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Mnova Training– Basics

For Mnova v14.2.0
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Main Topics

- Installation and Activation of Mnova NMR
- 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
- Saving the results

Note: This tutorial covers the NMR, NMRPredict and MS plugins of Mnova

Specifics for <xxxxxx> University (To be completed by instructor)

- The instructions for downloading, installing and activating Mnova:
  - <Link to instruction page>

- The Mnova licenses that <XXXX> University has:
  - Mnova Suite (NMR, NMRPredict & MS), unlimited
  - Etc.

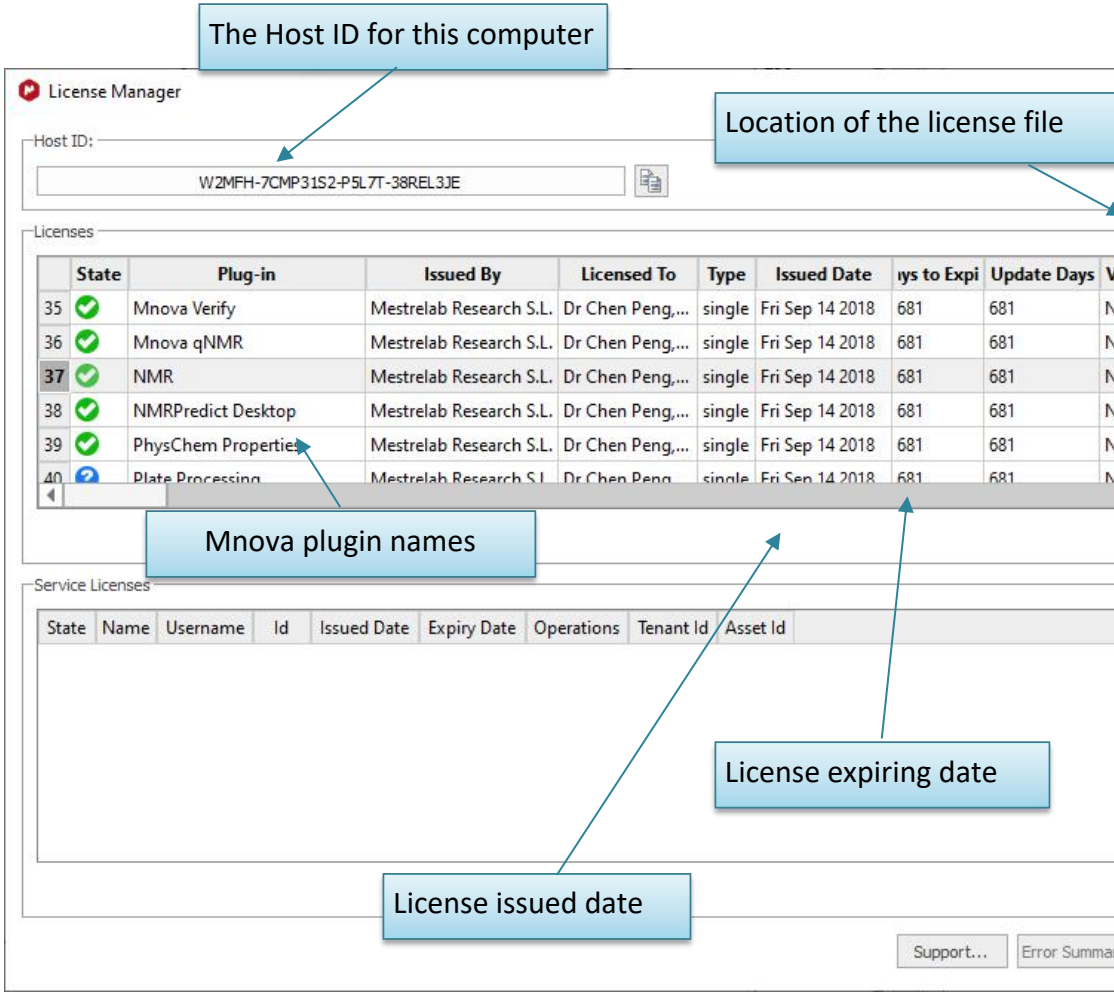
- The sample data used in this tutorial are located at:
  - <Link to data folder>.

Installation and Activation of Mnova, and General Setup*

*You will need to have Mnova Suite (NMR, NMRPredict Desktop and MS) licenses for this tutorial. For the Advanced tutorial, you will also need Mnova DB and Wiley DB licenses.

Install and activate Mnova in General

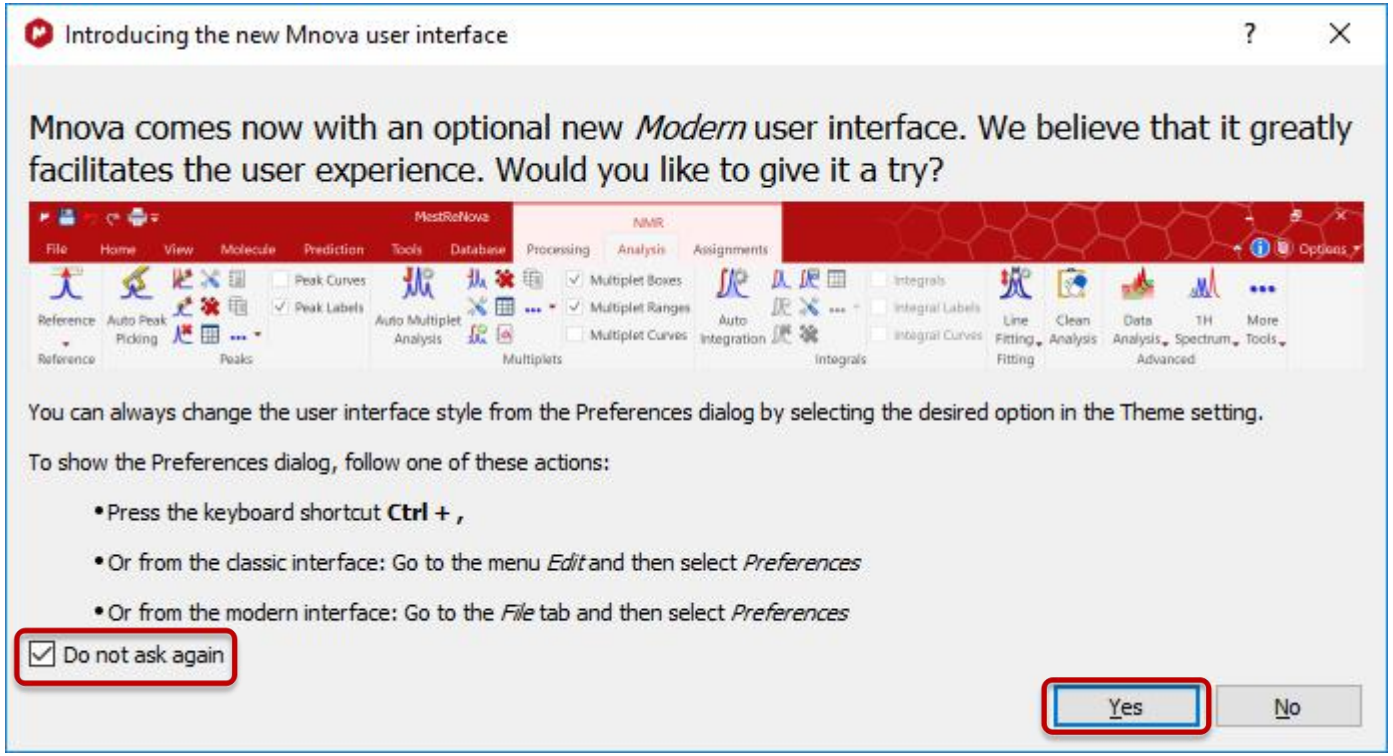
- Download and install Mnova from www.mestrelab.com. Choose ***File > Help > License Manager*** to open the License Manager dialog.
- Activate Mnova using your purchased license files, or apply for 45 day free trial licenses (Click ***Get/Install Licenses***)
- Make sure that there are green checkmarks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



PREFERENCES

Use the New Graphical User Interface (GUI)

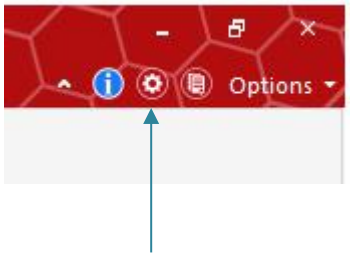
The first time you start Mnova, it asks if you want to use the “Modern” GUI. Choose it and check “Do not ask again”. Restart Mnova, you will enjoy the modular ribbon GUI introduced since version 12.



*Note: This instruction is based on the Modern GUI. You can always switch back to the “Classic” GUI from **”File/Preferences”.***

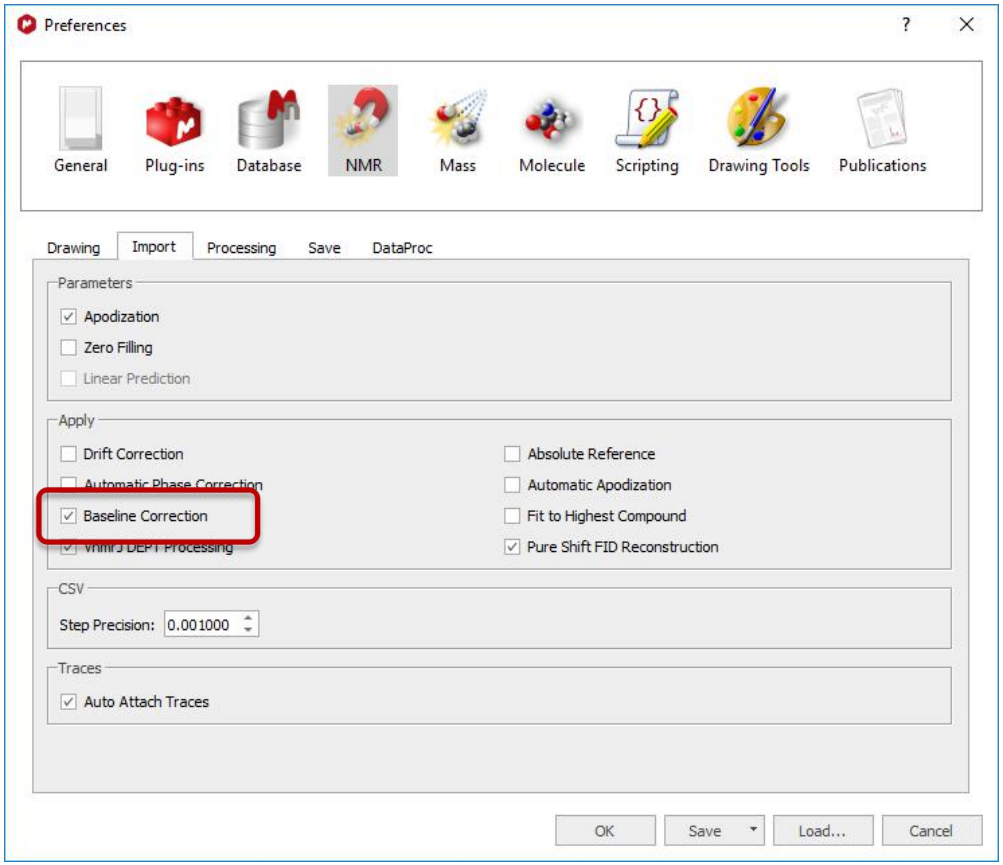
Turn on Auto Baseline Correction

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



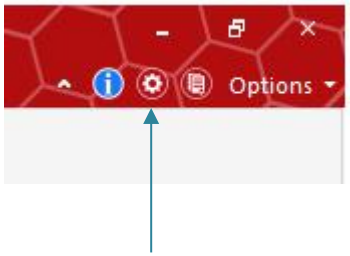
Note: Automatic Baseline Correction use the default algorithm of "Bernstein Polynomial with order of 3", or the one that you used previously. This option may make manual phasing of 2D NMR sluggish. In that case, turn baseline off from Processing .

Tip: There are many options and settings that you may change in the Preferences Dialog, especially the resolution of image copying and image exporting in the Drawing Tab.



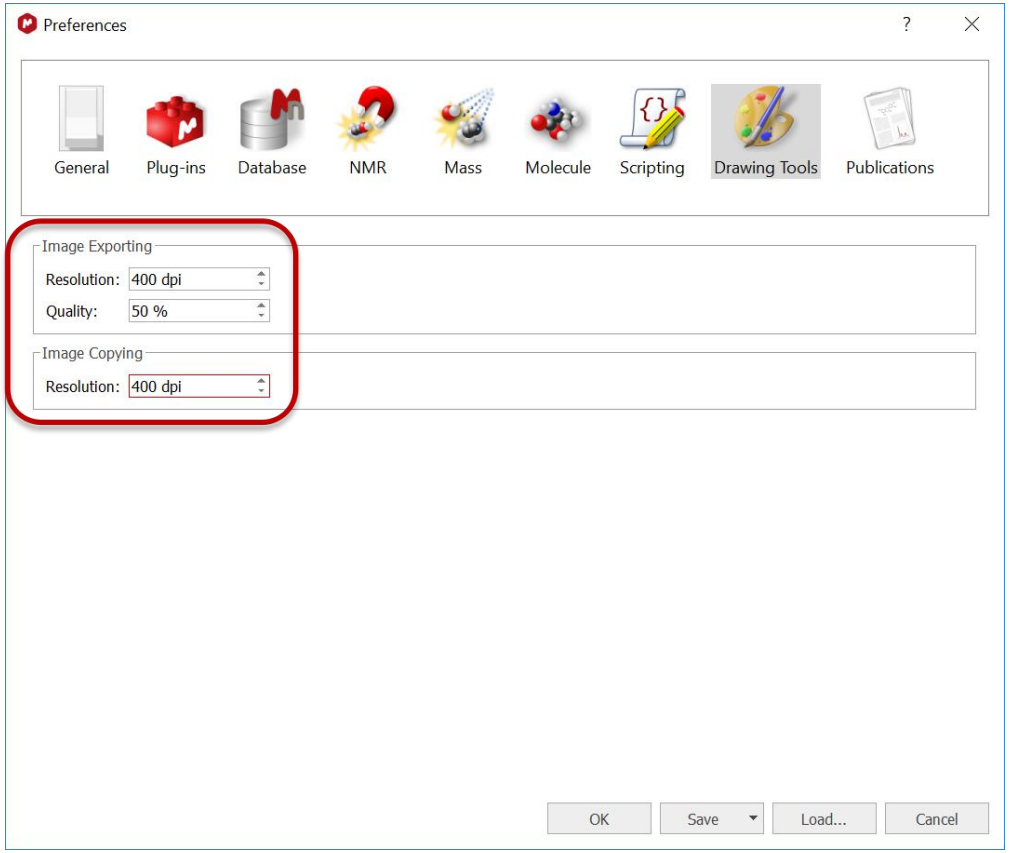
Setup the resolution for publishing spectra

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



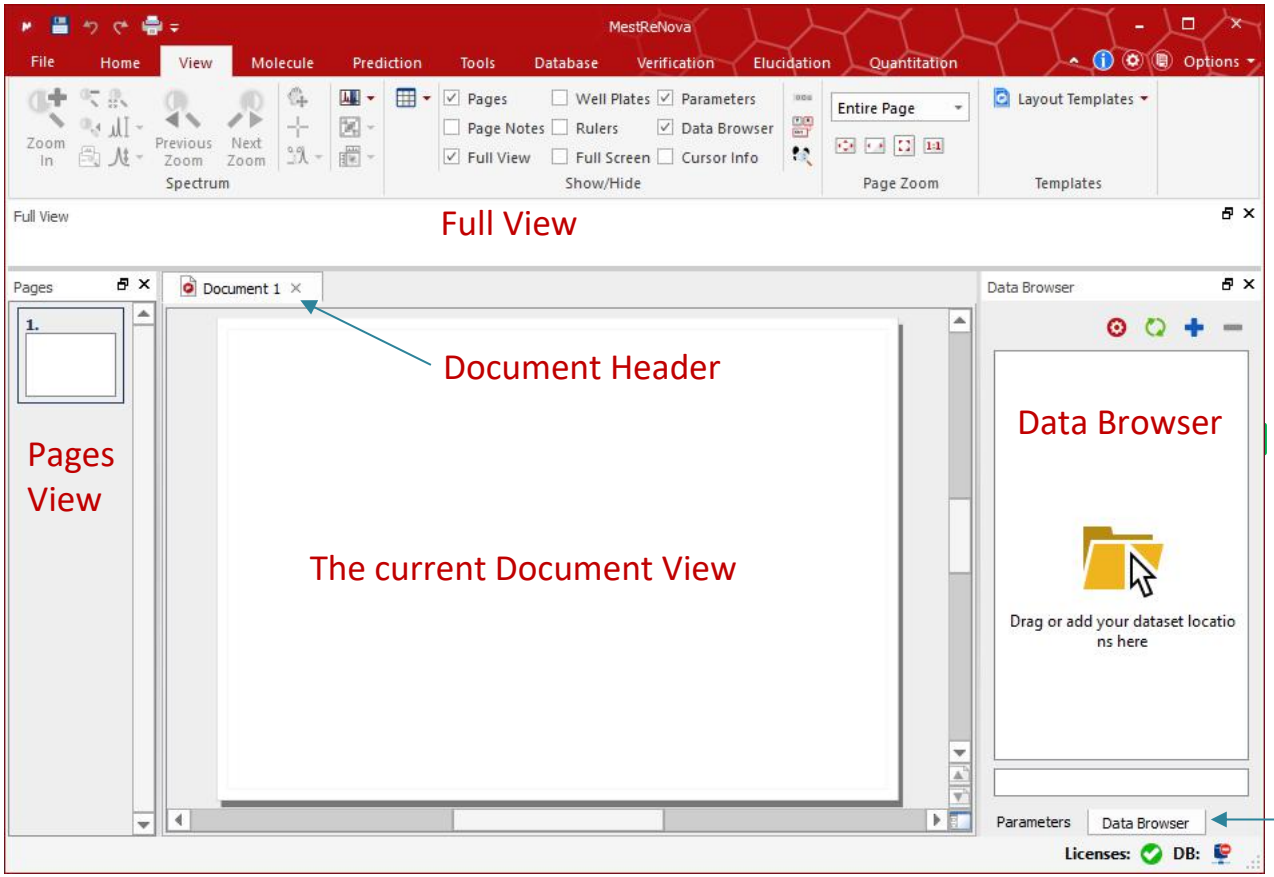
The resolution for Image Exporting is used when you choose File > Save As and save the selected objects in Mnova as a graphical image file.

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

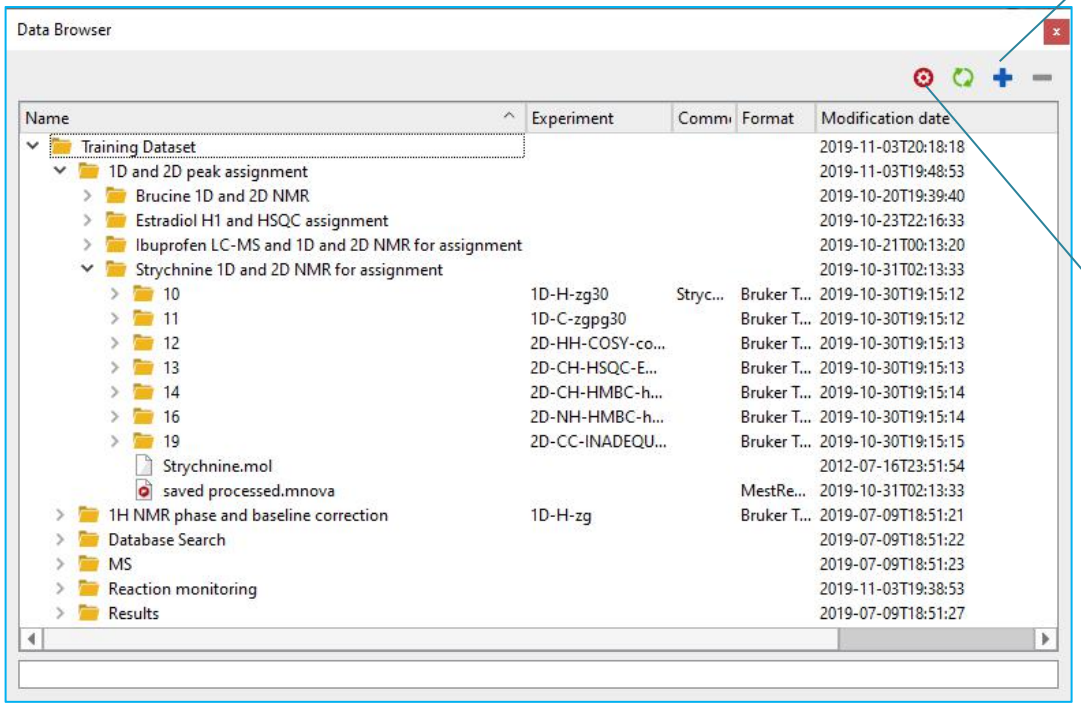


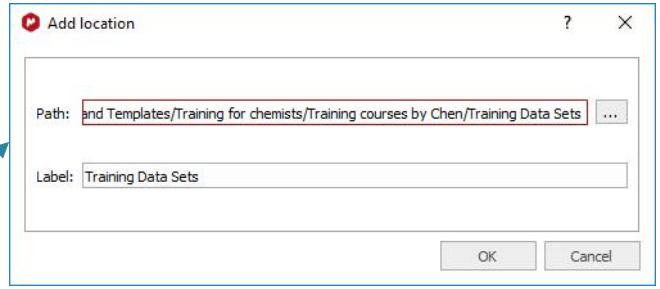
Click here to minimize the ribbon

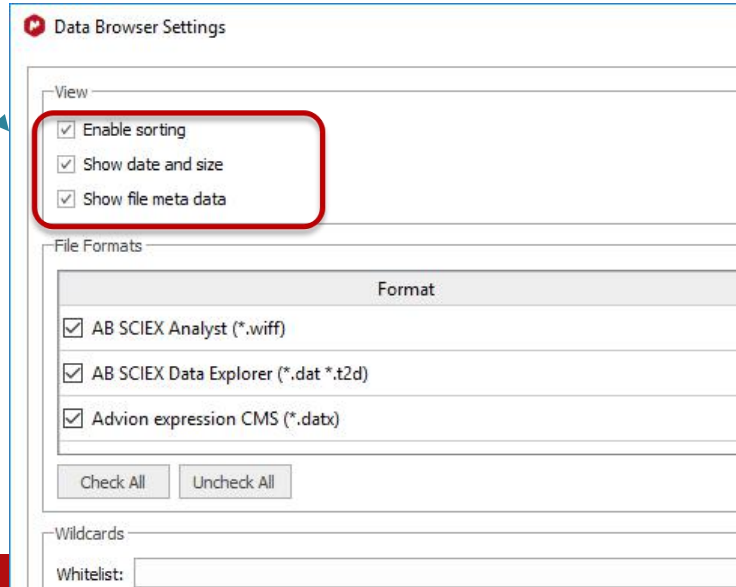
Click here to switch the panels or tables

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







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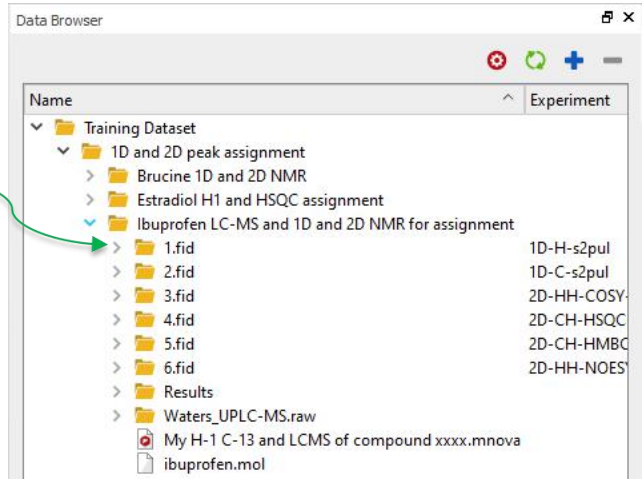
1D ^{1}H NMR Spectrum Processing, Analysis, and Reporting

Sample data



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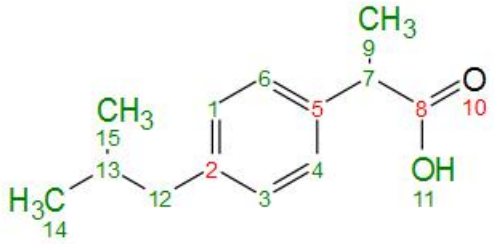
PROCEDURE

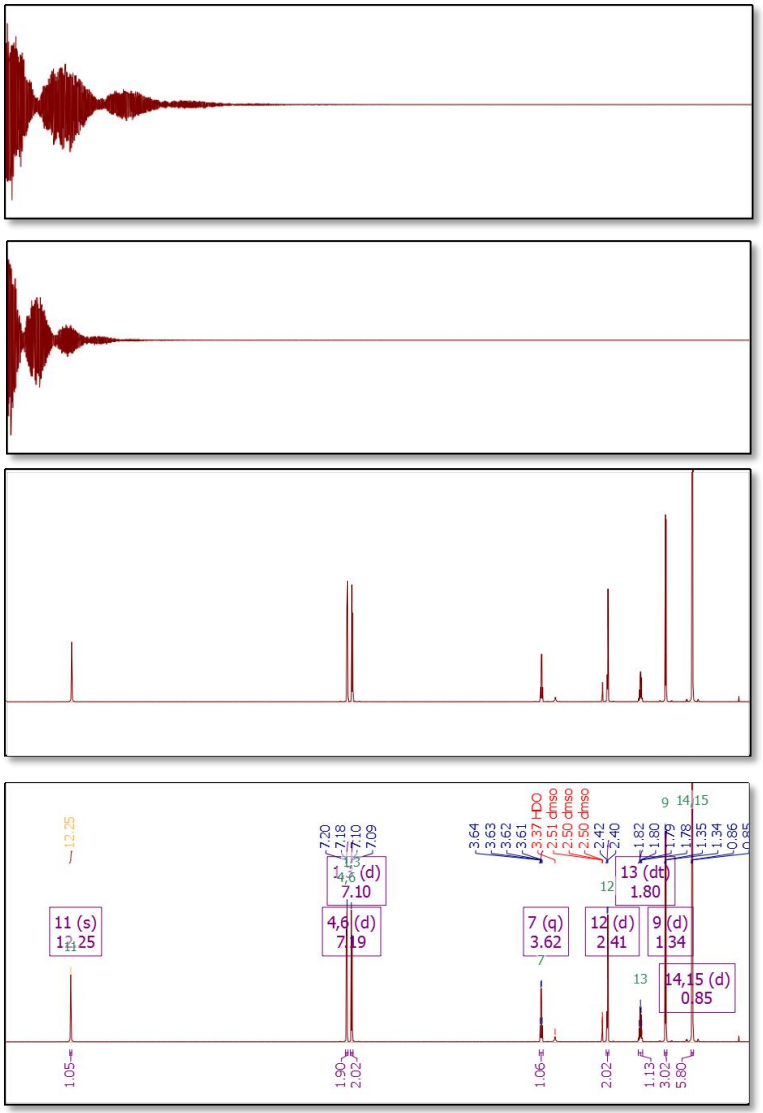
^{1}H processing and analysis: general procedure

- 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



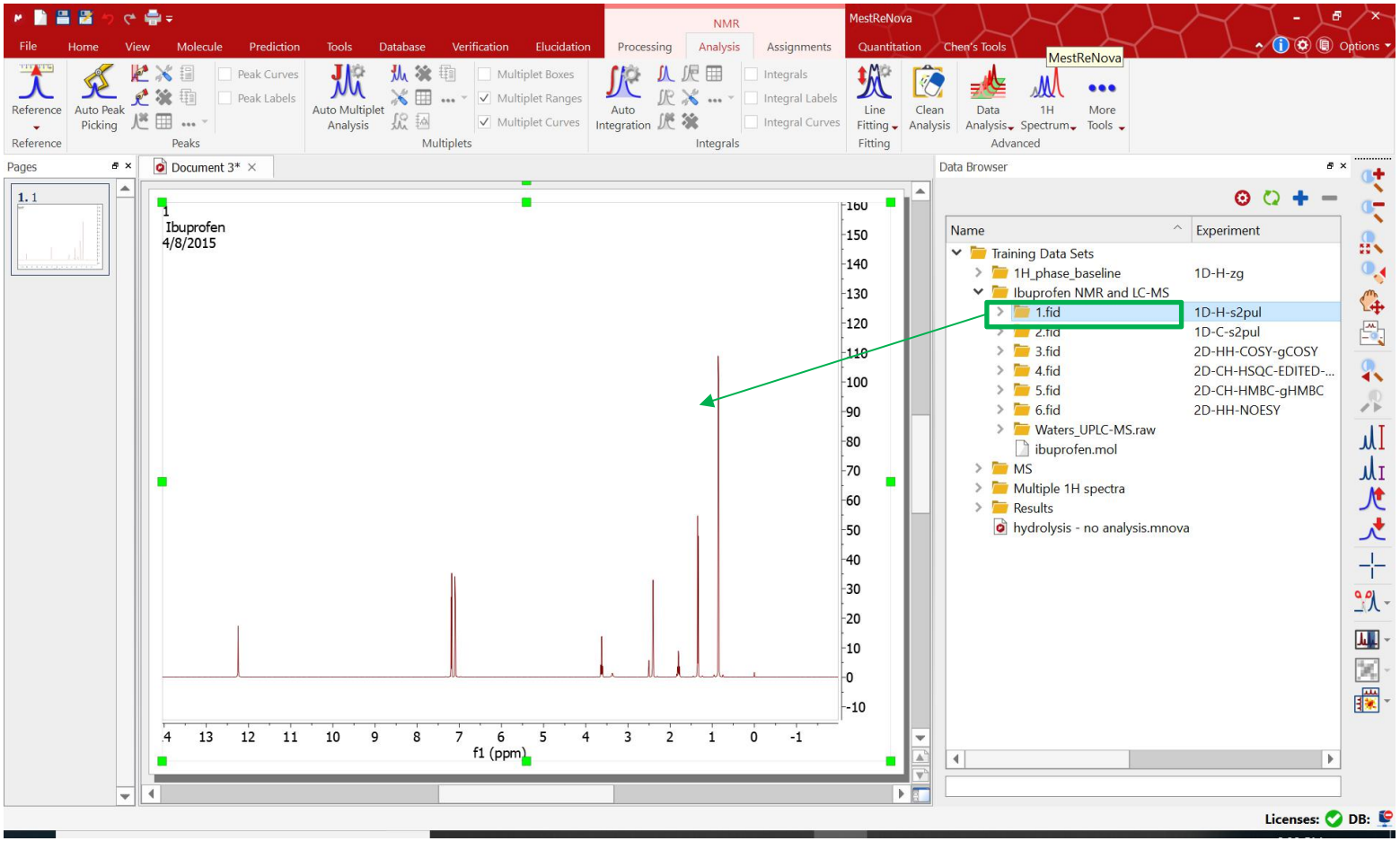
^{1}H NMR (600 MHz, DMSO-d_6) δ 12.25 (s, 1H), 7.19 (d, J = 7.8 Hz, 2H), 7.10 (d, J = 7.9 Hz, 2H), 3.62 (q, J = 7.1 Hz, 1H), 2.41 (d, J = 7.2 Hz, 2H), 1.80 (dt, J = 13.5, 6.8 Hz, 1H), 1.34 (d, J = 7.1 Hz, 3H), 0.85 (d, J = 6.7 Hz, 6H).

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



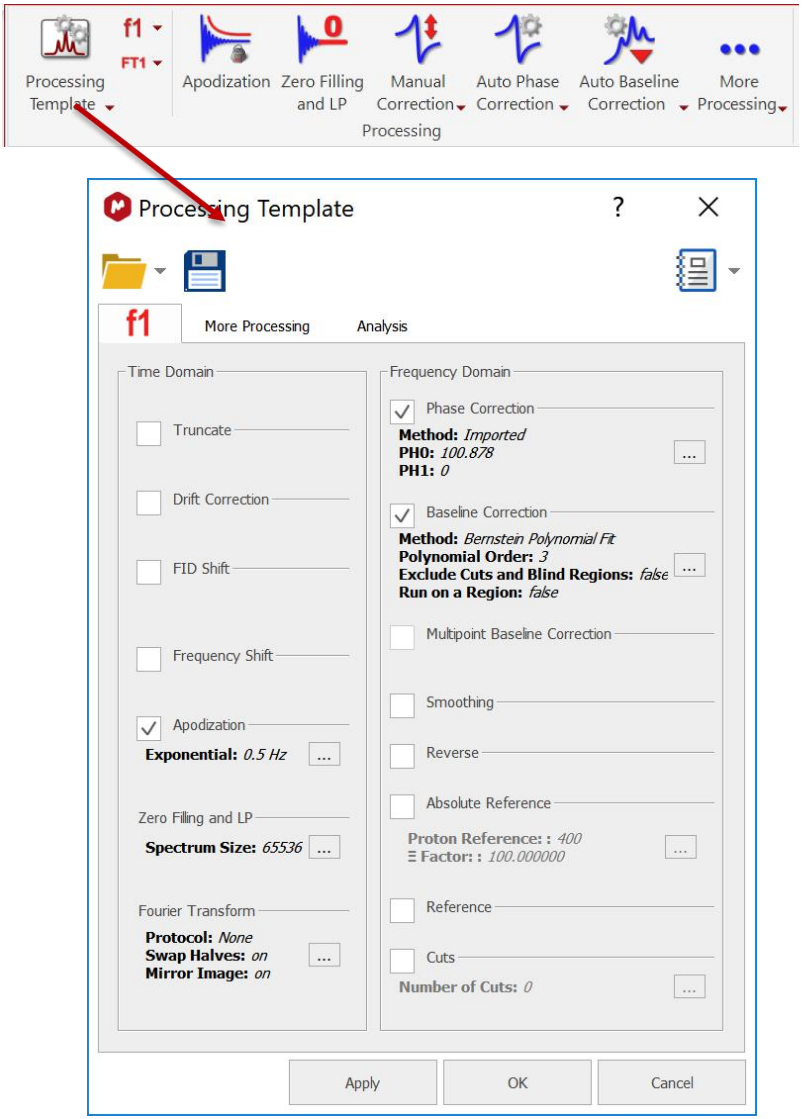
Open a H-1 spectrum

- 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.



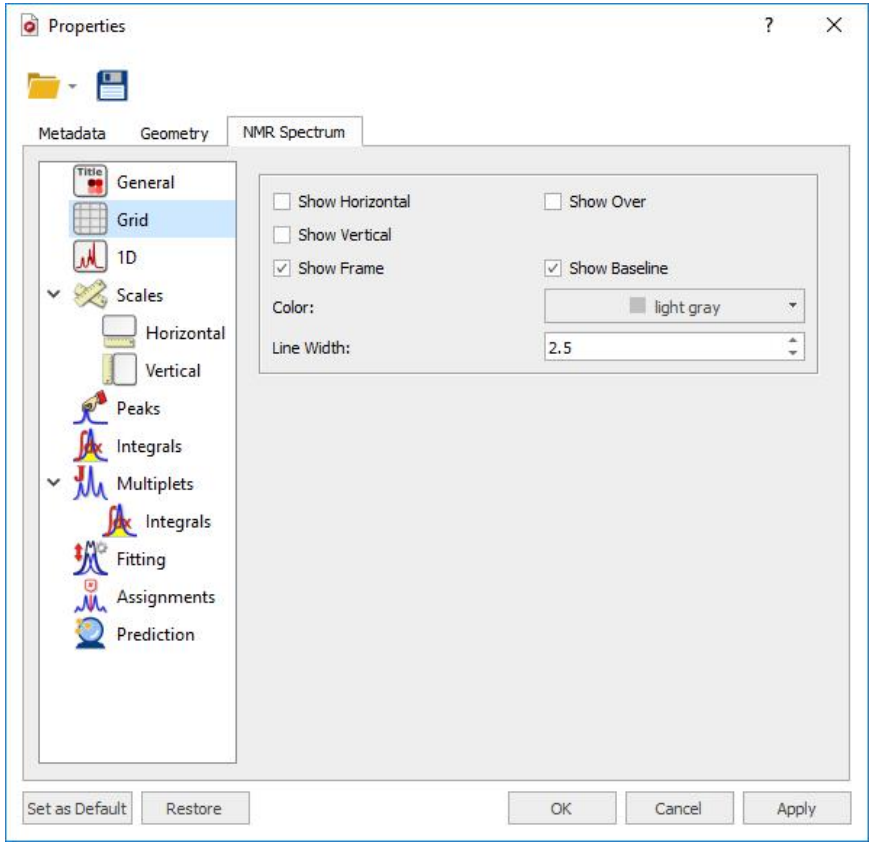
Verify the processing parameters

- 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

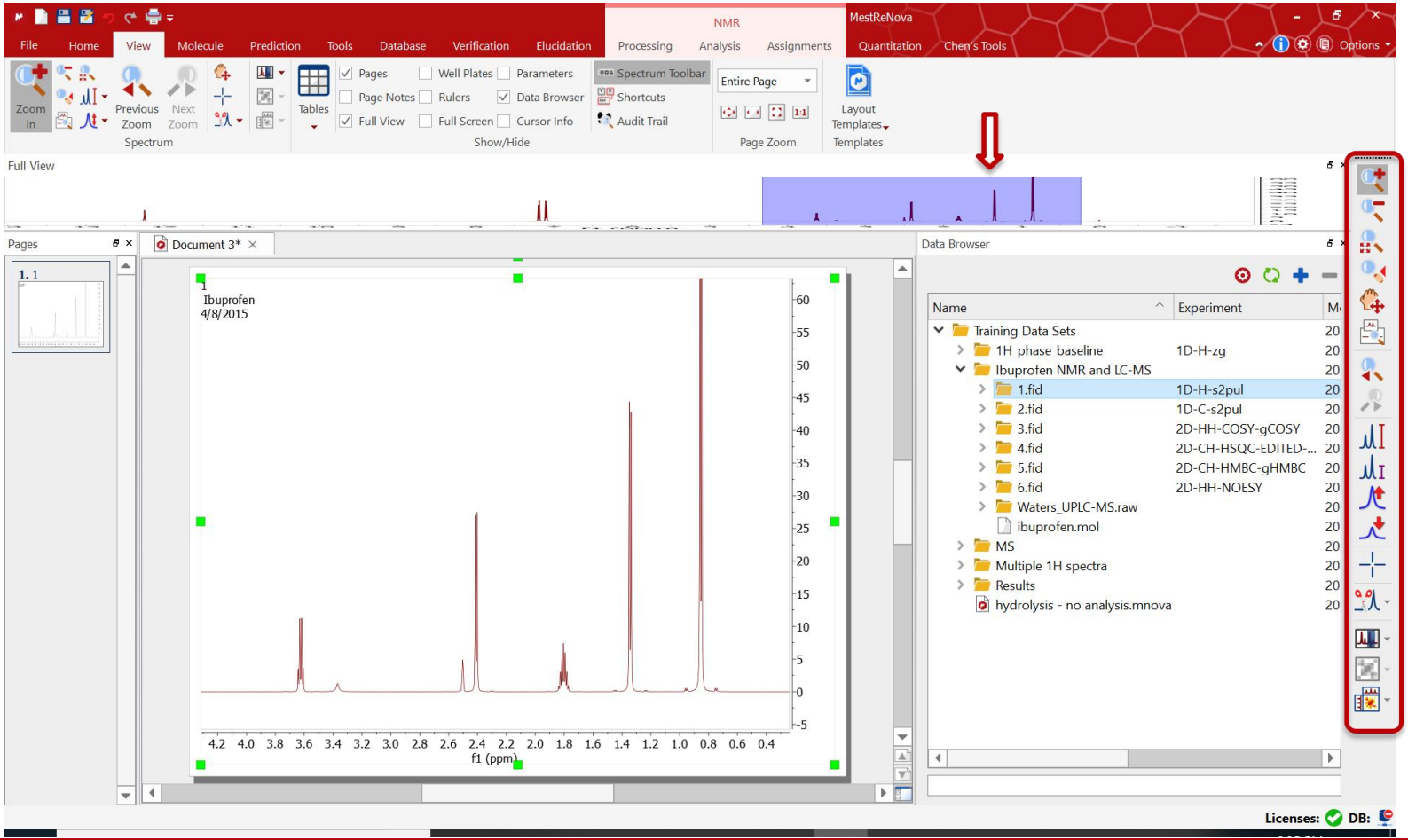
- Right click on the spectrum* and choose Properties to open the Properties Dialog, view the properties that can be changed.
- In the Grid Category, uncheck Show Horizontal, and Show Vertical, check Show Baseline
- Click Apply, and then Set as Default to apply the settings to 1D spectra opened in the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



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

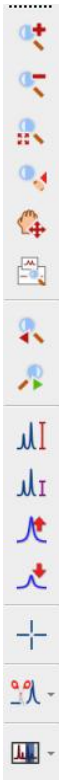
Navigate in the H-1 Spectrum

- 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)

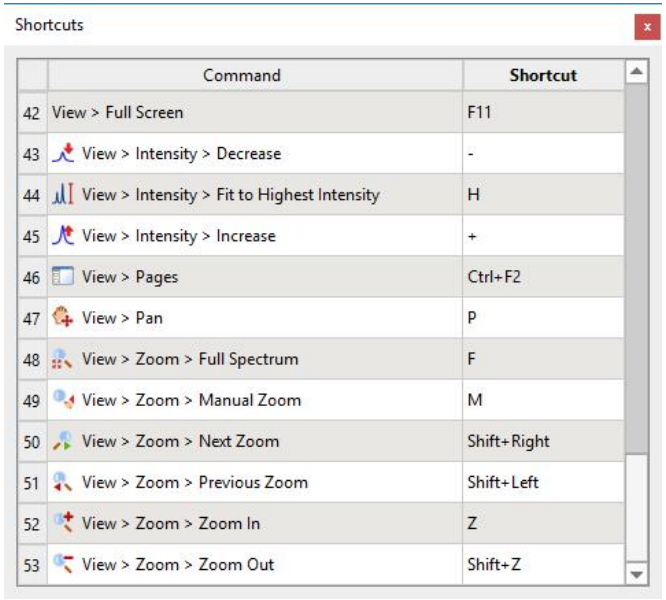


Spectrum visualization tools

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



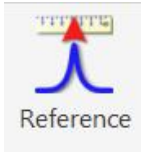
Zoom in/Zoom out (or press Z) *
Zoom out**
Full spectrum (or press F)
Manual Zoom in to defined ppm range
Pan spectrum (or press P) ***
Expansion – click&drag to draw an inset (or press E)
Previous Zoom level
Next Zoom level
Fit to Highest Intensity (or press H)
Fit to highest compound peak
Increase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



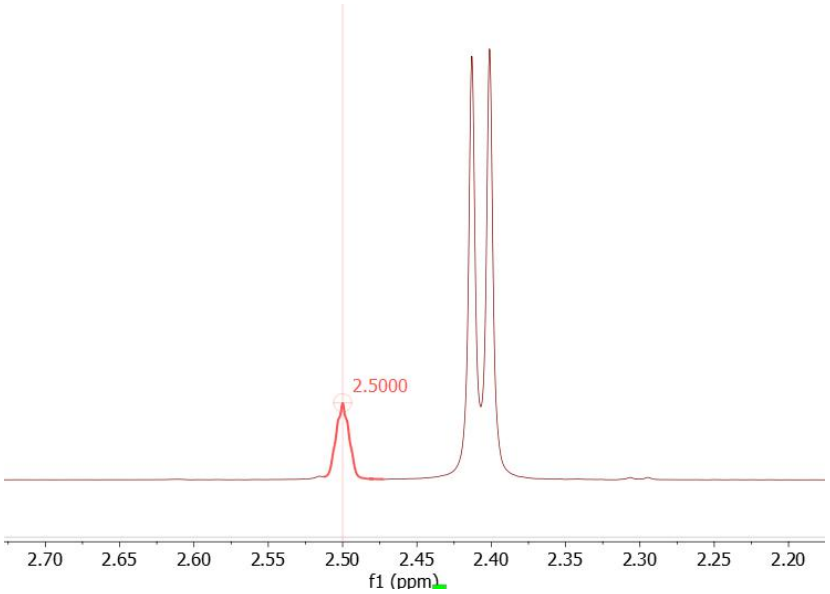
	Command	Shortcut
42	View > Full Screen	F11
43	View > Intensity > Decrease	-
44	View > Intensity > Fit to Highest Intensity	H
45	View > Intensity > Increase	+
46	View > Pages	Ctrl+F2
47	View > Pan	P
48	View > Zoom > Full Spectrum	F
49	View > Zoom > Manual Zoom	M
50	View > Zoom > Next Zoom	Shift+Right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

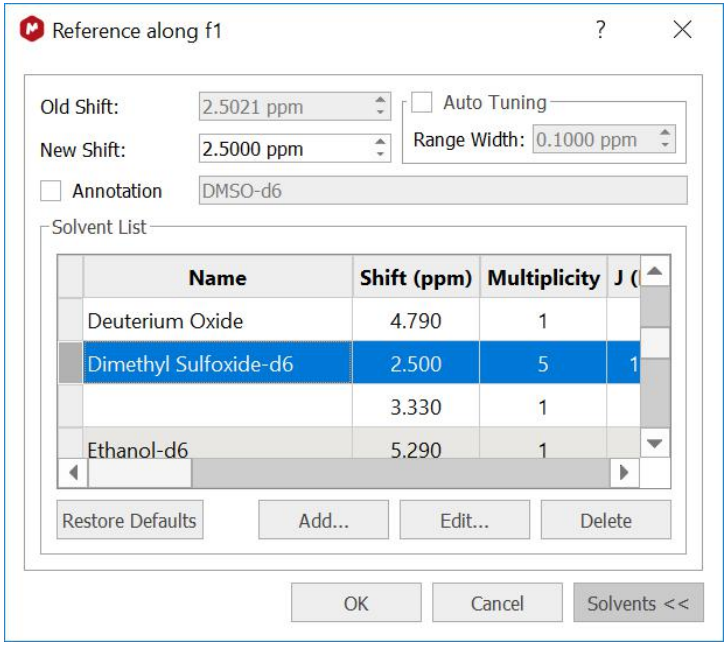
** Press **Z** several times to toggle between horizontal/vertical/box zoom*
*** Press **P** several times to toggle between free/horizontal/vertical panning*

Chemical Shift Referencing



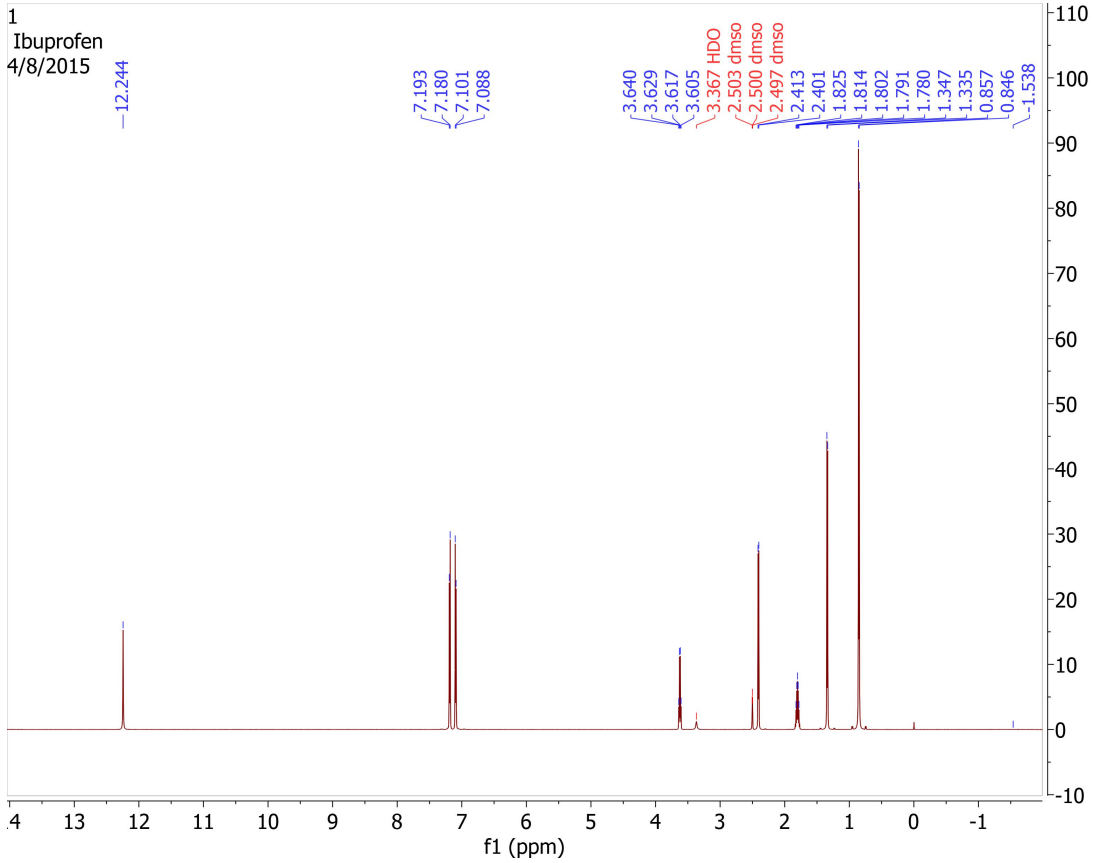
- This spectrum uses DMSO-d6 as the solvent. We can reference the chemical shifts by setting its middle peak to 2.5 ppm.
- Zoom to the DMSO peak at around 2.5 ppm. Choose Analysis > Reference, and click on the top of the middle peak.
- Set it to 2.5 ppm either manually or from the Solvent List.

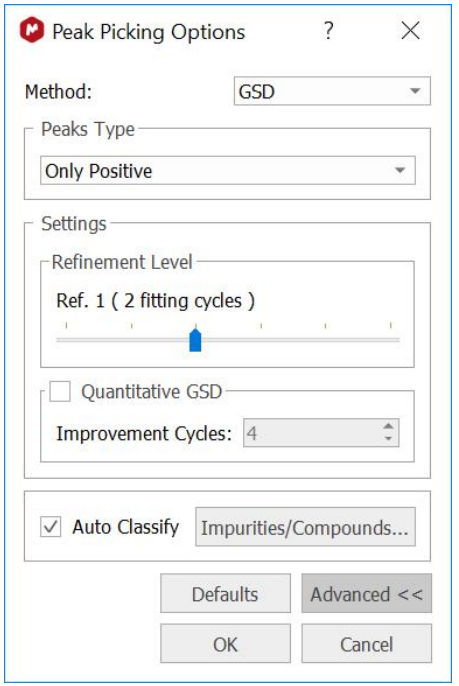




Peak picking

- 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.





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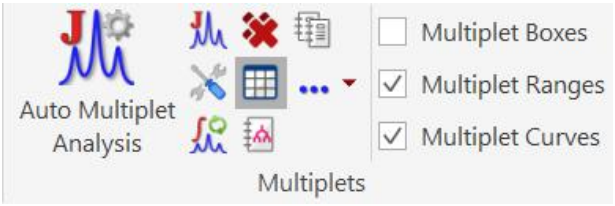
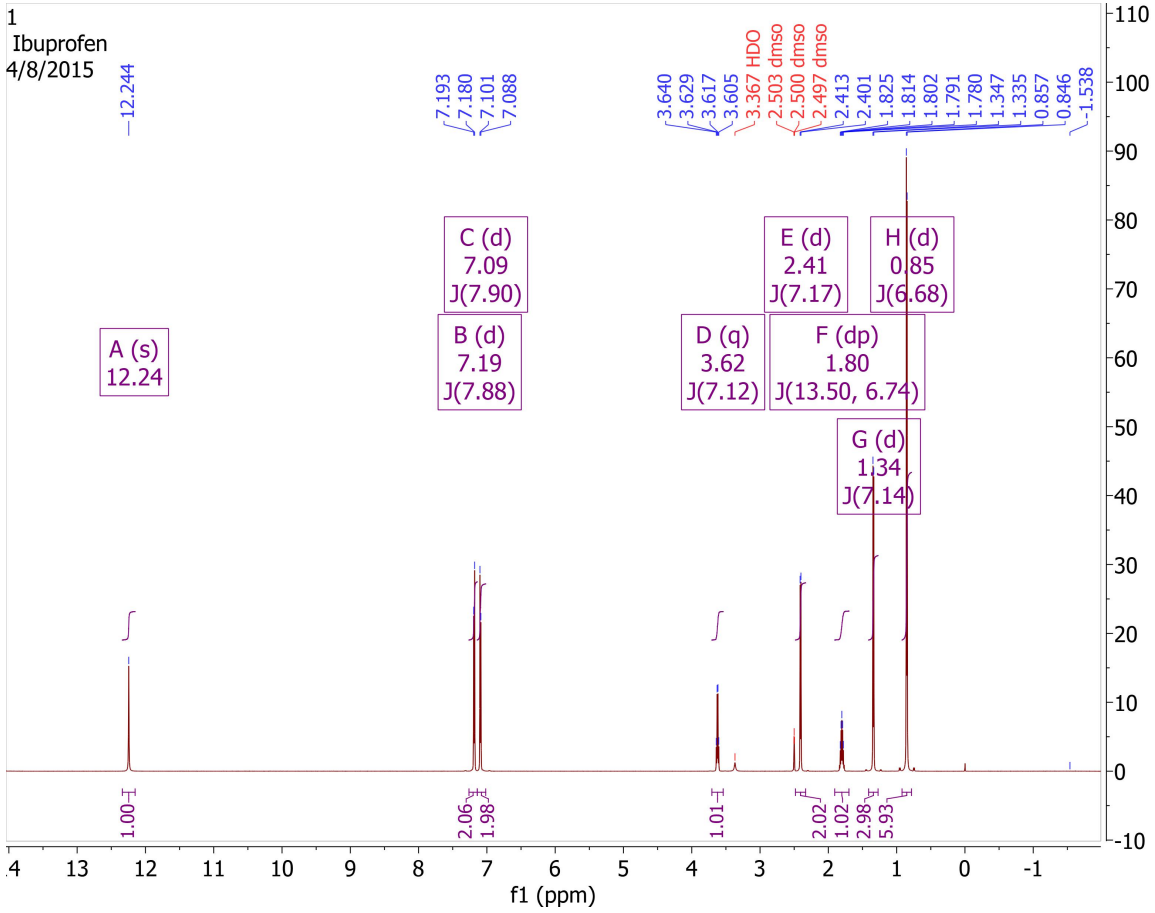
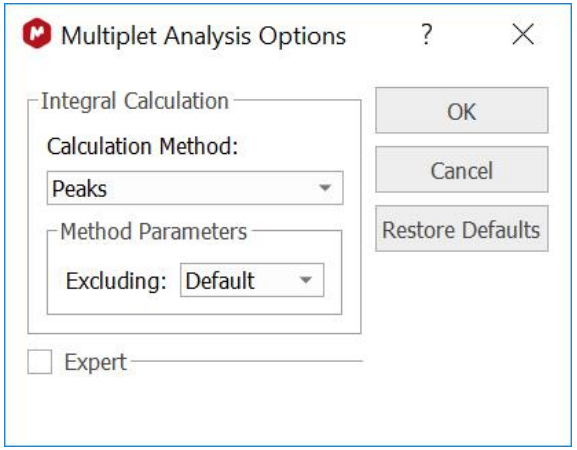
ANALYSIS

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

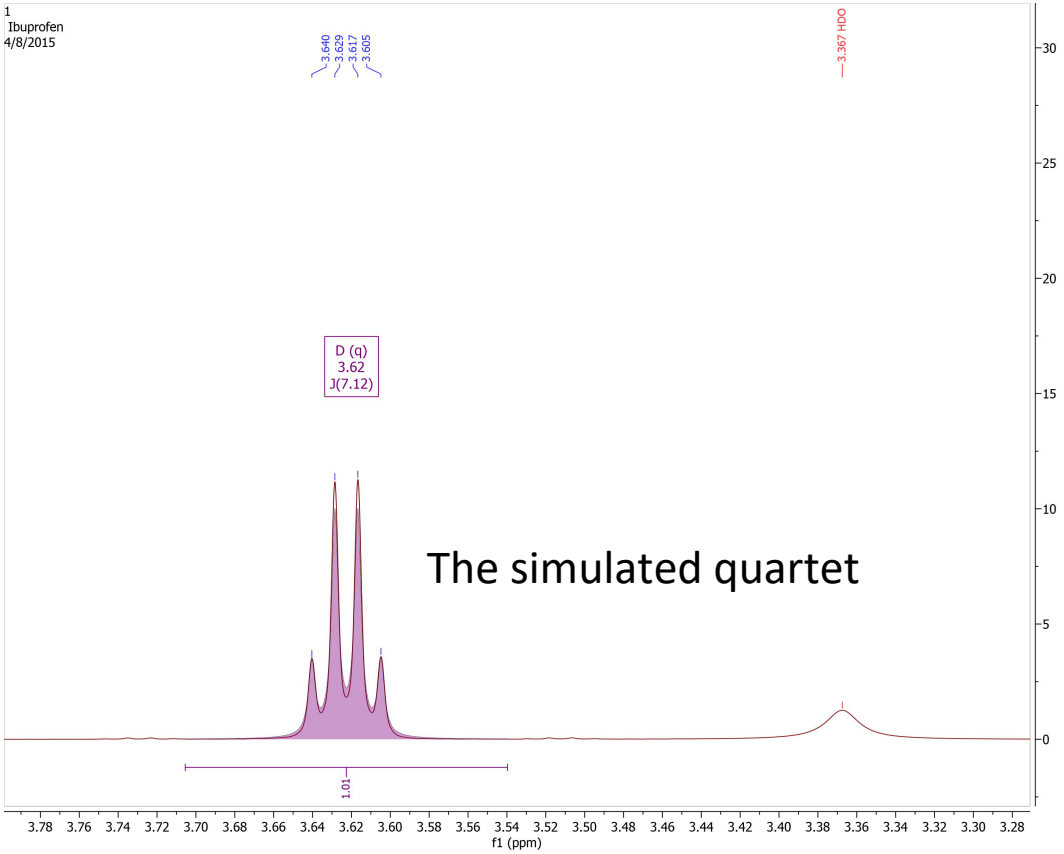


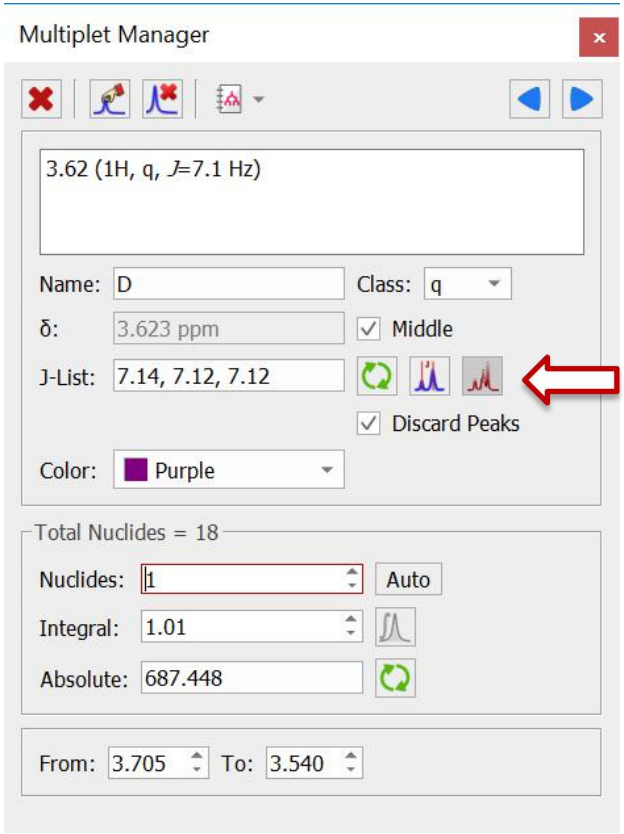




Multiplet Manager

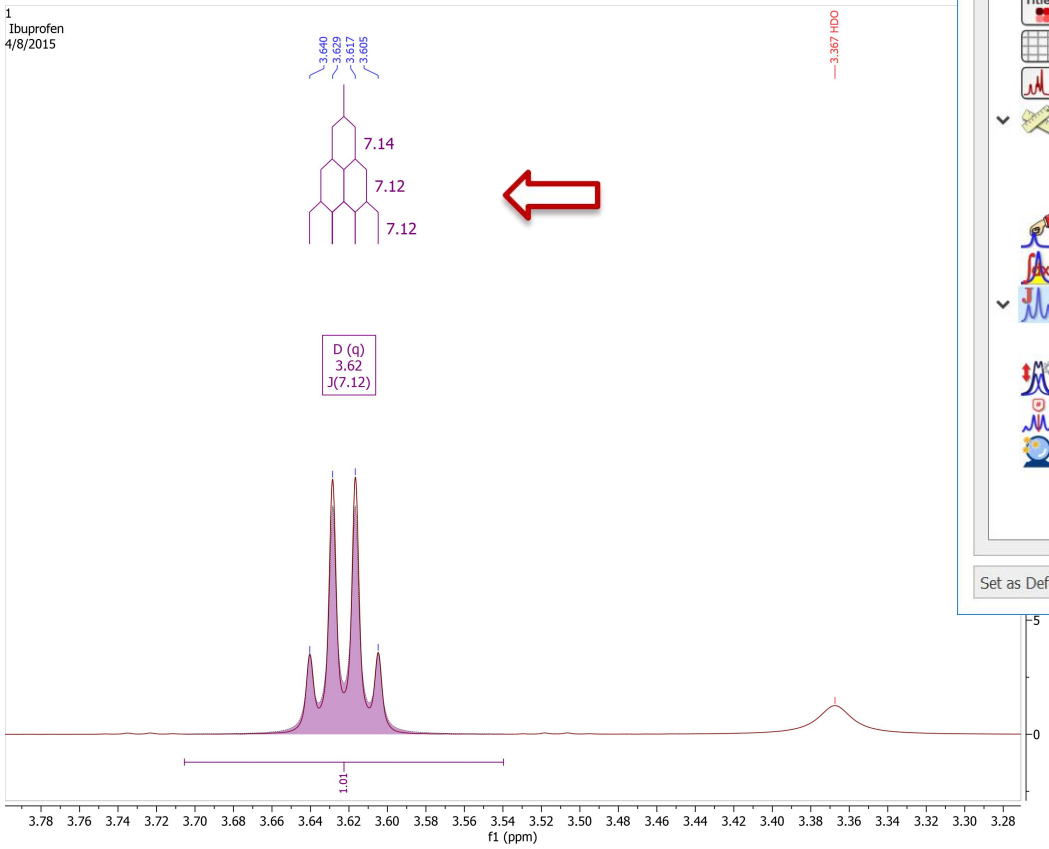
- Double click on a multiplet label to open the Multiplet Manager.
- Use the tools there to verify and change multiplet analysis results if needed.

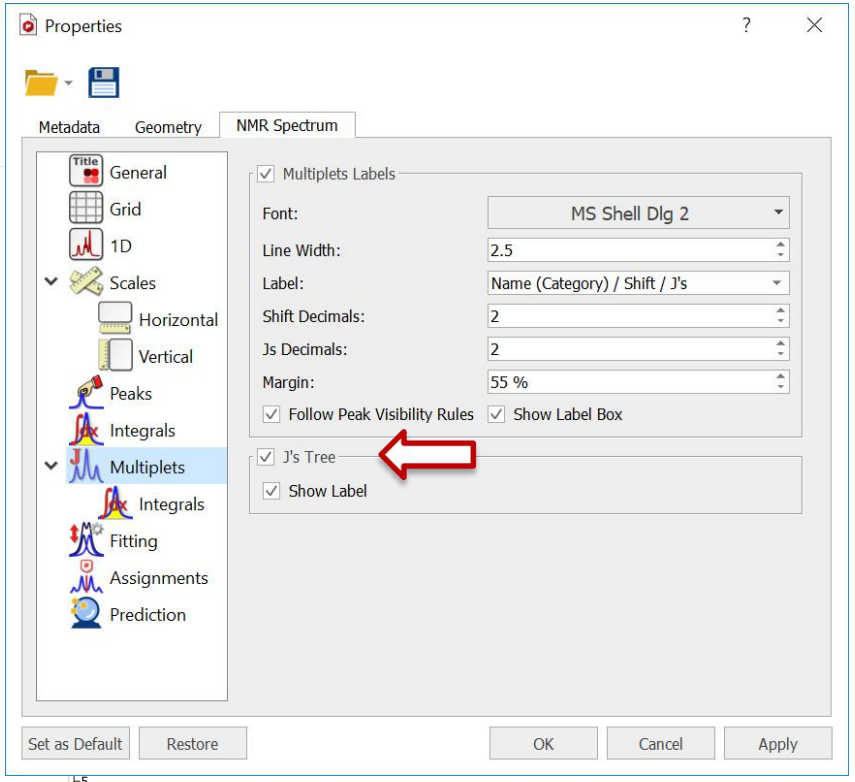




Multiplet Manager

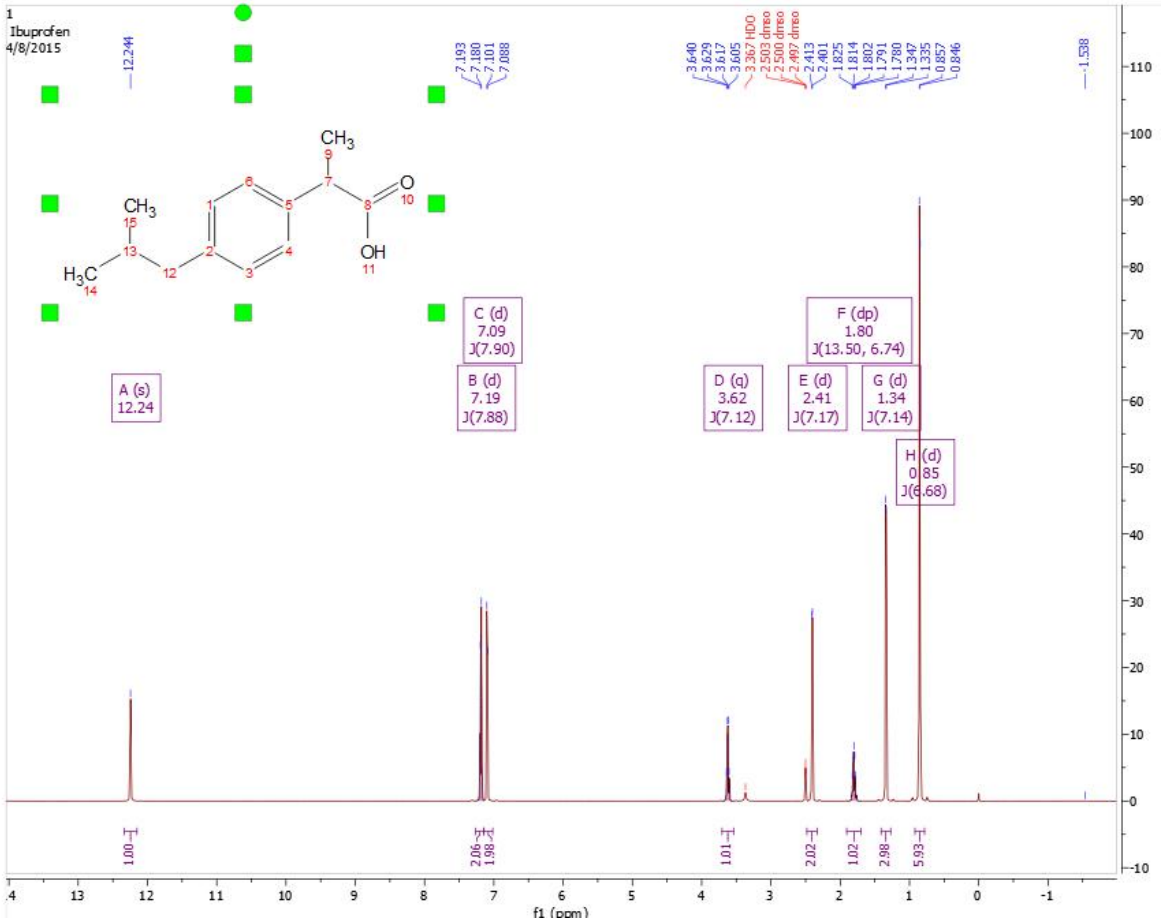
- Double click on the spectrum to open the Properties dialog.
- Choose Multiplets, and check J's Tree to display the J-coupling tree for visual verification of the multiplet analysis results.

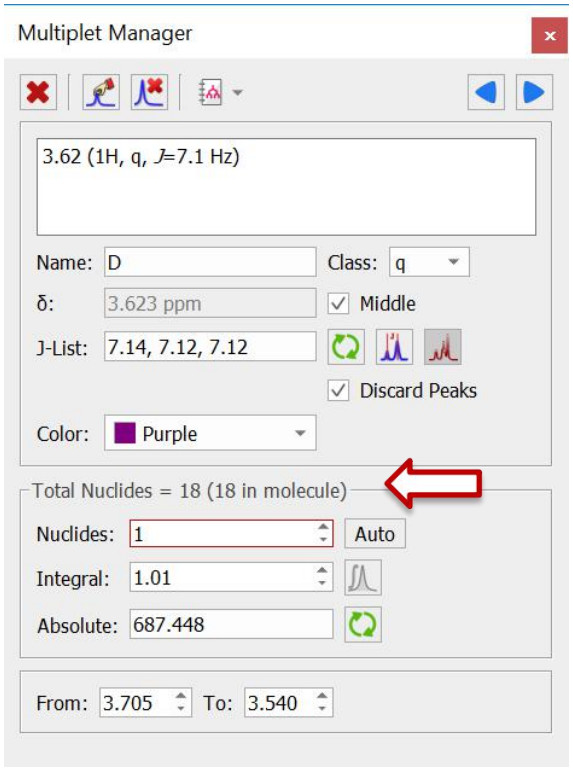




Verify the number of Hs

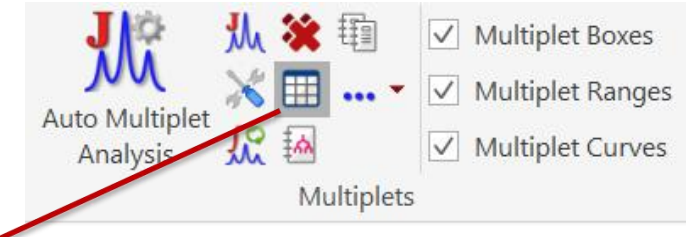
- Open the Ibuprofen.mol file from the Data Browser.
- Note the number of protons from multiplet analysis vs. that from the structure

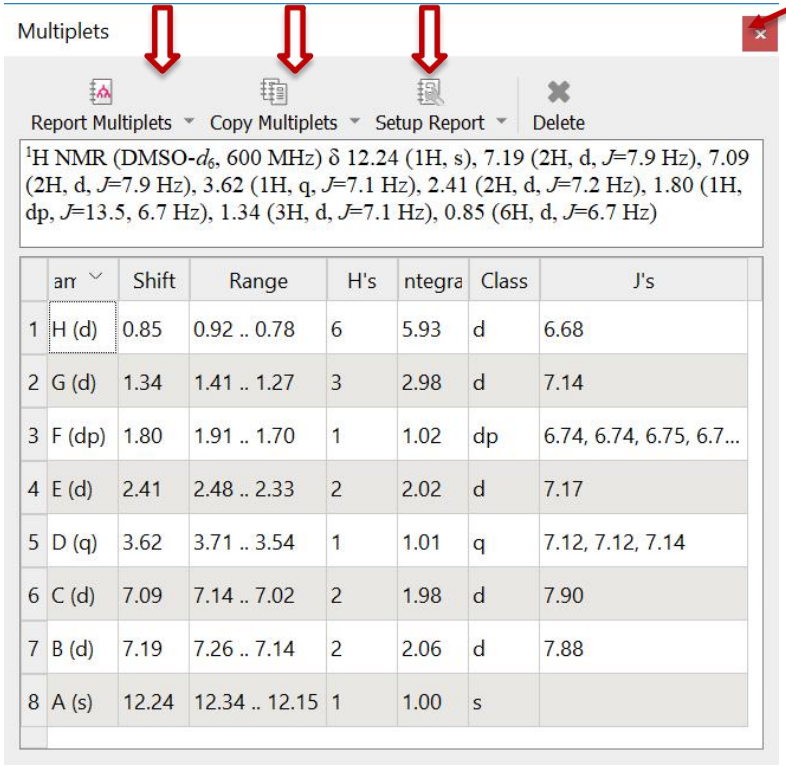




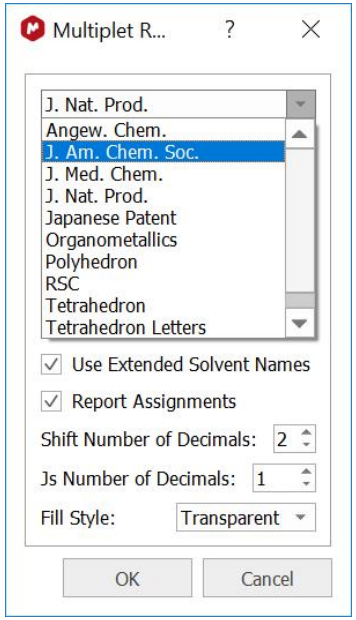
Report the multiplets

- 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





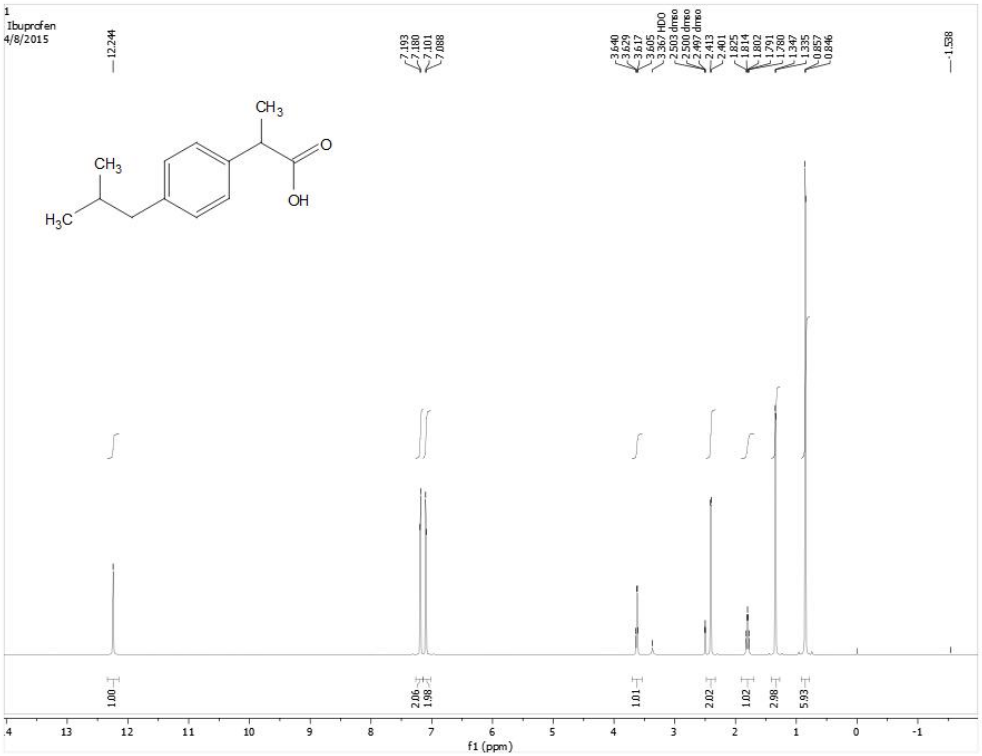
	arr	Shift	Range	H's	ntegra	Class	J's
1	H (d)	0.85	0.92 .. 0.78	6	5.93	d	6.68
2	G (d)	1.34	1.41 .. 1.27	3	2.98	d	7.14
3	F (dp)	1.80	1.91 .. 1.70	1	1.02	dp	6.74, 6.74, 6.75, 6.7...
4	E (d)	2.41	2.48 .. 2.33	2	2.02	d	7.17
5	D (q)	3.62	3.71 .. 3.54	1	1.01	q	7.12, 7.12, 7.14
6	C (d)	7.09	7.14 .. 7.02	2	1.98	d	7.90
7	B (d)	7.19	7.26 .. 7.14	2	2.06	d	7.88
8	A (s)	12.24	12.34 .. 12.15	1	1.00	s	

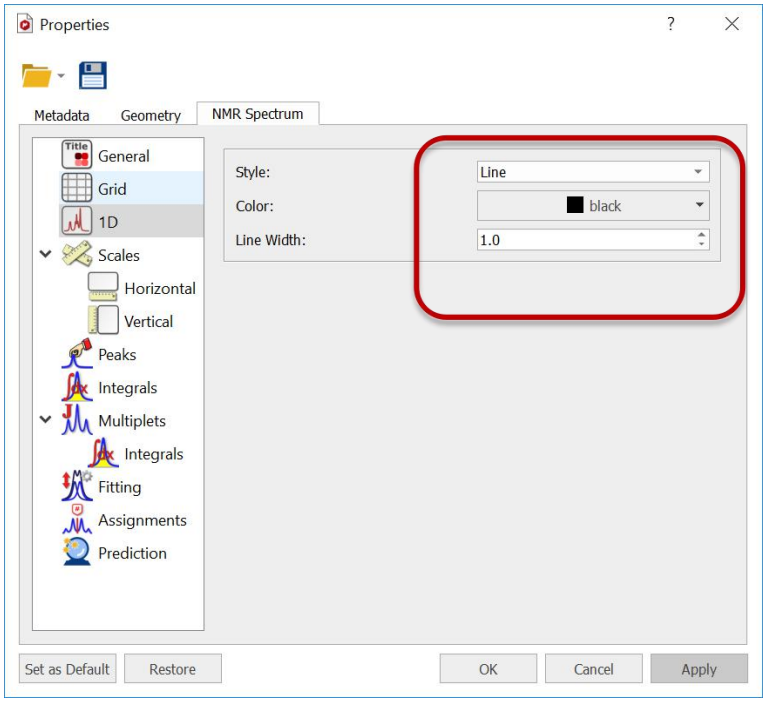


¹H NMR (DMSO-d_6, 600 MHz) δ 12.24 (1H, s), 7.19 (2H, d, J=7.9 Hz), 7.09 (2H, d, J=7.9 Hz), 3.62 (1H, q, J=7.1 Hz), 2.41 (2H, d, J=7.2 Hz), 1.80 (1H, dp, J=13.5, 6.7 Hz), 1.34 (3H, d, J=7.1 Hz), 0.85 (6H, d, J=6.7 Hz)

Publishing a spectrum

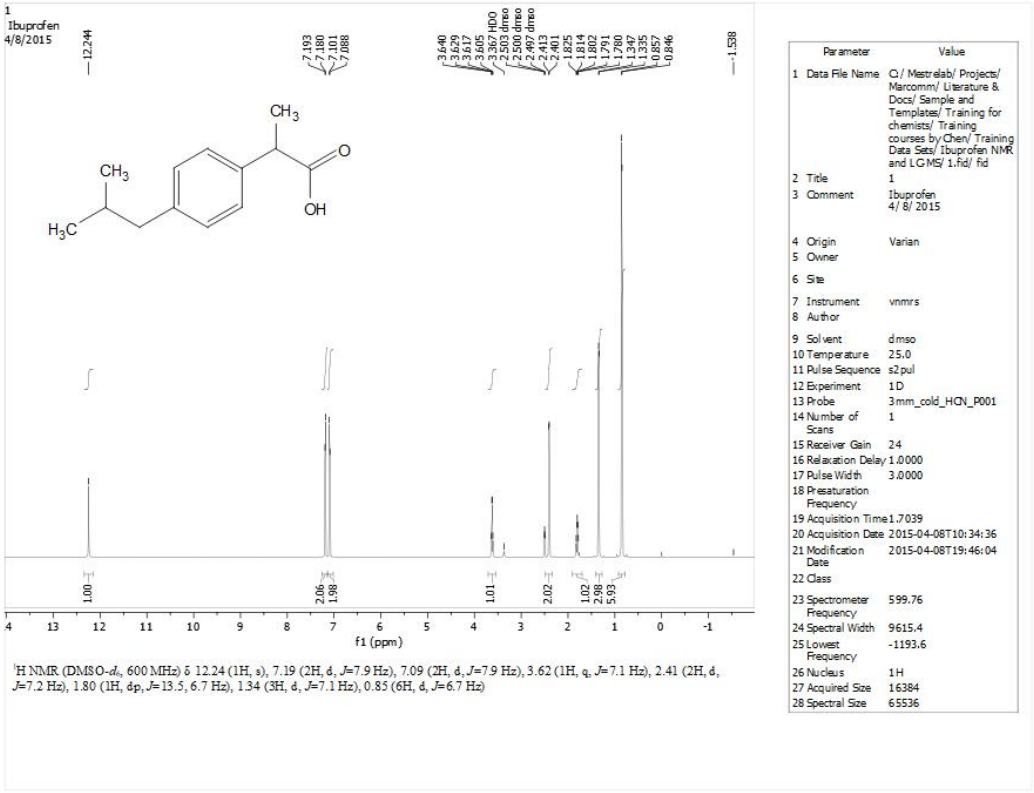
- To publish the spectrum on a black and white journal, double click the spectrum to open the Properties Dialog, and set the 1D properties to as shown on the right.
- Choose other properties to display, such as the peak labels, multiplet labels, integrals, etc.
- Copy the spectrum and structure objects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

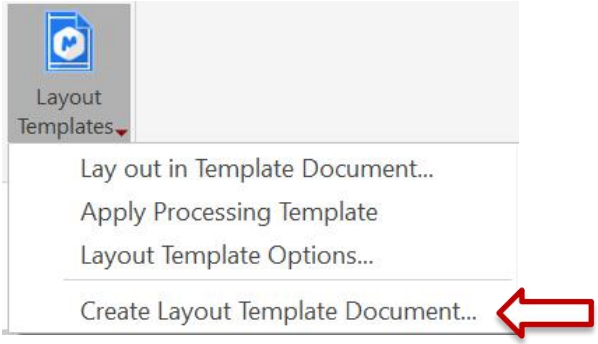
Parameters

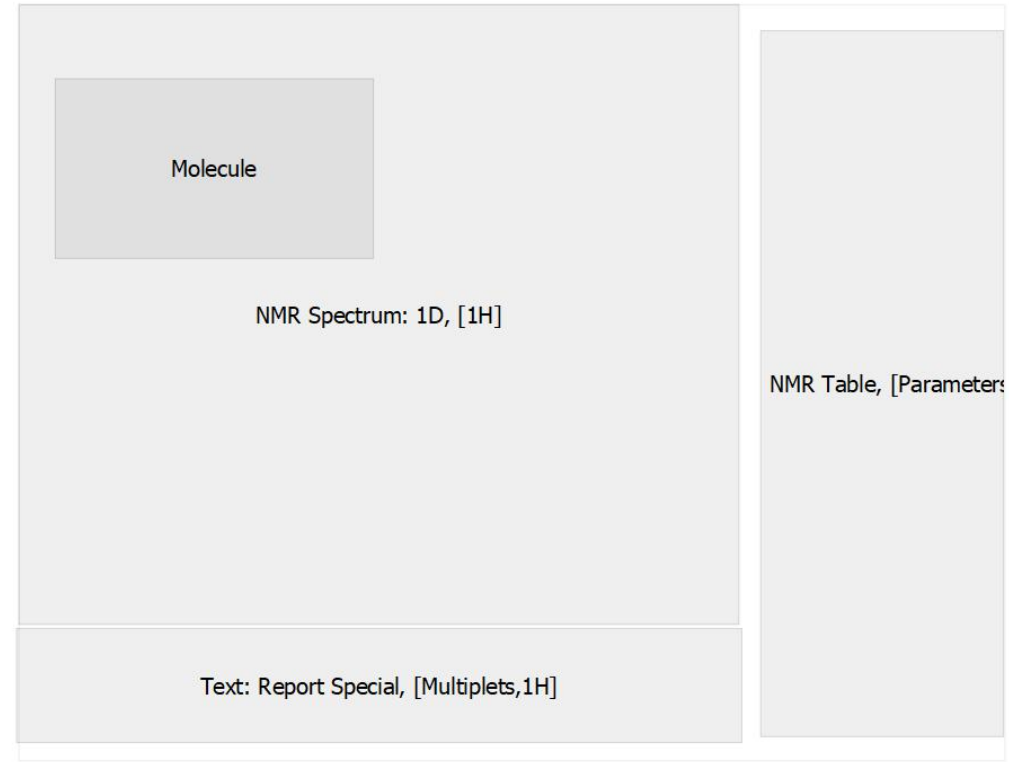
Report Copy Setup Customize

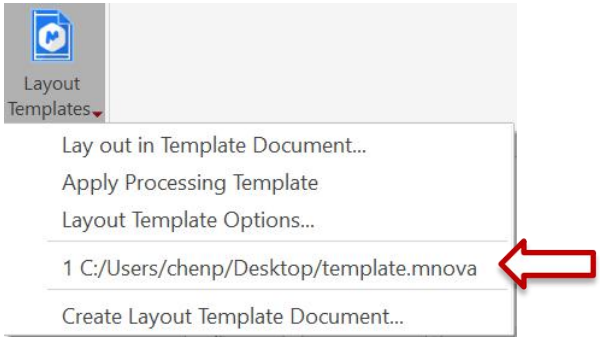
	Parameter	Value
1	Data File Name	C:/Mestrelab/Projects/Marcomm/Liter...
2	Title	1
3	Comment	Ibuprofen 4/8/2015
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	vnmrs
8	Author	
9	Solvent	dmso
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	3mm_cold_HCN_P001
14	Number of Scans	1
15	Receiver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



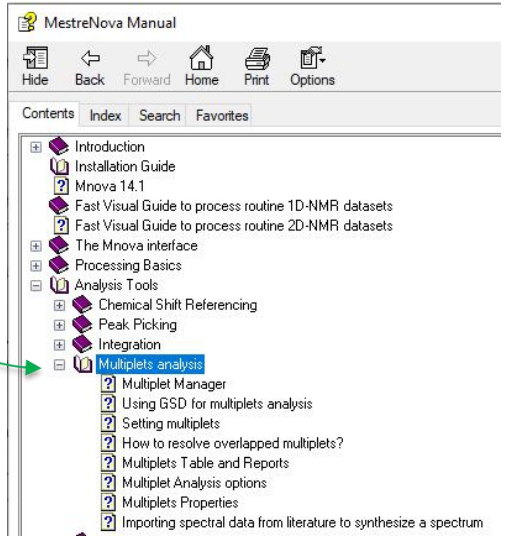




Tip: Mnova uses all pages in the document to create the layout template. So if you have multiple pages, make sure you delete the unwanted ones before creating the layout template.

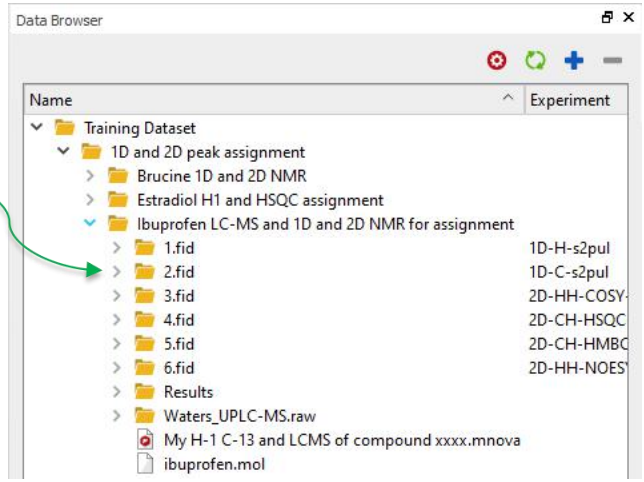
More about H-1 processing

- 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.



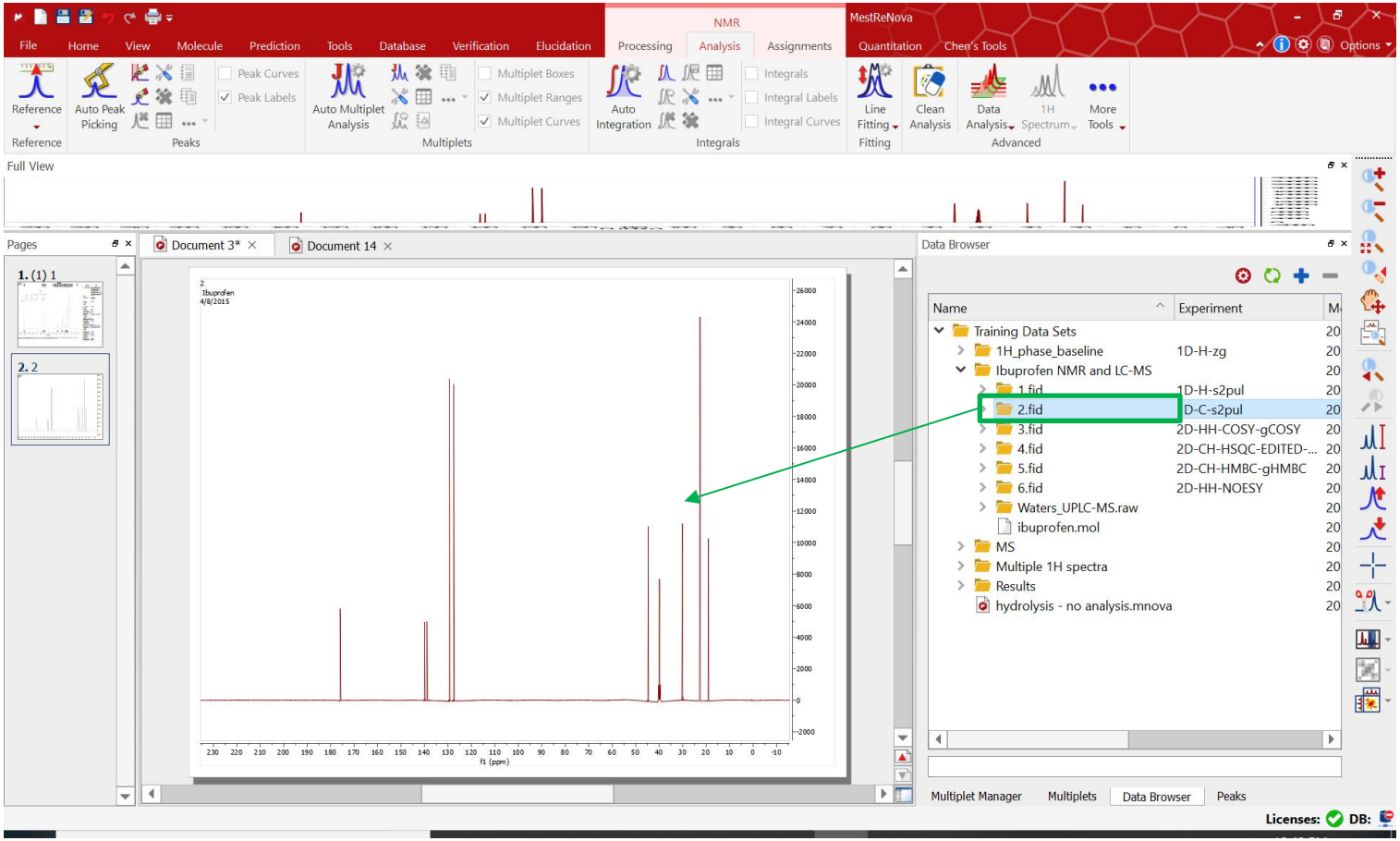
1D ^{13}C NMR Spectrum Processing, Analysis, and Reporting

Sample data



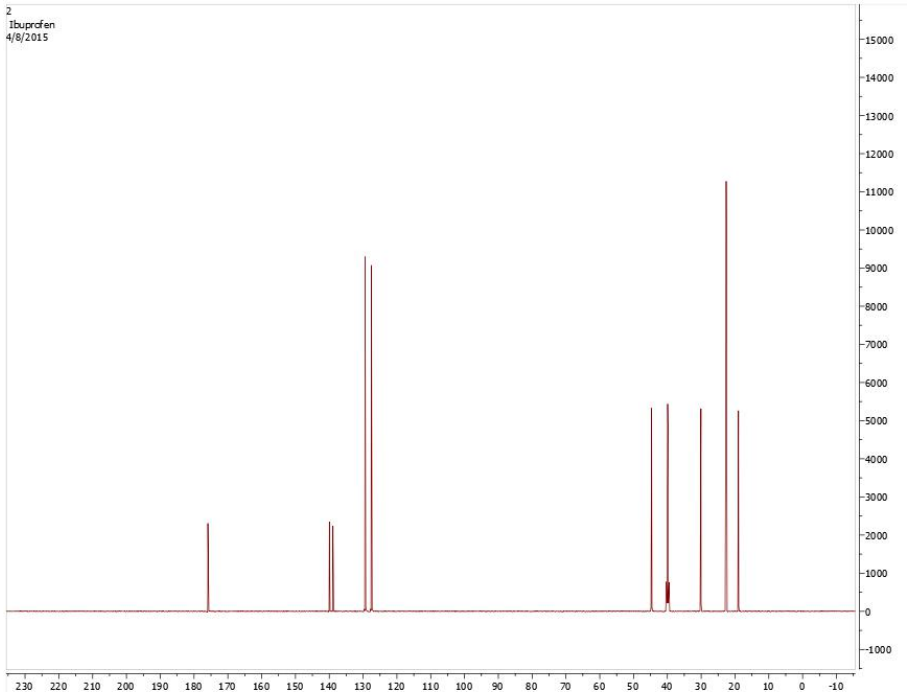
Open a C-13 spectrum

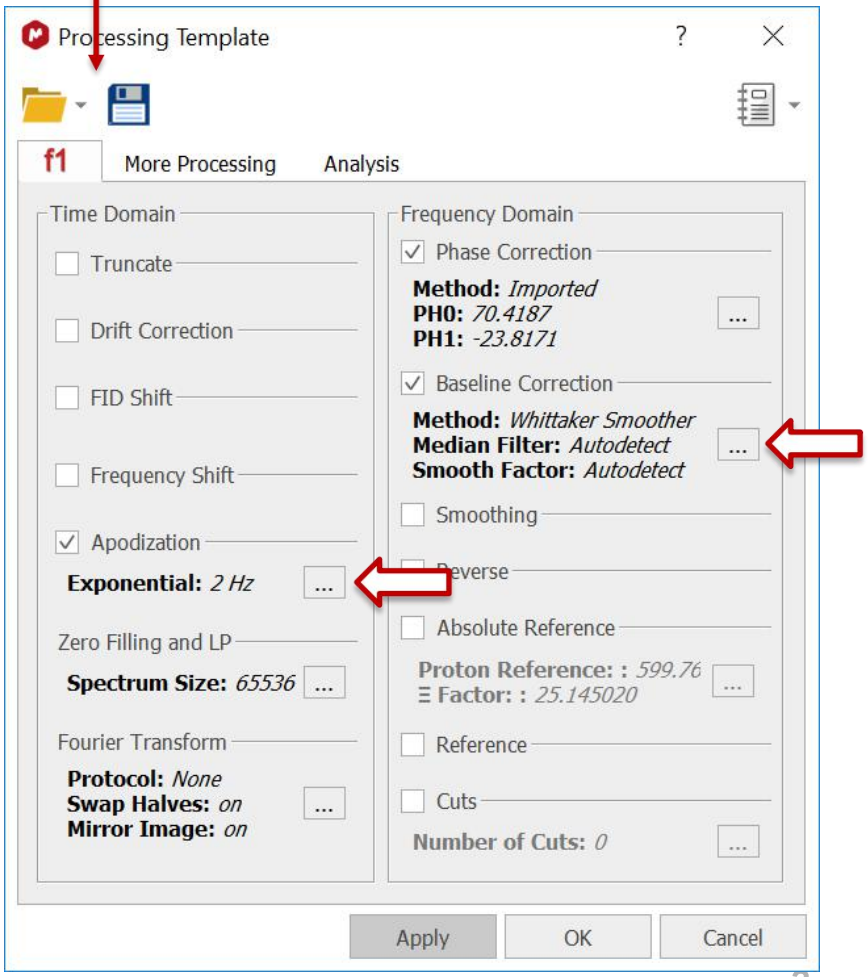
➢ In Data Browser, open the C-13 spectrum of Ibuprofen.



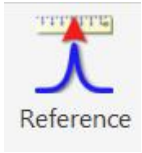
Verify the processing parameters

- 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.

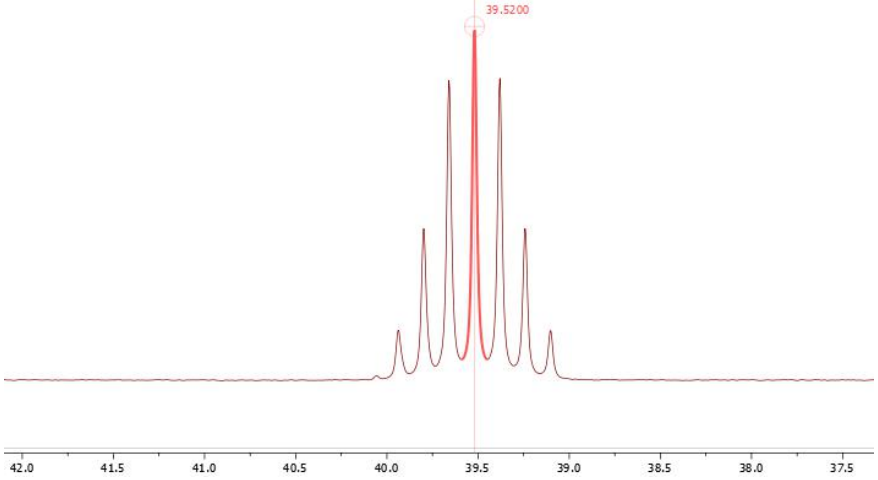


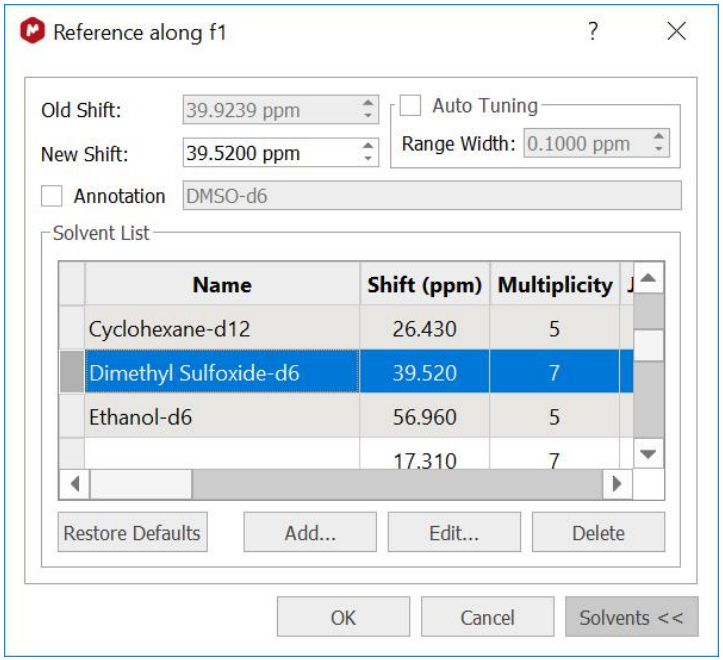


Chemical Shift Referencing



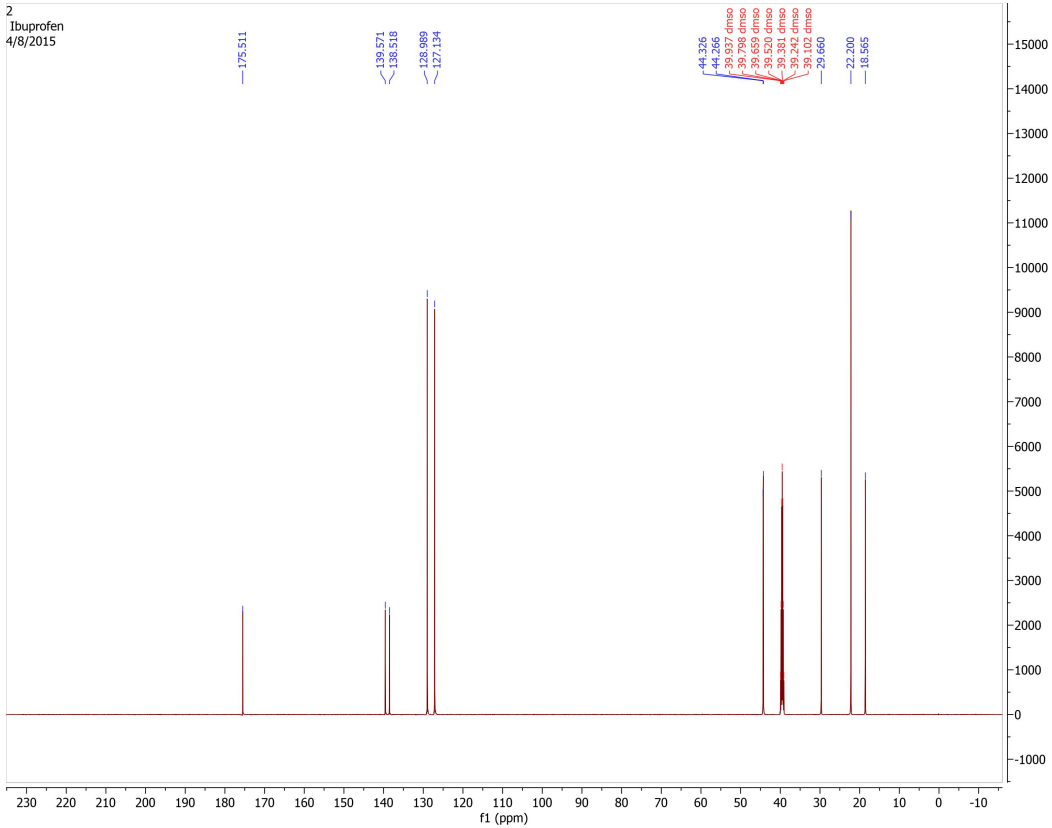
- This spectrum uses DMSO-d6 as the solvent. We can reference the chemical shifts by setting its middle peak to 39.52 ppm.
- Zoom to the DMSO peak at around 39 ppm. Choose Analysis > Reference, and click on the top of the middle peak.
- Set it to 39.52 ppm either manually or from the Solvent List.

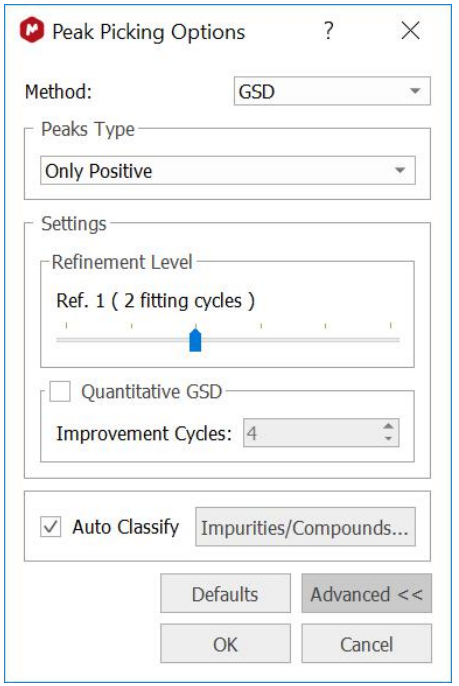




Peak picking

- 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.





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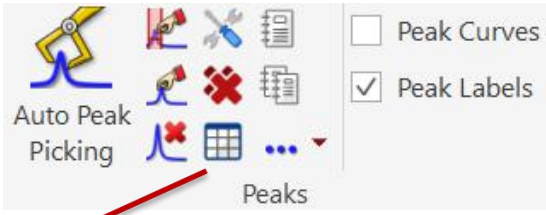
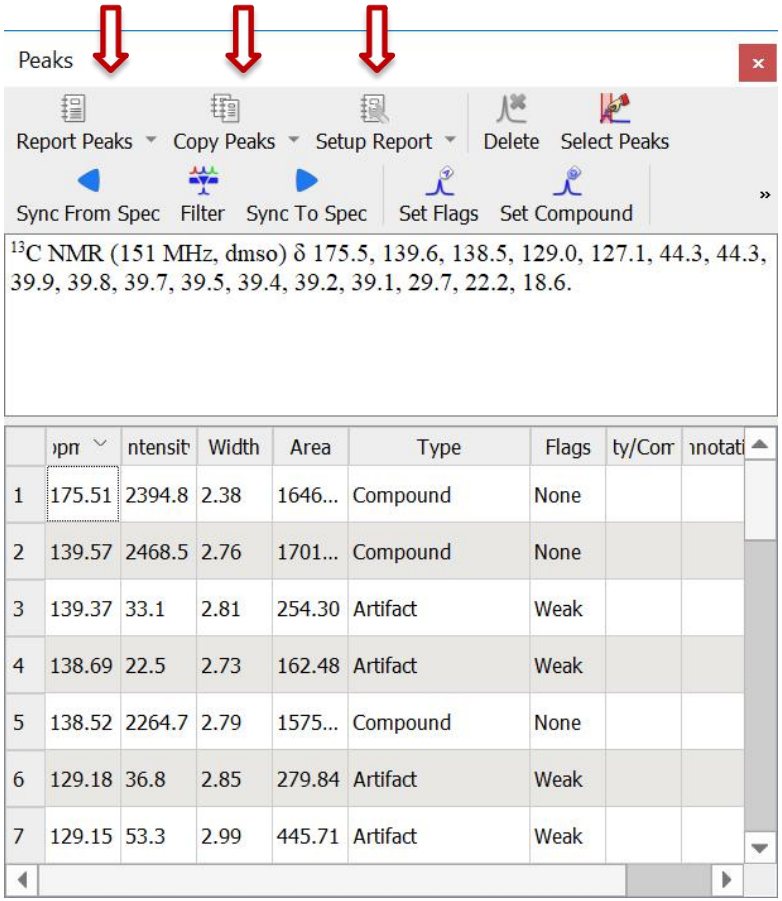
PUBLISHING

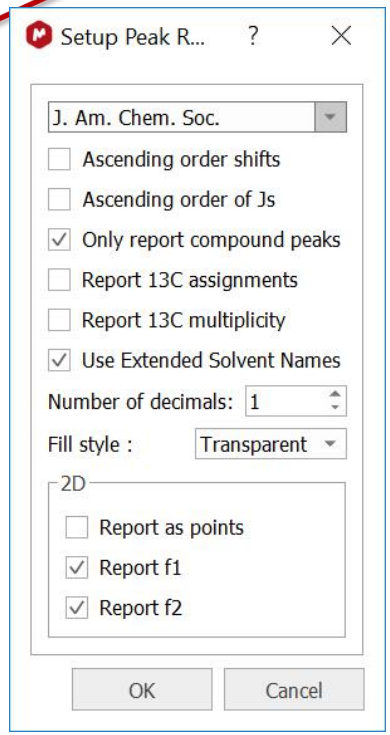
Report the C-13 peaks

- 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	Purity/Comp	Annotation
1	175.51	2394.8	2.38	1646...	Compound	None		
2	139.57	2468.5	2.76	1701...	Compound	None		
3	139.37	33.1	2.81	254.30	Artifact	Weak		
4	138.69	22.5	2.73	162.48	Artifact	Weak		
5	138.52	2264.7	2.79	1575...	Compound	None		
6	129.18	36.8	2.85	279.84	Artifact	Weak		
7	129.15	53.3	2.99	445.71	Artifact	Weak		

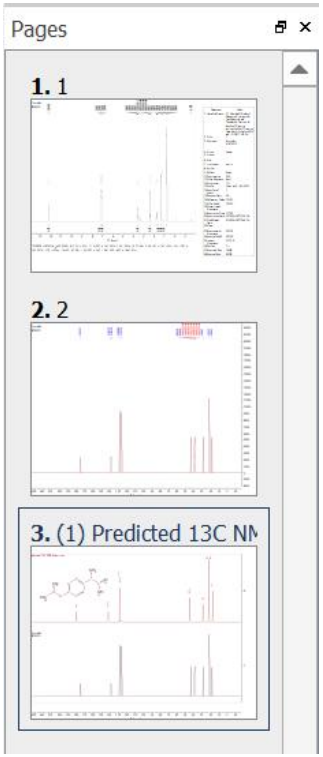


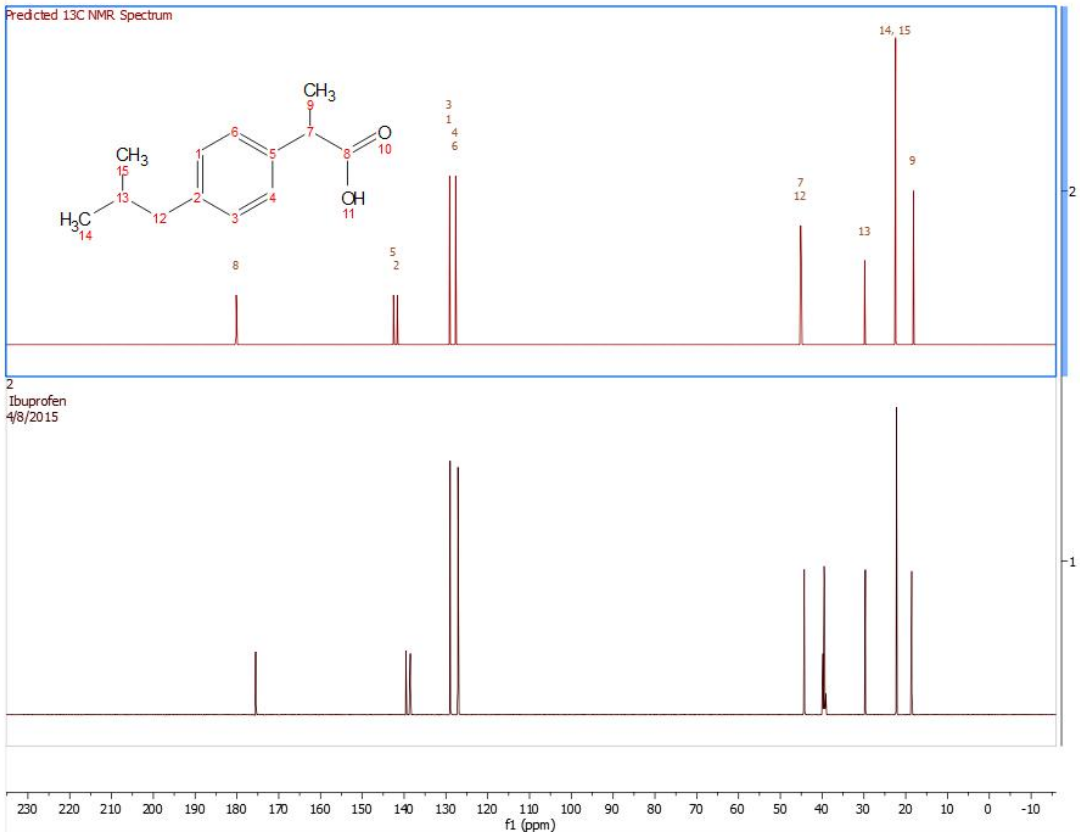
^{13}C NMR (151 MHz, DMSO-d_6) δ 175.5, 139.6, 138.5, 129.0, 127.1, 44.3, 44.3, 29.7, 22.2, 18.6.

PREDICTION

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.





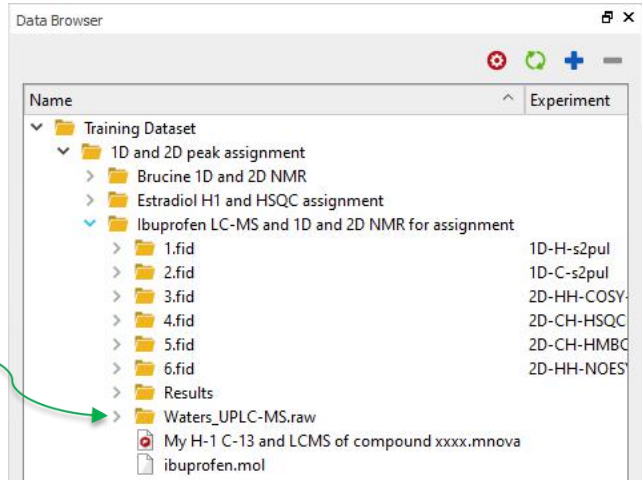
Tip: if you want to delete the predicted C-13 spectrum from the stack, choose Stacked > Stacked Items Table, and use the Delete tool in the Table to delete the predicted C-13 spectrum.

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



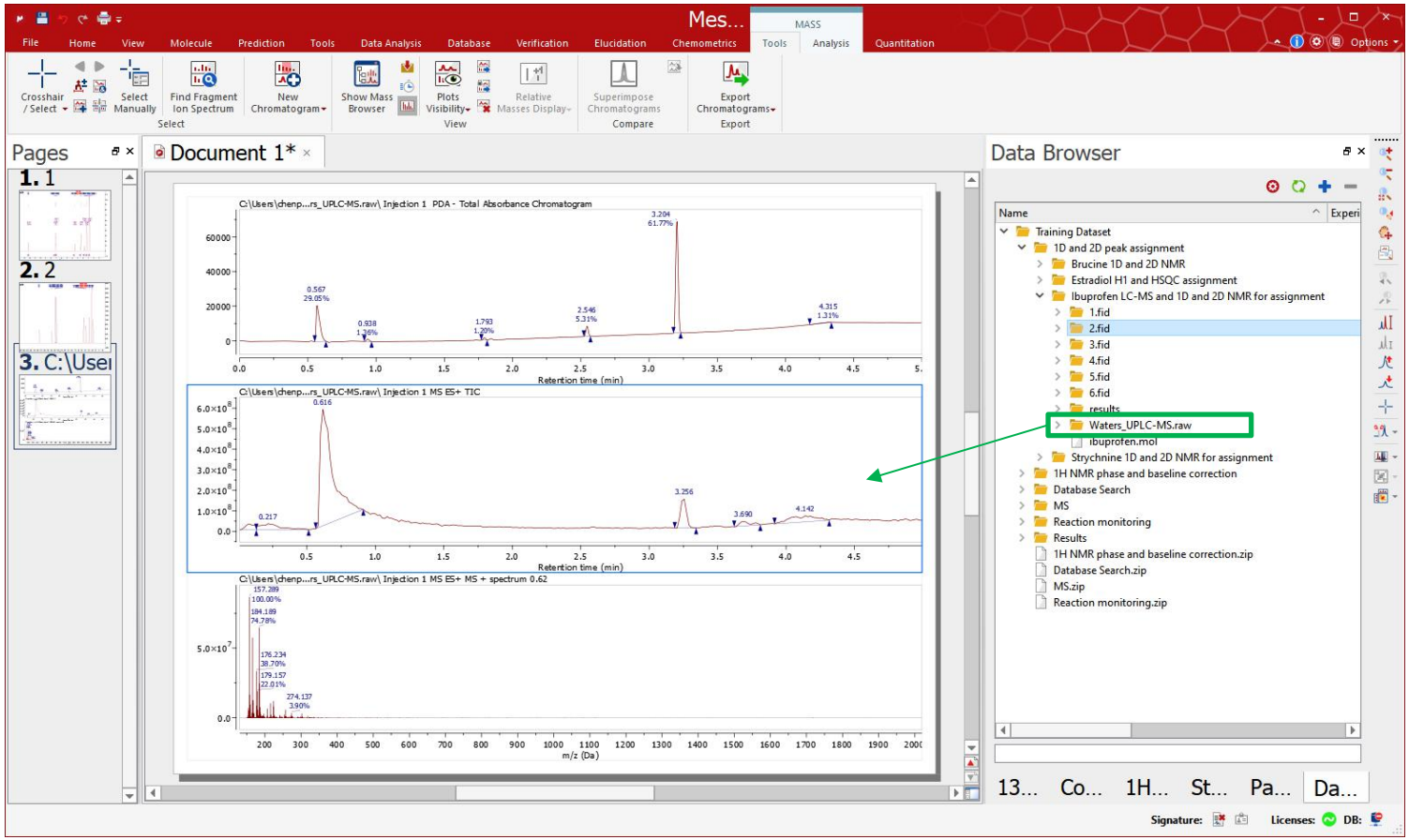
Open the LC-MS data

- 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

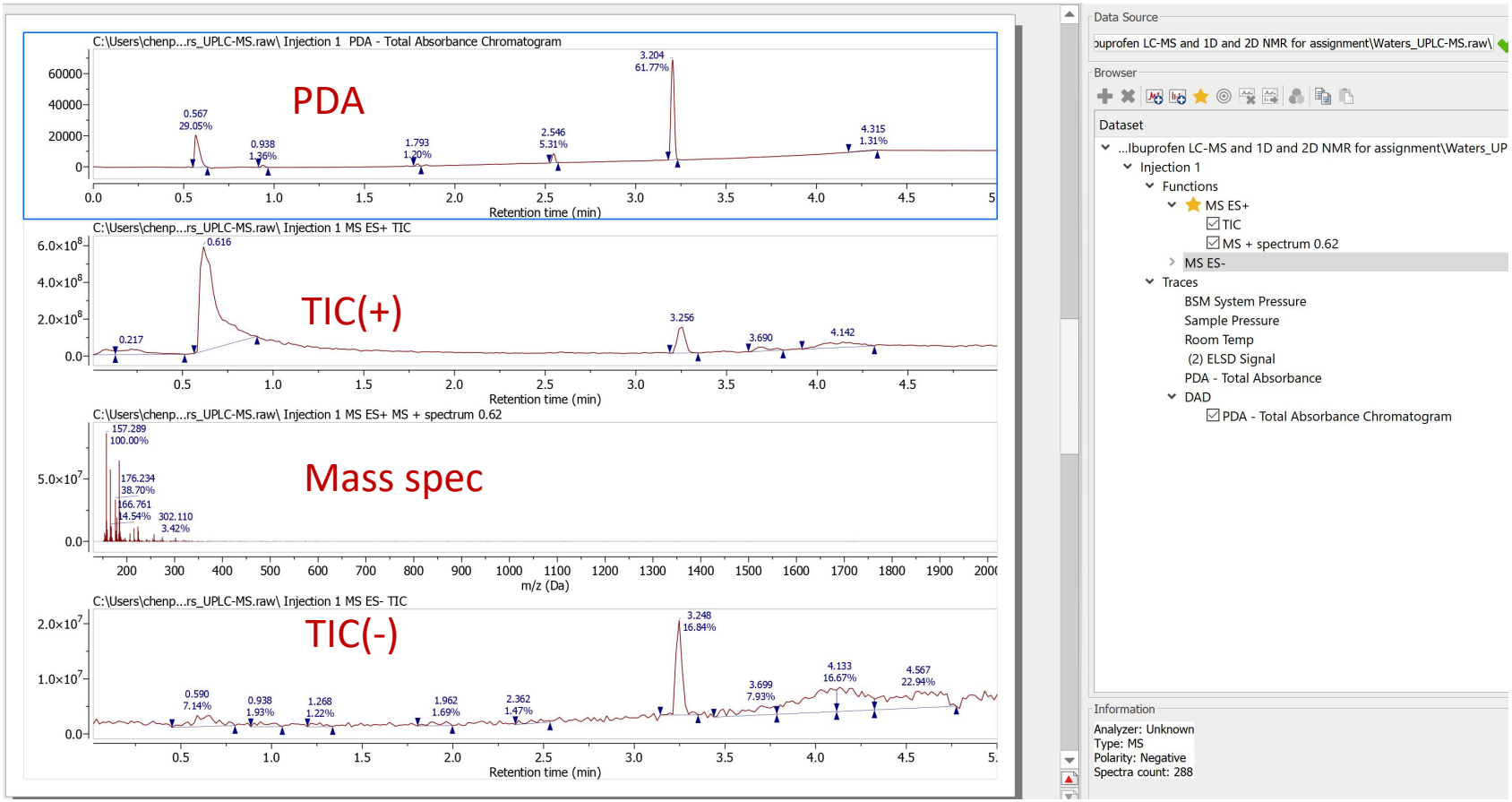
C-13

MS



Display chromatograms

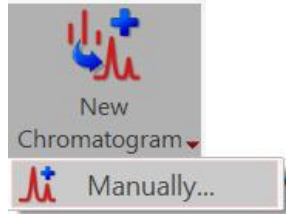
- The Mass Browser is automatically displayed.*
- Open the negative polarization TIC by double clicking on “MS ES-”
- Right on the PDA and choose Hide Plot to hide PDA.

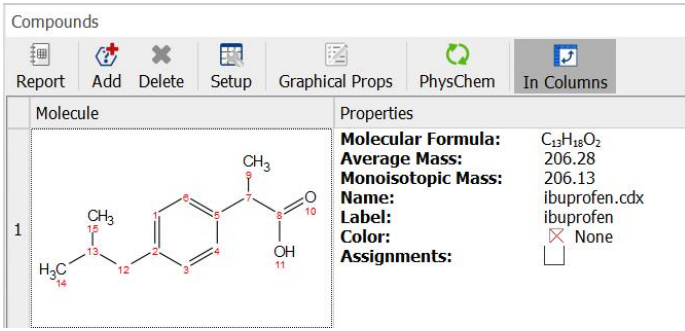


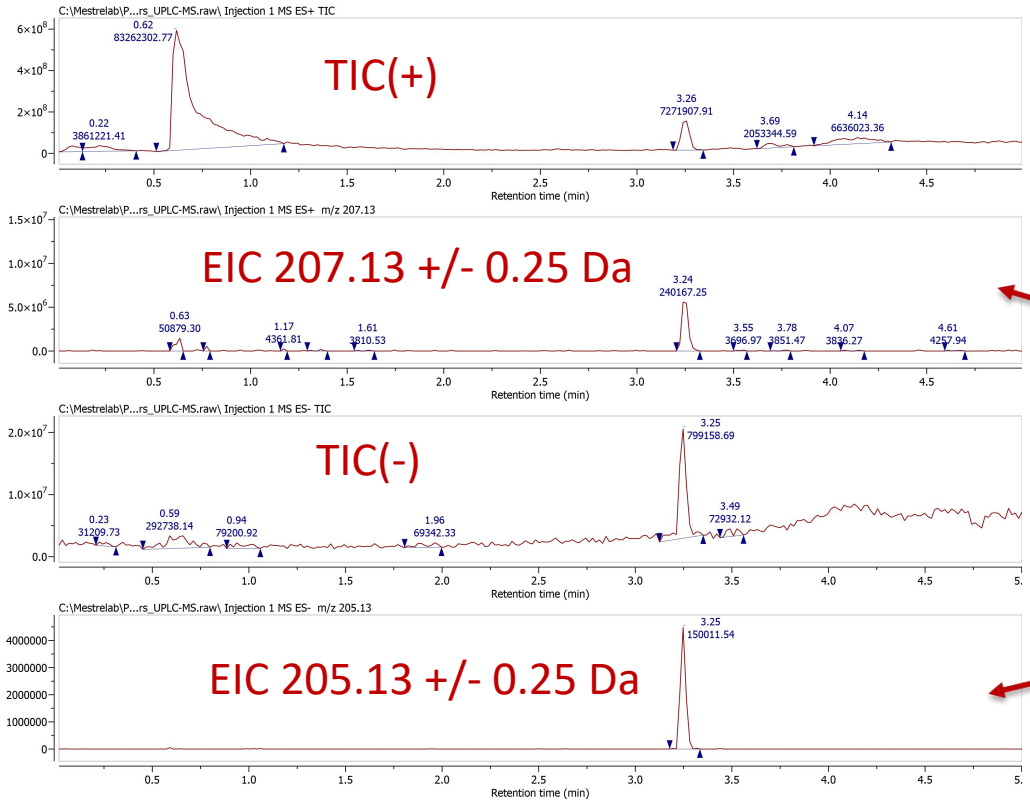
If the Mass Browser is closed, you can open it using the Show Mass Browser tool in the MASS Tools ribbon.

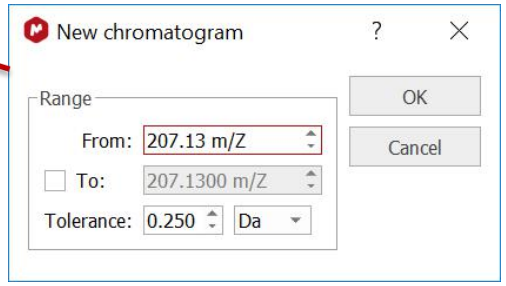
Verify the elemental composition

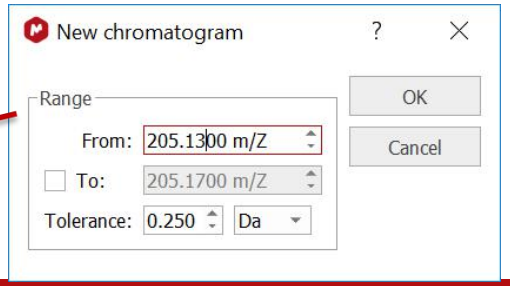
- Open the Ibuprofen.mol file from the Data Browser.
- Choose Molecule > Compound Table to find its monoisotopic mass: 206.13
- Hight the TIC(+), click Mass > New Chromatogram > Manually, and enter a value of 207.13 +/- 0.25 Da to display the new chromatogram (also called Extracted Icon Chrom., EIC)





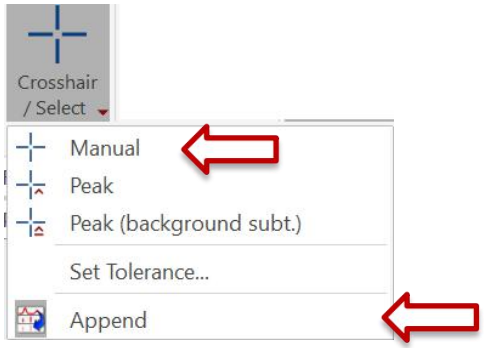


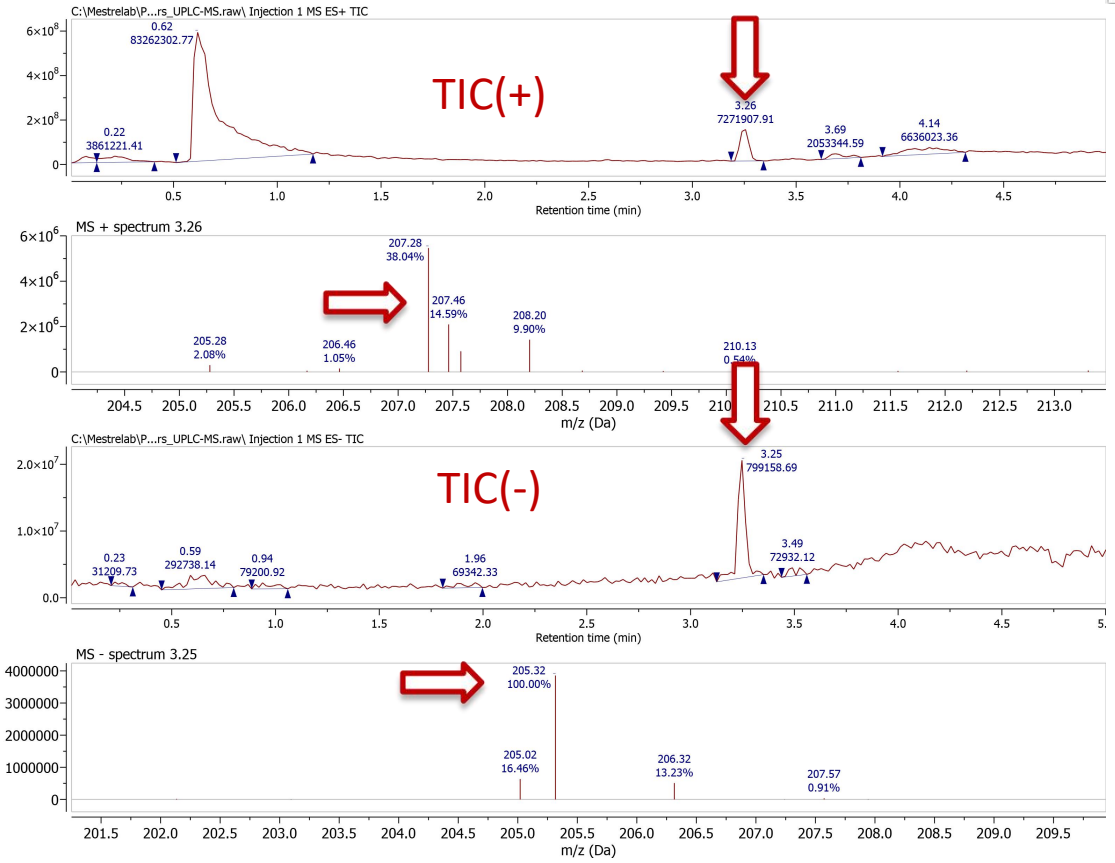




Find the molecule ion peaks

- 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.

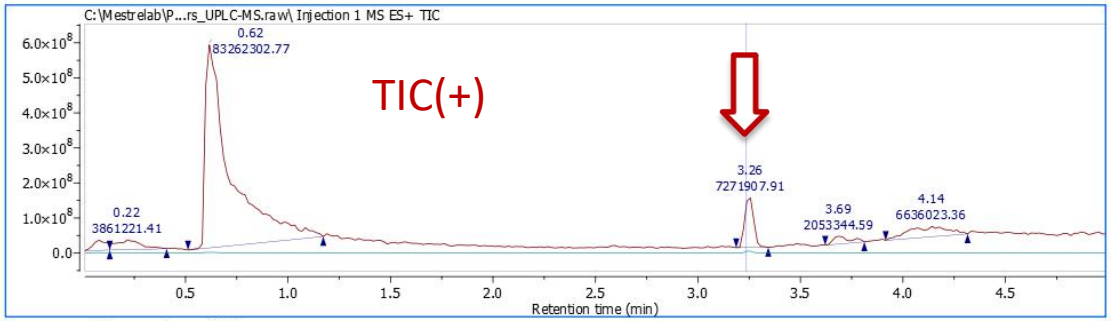


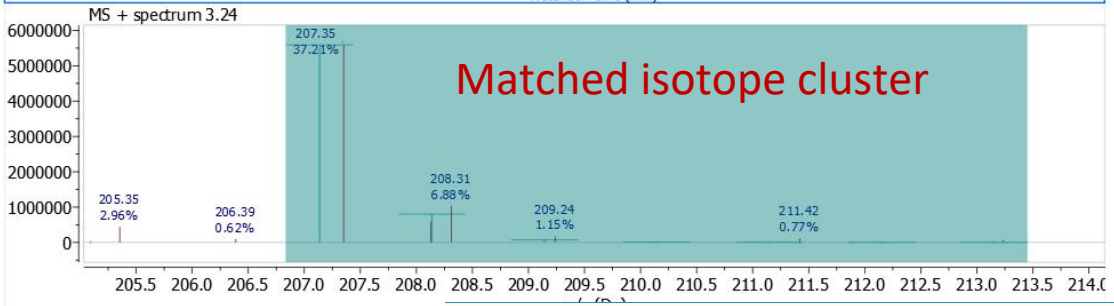


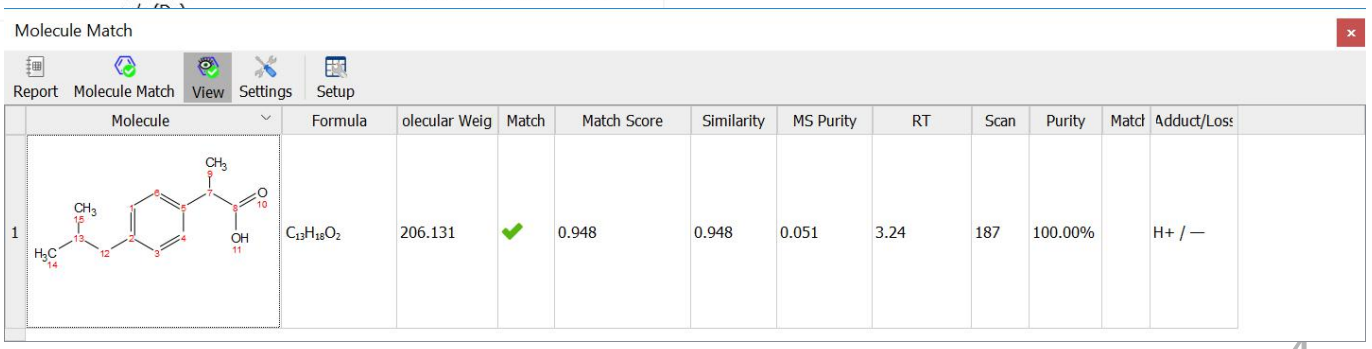
Tip: Use the Mass Browser to hide or delete unwanted plots. Right-click on a plot and choose Move up/Move Down etc. to re-order of the plots

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

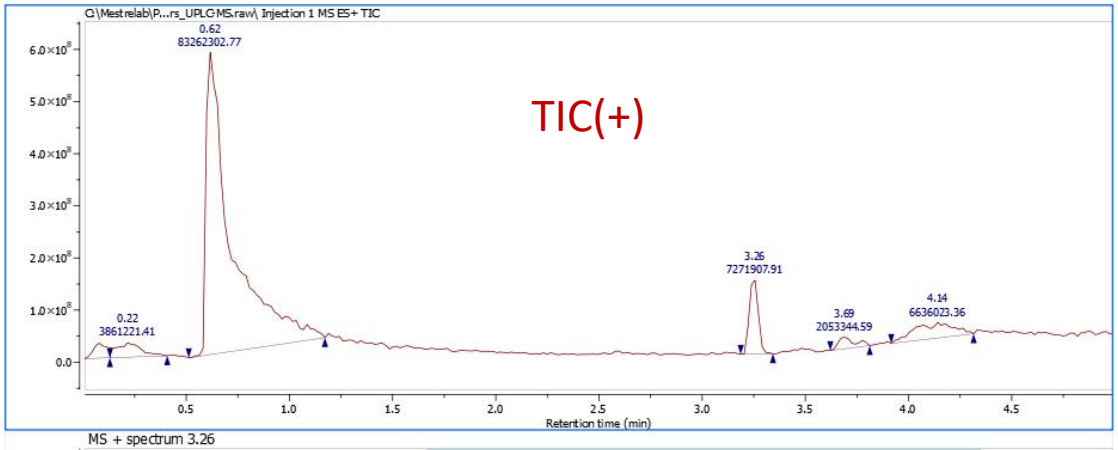


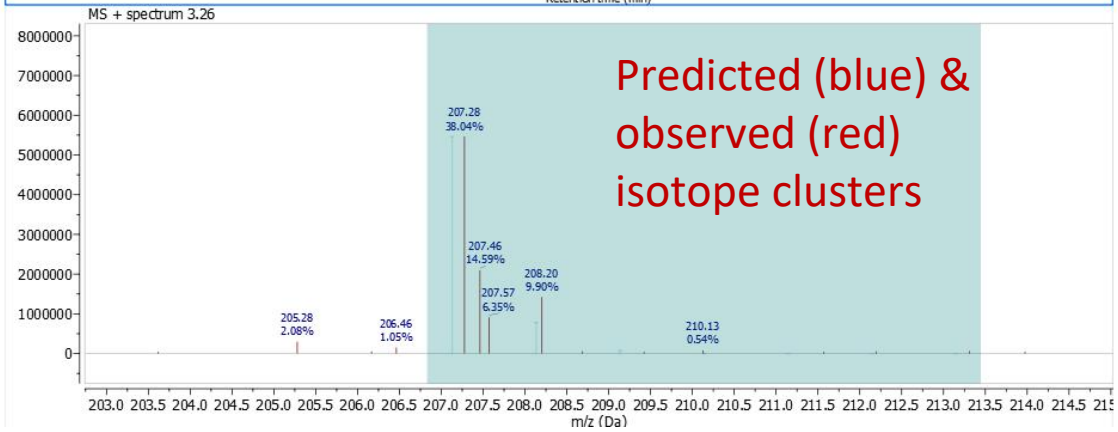


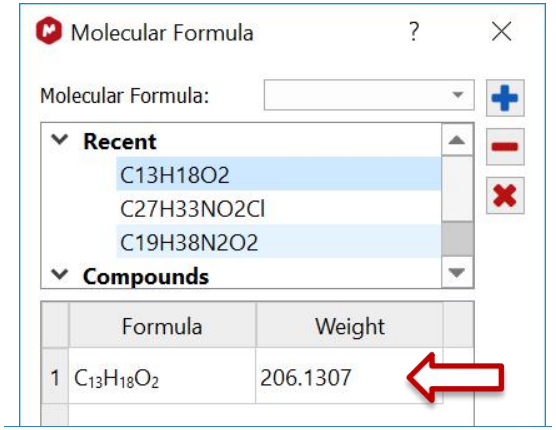


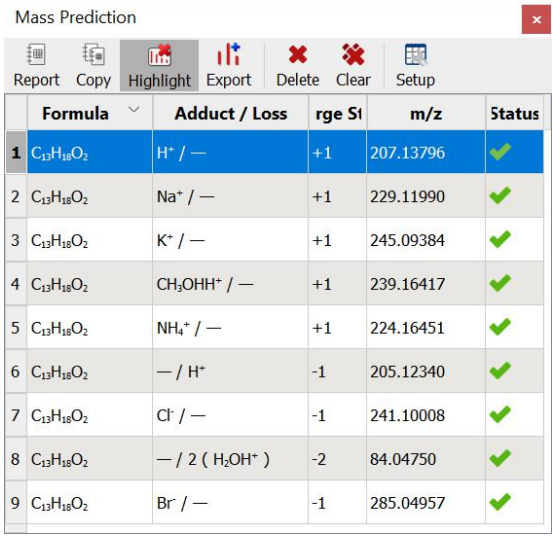
Predict and verify the molecule ion peaks

- 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.







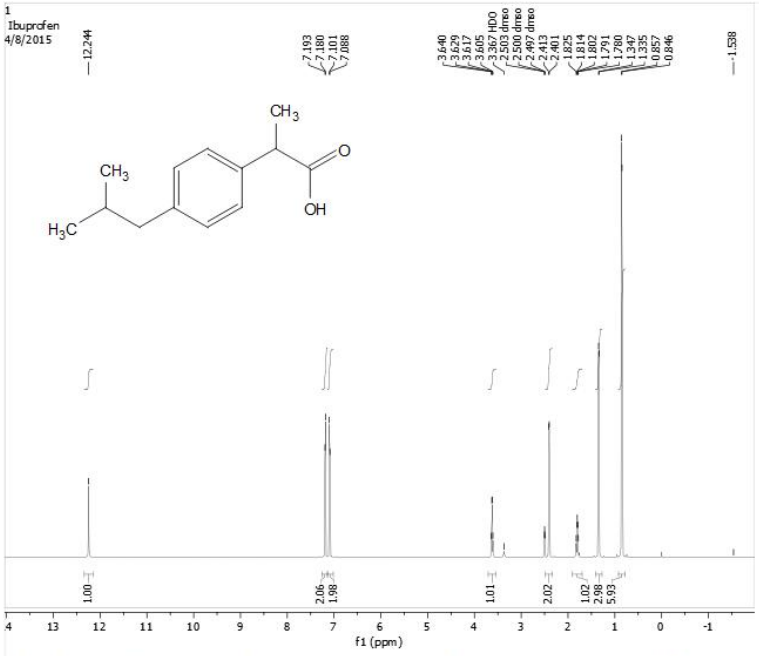


	Formula	Adduct / Loss	rge St	m/z	Status
1	$C_{13}H_{18}O_2$	H^+ / —	+1	207.13796	✓
2	$C_{13}H_{18}O_2$	Na^+ / —	+1	229.11990	✓
3	$C_{13}H_{18}O_2$	K^+ / —	+1	245.09384	✓
4	$C_{13}H_{18}O_2$	CH_3OHH^+ / —	+1	239.16417	✓
5	$C_{13}H_{18}O_2$	NH_4^+ / —	+1	224.16451	✓
6	$C_{13}H_{18}O_2$	— / H^+	-1	205.12340	✓
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	✓

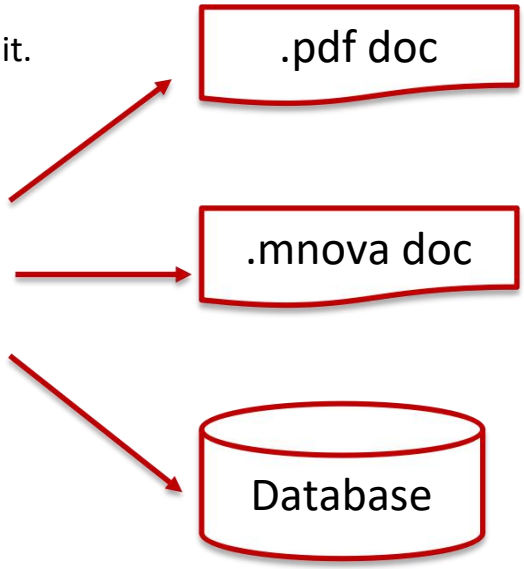
SAVING RESULTS

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.
- Now can close the document or continue to add other spectra to it.



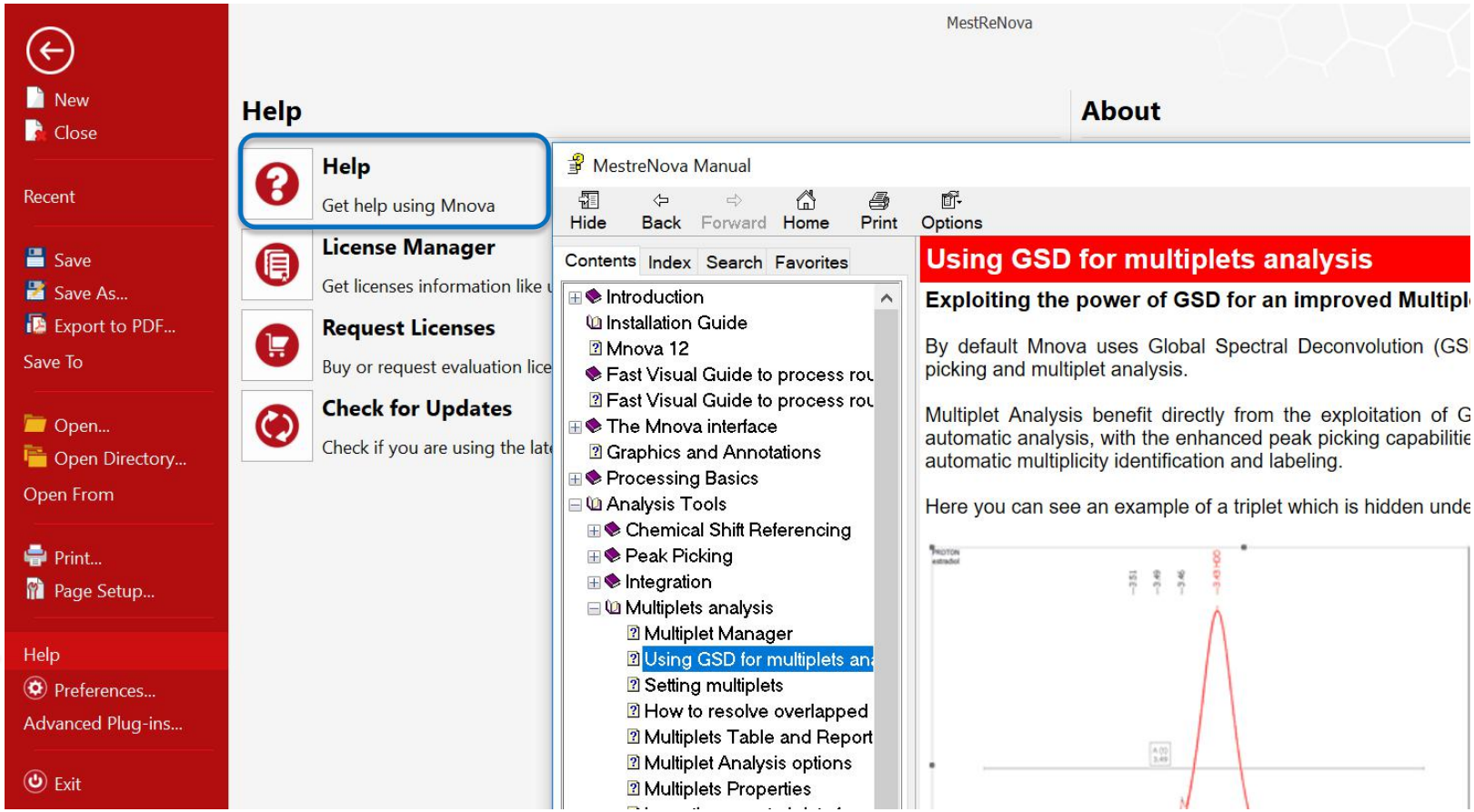
	Parameter	Value
1	Data File Name	C:/ Mestrelab/ Projects/ Marcomm/ Literature & Docs/ Sample and Templates/ Training for chemists/ Training courses by Chen/ Training Data Sets/ Ibuprofen NMR and LCMS/ 1.fid/ fid
2	Title	1
3	Comment	Ibuprofen 4/ 8/ 2015
4	Origin	Varian
5	Owner	
6	Site	
7	Instrument	vnmrs
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



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Mnova Training– Advanced

For Mnova v14.2.0
Oct. 2020

Chen Peng, PhD,
VP of Business Development, North America & Asia
Mestrelab Research SL
chen.peng@mestrelab.com
858.736.4563

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Main Topics

- Opening and processing 2D NMR
- Assigning peaks to atoms
- Reporting assignment results
- Creating a database to save the data
- Searching Wiley C & H databases
- Analyzing arrayed spectra for reaction monitoring

Note: This tutorial covers the NMR, NMRPredict, MS, DB plugins of Mnova, and Wiley DBs

Specifics for <xxxxxx> University (To be completed by instructor)

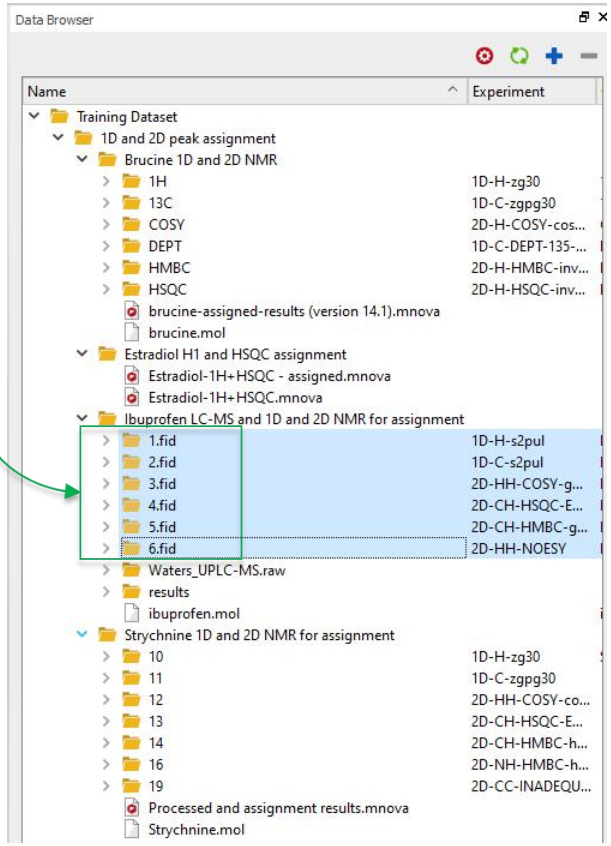
- The instructions for downloading, installing and activating Mnova:
  - <Link to instruction page>

- The Mnova licenses that <XXXX> University has:
  - Mnova Suite (NMR, NMRPredict & MS), unlimited
  - Etc.

- The sample data used in this tutorial are located at:
  - <Link to data folder>.

Processing 1D & 2D NMR Spectra Together

Sample data

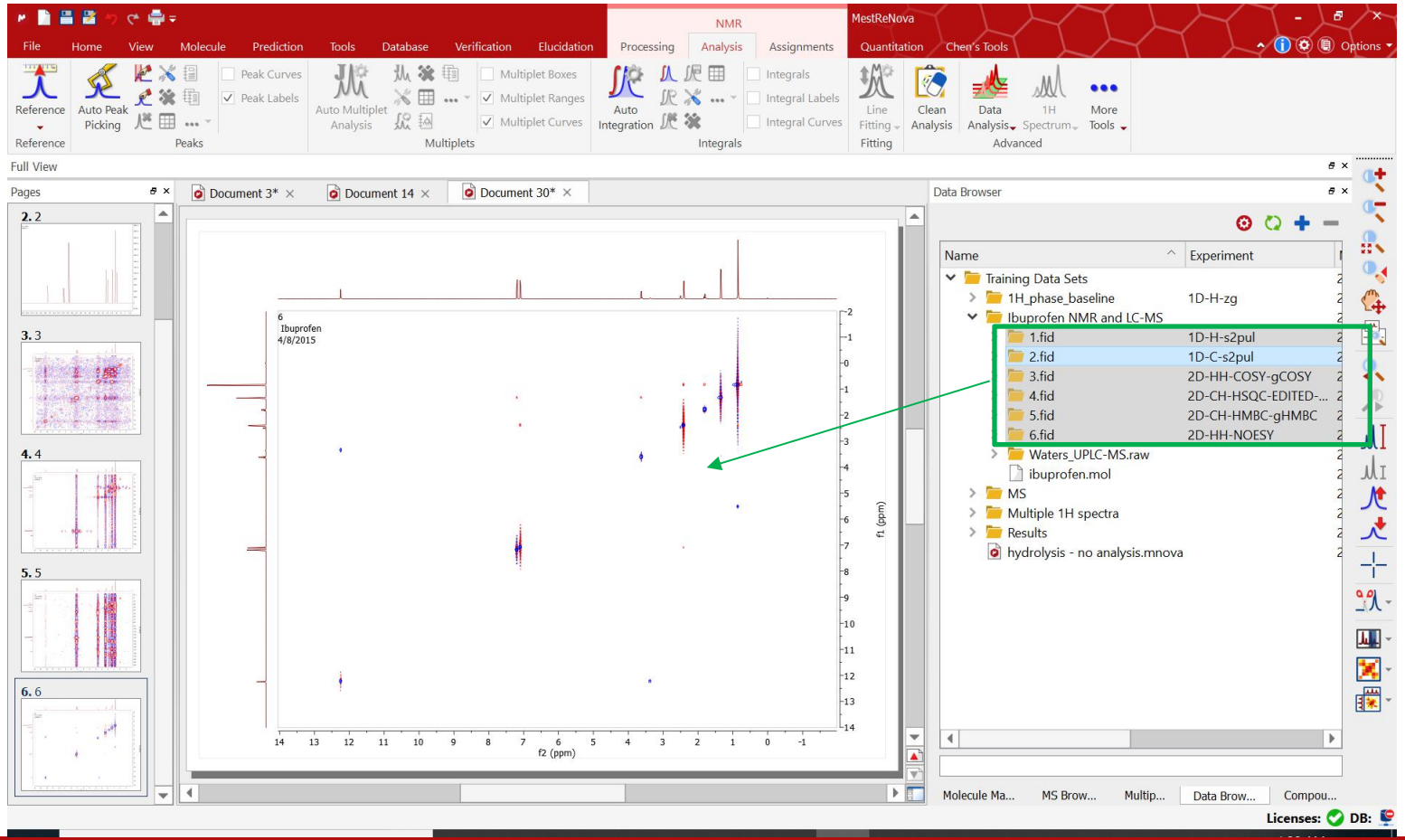


Tip: There are a total of 4 datasets with 1D and 2D NMR spectra for practicing spectral processing, peak assignment (and structure elucidation, which is not covered in this tutorial). The Ibuprofen one used here is the simplest one compared to the others (Brucine, Strychnine and Estradiol).

PROCESSING

Open a 1D and 2D spectra of Ibuprofen

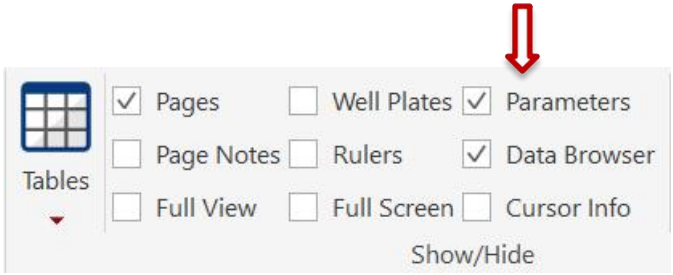
- Choose File > New to open a new blank document.
- In Data Browser, choose the 1D H/C, 2D HSQC, HMBC, COSY, and NOESY spectra and drag all of them to the main window.
- Re-process and analyze the H-1 and C-13 spectra according to the Basic Tutorial.

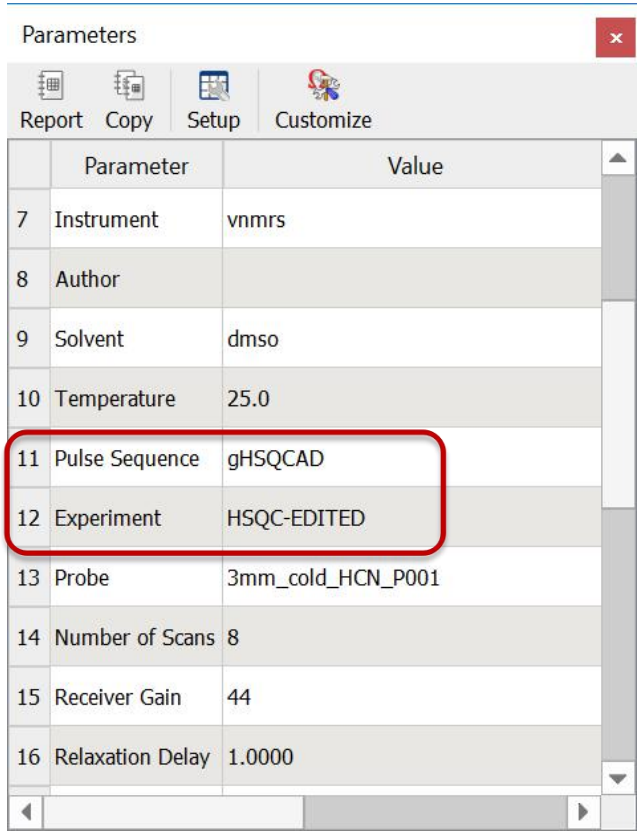


PARAMETERS

Which is which?

- Check View > Parameters Table to display the Parameters Table
- The Experiment and Pulse Sequence parameters usually indicate the type of NMR data

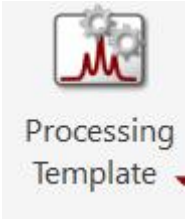




	Parameter	Value
7	Instrument	vnmrs
8	Author	
9	Solvent	dmso
10	Temperature	25.0
11	Pulse Sequence	gHSQCAD
12	Experiment	HSQC-EDITED
13	Probe	3mm_cold_HCN_P001
14	Number of Scans	8
15	Receiver Gain	44
16	Relaxation Delay	1.0000

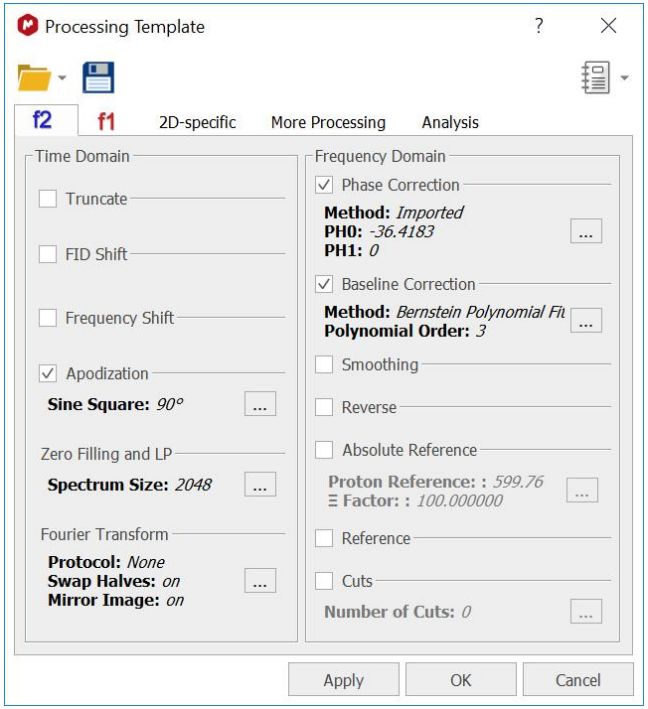
Tip: You can display the Experiment as part of the spectrum title. Double click on the spectrum and setup the Title in the Properties Dialog.

Rules of thumb for 2D processing

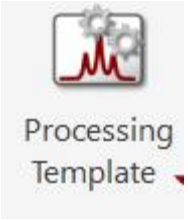


When a 2D is opened in Mnova, it is automatically processed starting from the raw data (*ser* or *fid*) with the parameters from the instrument. If the results are not satisfactory, you may need to adjust the following parameters to improve the results:

- Apodization: To improves the line shape, resolution and S/N ratio
  - COSY: Use Sine Square 0 for F2 & F1
  - Others: Use Since Square 90 F2 & F1
- Zero Fill and LP (Linear Prediction): To improve resolution
  - F2: at least double of the original datapoints, 2048 or 4096
  - F1: At least double of the original datapoints, 1024 or 2048
  - F1: Do LP if original datapoints <= 128 (optional)
- Phase Correction: To improve line shape
  - Use Imported or Automated (Regions) first
  - Do manual correction if needed.
- Baseline Correction: To reduce noise
  - Use Bernstein Polynomial Fit on either dimension
- Other 2D-Specific parameters (optional):
  - COSY, NOESY: Use Symmetrize with caution
  - HSQC, HMBC: Use Reduce T1 Noise Reduction when needed.



Rules of thumb for 2D processing

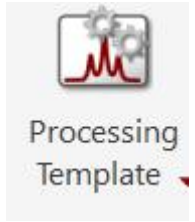


The 2D processing parameters that you may want to adjust and their recommended values*

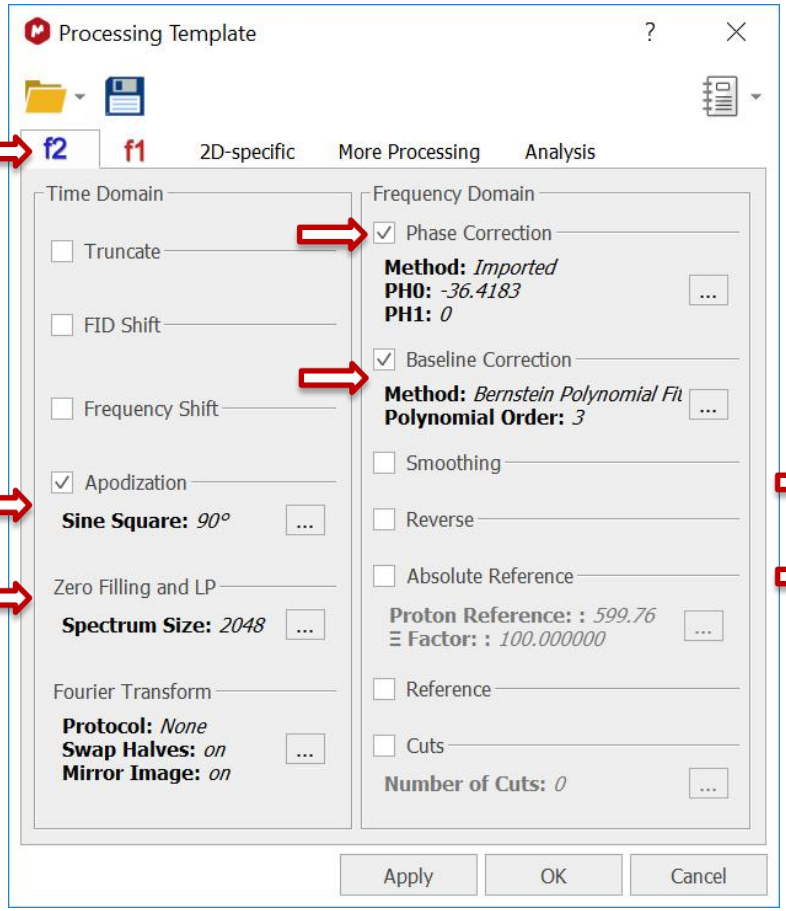
	Apodi -zation	Zero-fill & Linear Prediction	Phase Correction	Baseline Correction	Others
COSY	Sine square 0 on both F2 and F1	At least double to 2K or 4K on F2; or 1K or 2K on F1. Do linear prediction on F1 if # of increments < 128	Use imported parameters first. Use auto or manual phasing if needed on both F1 and F2	Use Bernstein Polynomial Fitting (3rd order) for F2 and F1	Do COSY-style symmetrization with caution
HSQC	Sine square 90 on both F2 and F1	Same as above	Same as above	Same as above	Use Reduce T1 Noise to reduce T1 noises with caution
HMBC	Same as above	Same as above	Same as above	Same as above	Same as above
NOESY/ROESY	Same as above	Same as above	Same as above	Same as above	Do COSY-style symmetrization with caution

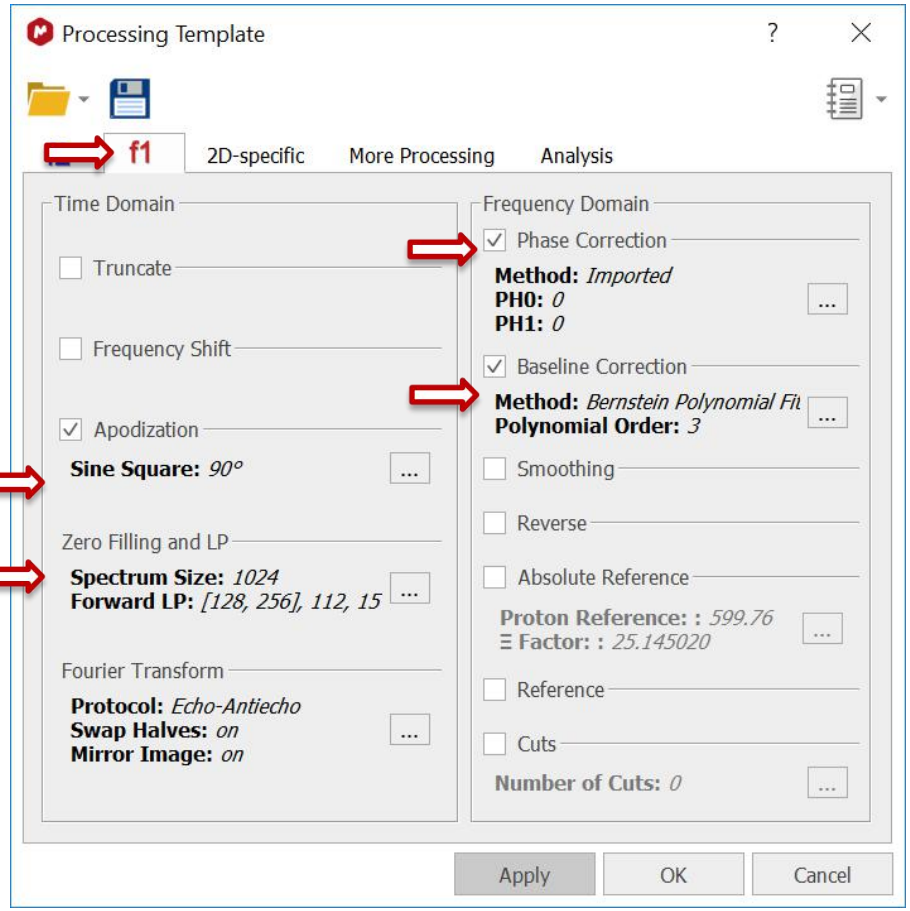
**These are recommended starting points for conventional 2D NMR processing. You can try many of other combinations as appropriate. Once you are satisfied with the results, you can save all the parameters as a processing template, and apply it to similar spectra later.*

Re-process HSQC spectrum



- Reprocess the HSQC spectrum as shown below.
- Note the apodization functions for F2 and F1
- Note the forward linear prediction for F1 applied here

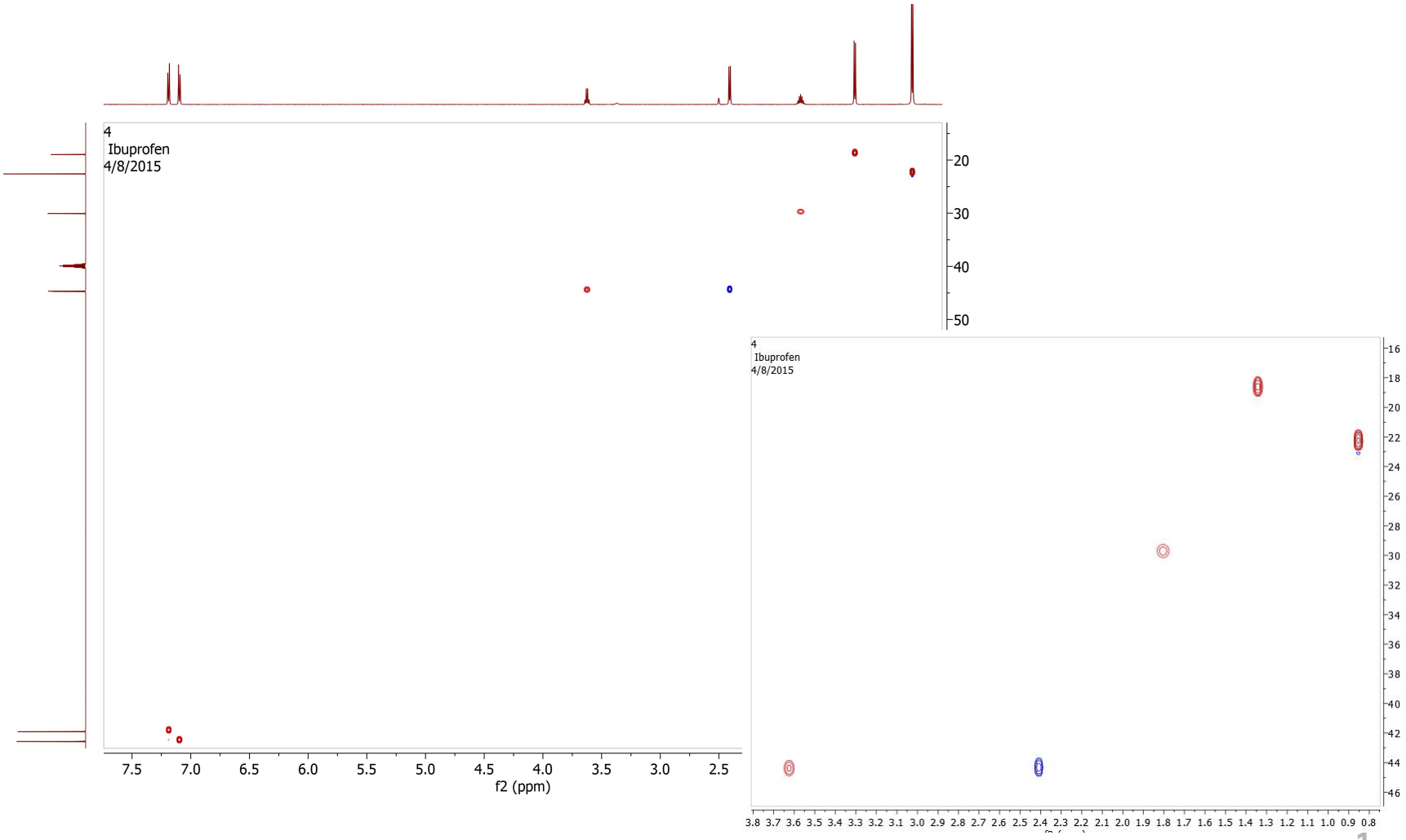




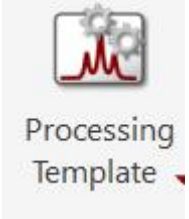
Note: The Fourier Transform method is automatically set and normally you don't need to change it.

Re-process HSQC spectrum

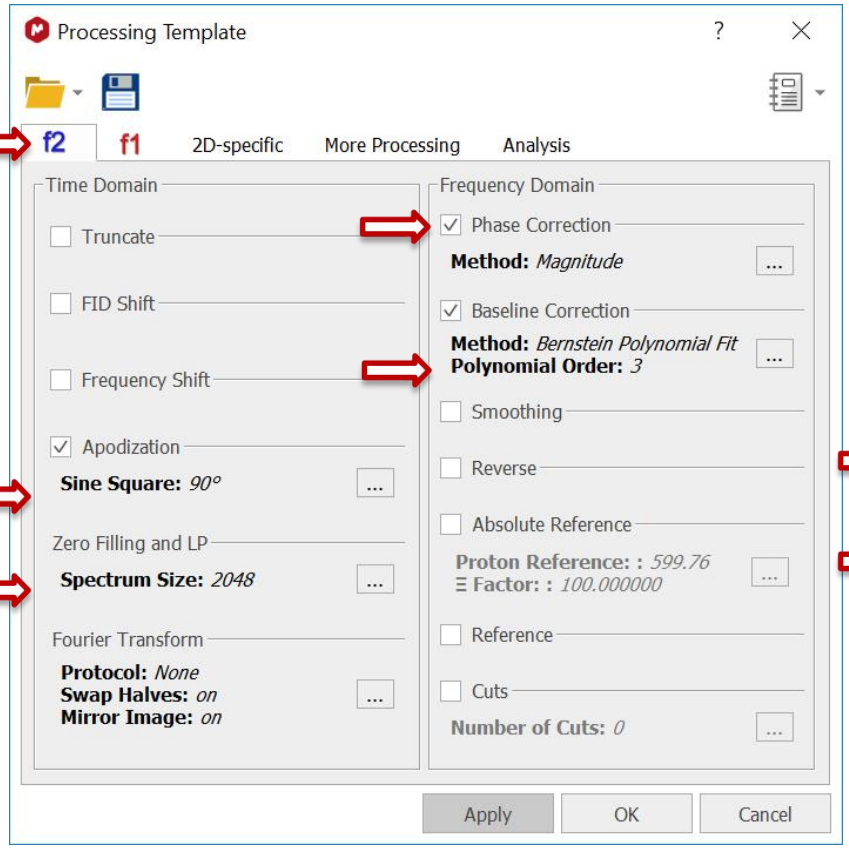
➢ The re-processed HSQC spectrum shows better line shape, and higher resolution on the F1 dimension

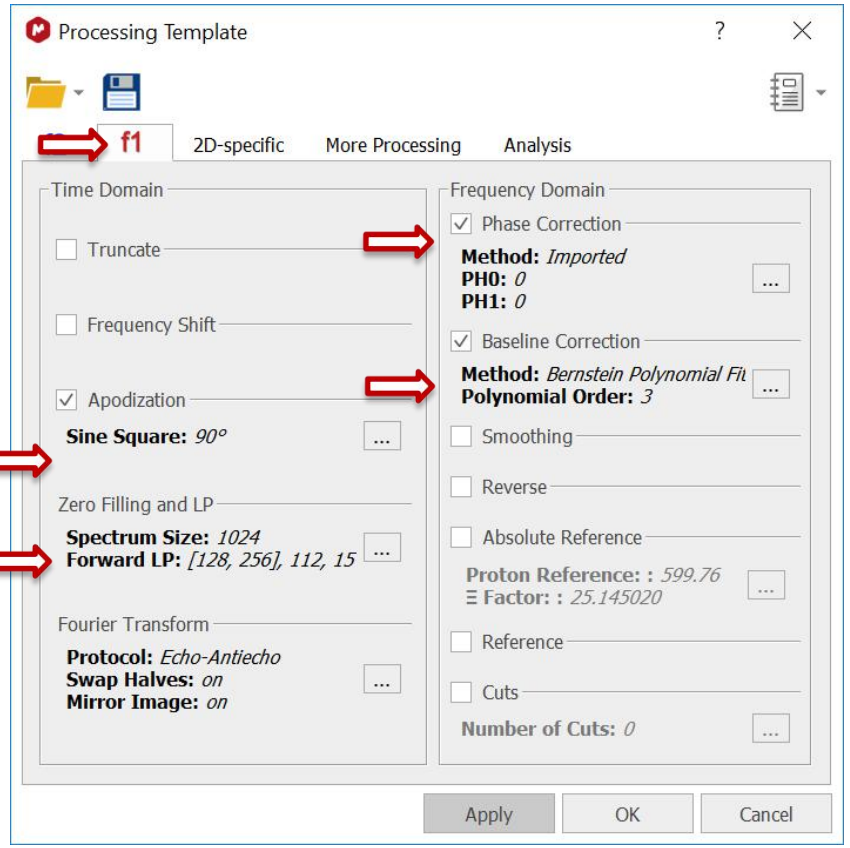


Re-process HMBC spectrum



- Reprocess the HMBC spectrum as shown below.
- Note the apodization functions for F2 and F1
- Note the forward linear prediction for F1 applied here

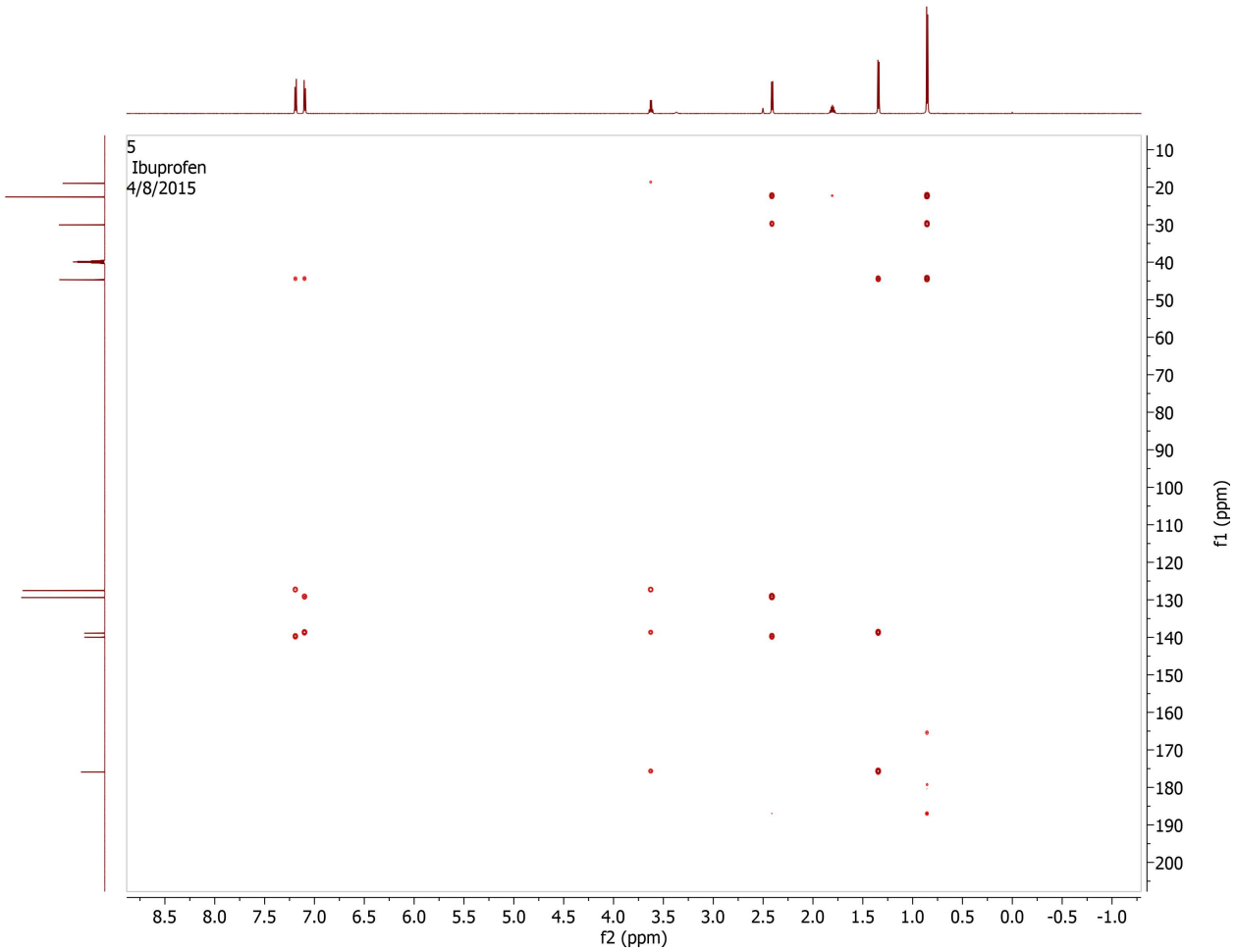




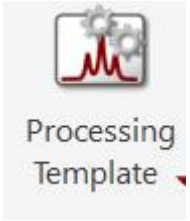
Note: The Fourier Transform method is automatically set and normally you don't need to change it.

Re-process HMBC spectrum

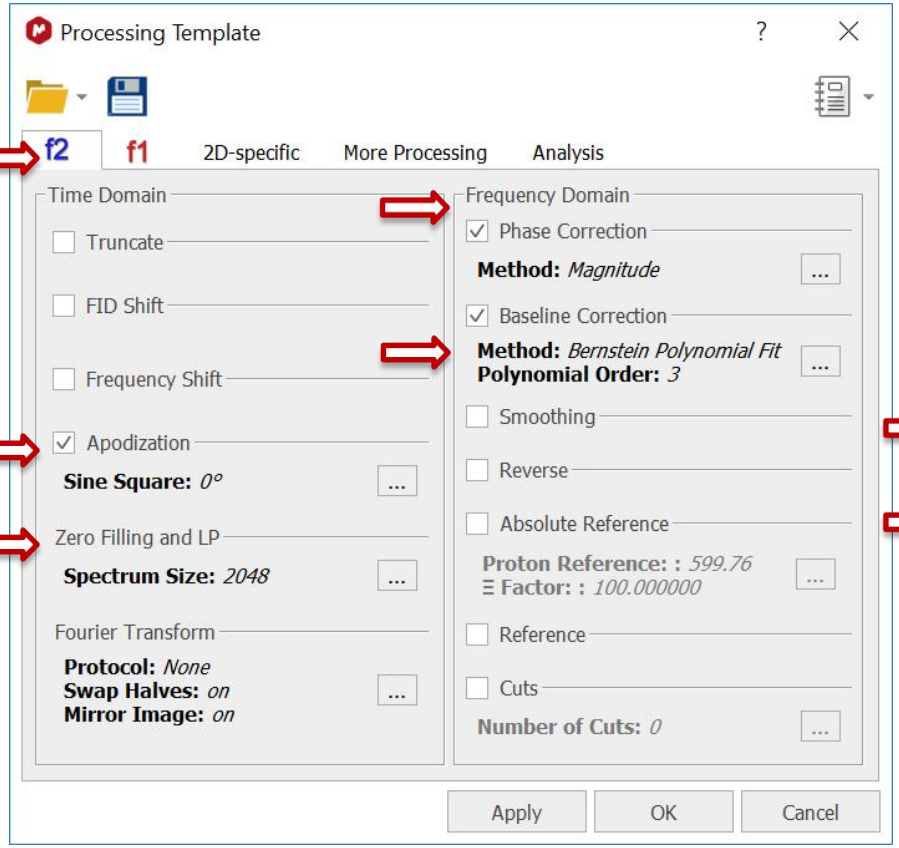
➢ The re-processed HSQC spectrum shows better line shape, and higher resolution on the F1 dimension

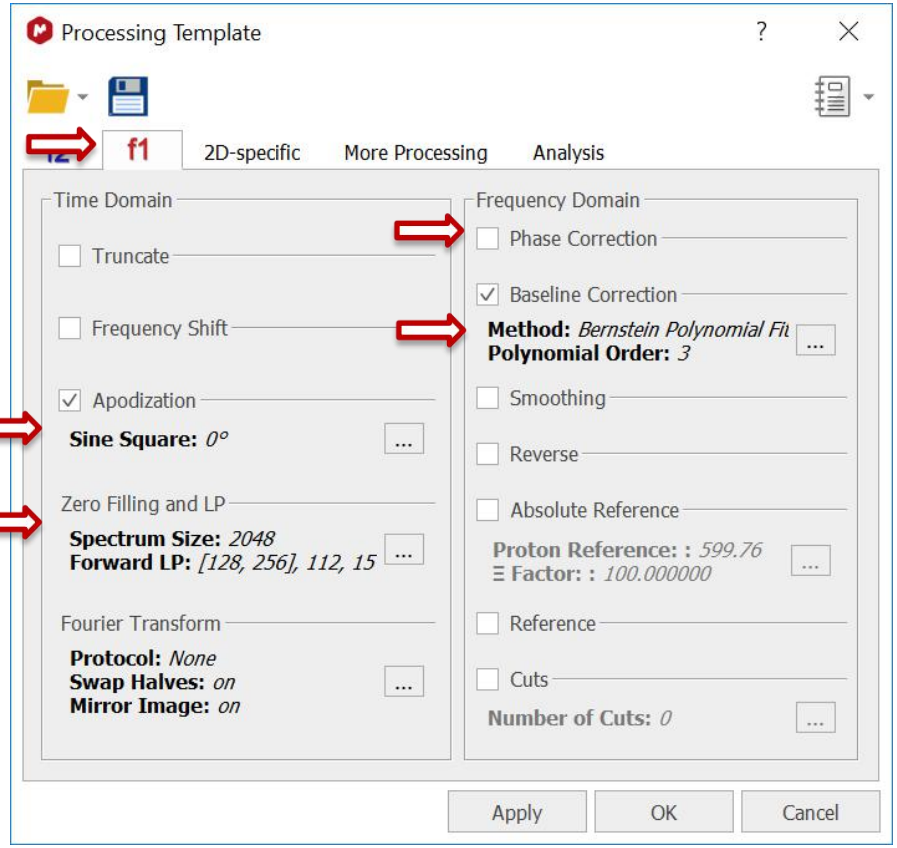


Re-process COSY spectrum



- Reprocess the COSY spectrum as shown below.
- Note the apodization functions for F2 and F1
- Note the forward linear prediction for F1 applied here
- Turn off Symmetrize in the 2D-specific Tab

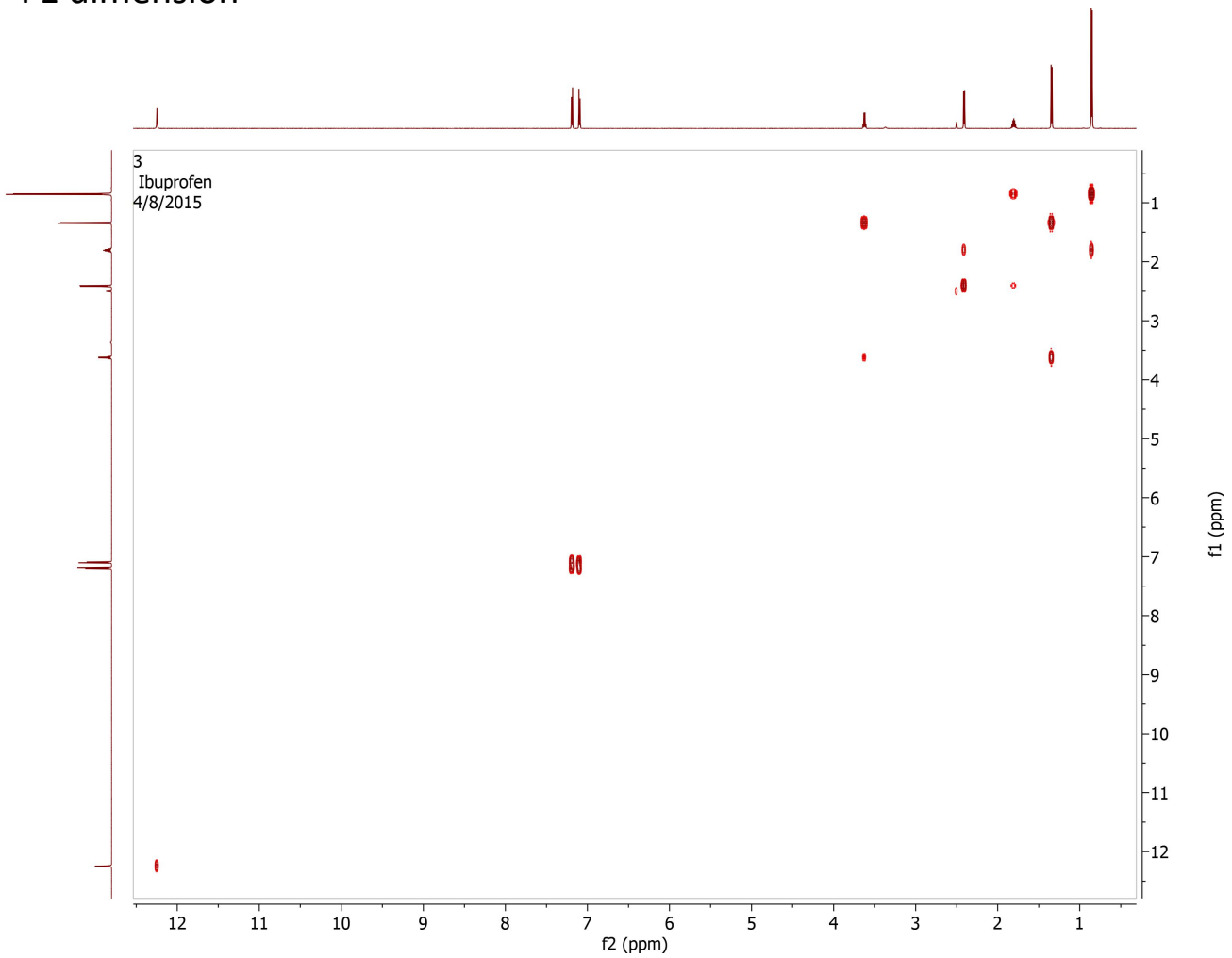




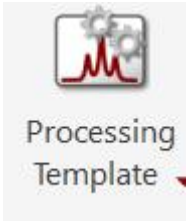
Note: The Fourier Transform method is automatically set and normally you don't need to change it.

Re-process COSY spectrum

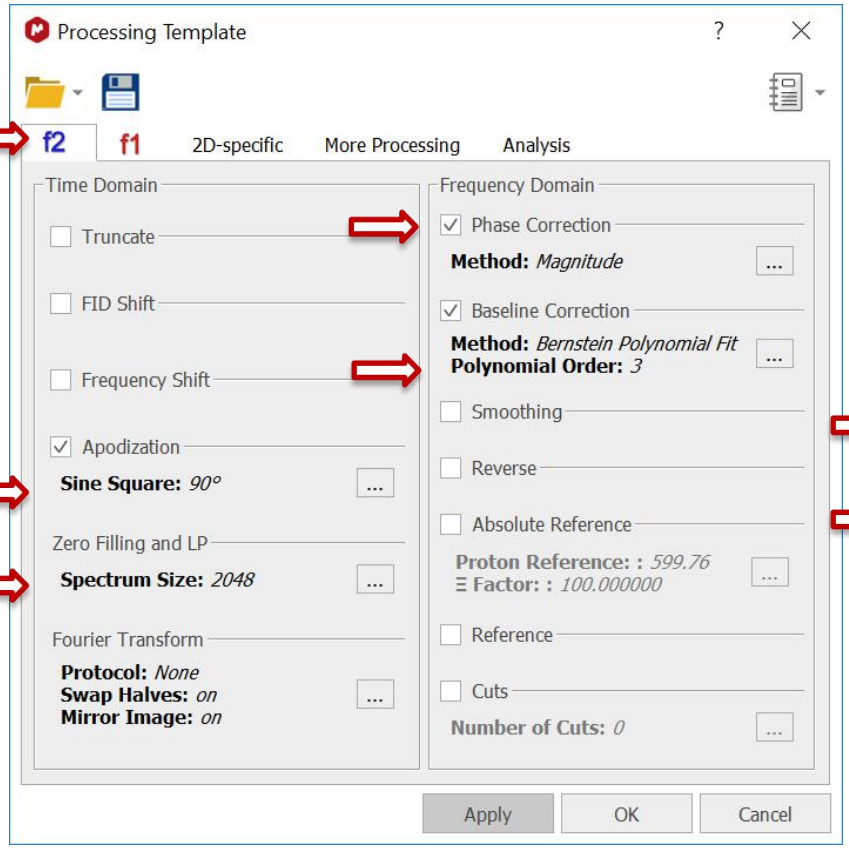
➢ The re-processed COSY spectrum shows better line shape, and higher resolution on the F1 dimension

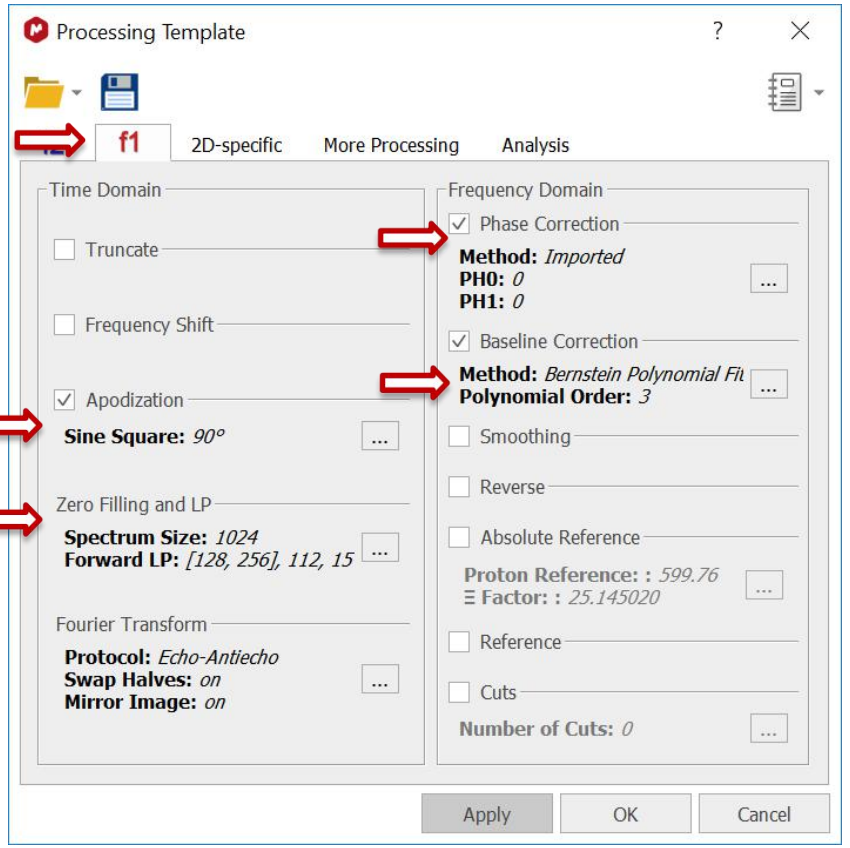


Re-process NOESY spectrum



- Reprocess the NOESY spectrum as shown below.
- Note the apodization functions for F2 and F1
- Note the forward linear prediction for F1 applied here

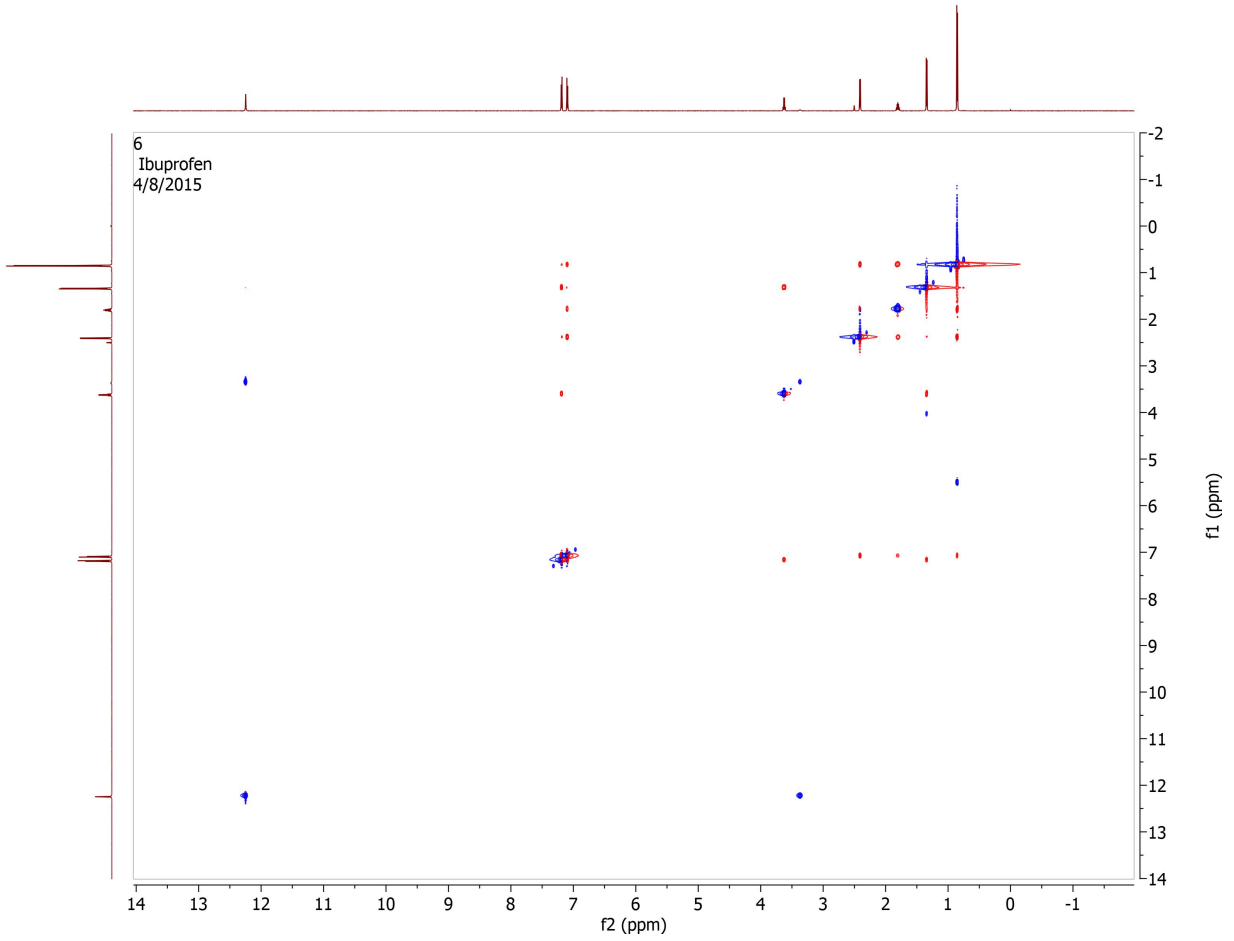




Note: The Fourier Transform method is automatically set and normally you don't need to change it.

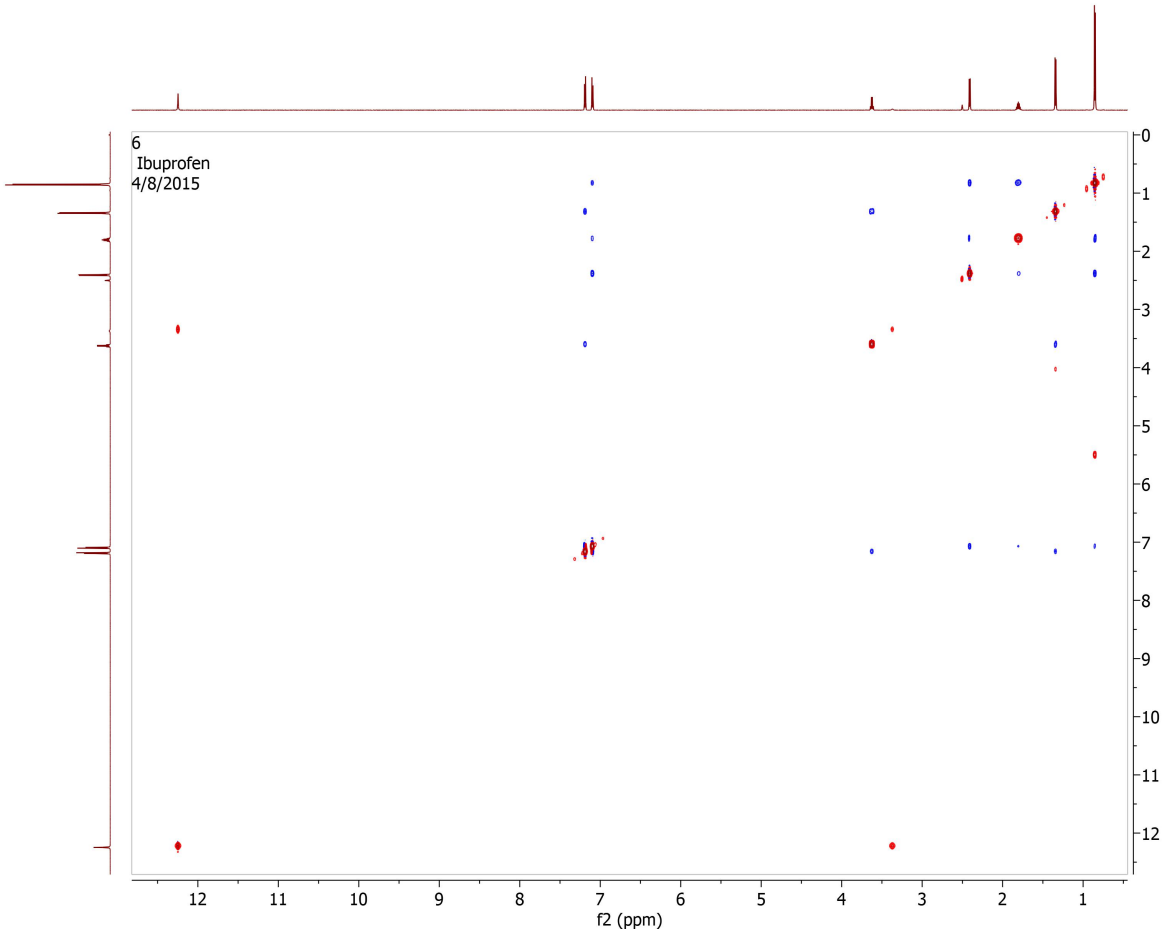
Re-process NOESY spectrum

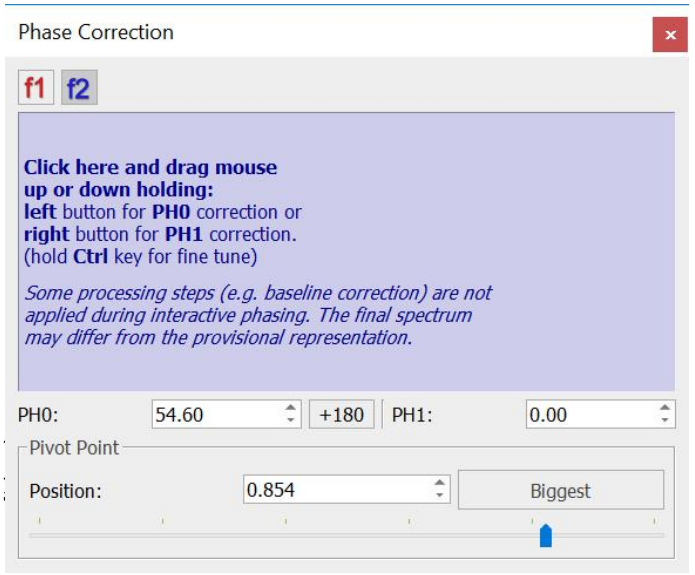
➢ The re-processed NOESY spectrum shows better line shape, and higher resolution on the F1 dimension, though there still some phase errors



Phase correction for NOESY spectrum

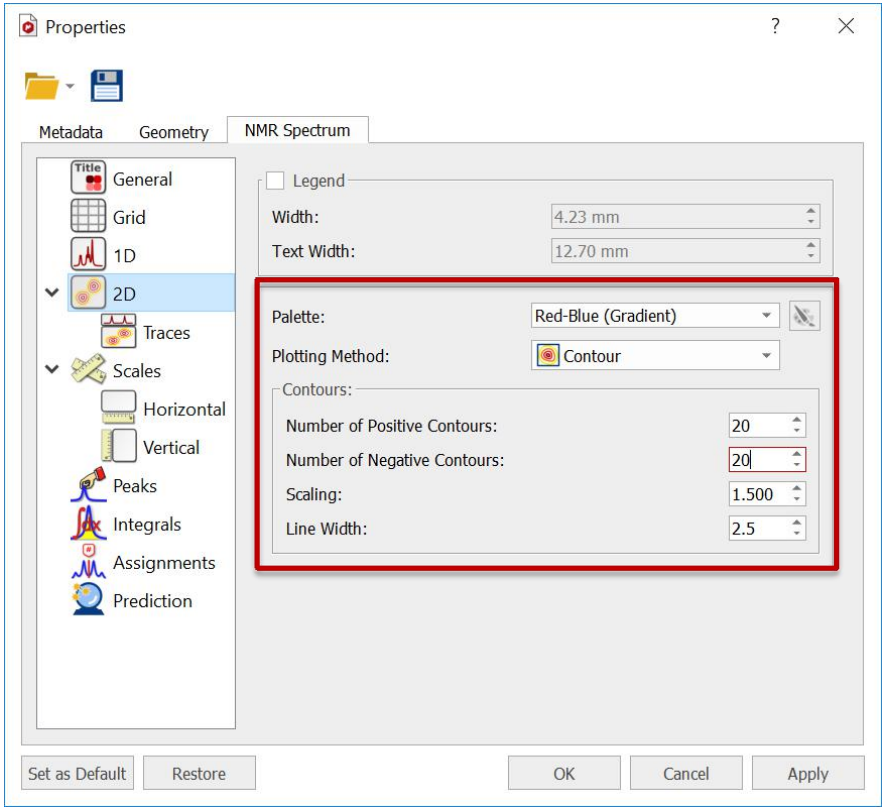
- Do Manual phase correction for either both dimensions.
- Also applied +180 for PH0 to make the cross peaks negative and diagonal peaks positive

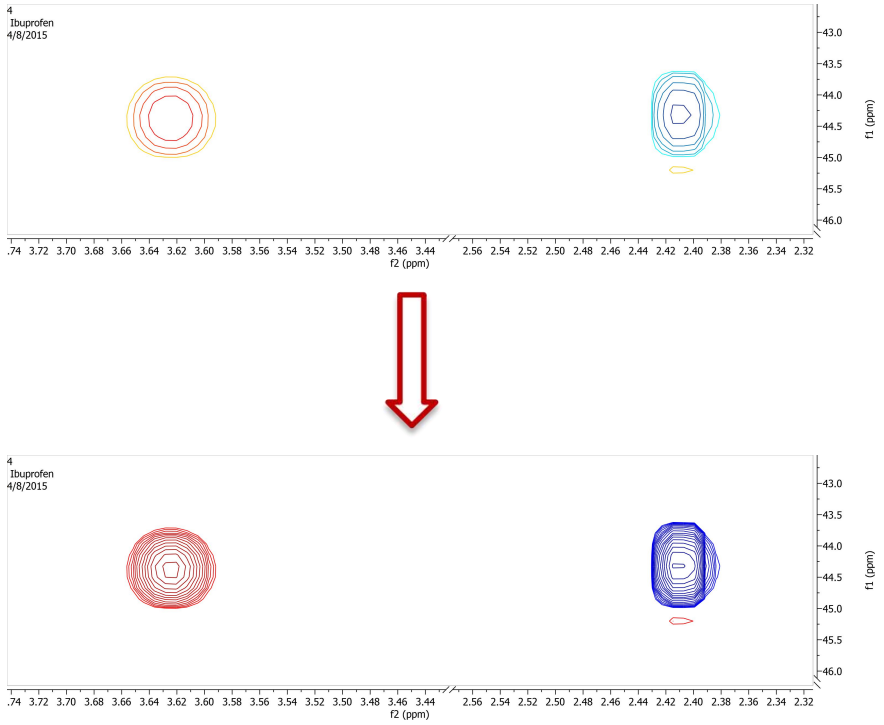




Change the Display Properties

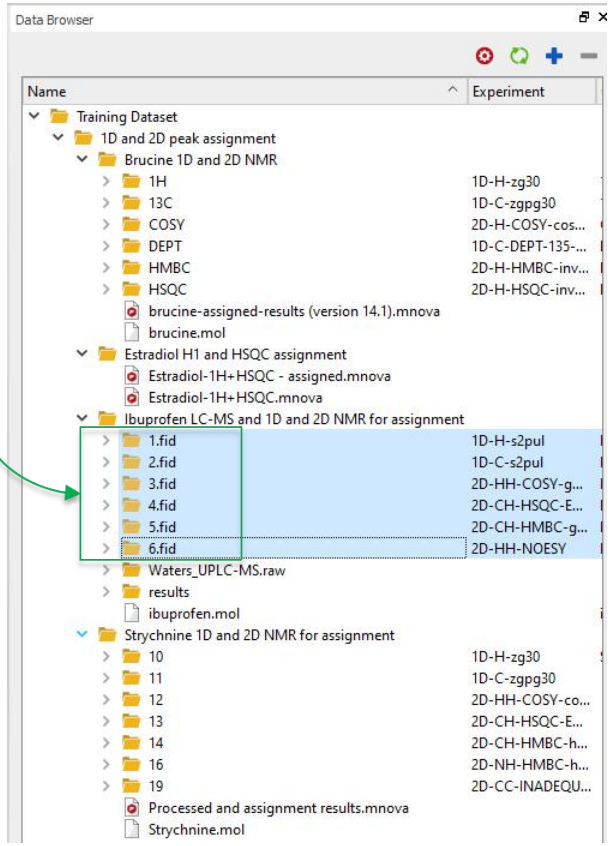
- Right click on the spectrum to open the Properties Dialog, view the properties that can be changed
- In the 2D Category, adjust the highlighted parameters and click Apply to see the effects
- Click Set as Default to retain the settings for 2D spectra display in the future





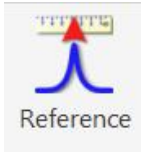
Peak Assignment Using 1D & 2D NMR Spectra Together

Sample data

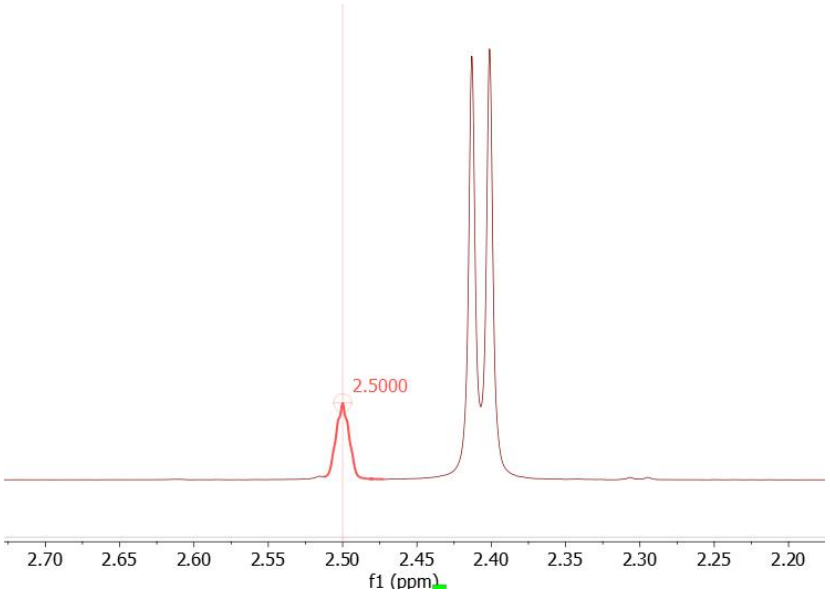


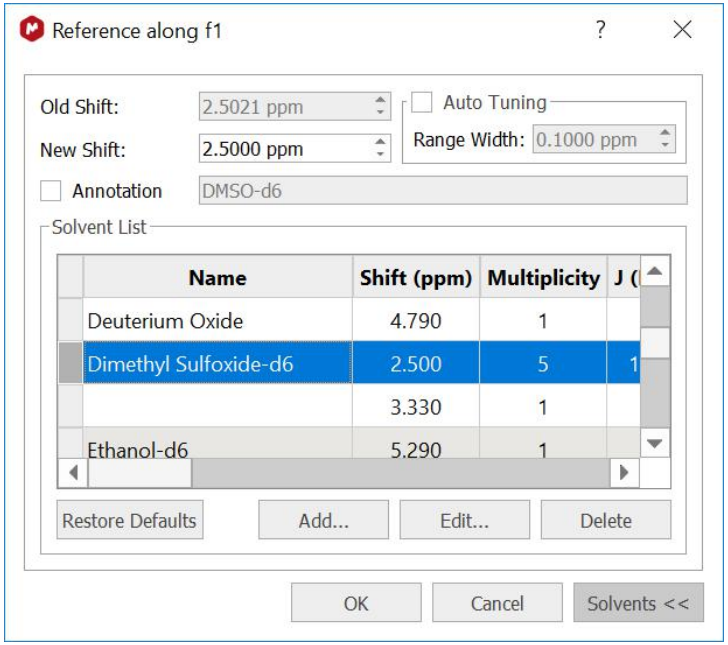
Tip: There are a total of 4 datasets with 1D and 2D NMR spectra for practicing spectral processing, peak assignment (and structure elucidation, which is not covered in this tutorial). The Ibuprofen one here is the simplest one compared to the others (Brucine, Strychnine and Estradiol).

Chemical shift referencing for H-1



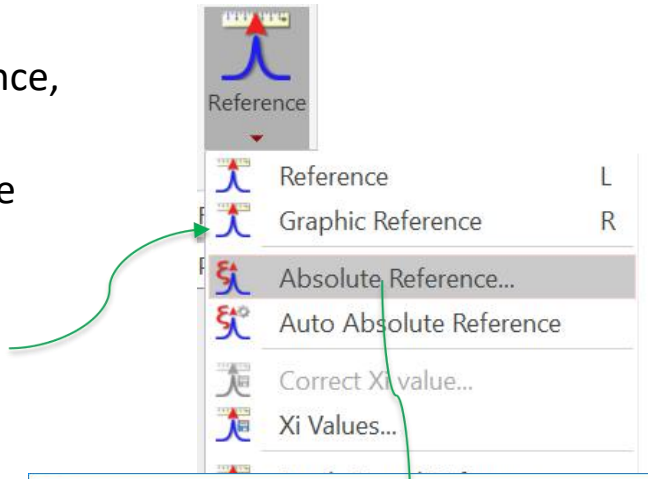
- This spectrum uses DMSO-d6 as the solvent. We can reference the chemical shifts by setting its middle peak to 2.5 ppm.
- Zoom to the DMSO peak at around 2.5 ppm. Choose Analysis > Reference, and click on the top of the middle peak.
- Set it to 2.5 ppm either manually or from the Solvent List.

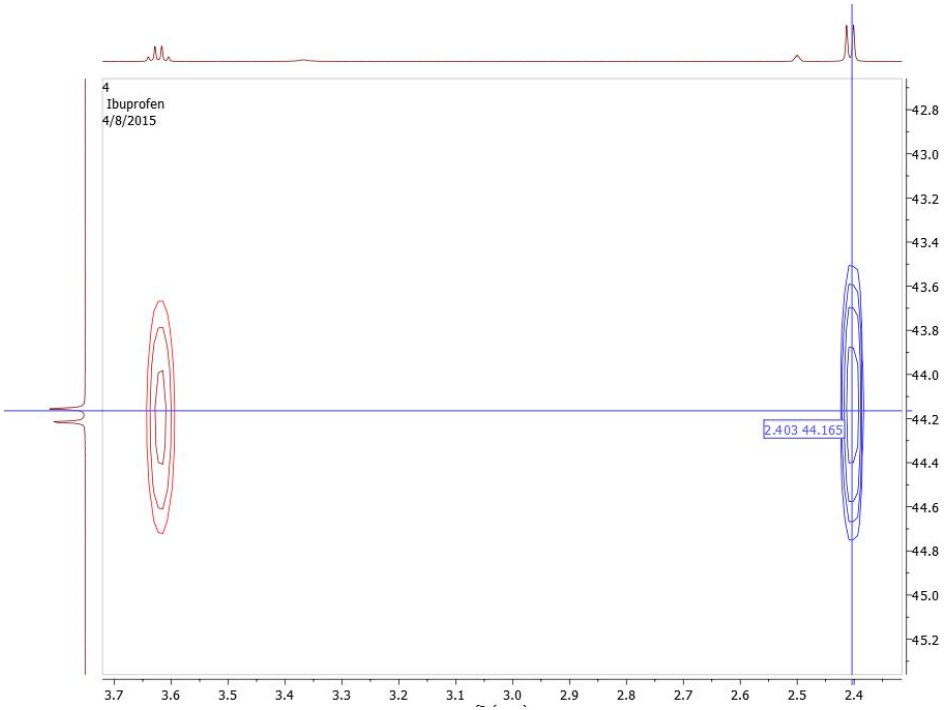


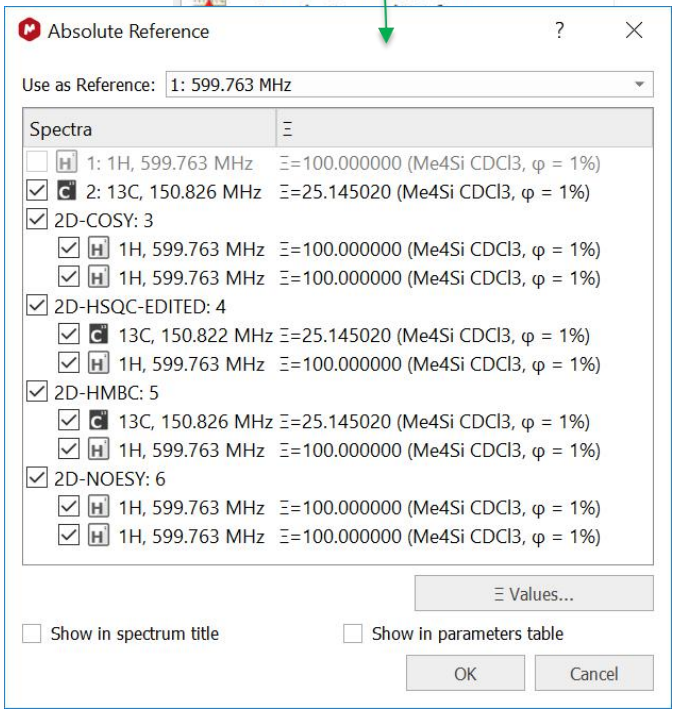


Chemical shift referencing for other spectra

- Choose Analysis > References > Absolute Reference, and click OK to the dialog.
- This applies referencing to all other spectra in the document using the H-1 spectrum as a standard.
- If needed, further align the 1D and 2D spectra manually using the Graphic Reference tool.







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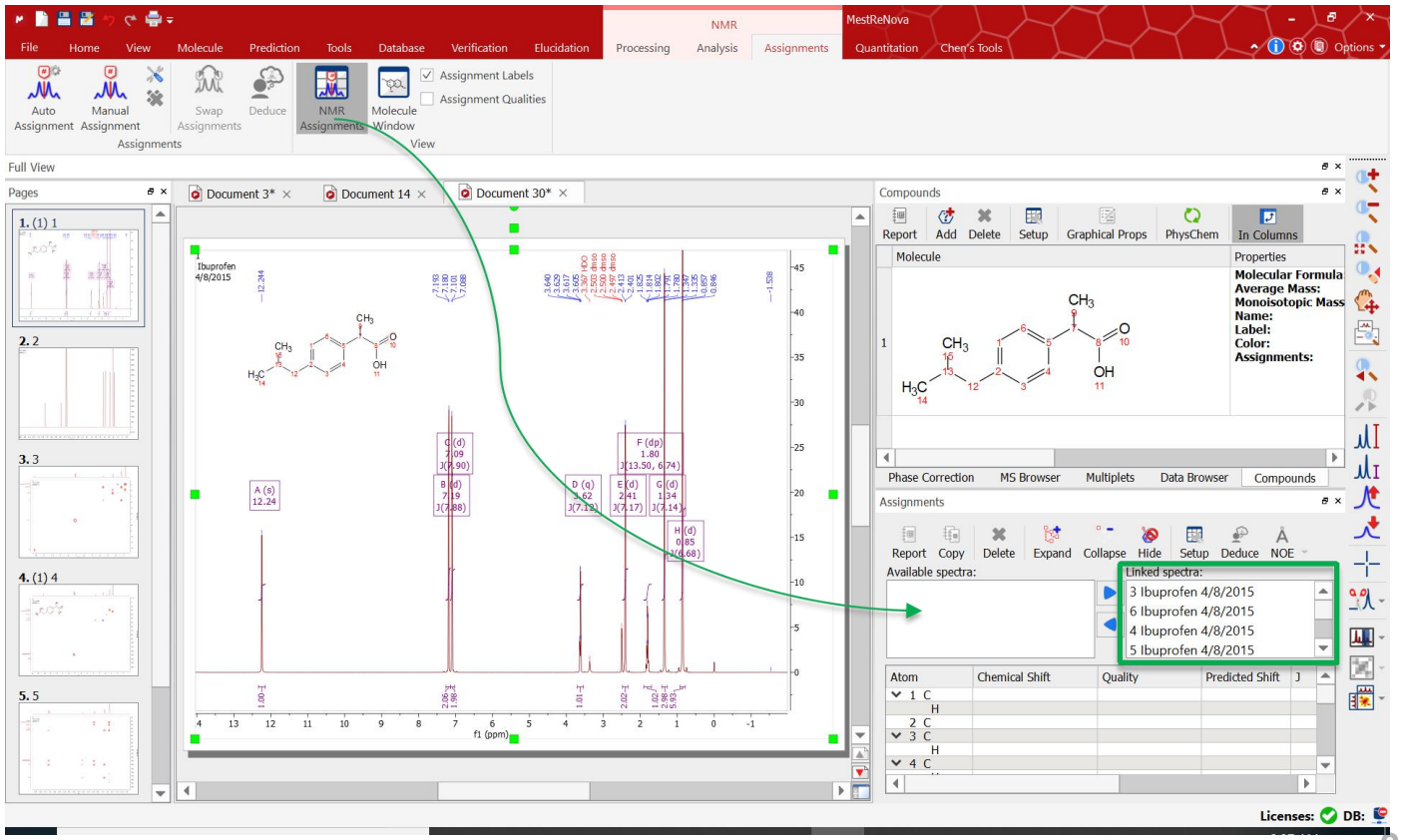
ANALYSIS

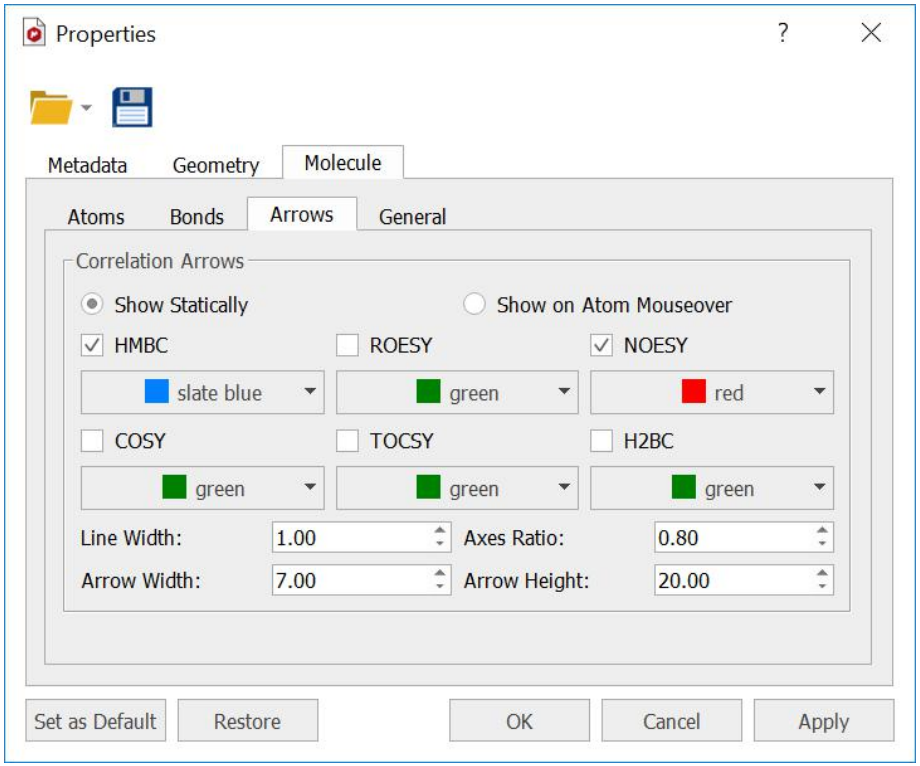
Open the structure for peak assignment

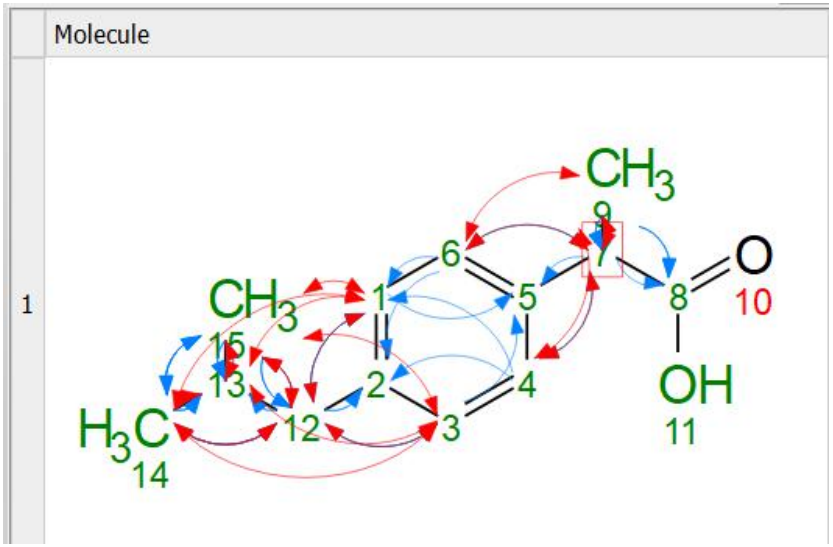
- Open the Ibuprofen.mol file from the Data Browser.
- Choose Molecule > Compound Table to show the structure on the side.
- Note: Open the same molecule only once. If needed, use Report on the Compound Table to report the structure to other pages. Do not open the same structure multiple times.
- Display the Assignment Table. Make sure all spectra are “linked” in it.



Show 2D correlation as arrows

- Right-click on the structure (or click on Graphical Props in the Compounds Table)
- In the Arrows Tab, turn on the display of HMBC and NOESY correlation as different colors
- The correlations will be displayed when the assignments are added later





Tip: Click Save as Default button to save the settings

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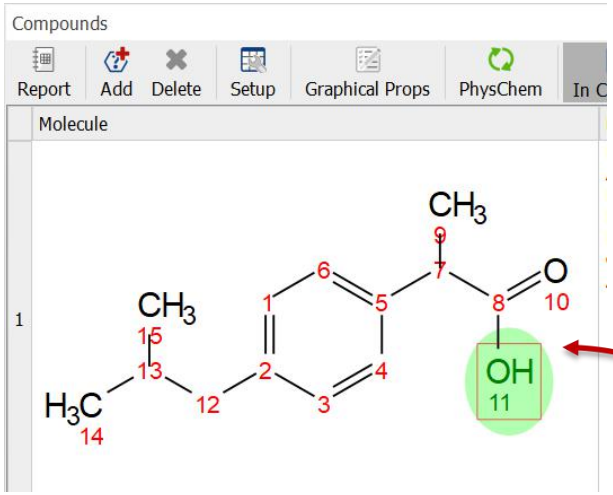
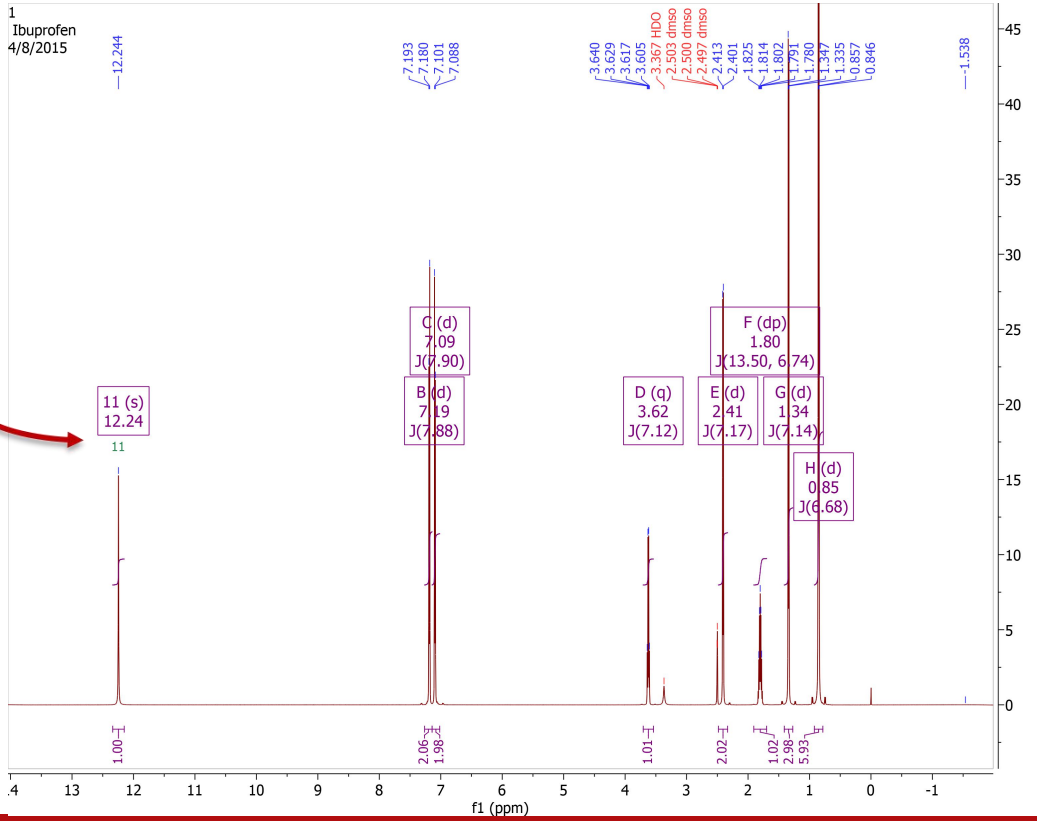
ANALYSIS

Assign H-1 multiplets

- Click A key to switch to Manual Assignment mode
  - Click on a multiplet label and assign it to an atom (This is the most common way to assign H-1 peaks)
  - Click on a peak and assign it to an atom
  - Click and drag on the spectrum, and assign the range to an atom
- View chemical shift assignment grids on the other “linked” spectra

Shortcut = A





**This tutorial is focused on manual assignment, although it is possible to try the Auto Assignment first, and then do manual correction.*

Predict and Compare for H-1 assignment

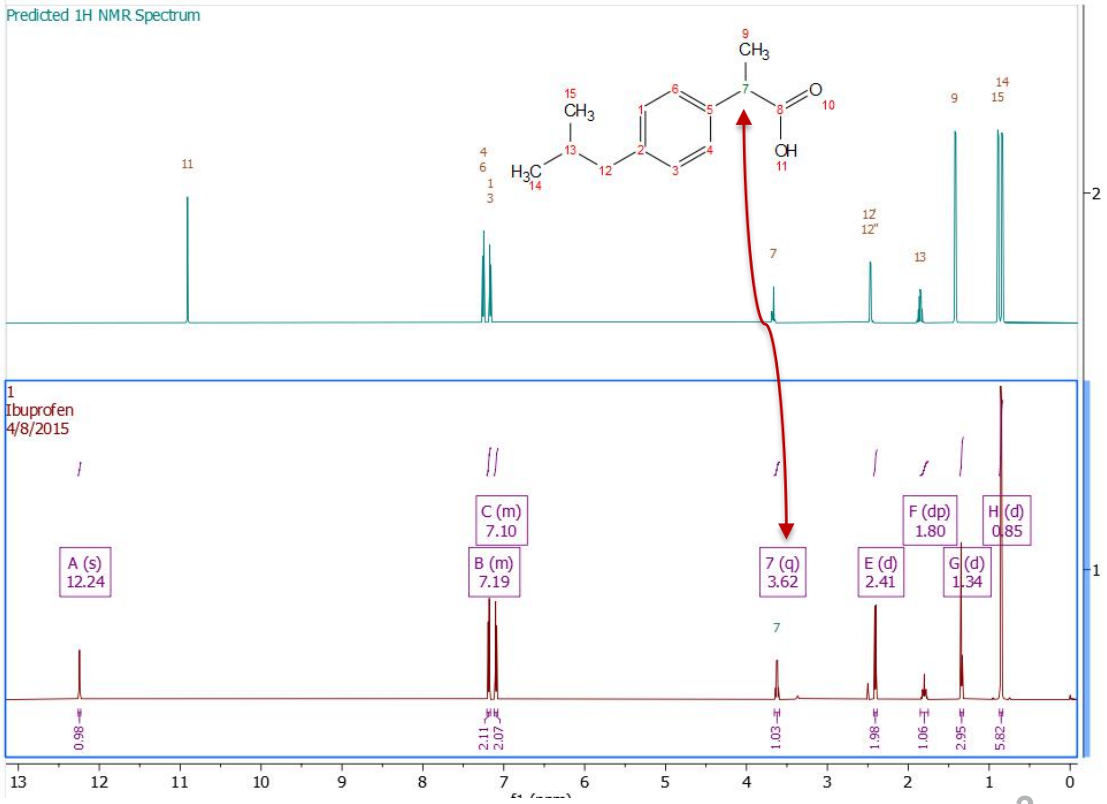
Shortcut = A

- Optionally, you can choose Predict > Predict and Compare to have a predicted H-1 spectrum stacked above the experimental one to guide your assignment of some peaks
- For example, the predicted quartet for H-7 is very close to the quartet observed at around 3.62ppm, so we can assign that observed quartet to H-7, by clicking the atom and then the multiplet label in the Manual Assignment mode.
- You can assign more multiplets in this way.

Tip: Use the following short cut keys to accelerate your assignment:
A: Assignment mode
Z: Zoom in mode
S: Swap the assignments of two atoms
<Ctrl+Space>: Switch to Zoom in mode temporarily
<ESC>: Exit from any of the modes above

If you need a copy of the structure in a page, click the structure in the Compounds Table and click Report.

To delete the predicted C-13 spectrum, choose Stack > Stacked Items Table, and delete it from the Table.



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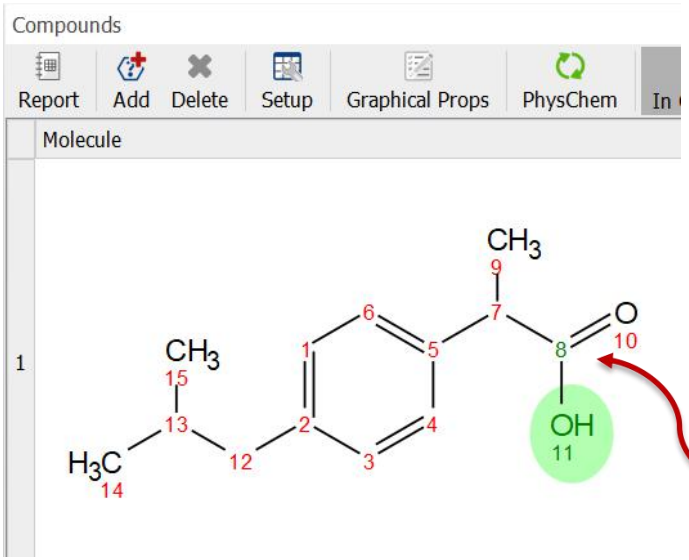
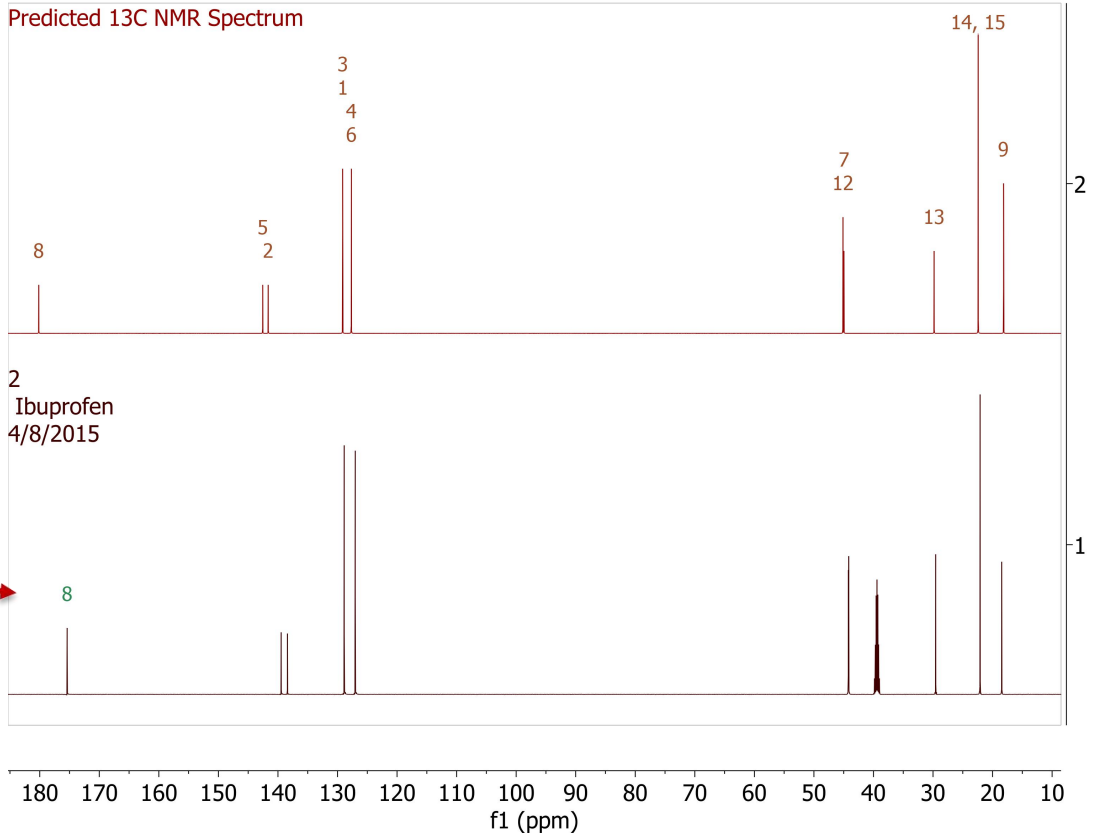
ANALYSIS

Assign C-13 peaks

- Make a copy of the C-13 spectrum.
- Choose Predict > Predict Compare to predict the 13C spectrum
- Use the prediction to guide the manual assignment

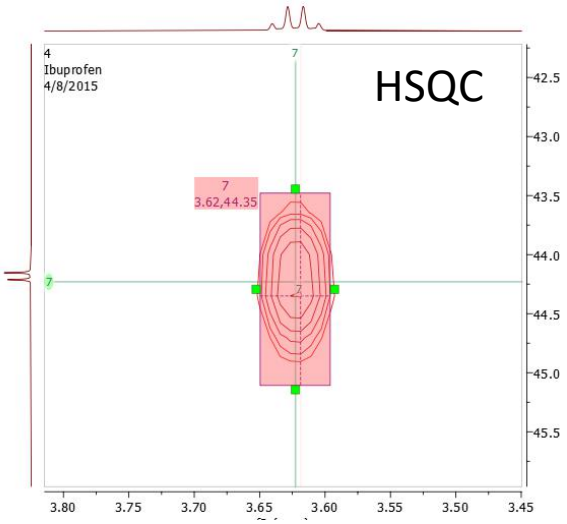
Shortcut = A



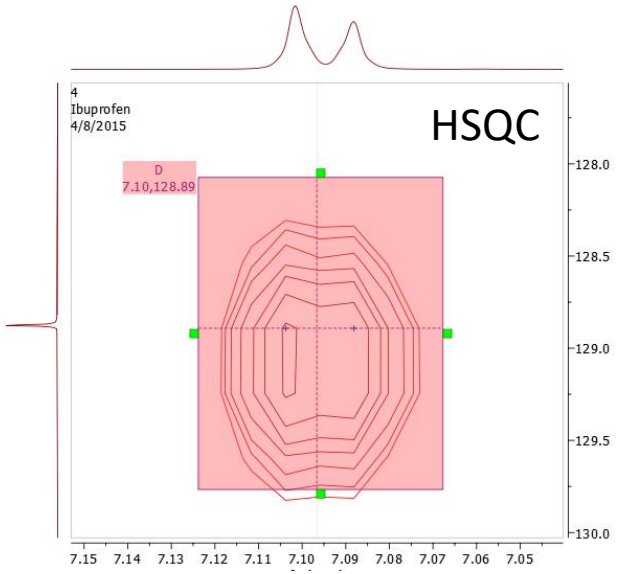


General guidance for assigning 2D spectra

- Since Mnova version 14.1, the assignment of a 2D peak is based on a “2D multiplet”, which can be either a single peak or a group of peaks.
- 2D multiplets can be automatically picked using Analysis > Auto Multiplet Analysis, and then manually corrected.
- If you don’t pick any multiplets before assigning a 2D peak, it will automatically pick a multiplet around where you clicked in the 2D spectrum during the assignment.
- A 2D multiplet can be manually resized using the green blocks shown around it when you hover the cursor on it.



A HSQC multiplet with a single peak. It is assigned to CH(7)



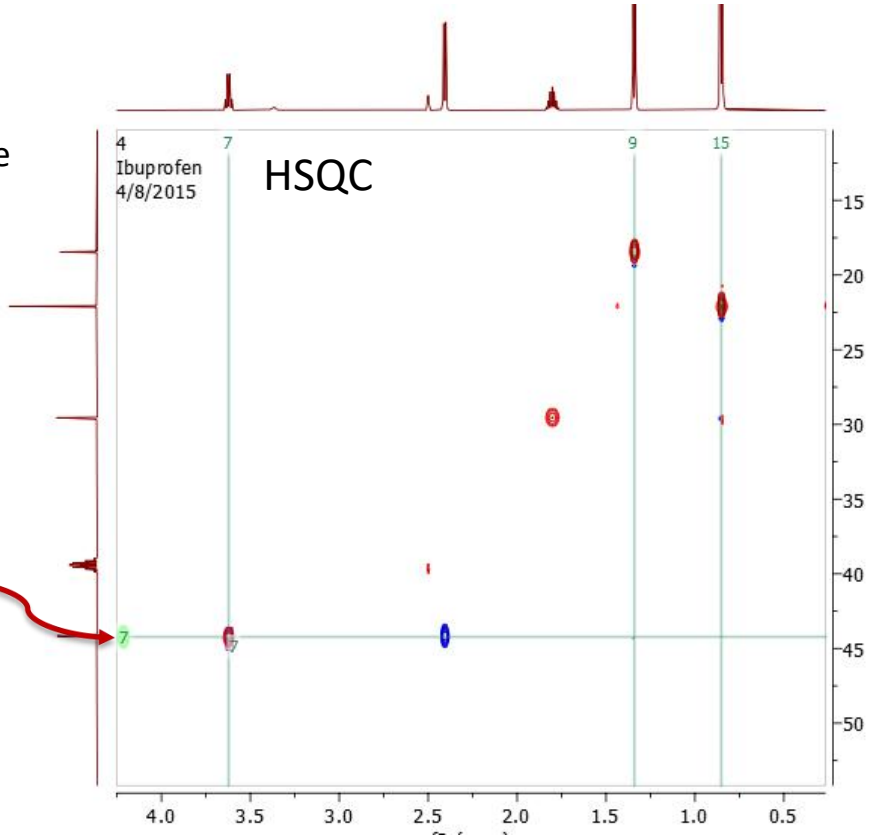
A HSQC multiplet with two peaks. It is not assigned to any atoms yet

Tip: For better visualization of the assignment results on a 2D spectrum, it is better to suppress the display of the 2D peaks and 2D multiplet labels. Right click on the spectrum and choose Properties, and turn off those options.

Assignment lines across the spectra

- If you assign a peak from a 1D H-1 or C-13 spectrum, the assignment is displayed for the same nucleus on the 2D spectra automatically
- If you assign a cross peak from a 2D spectrum, the assignments for the corresponding nuclei/dimensions are also displayed on the corresponding 1D and 2D spectra, automatically
- The 1D and 2D assignment results are recorded in the Assignment Table (Assignment > NMR Assignments)
- You can click and drag an assignment line to change the chemical shift.

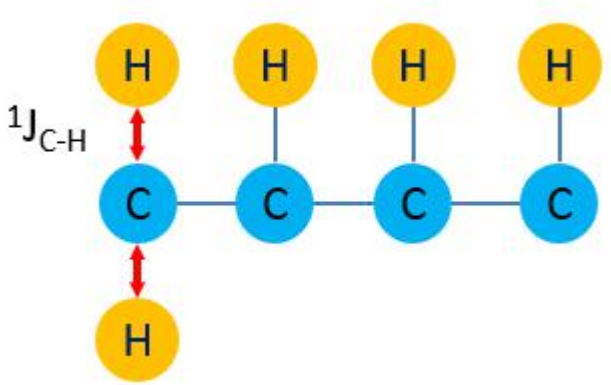
Shortcut = A

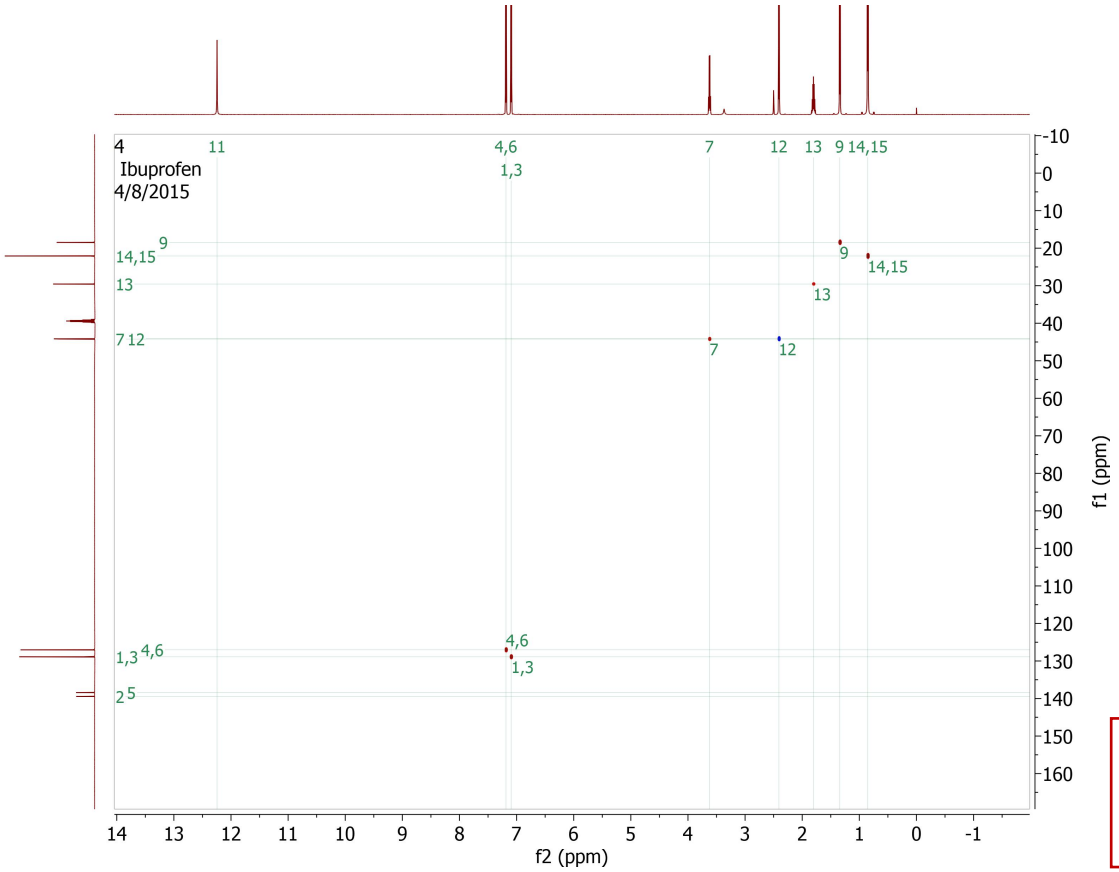


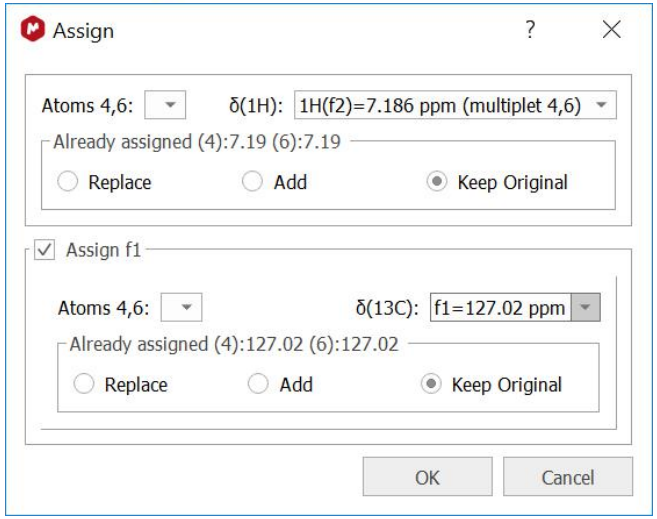
Tip: Click and drag the number ("7") to adjust the chemical shift value of this assigned peak in the C-13 dimension. The change will be reflected in all other spectra, as well as in the Assignment Table. You can do this on 1D spectra too.

Assign HSQC peaks

- Assign a cross peak to connected H-C atom pair: Click the peak first, then the assigned CH group (or, if H is drawn explicitly, the H first, and C next)
- Hold Alt key to display the Assign Dialog for more choices. Use "original" 1D H or C chemical shifts if available*



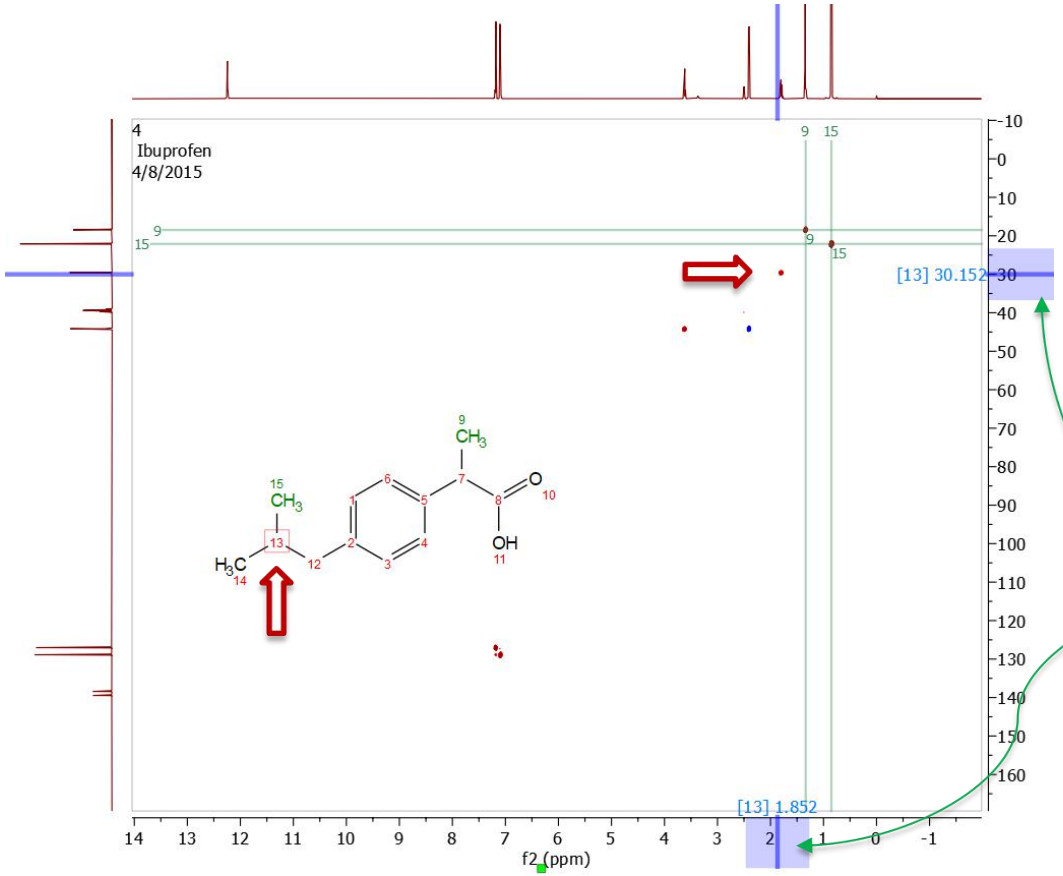




**The assigned chemical shifts can be from 1D or 2D peaks. Since a 1D spectrum typically has higher resolution, it is recommended to use those from 1D. Note you can also fine tune the chemical shift by moving the atom number on an assignment line.*

Use Predict & Highlight to help assigning HSQC peaks

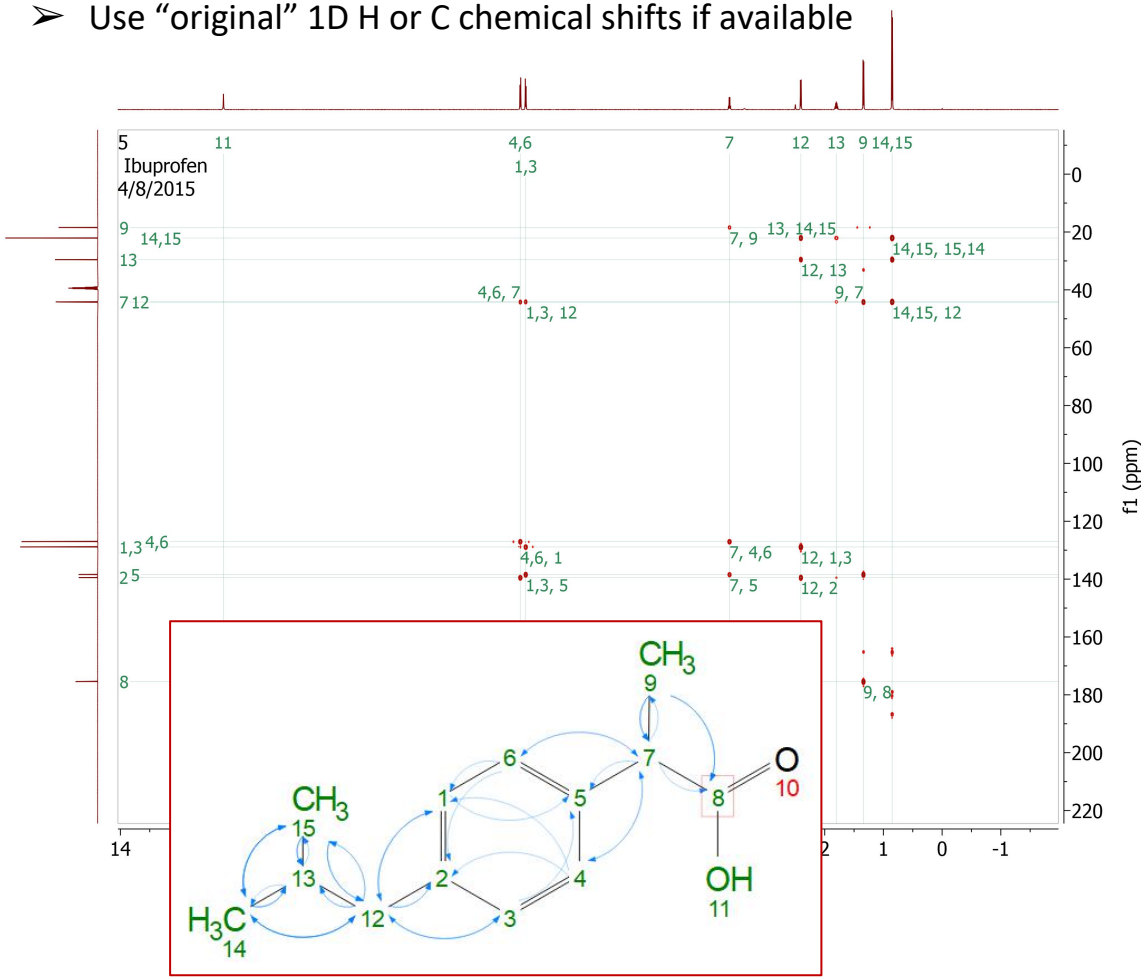
➢ Optionally, you can choose Predict > Predict and Highlight to display the predicted range of HSQC peaks for CH groups. The ranges can be helpful for assigning HSQC peaks to their corresponding CH groups

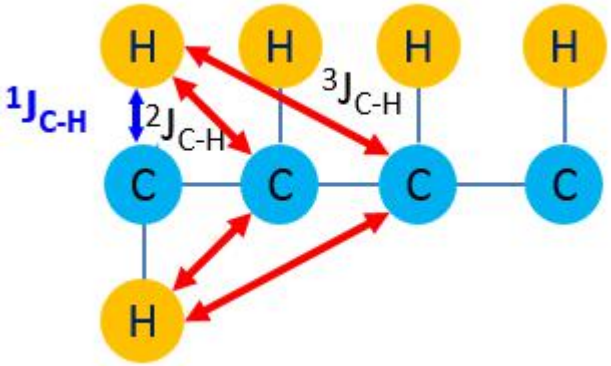


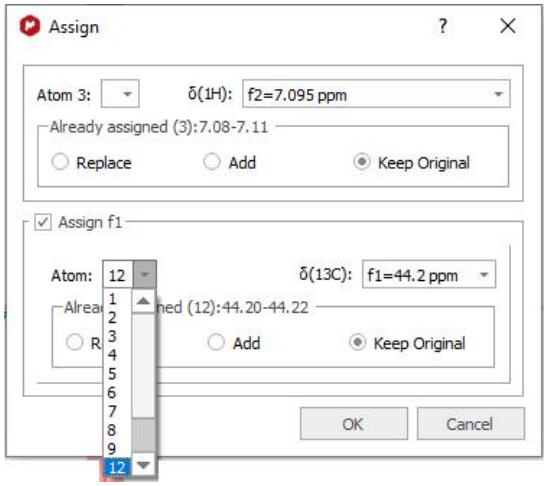
**Click on CH(13), it shows the value and error range of its predicted C-13 and H-1 shifts. This gives you an idea where to look for the cross peak to assign to this CH group.*

Assign HMBC peaks

- Assign a cross peak to connected H-C with 2 or 3 bonds in between: Click the peak first, then the assigned H. Mnova will popup an Assign Dialog for you to choose the assigned C.
- Use “original” 1D H or C chemical shifts if available

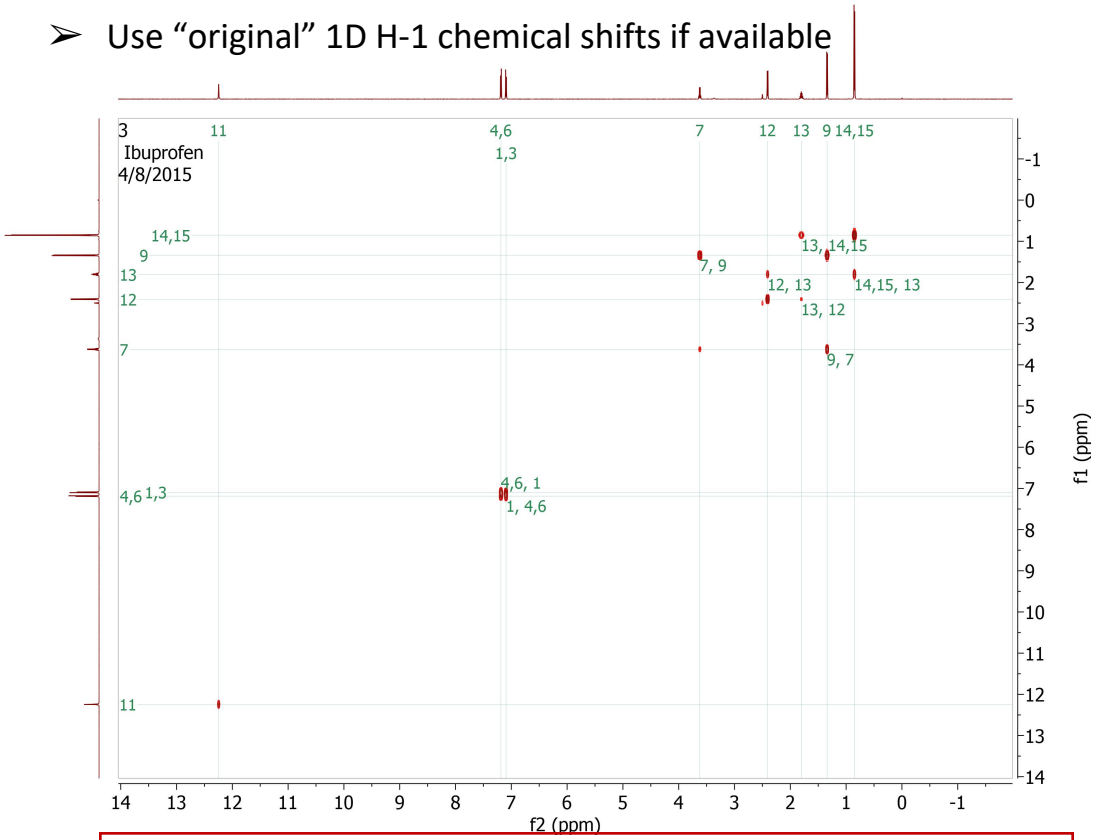


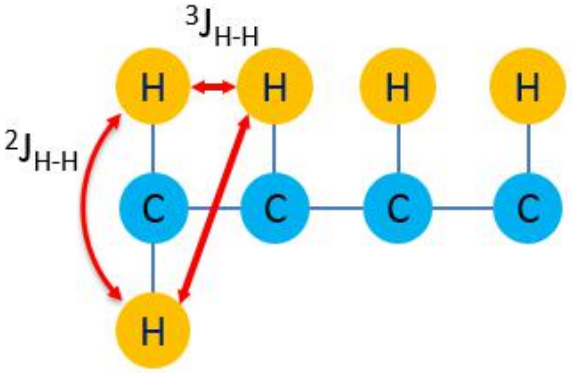


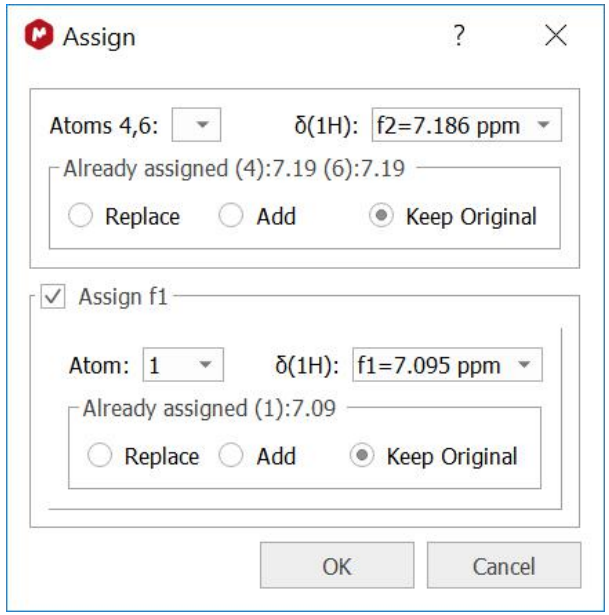


Assign COSY peaks

- Assign a cross peak to a H-H pair with 2 or 3 bonds in between: Click the peak first, then the assigned H on F2. Mnova will popup an Assign Dialog for you to choose the other H.
- Note weak couplings between 4-5 bonds is also possible
- Use “original” 1D H-1 chemical shifts if available



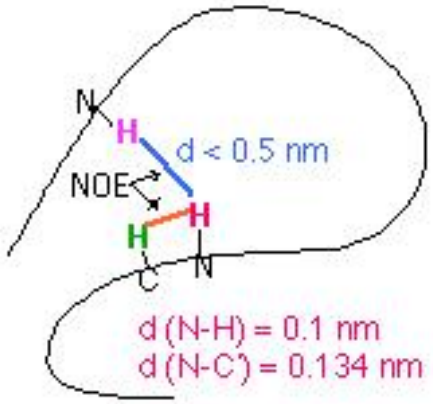


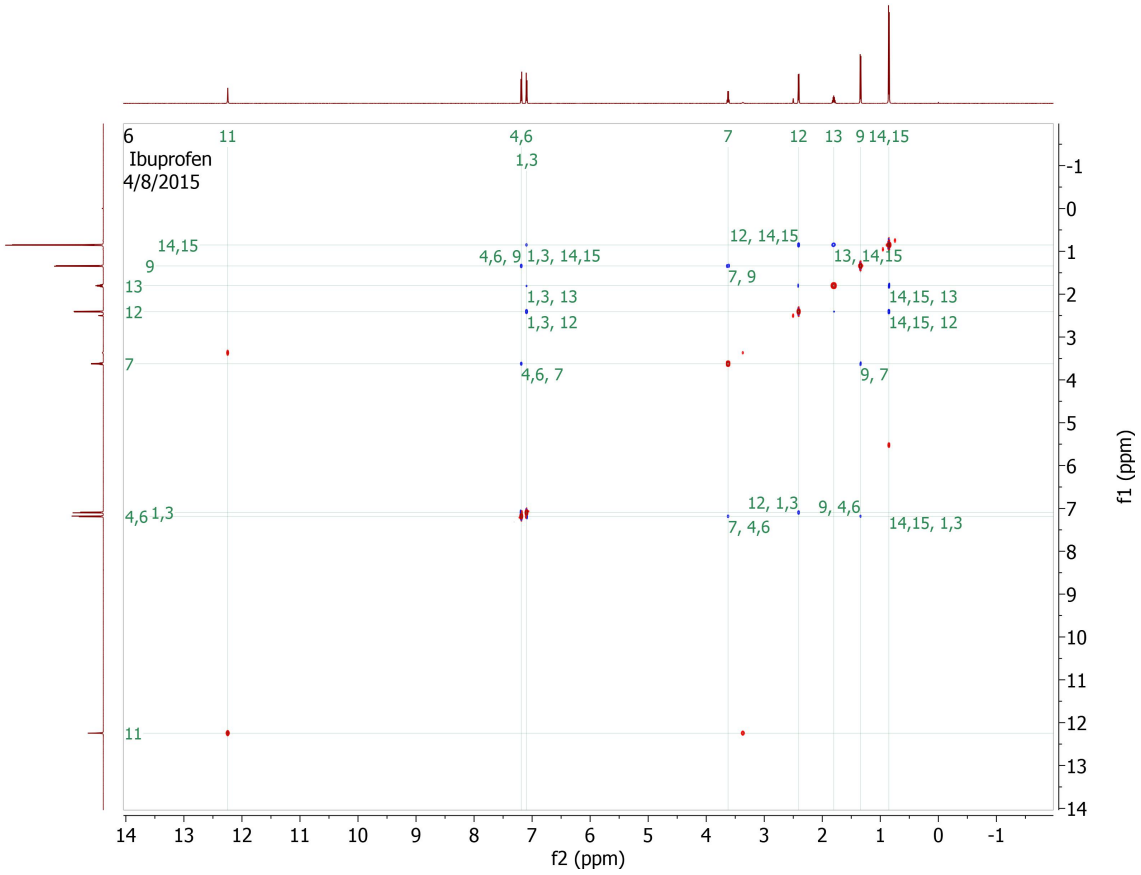


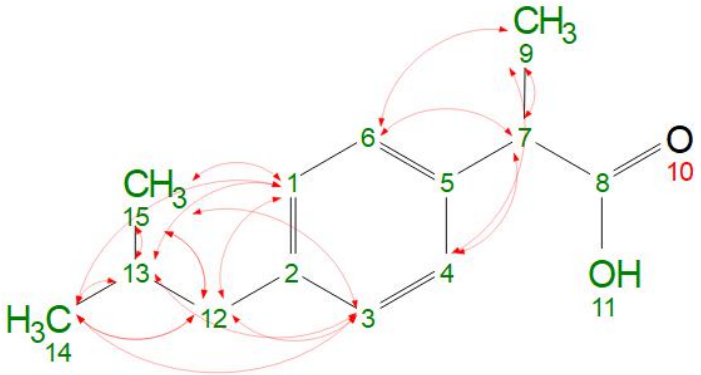
Tip: Displaying the diagonal line can be helpful to distinguish cross peaks and diagonal ones. To do that, right click and open the Properties Dialog, and check Grids > Show Diagonal.

Assign NOESY peaks

- Assign a cross peak to spatially approximate H-H pair (~5A or less): Click the peak first, then the assigned H on F2. Mnova will popup an Assign Dialog for you to choose the other H.
- For small molecules, NOE cross peaks are usually negative in phase. Positive one may be from J-couplings and should be ignored with caution.







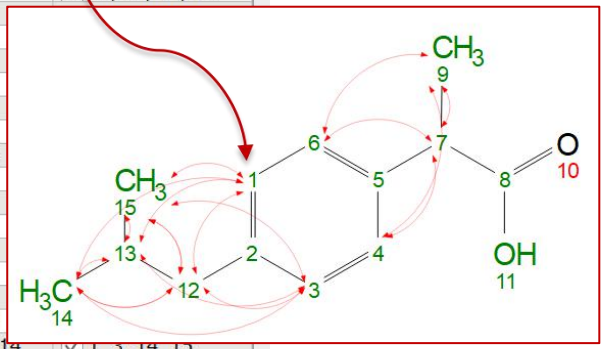
Assignments table

- Click Assignment > Assignment Table to display the Assignment Table
- The check boxes can be used to turn on/off the display of individual correlations on the structure

Assignments

Report Copy Delete Expand Collapse Hide Setup Deduce NOE

Atom	Chemical Shift	Quality	Predicted Shift	J	NOE	COSY	HSQC	HMBC	NOESY
1 C	128.88		129.12				1	✓ 4, 6, 12	
H	7.09	0.71				✓ 4, 6	1	✓ 5, 12	✓ 12, 13, 14, 15
2 C	139.46		141.62					✓ 4, 6, 12	
3 C	128.88		129.12				3	✓ 12	
H	7.09	0.71					3	✓ 5, 12	✓ 12, 13, 14, 15
4 C	127.02		127.66				4	✓ 7	
H	7.19	0.71				✓ 1	4	✓ 1, 2, 7	
5 C	138.41		142.54					✓ 1, 3, 7	
6 C	127.02		127.66				6	✓ 7	
H	7.19	0.71				✓ 1	6	✓ 1, 2, 7	
7 C	44.22		44.96				7	✓ 4, 6, 9	
H	3.62	0.71				✓ 9	7	✓ 4, 5, 6, 8, 9	
8 C	175.40		180.15					✓ 7, 9	
9 C	18.45		18.15				9	✓ 7	
H3	1.34	0.71				✓ 7	9	✓ 7, 8	
10 O									
11 O									
H	12.24	0.56							
12 C	44.16		45.12				12	✓ 1, 3, 14, 15	
H2	2.41	0.71				✓ 13	12	✓ 1, 2, 3, 13, 14,...	✓ 1, 3, 14, 15
13 C	29.55		29.81				13	✓ 12, 14, 15	
H	1.80	0.25				✓ 12, 14, 15	13	✓ 14, 15	✓ 1, 3, 14, 15
14 C	22.09		22.41				14	✓ 12, 13, 15	
H3	0.85	0.71				✓ 13	14	✓ 12, 13, 15	✓ 1, 3, 12, 13
15 C	22.09		22.41				15	✓ 12, 13, 14	
H3	0.85	0.71				✓ 13	15	✓ 12, 13, 14	✓ 1, 3, 12, 13



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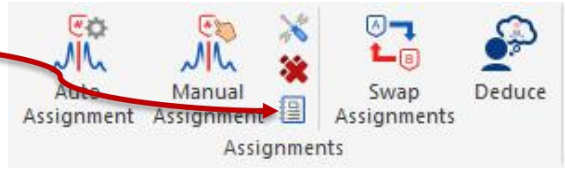
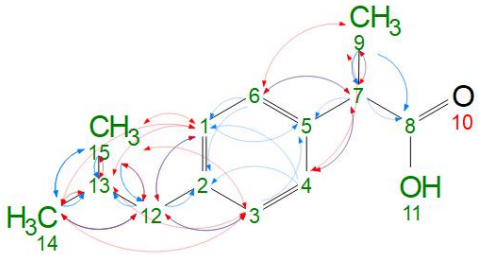
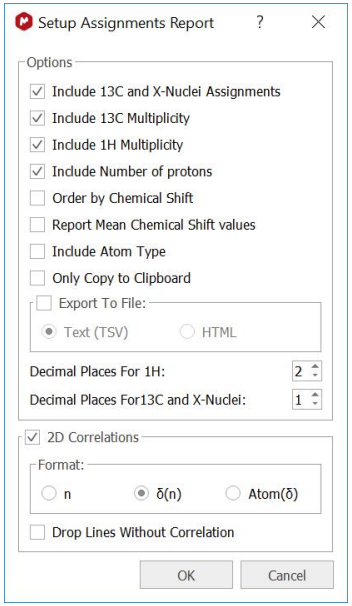
REPORT

Report assignments

- Choose Assignment > Report Assignments.
- Report the assignments on the spectrum or paste the table to another document



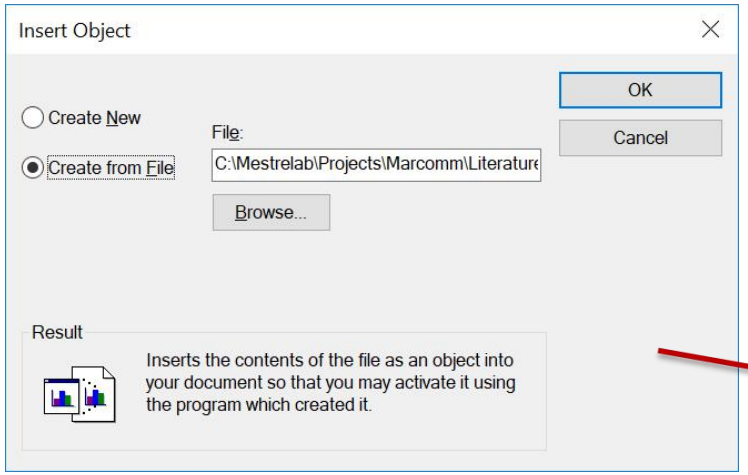


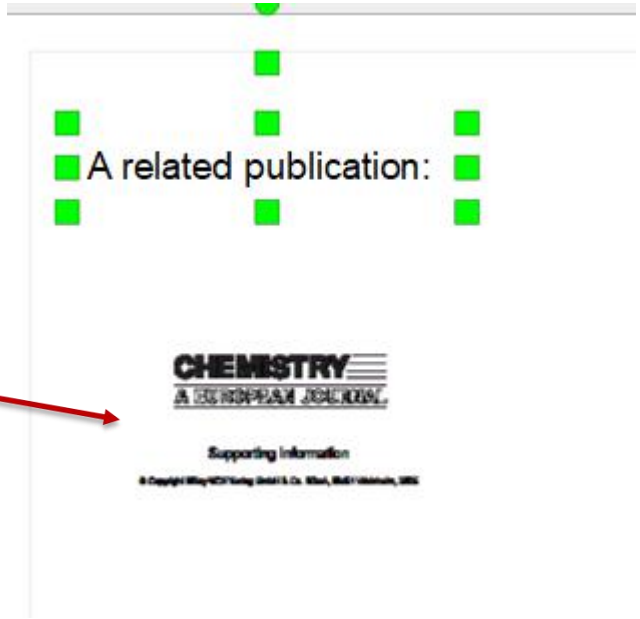


No	δ_H (Multiplicity, *J*, nH)	δ_C (Multiplicity, *J*)	HSQC-EDITED	HMBC	COSY	NOESY
1	7.09 (d, 7.9 Hz, 1H)	128.9(s)	128.9(1)	44.2(12),138.4(5)	7.19(4), 7.19(6)	0.85(14), 0.85(15), 1.80(13),2.41(12)
2	-	139.5(s)	-	-	-	-
3	7.09 (d, 7.9 Hz, 1H)	128.9(s)	128.9(3)	44.2(12),138.4(5)	-	0.85(14), 0.85(15), 1.80(13),2.41(12)
4	7.19 (d, 7.9 Hz, 1H)	127.0(s)	127.0(4)	44.2(7),128.9(1), 139.5(2)	7.09(1)	1.34(9),3.62(7)
5	-	138.4(s)	-	-	-	-
6	7.19 (d, 7.9 Hz, 1H)	127.0(s)	127.0(6)	44.2(7),128.9(1), 139.5(2)	7.09(1)	1.34(9),3.62(7)
7	3.62 (q, 7.1 Hz, 1H)	44.2(s)	44.2(7)	18.5(9),127.0(4), 127.0(6), 138.4(5), 175.4(8)	1.34(9)	1.34(9),7.19(4), 7.19(6)
8	-	175.4(s)	-	-	-	-
9	1.34 (d, 7.1 Hz, 3H)	18.5(s)	18.5(9)	44.2(7), 175.4(8)	3.62(7)	3.62(7),7.19(4), 7.19(6)
11	12.24 (s, 1H)	-	-	-	-	-
12	2.41 (d, 7.2 Hz, 2H)	44.2(s)	44.2(12)	22.1(14), 22.1(15), 29.6(13),128.9(1), 128.9(3), 139.5(2)	1.80(13)	0.85(14), 0.85(15),7.09(1), 7.09(3)
13	1.80 (dp, 13.5,6.7 Hz, 1H)	29.6(s)	29.6(13)	22.1(14), 22.1(15)	0.85(14), 0.85(14), 0.85(15),7.09(1), 0.85(15),2.41(12)	7.09(3)
14	0.85 (d, 6.7 Hz, 3H)	22.1(s)	22.1(14)	22.1(15), 29.6(13),44.2(12)	1.80(13)	1.80(13), 2.41(12),7.09(1), 7.09(3)
15	0.85 (d, 6.7 Hz, 3H)	22.1(s)	22.1(15)	22.1(14), 29.6(13),44.2(12)	1.80(13)	1.80(13), 2.41(12),7.09(1), 7.09(3)

Insert a PDF to the document

- Choose Home > Insert Object, choose Create from File, and insert a PDF to the document
- A preview logo of the document is displayed.
- Add a text box annotation to it
- You can double click on the preview to open it





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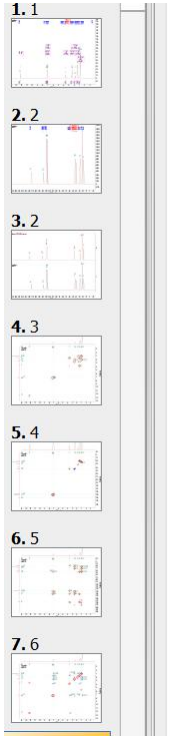
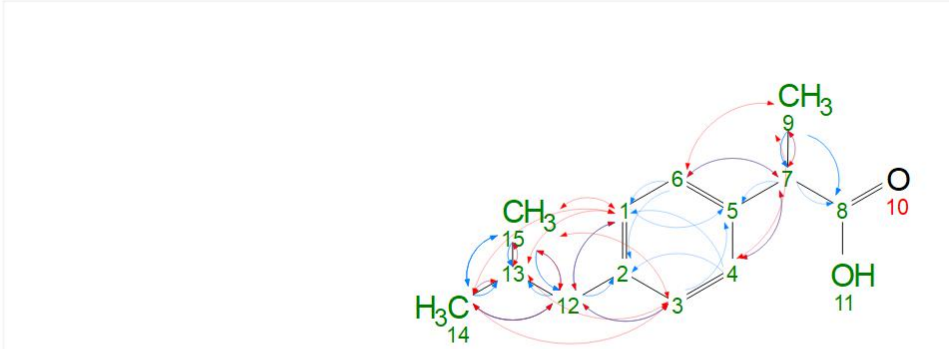
REPORT

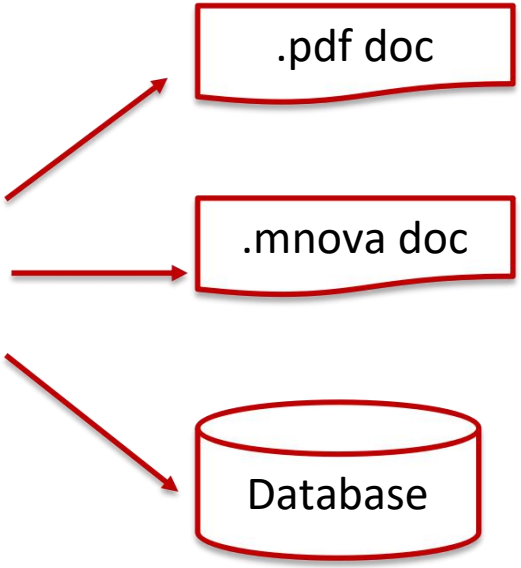
Save the results

- 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.
- Save all the results to a database (see steps later)
- Now you can close the document or continue to add other spectra to it.



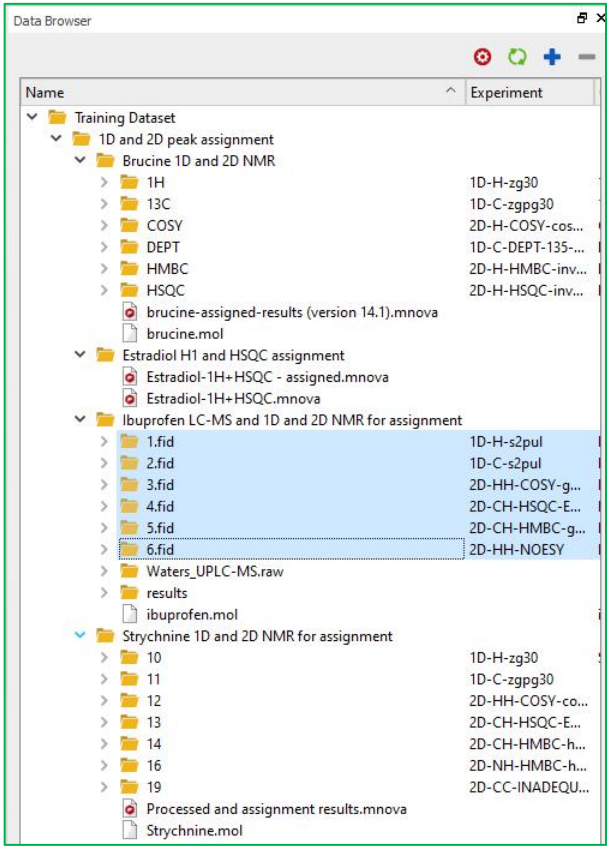


No	δ H (Multiplicity, J, nH)	δ C (Multiplicity, J)	HSQC-EDITED	HMBC	COSY	NOESY
1	7.09 (d, 7.9 Hz, 1H)	128.9(s)	128.9(1)	44.2(12),138.4(5)	7.19(4), 7.19(6)	0.85(14), 0.85(15), 1.80(13),2.41(12)
2	-	139.5(s)	-	-	-	-
3	7.09 (d, 7.9 Hz, 1H)	128.9(s)	128.9(3)	44.2(12),138.4(5)	-	0.85(14), 0.85(15), 1.80(13),2.41(12)
4	7.19 (d, 7.9 Hz, 1H)	127.0(s)	127.0(4)	44.2(7),128.9(1), 139.5(2)	7.09(1)	1.34(9),3.62(7)
5	-	138.4(s)	-	-	-	-
6	7.19 (d, 7.9 Hz, 1H)	127.0(s)	127.0(6)	44.2(7),128.9(1), 139.5(2)	7.09(1)	1.34(9),3.62(7)
7	3.62 (q, 7.1 Hz, 1H)	44.2(s)	44.2(7)	18.5(9),127.0(4), 127.0(6), 138.4(5), 175.4(8)	1.34(9)	1.34(9),7.19(4), 7.19(6)
8	-	175.4(s)	-	-	-	-
9	1.34 (d, 7.1 Hz, 3H)	18.5(s)	18.5(9)	44.2(7), 175.4(8)	3.62(7)	3.62(7),7.19(4), 7.19(6)
11	12.24 (s, 1H)	-	-	-	-	-
12	2.41 (d, 7.2 Hz, 2H)	44.2(s)	44.2(12)	22.1(14), 22.1(15), 29.6(13),128.9(1), 128.9(3), 139.5(2)	1.80(13)	0.85(14), 0.85(15),7.09(1), 7.09(3)
13	1.80 (dp, 13.5,6.7 Hz, 1H)	29.6(s)	29.6(13)	22.1(14), 22.1(15)	0.85(14), 0.85(15),2.41(12)	0.85(14), 0.85(15),7.09(1), 7.09(3)
14	0.85 (d, 6.7 Hz, 3H)	22.1(s)	22.1(14)	22.1(15), 29.6(13),44.2(12)	1.80(13)	1.80(13), 2.41(12),7.09(1), 7.09(3)
15	0.85 (d, 6.7 Hz, 3H)	22.1(s)	22.1(15)	22.1(14), 29.6(13),44.2(12)	1.80(13)	1.80(13), 2.41(12),7.09(1), 7.09(3)



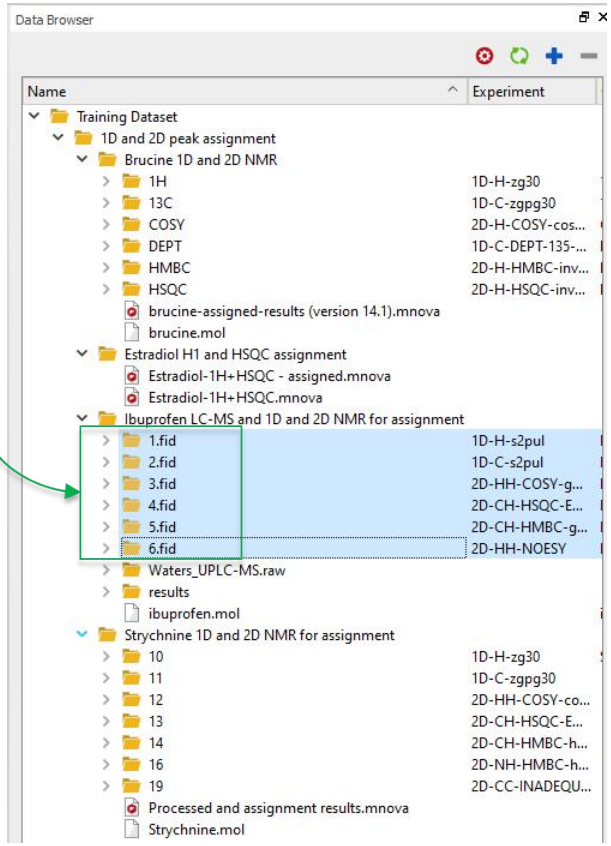
More about peak assignment

- Manual assignment of 1D and 2D peaks is not only an effective way to verify a proposed structure, but also a proven way to learn to understand and analyze 1D and 2D NMR.
- Usually you start with the 1H, 13C and HSQC spectra, if available, with the assistance of the predicted peaks or ranges as a guidance. Then you extend the assignment to the other 2D spectra such as COSY and HMBC. While assigning COSY or HMBC peaks, conflicts with the previous assignments may be discovered and hence corrections can be done. If the conflicts cannot be resolved, it may imply that the structure is wrong.
- There are a total of 4 datasets with 1D and 2D NMR spectra for practicing spectral processing, peak assignment that come with this tutorial: Ibuprofen, Brucine, Strychnine, and Estradiol, along with results of full assignments. You can use them for practice.



Saving Processed Spectra and Analysis Results to a Database

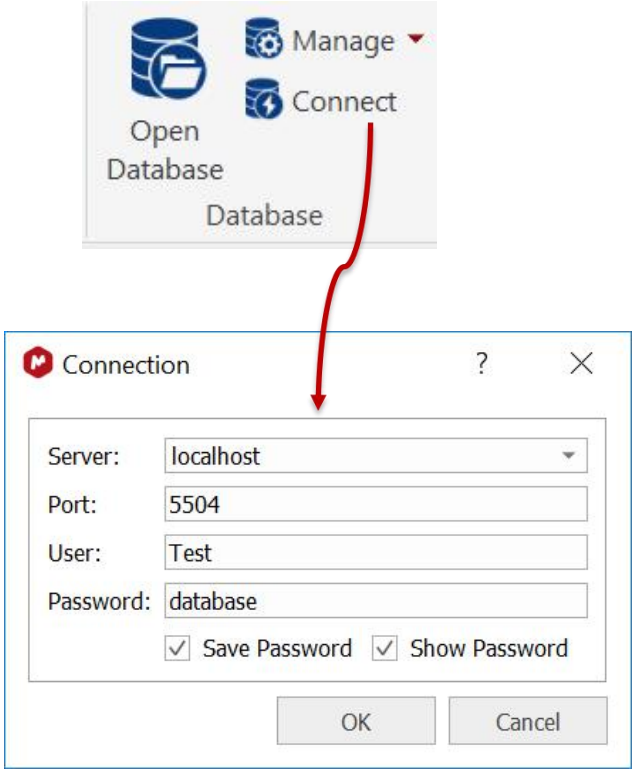
Sample data



Note: You will need a Mnova DB Client license and install Mnova MyData Server for this session

Install MyData DB Server

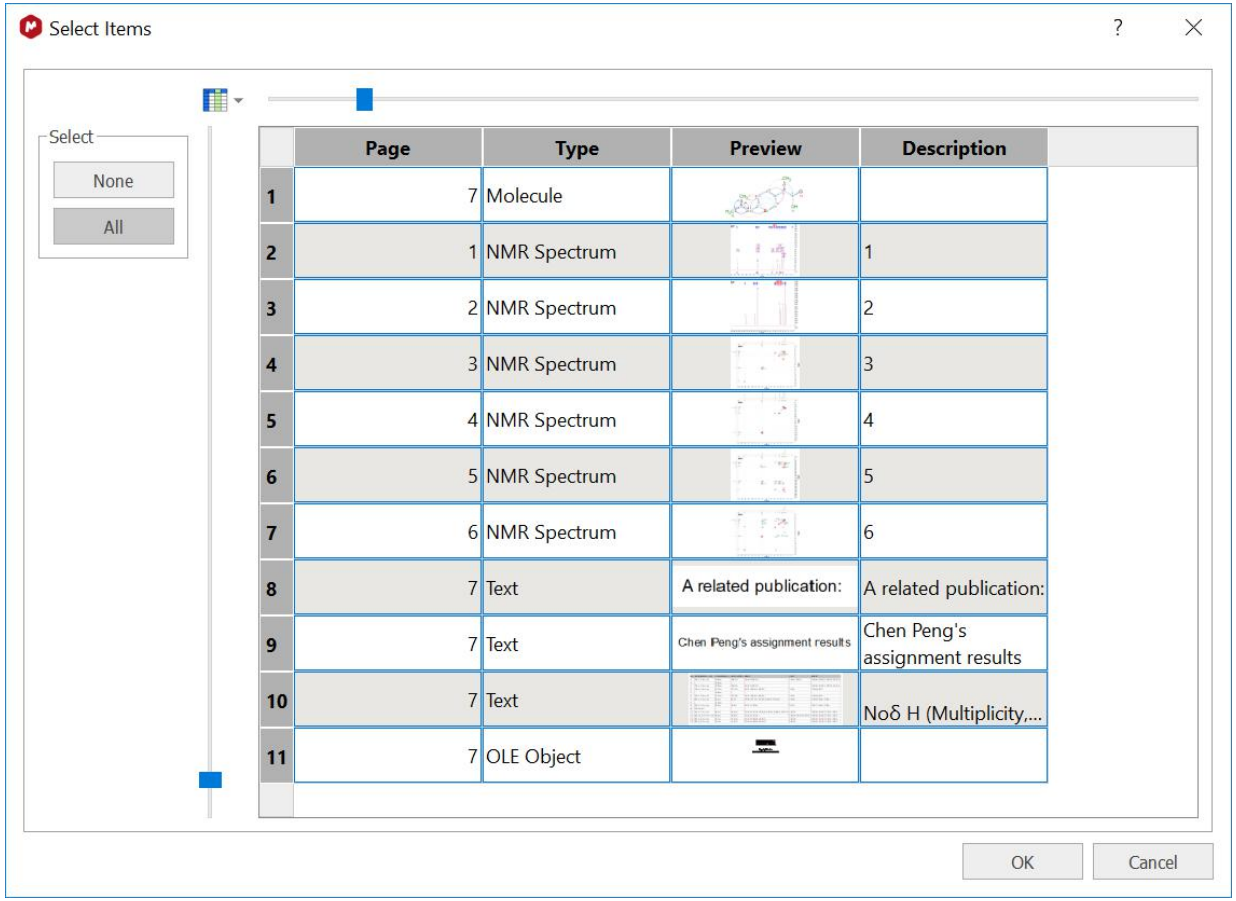
- Make sure MyData Server is installed and running as a service*
- Connect to MyData Server with the default account setting
- Create and open a new database (Database > Manage > Add)



**If not yet, download the DB MyData Server Installer from http://mestrelab.com/download/mnova/db/ and install it. You may need to download the latest Java too. No license is needed for MyData DB Server.*
Note: MyData is a personal version of Mnova DB Group or Enterprise Server.

Save data to database

- Choose Database > Save to Database
- Click All in the Select Items dialog
- Click OK to save all items to the new database



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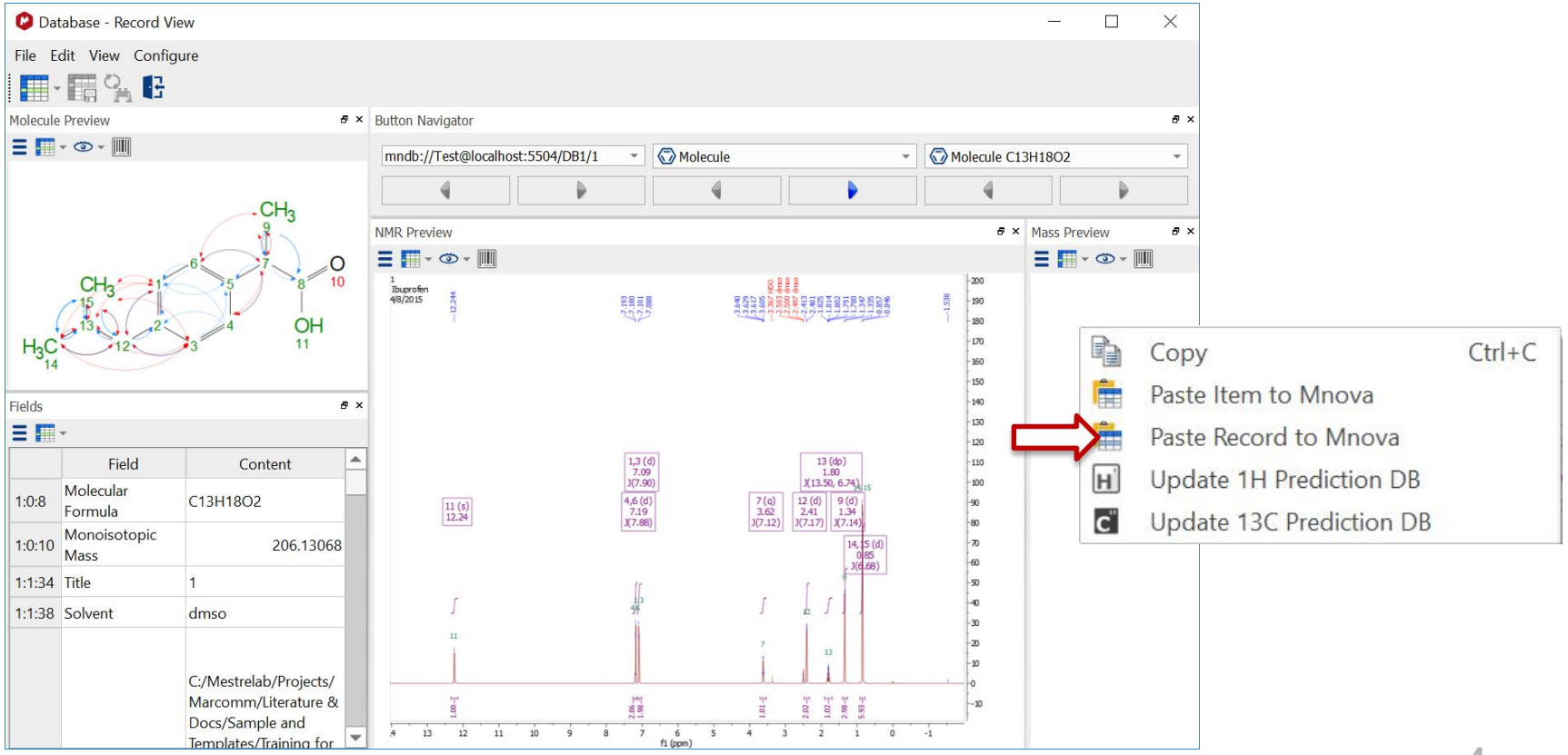
DATABASE

Browse and download from database

- Choose Database > Browse or Show Record
- Display the contents in Record View (or Table View)
- Choose File > New in Mnova to open a new document
- Right click on the spectrum in the Database Dialog and choose Paste Record to Mnova to download the whole record to Mnova

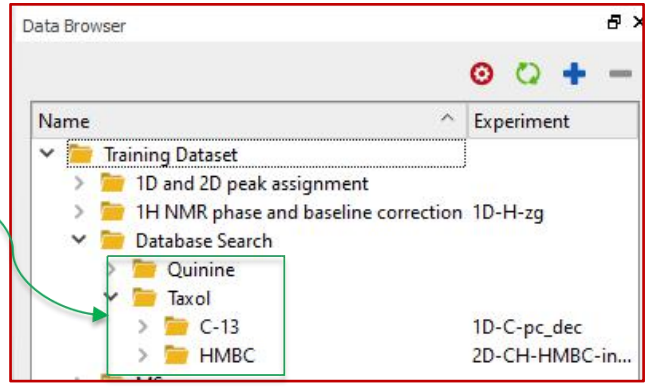


Search your own database

- Search by text
- Search by peaks
- Search by multiplets
- Search by 2D peaks
- Search by structure/substructure

Searching Wiley C-13 and H-1 Databases from Mnova

Sample data



Note: You will need a subscription to Wiley Databases from Mestrelab.

Search Wiley databases

- Wiley C-13 and H-1 databases are collection of published C13 and H-1 spectra of known organic compounds. They are usually installed on a central server (Mnova DB Enterprise Server) for remote access.
- Make sure you have an account to access the Wiley databases. Contact your library administrators if you don't have it.
- Once connected to the server, the searching methods are the same as with MyData DB Server.

Wiley C-13 database

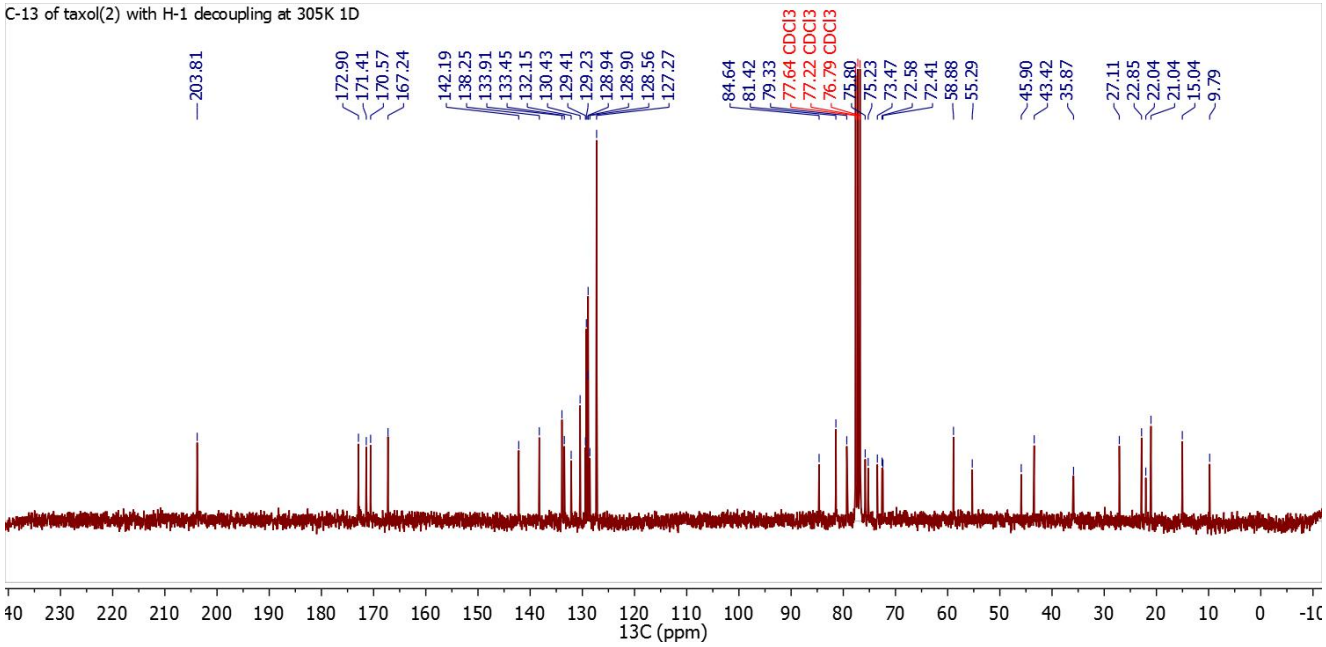
- 13C NMR Spectra: 268,000
- Structures: 268,000
- Compounds: 228,000
- Replicate Spectra: 40,000
- Collected and reviewed by Wolfgang Robien, with carefully reviewed peak assignments, specific measurement and instrument parameters, where available.
- Using proprietary quality assurance measures developed by the author and Wiley, this is the finest collection of 13C NMR spectra available

Search Wiley database

- 1H NMR Spectra: 157,000
- Structures: 157,000
- Compounds: 155,000
- Replicate Spectra: 2,000
- Collected and reviewed by Alexander Yarkov, with carefully reviewed peak assignments, and specific measurement and instrument parameters, where available.
- Using proprietary quality assurance measures developed by the author and Wiley, this is the finest and largest collection of 1H NMR spectra available.

Search a C-13 spectrum

- Open Training Data Sets > Database Search > Taxol > C-13 > fid
- Do Analysis > Auto Peak Picking, right click and choose peak search
- Peak Search Settings:
  - *Reverse to penalize only unmatched query peaks.*
  - *Tolerance = +/- 1.0 ppm*
- Choose the top hits with score > 800 (out of 1000)
- Taxol has the highest score 948



WILEY DB

C-13 search results

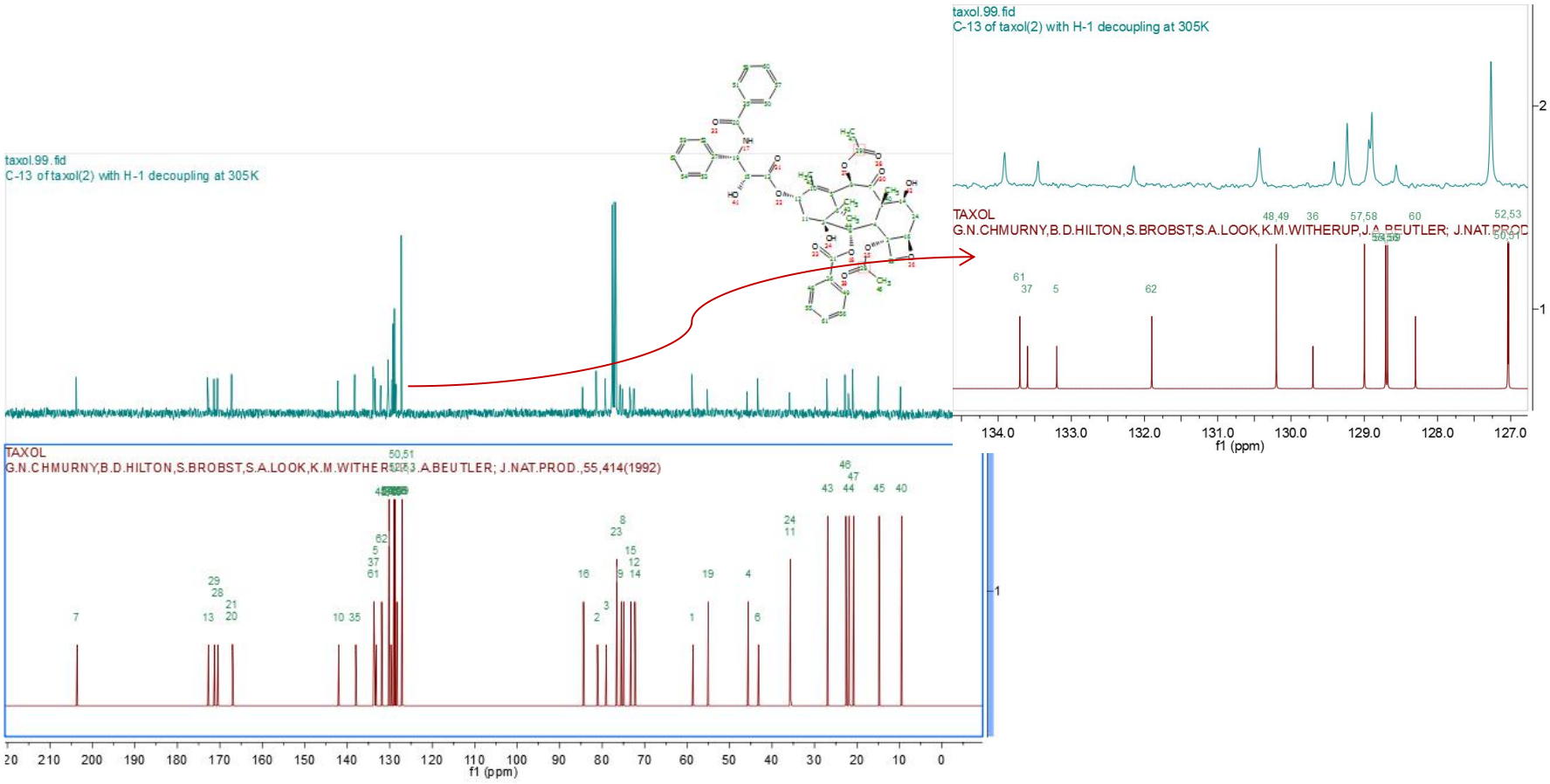
- Hit list, and preview of hits

Mestrelab Research
chemistry software solutions

WILEY DB

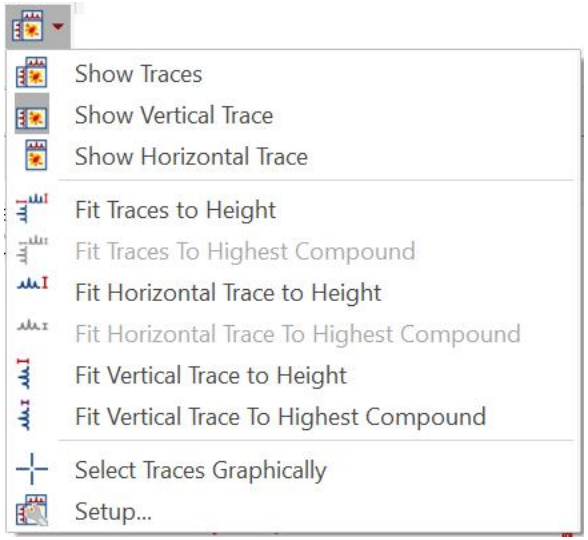
Search a C-13 spectrum

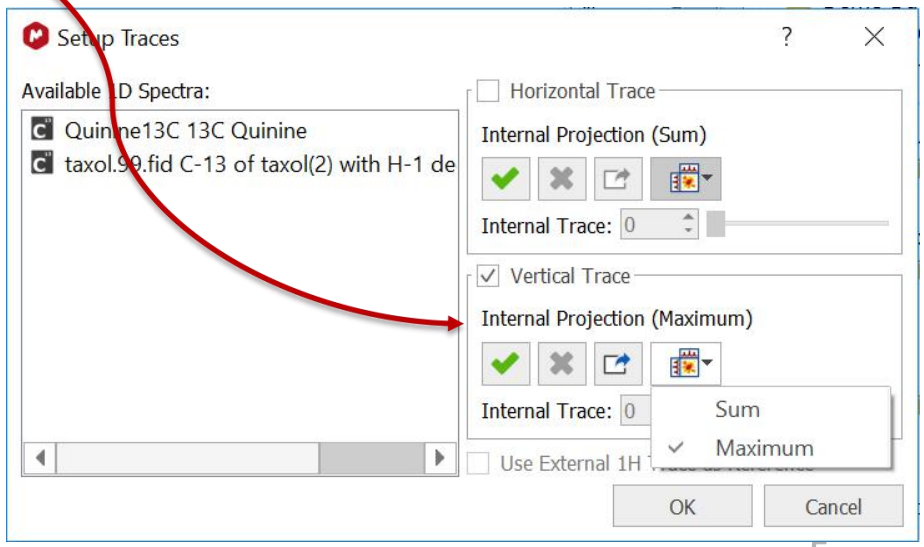
- Right click on the spectrum, choose Paste Record to Mnova to download the hit spectrum and compare with the experimental one



Search C-13 peaks from HMBC

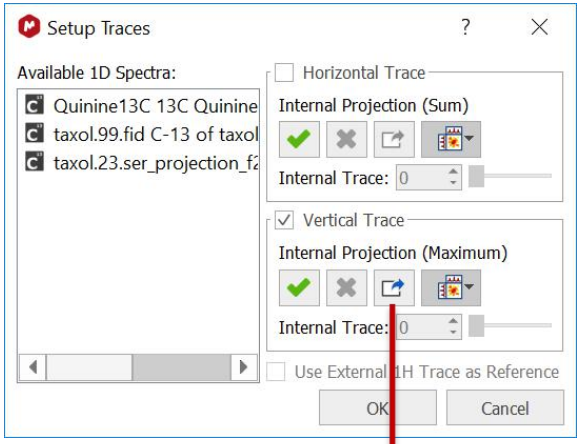
- Open Training Data Sets > Database Search > Taxol > HMBC > ser
- Choose Processing > More Processing > Reduce t1 Noise.
- Choose View > 2D Traces > Setup
- In the Setup Traces dialog, choose to display Internal Projection (Maximum) as Vertical Trace

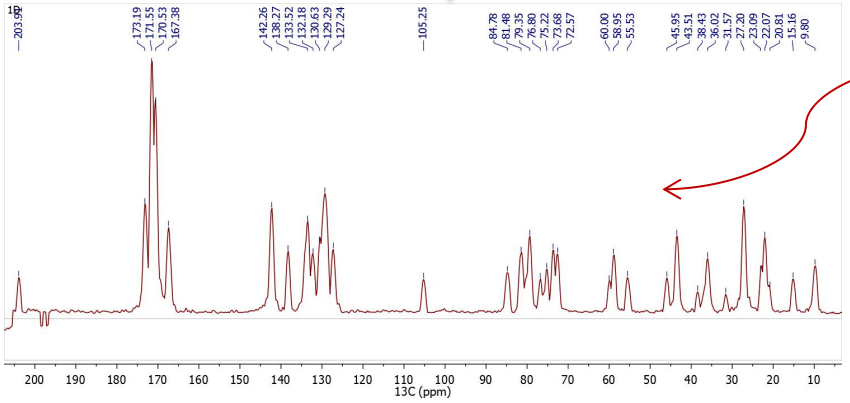


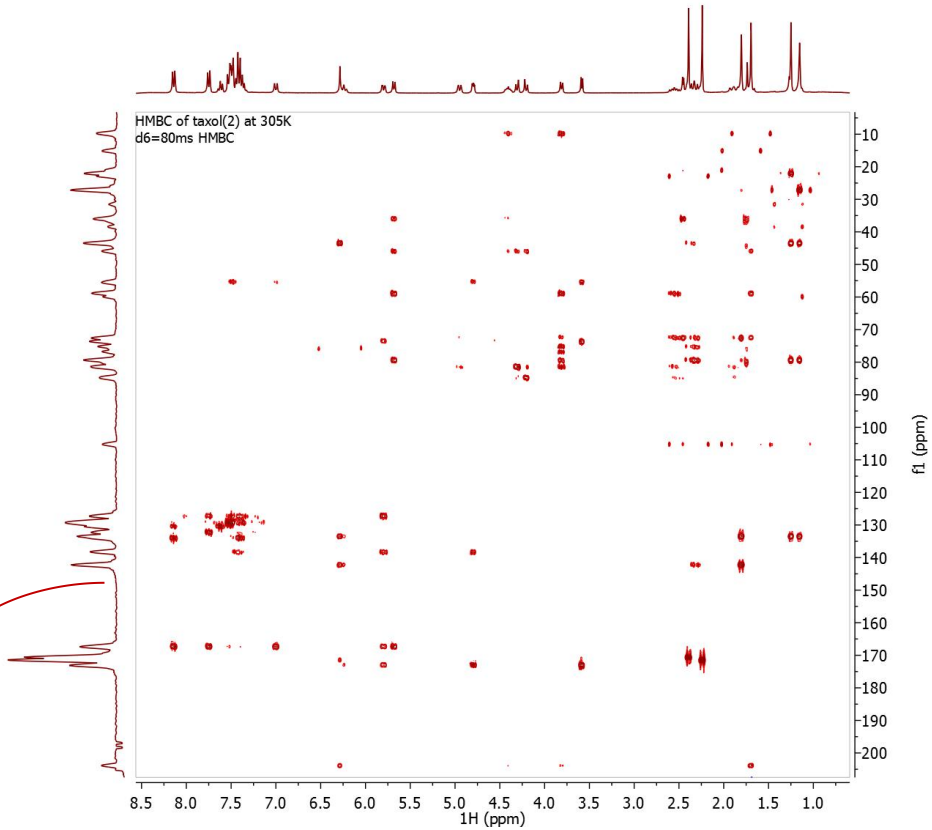


Search C-13 peaks from HMBC

- Click Extract in the Setup Trace Dialog to generate a pseudo 1D C13 spectrum in a new page, and do auto peak picking on the pseudo C13 spectrum.

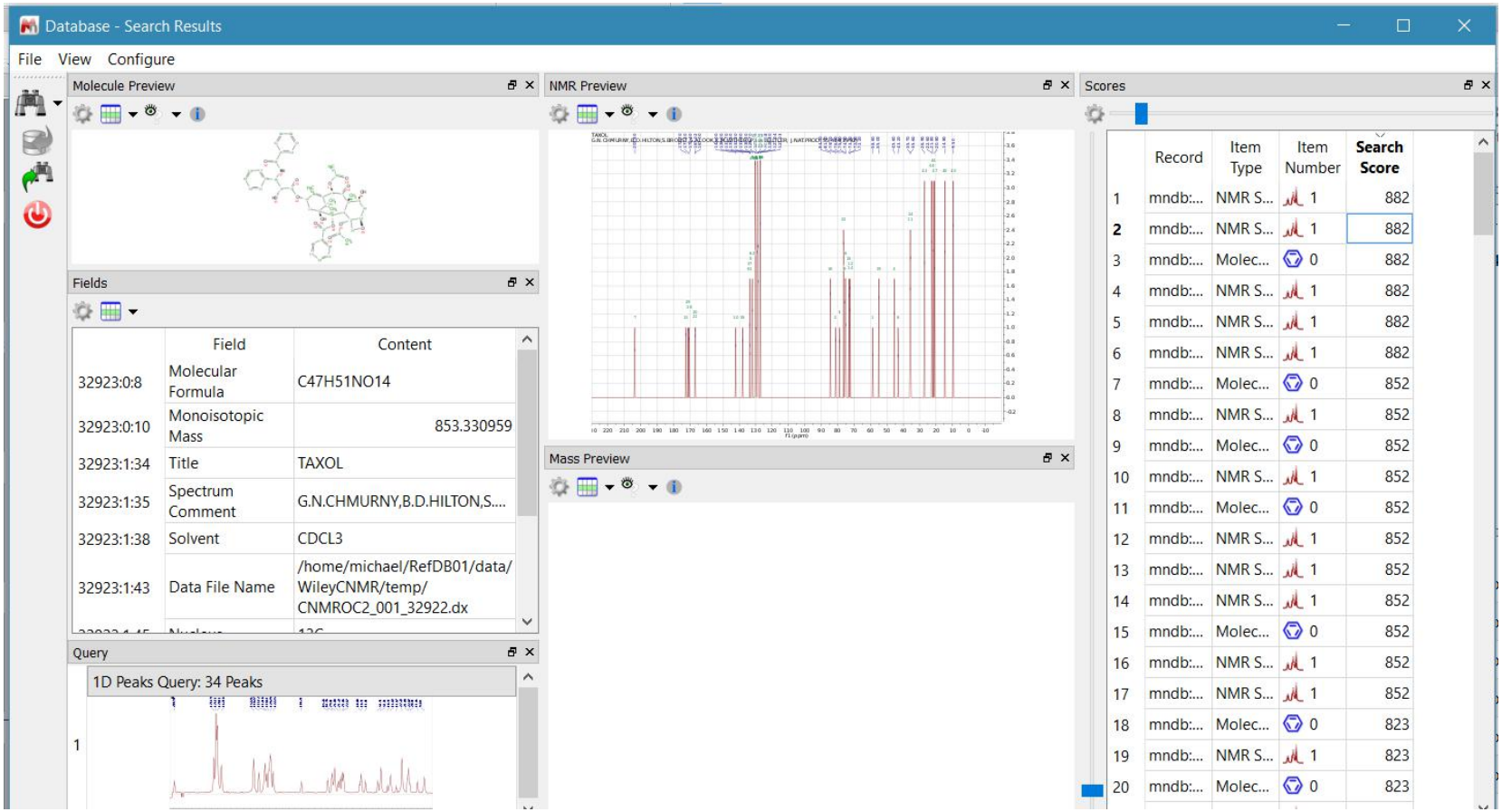






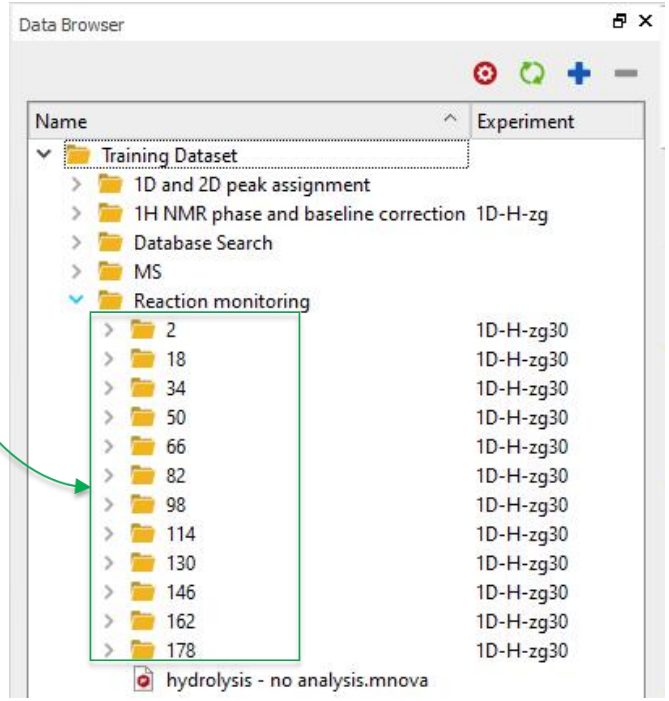
Search C-13 peaks from HMBC

- Right click on the C-13 spectrum and do a peak search again. Taxol is listed as one of the top hits again



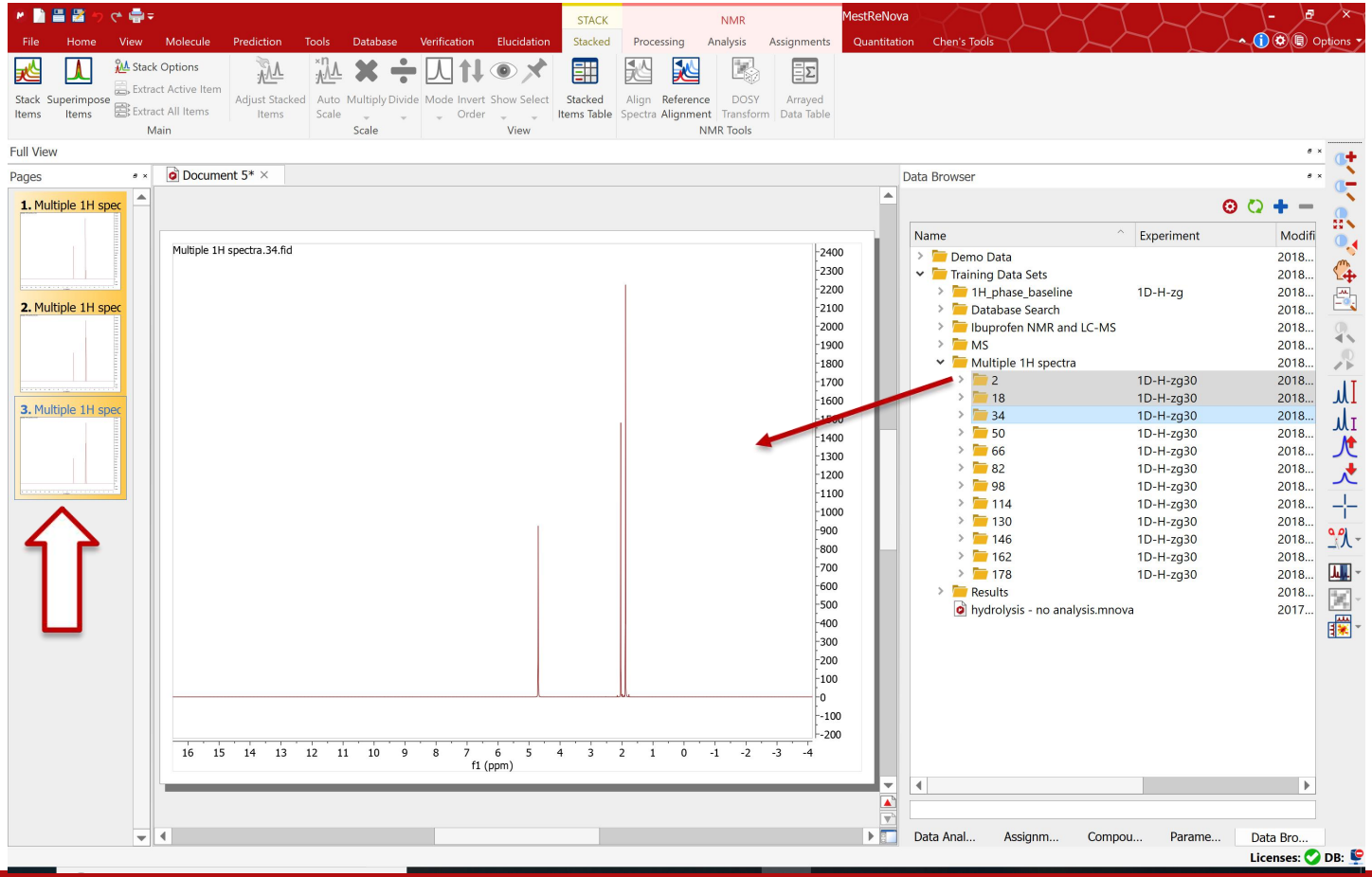
Processing Arrayed Spectra for Reaction Monitoring

Sample data

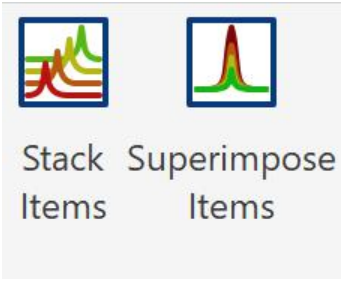


Stack a few spectra

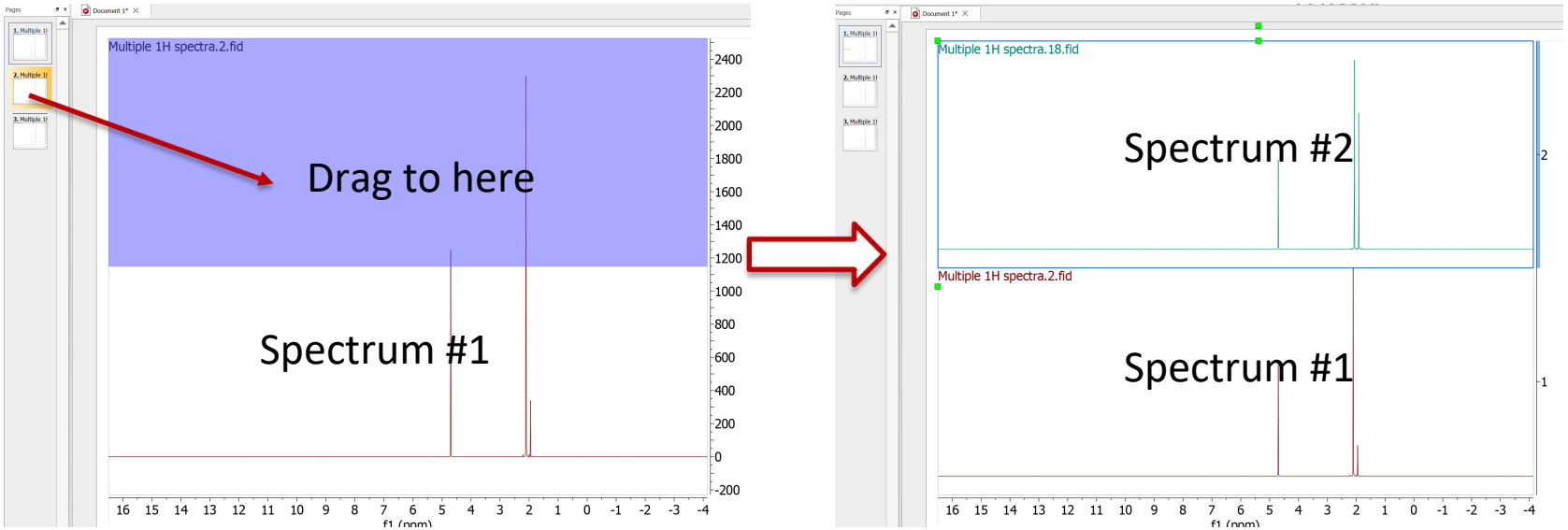
- Open the first 3 spectra from the Multiple 1H spectra folder in Data Browser
- The Stacked Ribbon is visible if you highlight multiple spectra in the Pages View



Stack a few spectra

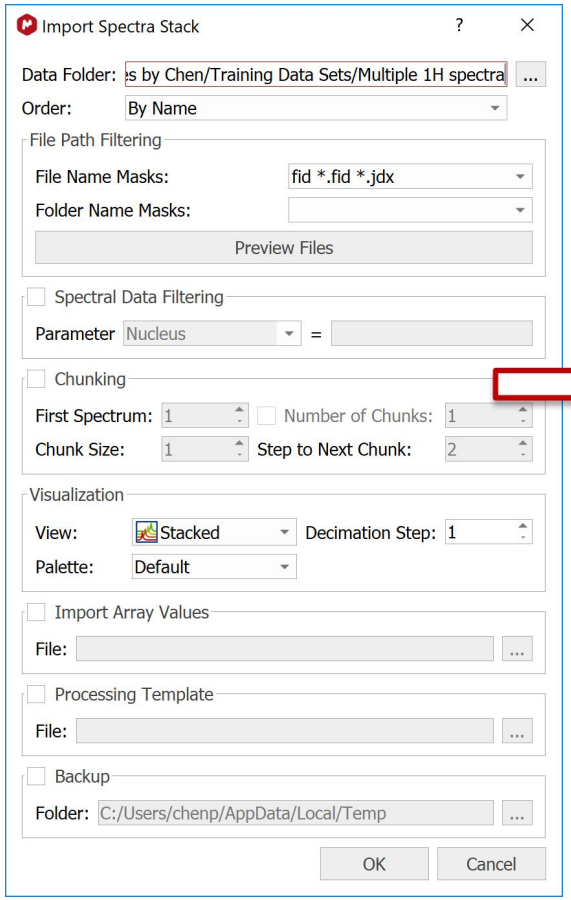


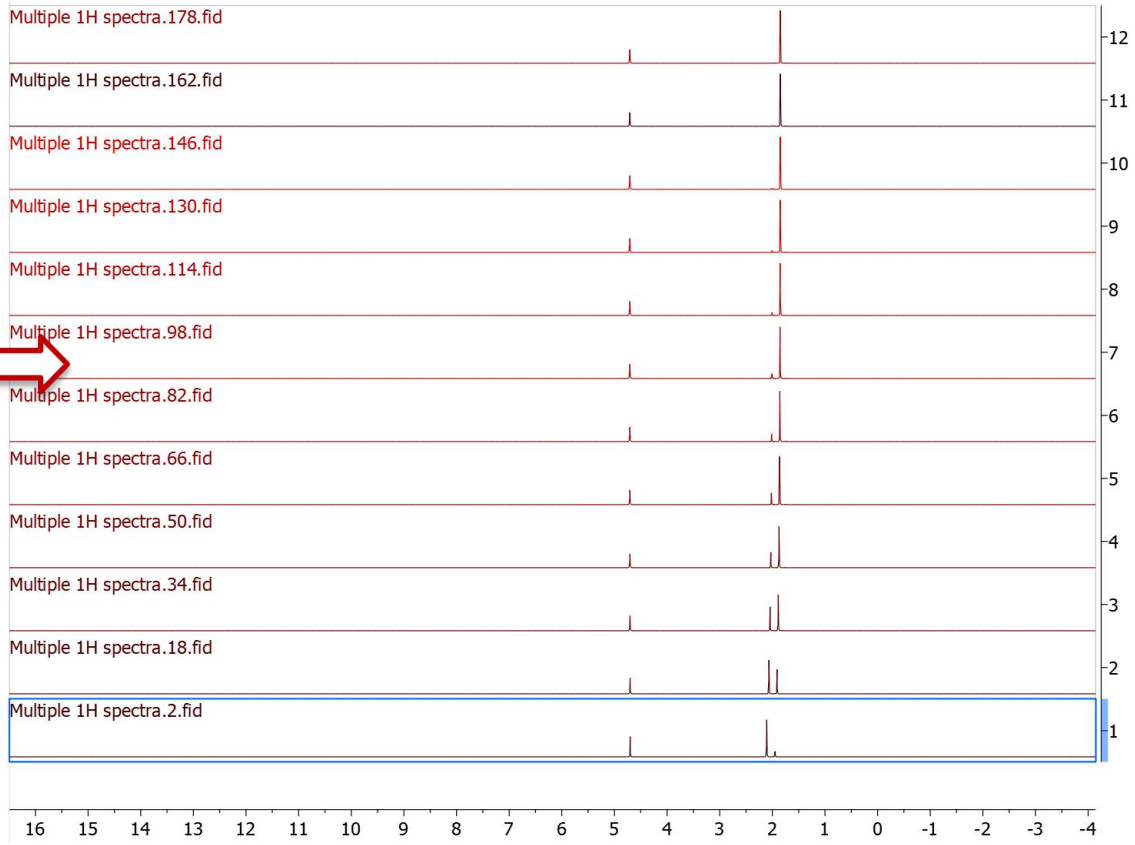
- You can use the Stack Items or Superimpose Items tools to stack or superimpose the highlighted spectra in the Pages View, or:
- Drag the thumbnail of another spectra from the Pages View to the current spectrum to stack them in desired way.
- Continue to drag the 3rd spectrum to the stack. Note you can put the spectrum to the top, middle or bottom, or to replace an existing spectrum in the stack.
- Try the different Stacking Mode, and other tools in the Stacked Ribbon



Stack many spectra

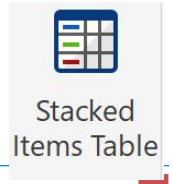
➢ Choose Tools > Loaded Scripts > Directory Spectra Stack, navigate to the directory "Multiple H-1 Spectra" in the training dataset. Click OK to import and stack all of them.

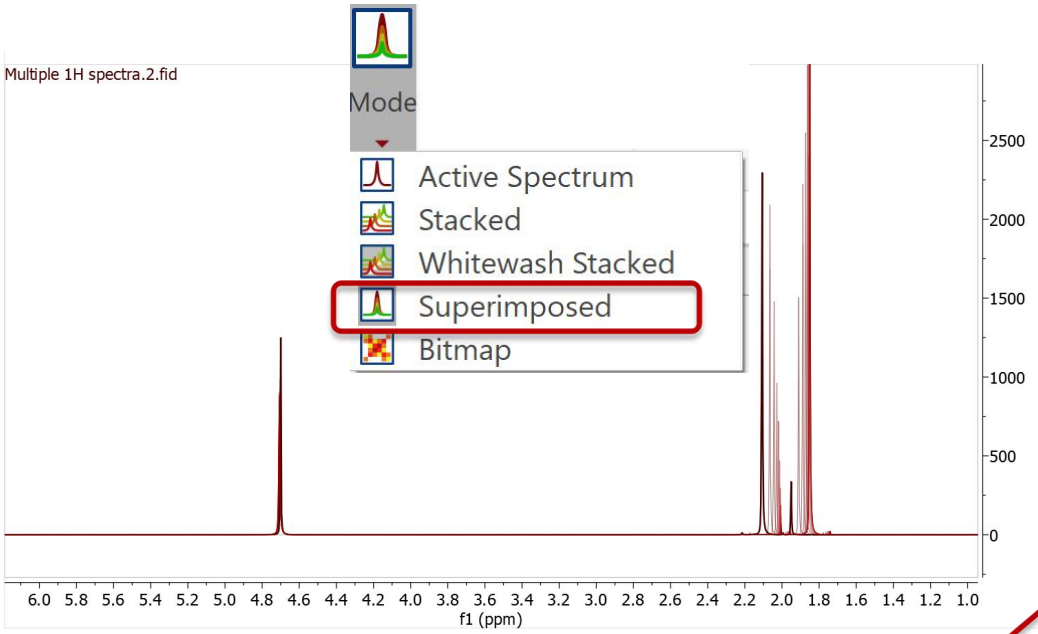


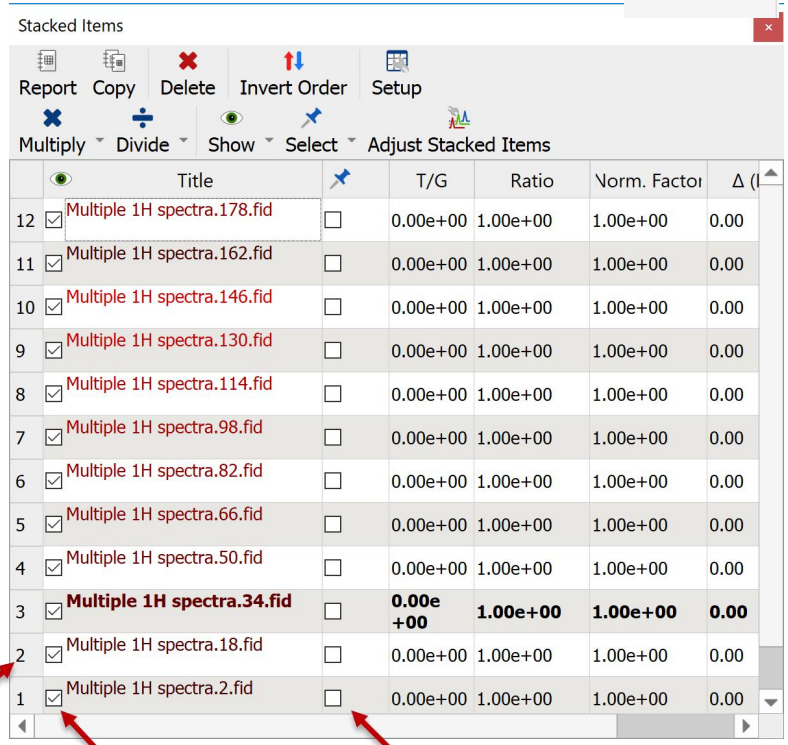


Stacking mode and Stacked Items Table

- Choose Stacked > Mode to try different display modes. Choose Superimposed mode to make sure the baseline and phasing is OK for all spectra.
- Choose Stacked > Stacked Items Table to display the Table. You can manipulate the spectra in many ways using the tools on this Table.
- If needed, you can reprocess all or selected spectra







	Title	T/G	Ratio	Norm. Factor	Δ (I
12	Multiple 1H spectra.178.fid	0.00e+00	1.00e+00	1.00e+00	0.00
11	Multiple 1H spectra.162.fid	0.00e+00	1.00e+00	1.00e+00	0.00
10	Multiple 1H spectra.146.fid	0.00e+00	1.00e+00	1.00e+00	0.00
9	Multiple 1H spectra.130.fid	0.00e+00	1.00e+00	1.00e+00	0.00
8	Multiple 1H spectra.114.fid	0.00e+00	1.00e+00	1.00e+00	0.00
7	Multiple 1H spectra.98.fid	0.00e+00	1.00e+00	1.00e+00	0.00
6	Multiple 1H spectra.82.fid	0.00e+00	1.00e+00	1.00e+00	0.00
5	Multiple 1H spectra.66.fid	0.00e+00	1.00e+00	1.00e+00	0.00
4	Multiple 1H spectra.50.fid	0.00e+00	1.00e+00	1.00e+00	0.00
3	**Multiple 1H spectra.34.fid**	**0.00e+00**	**1.00e+00**	**1.00e+00**	**0.00**
2	Multiple 1H spectra.18.fid	0.00e+00	1.00e+00	1.00e+00	0.00
1	Multiple 1H spectra.2.fid	0.00e+00	1.00e+00	1.00e+00	0.00

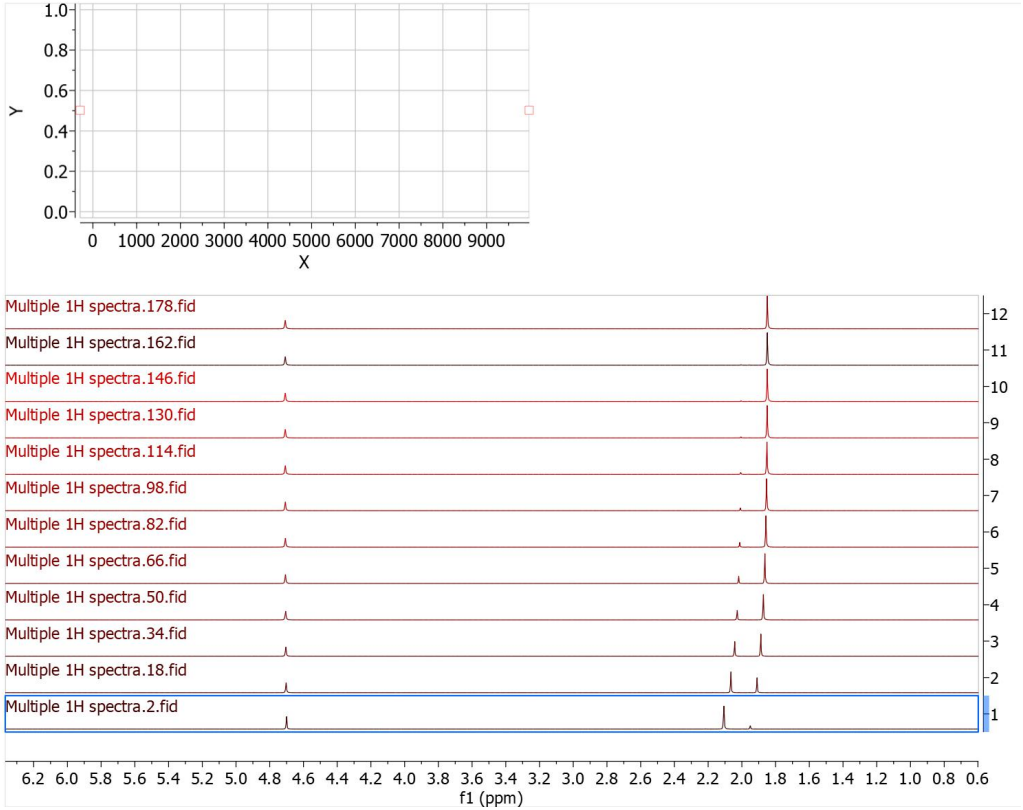
Click and drag here to change the order

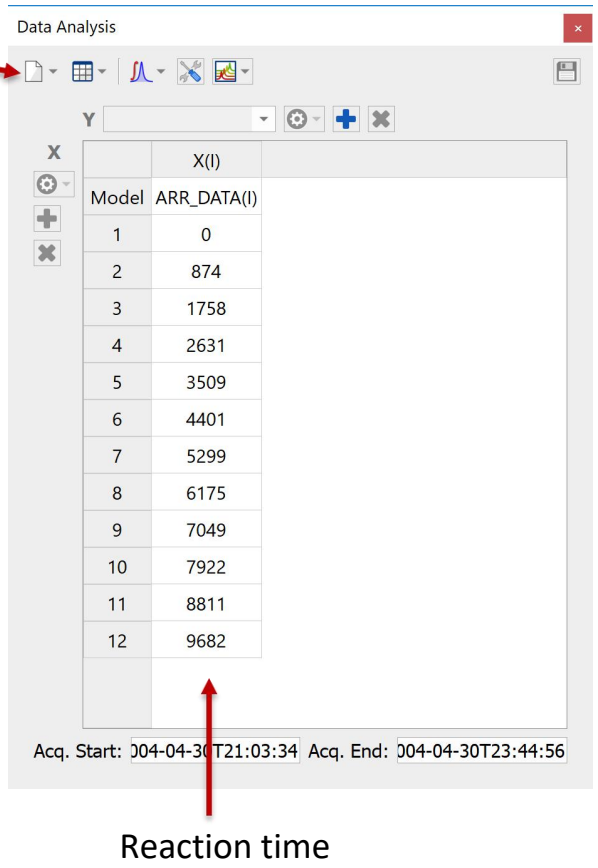
Check/uncheck these to show/hide spectra

Check these to choose spectra to change

Analyze arrayed spectra

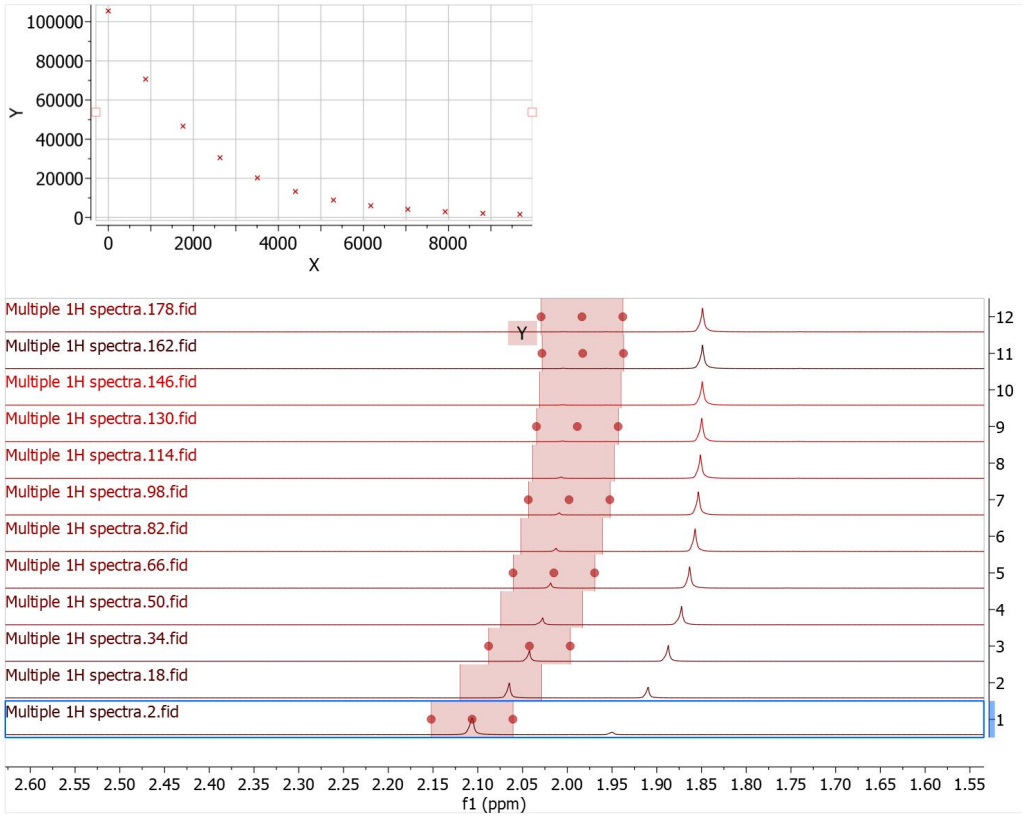
- Choose Analysis > Data Analysis > Show Table to display the Data Analysis Table.
- Click on the Empty Graph to import the X values (reaction time in this case) and display an empty XY graph.

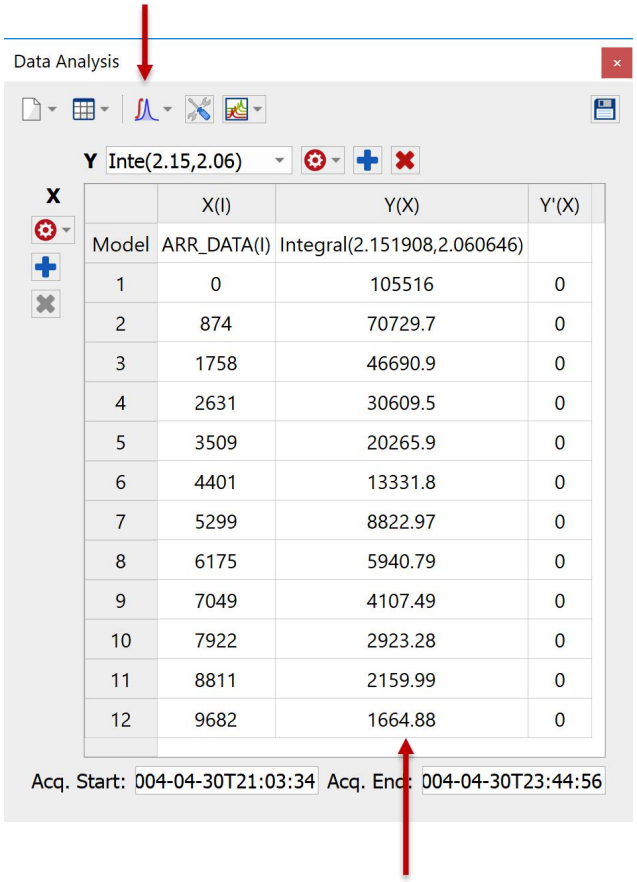




Integrate arrayed spectra

- Click the Pick Integral tool.* Click and drag on first (bottom) spectrum to define the integration range
- If needed, adjust the handlers to change the integration range **
- The integrals are displayed on the XY graph and in the Data Analysis Table.





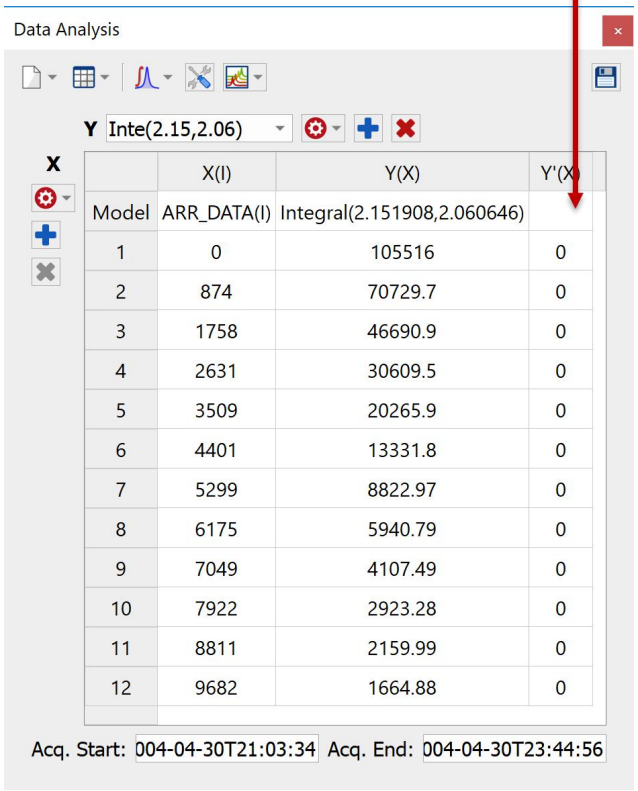
Integrals

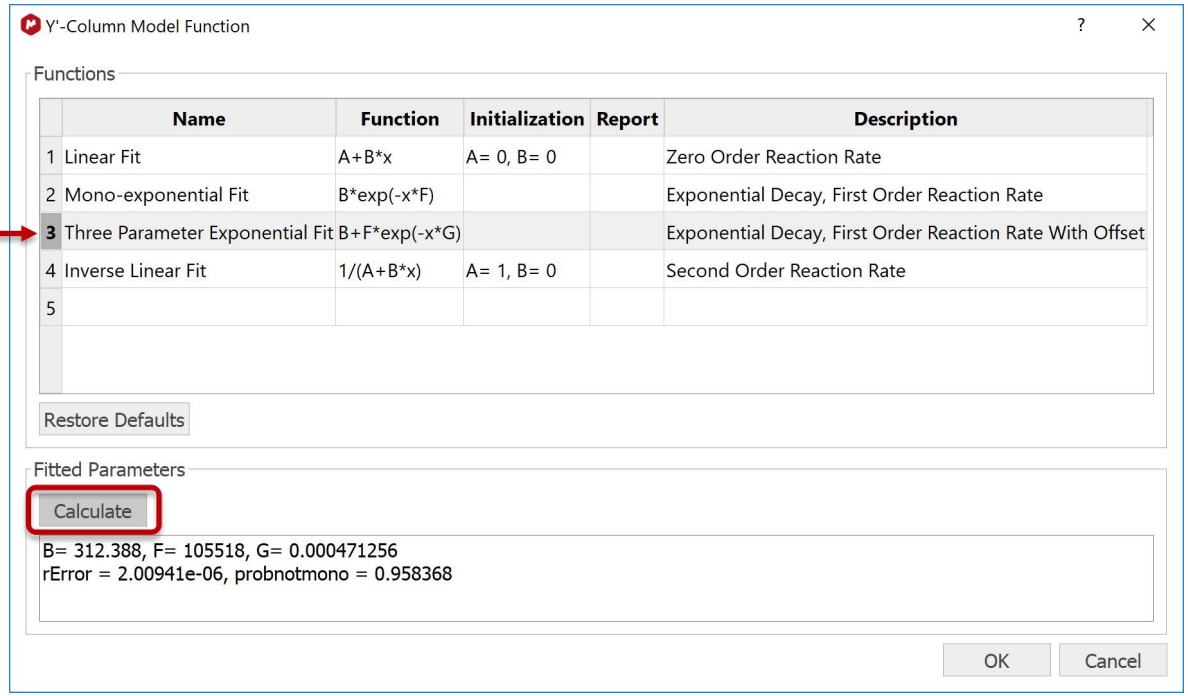
**Use Sum Method (default) for integration unless you are integrating overlapped peaks. Click Options for Integration in the Analysis Ribbon to verify. ** You can increase the # of handlers by using the Edit Model Option Tool.*

Fit XY to a function

- Click the Model cell under Y'(X) in Data Analysis.
- Choose the 3rd function, and click Calculate to fit the XY values to a first order reaction (with offset)

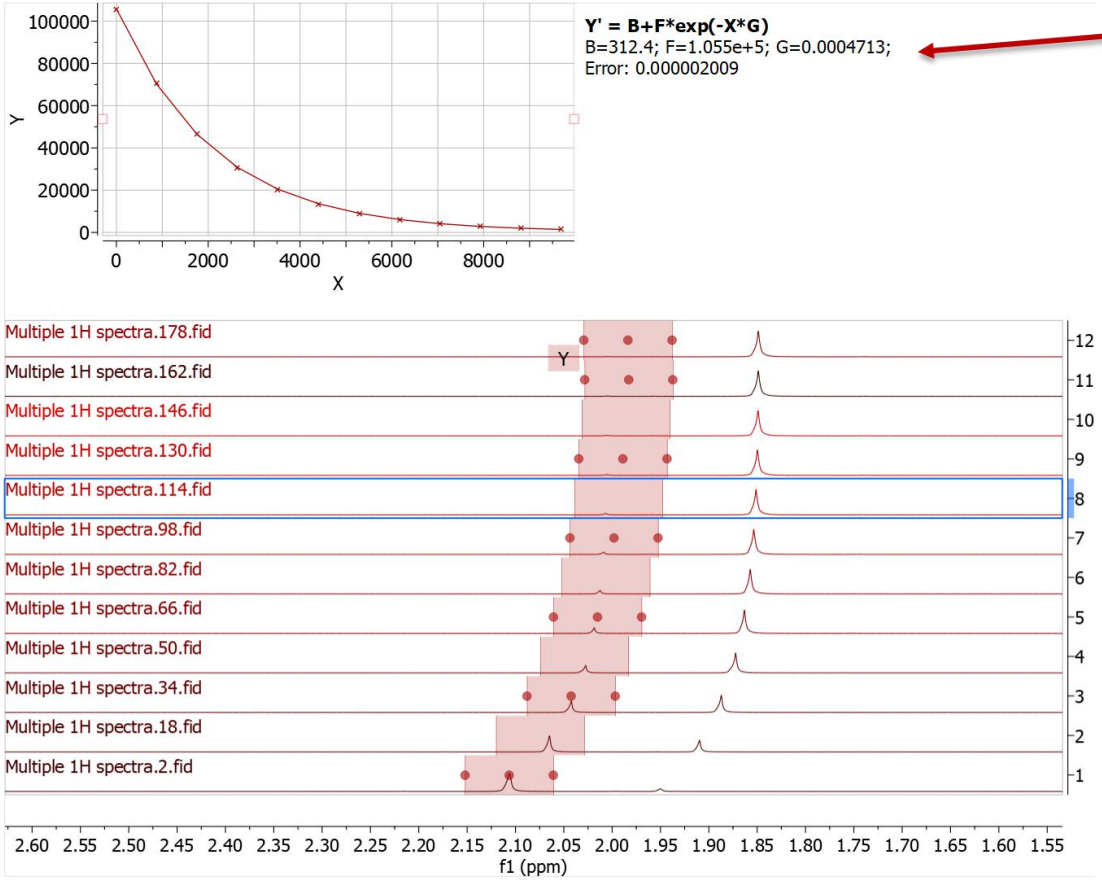
Double click here

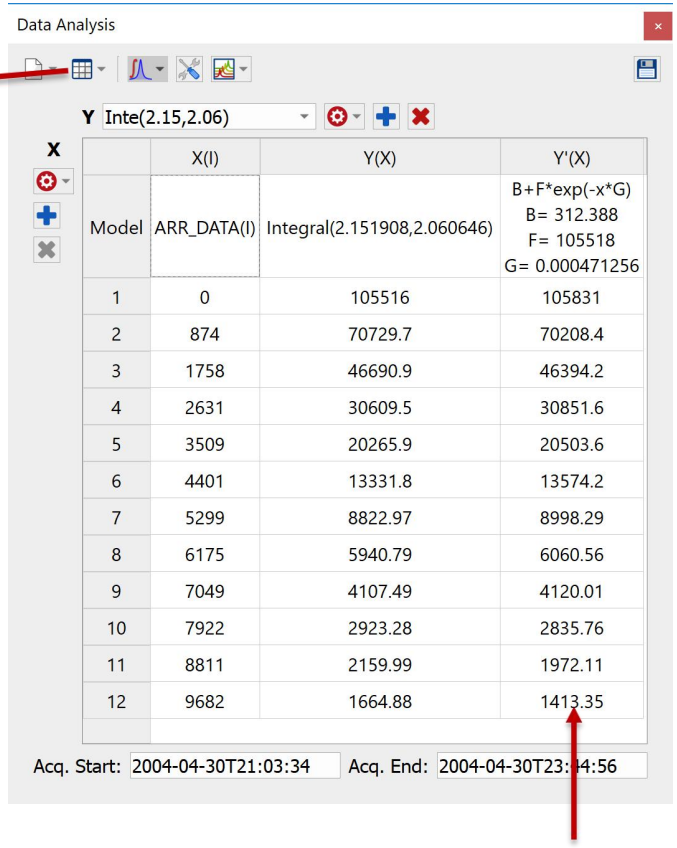




Report kinetic parameters

- Click the Report tools from the Data Analysis Panel to report the results next to the XY Graph
- Choose Report to Clipboard and paste the results to another document
- Repeat these steps for the other peaks around 1.91 ppm.





	X(I)	Y(X)	Y'(X)
Model	ARR_DATA(I)	Integral(2.151908,2.060646)	B+F*exp(-x*G) B= 312.388 F= 105518 G= 0.000471256
1	0	105516	105831
2	874	70729.7	70208.4
3	1758	46690.9	46394.2
4	2631	30609.5	30851.6
5	3509	20265.9	20503.6
6	4401	13331.8	13574.2
7	5299	8822.97	8998.29
8	6175	5940.79	6060.56
9	7049	4107.49	4120.01
10	7922	2923.28	2835.76
11	8811	2159.99	1972.11
12	9682	1664.88	1413.35

Fitting results

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