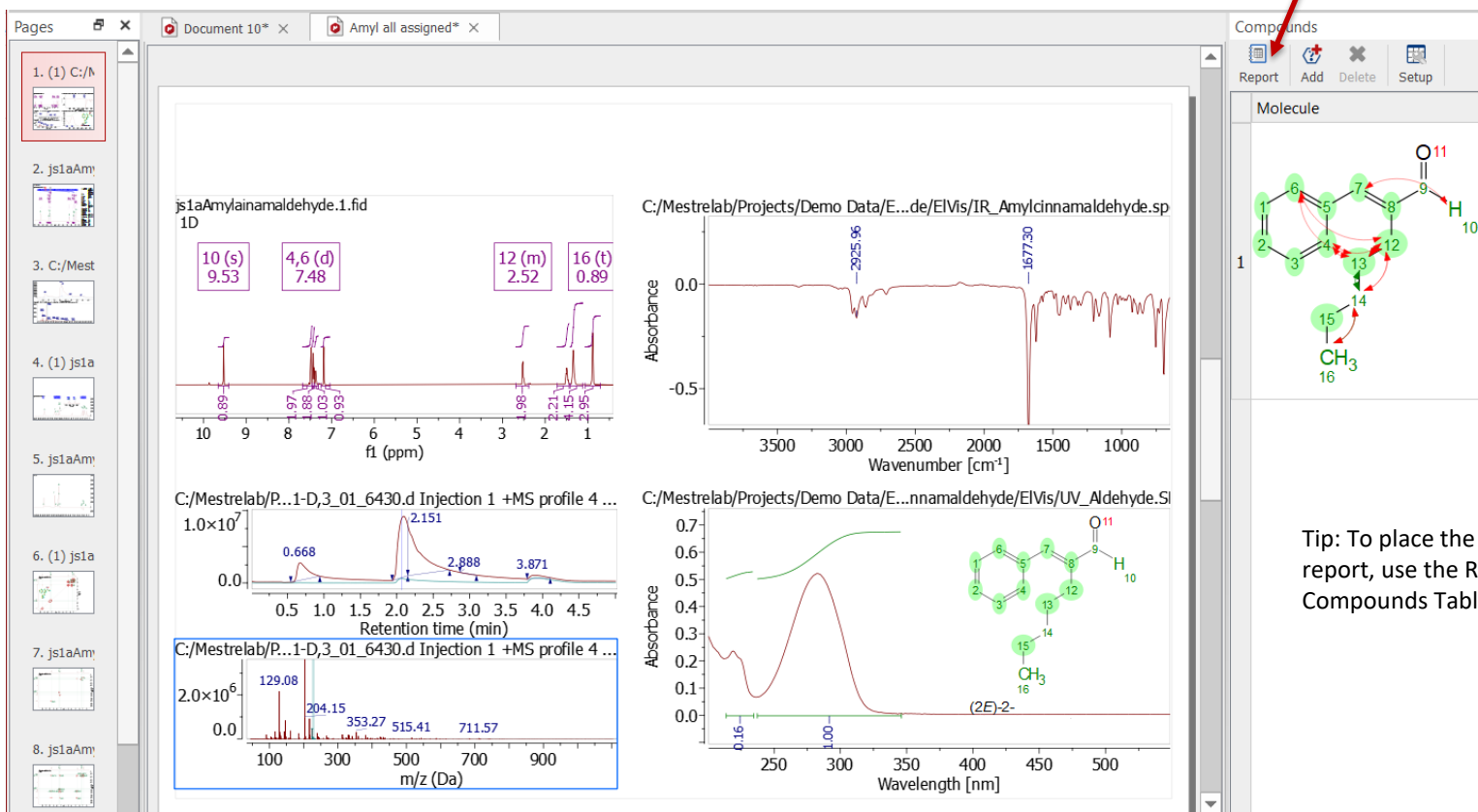
- In Data Browser, open ^1H NMR and LCMS data of Amylinalmaldehyde.
- Open the mol file of Amylinalmaldehyde.
- Do the routine analysis of them, such as multiplet analysis, mol match, peak assignment etc.



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

UV

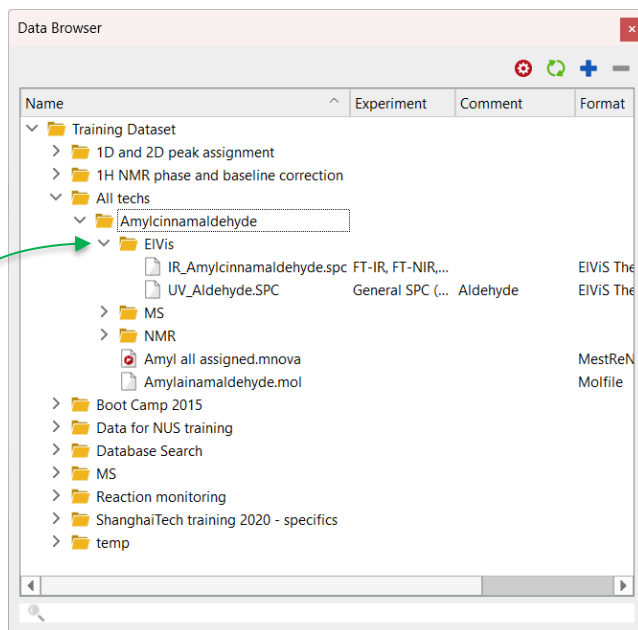
- Choose Home > New Page to open a new page.
- Copy and paste the IR, UV, ¹H NMR, and LC-MS to the new page one by one.
- Resize and arrange the objects similar to as shown below:



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

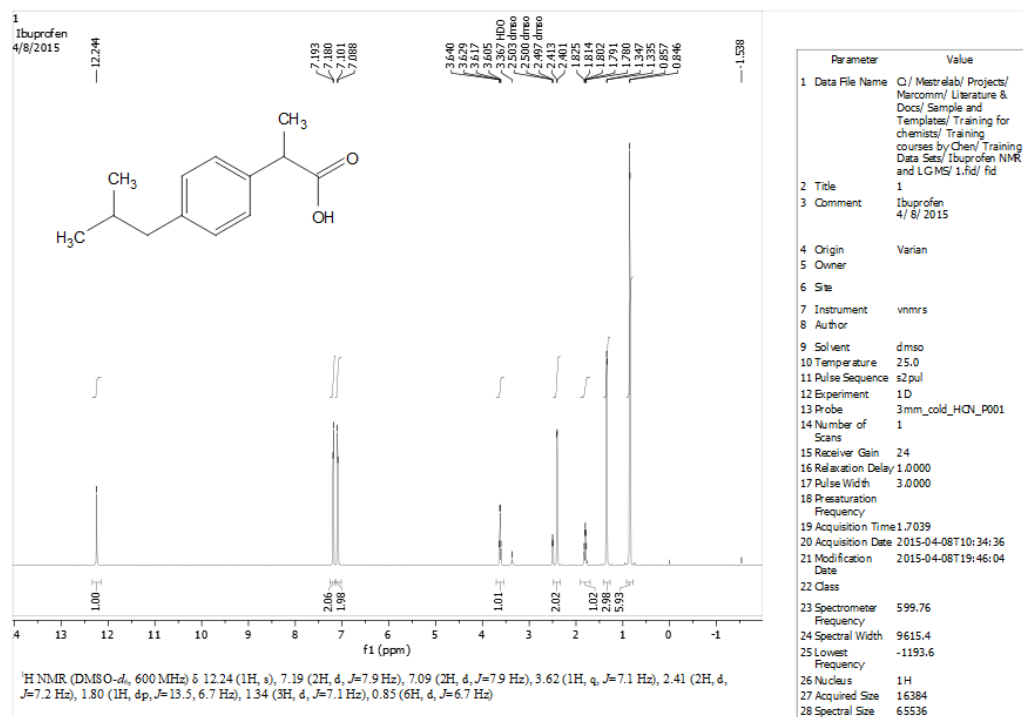
Saving the Results

Sample data



SAVING RESULTS

- 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.



Save the results

.pdf doc

.mnova doc

Database

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

The screenshot displays the MestReNova software interface. On the left, a red sidebar contains a menu with options: New, Close, Recent, Save, Save As..., Export to PDF..., Save To, Open..., Open Directory..., Open From, Print..., Page Setup..., Help (highlighted with a red arrow), Preferences..., Advanced Plug-ins..., and Exit. The main window is titled 'MestReNova' and features a 'Help' tab. The 'Help' tab is active, showing a 'MestReNova Manual' window. The manual's table of contents is visible, with 'Using GSD for multiplets analysis' highlighted. The right pane of the manual shows the title 'Using GSD for multiplets analysis' in a red header, followed by the text: 'Exploiting the power of GSD for an improved Multiplet Analysis'. Below this, it states: 'By default Mnova uses Global Spectral Deconvolution (GSD) for automatic analysis, with the enhanced peak picking capabilities and multiplet analysis.' Further down, it says: 'Multiplet Analysis benefit directly from the exploitation of GSD for automatic analysis, with the enhanced peak picking capabilities and automatic multiplicity identification and labeling.' At the bottom, it begins: 'Here you can see an example of a triplet which is hidden under'. A spectral plot is shown at the bottom right, displaying a red curve with a peak labeled 'A.00 3.49' and a red vertical line at '3.49'.