



Mestrelab Research

chemistry software solutions

Mnova Training - Basics

Version 12.0.3

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Main Topics

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



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

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>

The Host ID for this computer

Location of the license file

Mnova plugin names

License expiring date

License issued date

License Manager

Host ID:
X2PNM-JB2...-605T6-Δ7L9CZWT

Licenses

State	Plug-in	Issued By	Licensed To	Type	Issued Date	Days to Expir
✓	Mnova Verify	Mestrelab Research S.L.	Laptop	single	lu. abr. 25 2016	Never
?	Mnova qNMR	Mestrelab Research S.L.	Laptop	single	lu. abr. 25 2016	Never
✓	NMR	Mestrelab Research S.L.	Laptop	single	lu. abr. 25 2016	Never
✓	NMRPredict Desktop	Mestrelab Research S.L.	Laptop	single	lu. abr. 25 2016	Never
✓	Random Forest Predictor	Mestrelab Research S.L.	Laptop	single	lu. abr. 25 2016	Never
?	Reaction Monitoring	Mestrelab Research S.L.	Laptop	single	lu. abr. 25 2016	Never
?	Str...	Mestrelab Research S.L.	Laptop	single	lu. abr. 25 2016	Never

Service Licenses

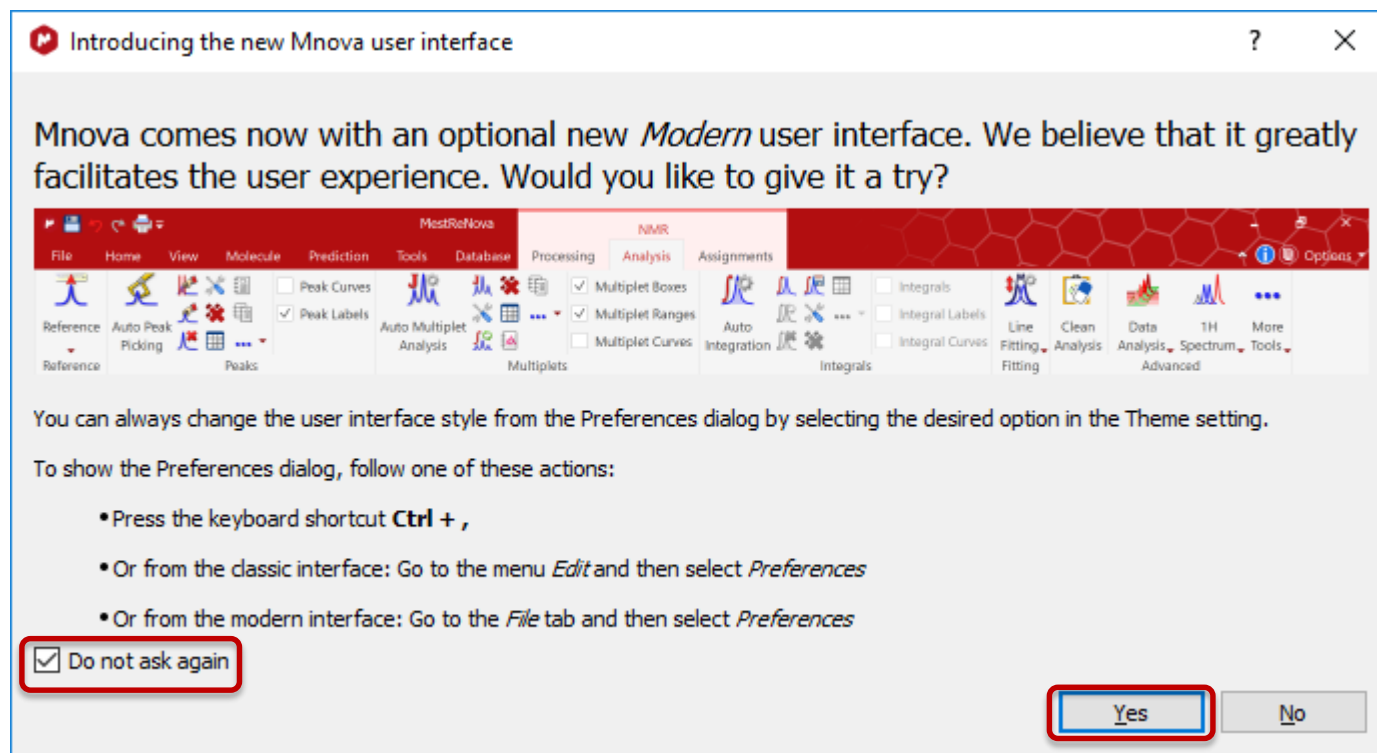
State	Name	Username	Id	Issued Date	Expiry Date	Operations	Tenant Id	Asset Id

Support... Error Summary... Close

Use the New Graphical User Interface (GUI)

PREFERENCES

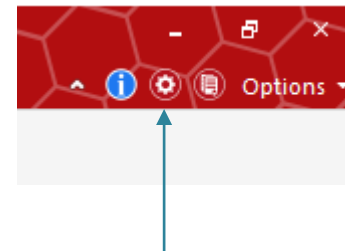
The first time you start Mnova, it asks if you want to use the “Modern” GUI. Choose it and check “Do not ask again”. Restart Mnova, you will enjoy the modular ribbon GUI introduced since version 12.



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

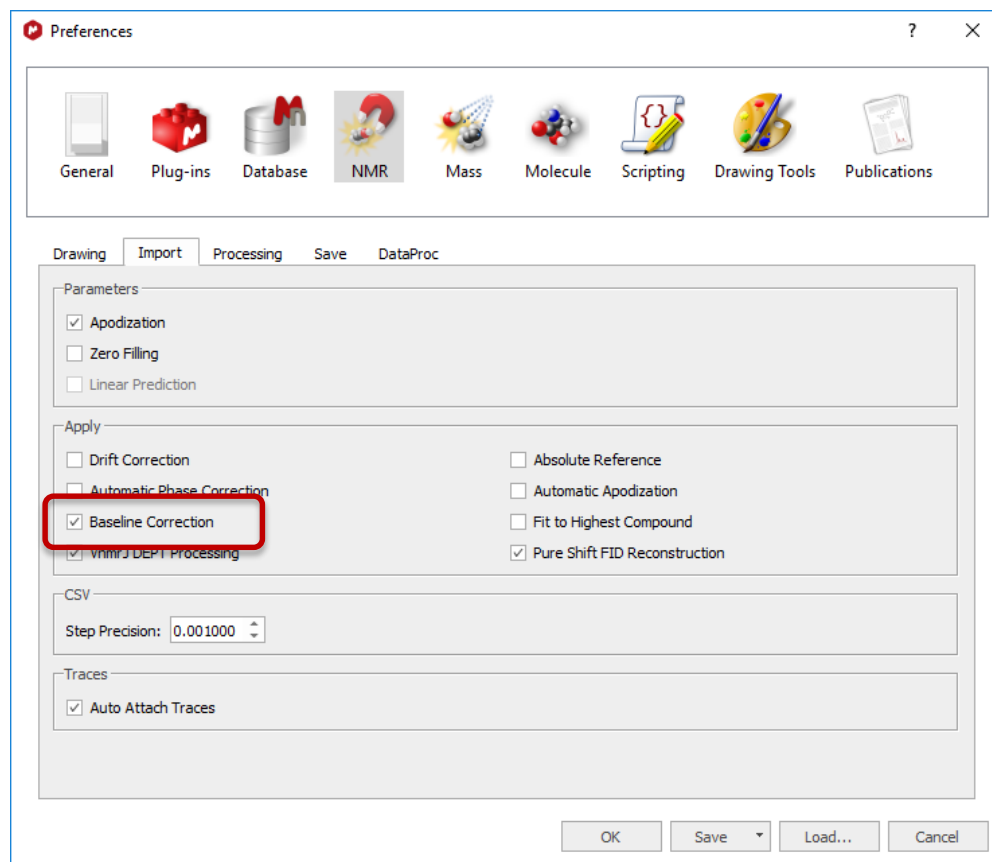
Turn on Auto Baseline Correction

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". This option may make manual phasing of 2D NMR sluggish. In that case, turn baseline off from Processing .

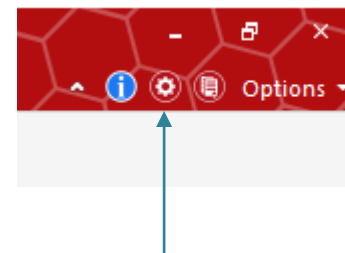
Tip: There are many options and settings that you may change in the Preferences Dialog, especially the resolution of image copying and image exporting in the Drawing Tab.



PREFERENCES

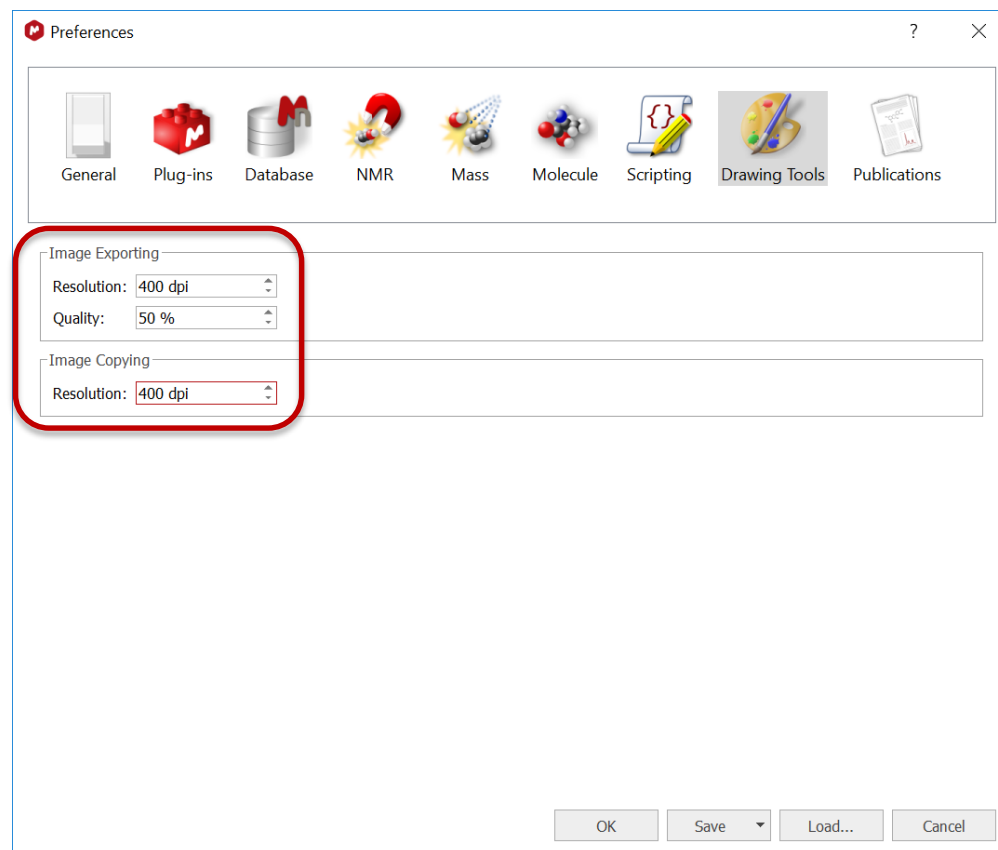
Setup the resolution for publishing spectra

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



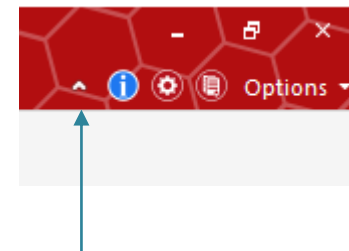
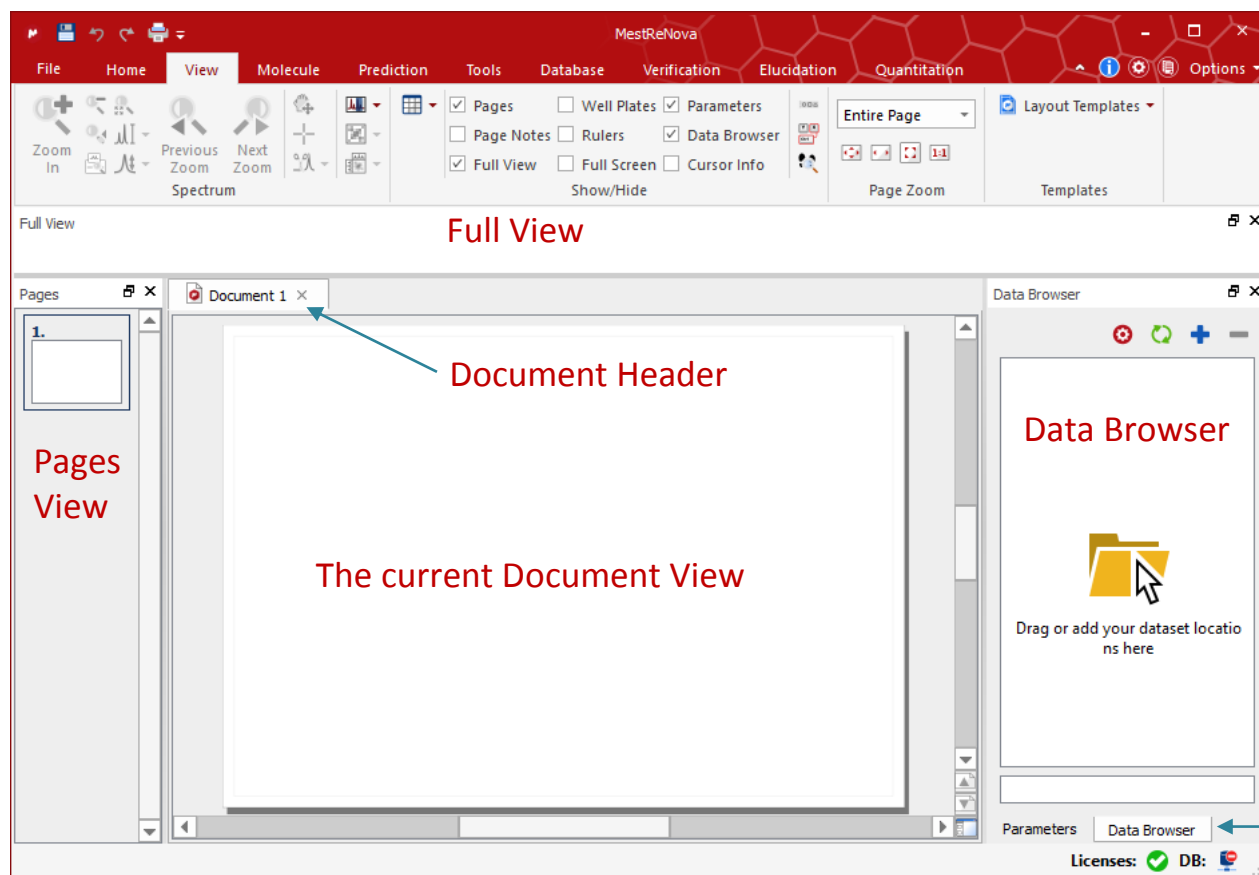
The resolution for Image Exporting is used when you choose File > Save As and save the selected objects in Mnova as a graphical image file.

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

SETUP

- 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	Modification date	Comment	Format
Training Data Sets		2018-10-30T1...		
1H_phase_baseline	1D-H-zg	2018-05-29T0...		Bruker UXNMR/XW...
Ibuprofen NMR and LC-MS		2018-10-30T1...		
1.fid	1D-H-s2pul	2018-10-30T1...	Ibuprofen 4/8/2015	Varian VNMR
2.fid	1D-C-s2pul	2018-10-30T1...	Ibuprofen 4/8/2015	Varian VNMR
3.fid	2D-HH-COSY-gCOSY	2018-10-30T1...	Ibuprofen 4/8/2015	Varian VNMR
4.fid	2D-CH-HSQC-EDITED...	2018-10-30T1...	Ibuprofen 4/8/2015	Varian VNMR
5.fid	2D-CH-HMBC-gHMBC	2018-10-30T1...	Ibuprofen 4/8/2015	Varian VNMR
6.fid	2D-HH-NOESY	2018-10-30T1...	Ibuprofen 4/8/2015	Varian VNMR
Waters_UPLC-MS.raw		2018-10-30T1...		
ibuprofen.mol		2011-05-06T0...	ibuprofen.cdx	Molfile
MS		2018-10-30T1...		
Multiple 1H spectra		2018-05-29T0...		
Results		2018-06-07T1...		
hydrolysis - no analysis.mnova		2017-02-05T1...		MestReNova Docu...

Add location

Path: ...

Label:

OK Cancel

Data Browser Settings

View

- Enable sorting
- Show date and size
- Show file meta data

File Formats

Format
<input checked="" type="checkbox"/> AB SCIEX Analyst (*.wiff)
<input checked="" type="checkbox"/> AB SCIEX Data Explorer (*.dat *.t2d)
<input checked="" type="checkbox"/> Advion expression CMS (*.datx)

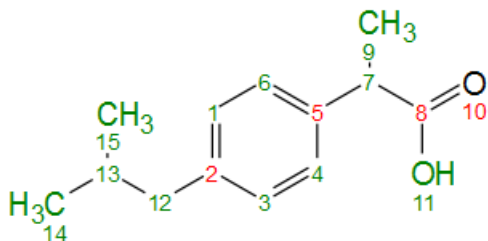
Check All Uncheck All

Wildcards

Whitelist:

PROCEDURE

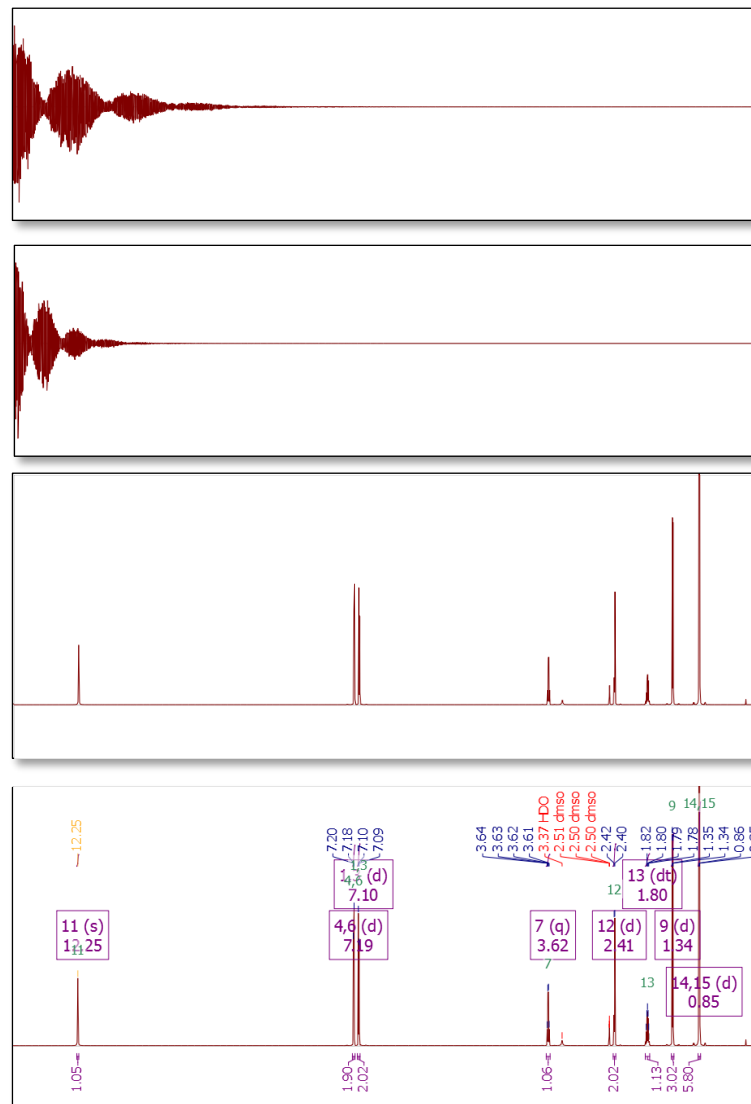
- Open the raw data
- Pre-process the FID: drift correct, apodize, zero fill, linear predict, etc.
- Fourier transform
- Phase correct and baseline correct
- Chemical shift reference
- Peak-pick, integrate, multiplet analysis
- Structure verification and peak assignment
- Report and publish



^1H NMR (600 MHz, $\text{DMSO-}d_6$) 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

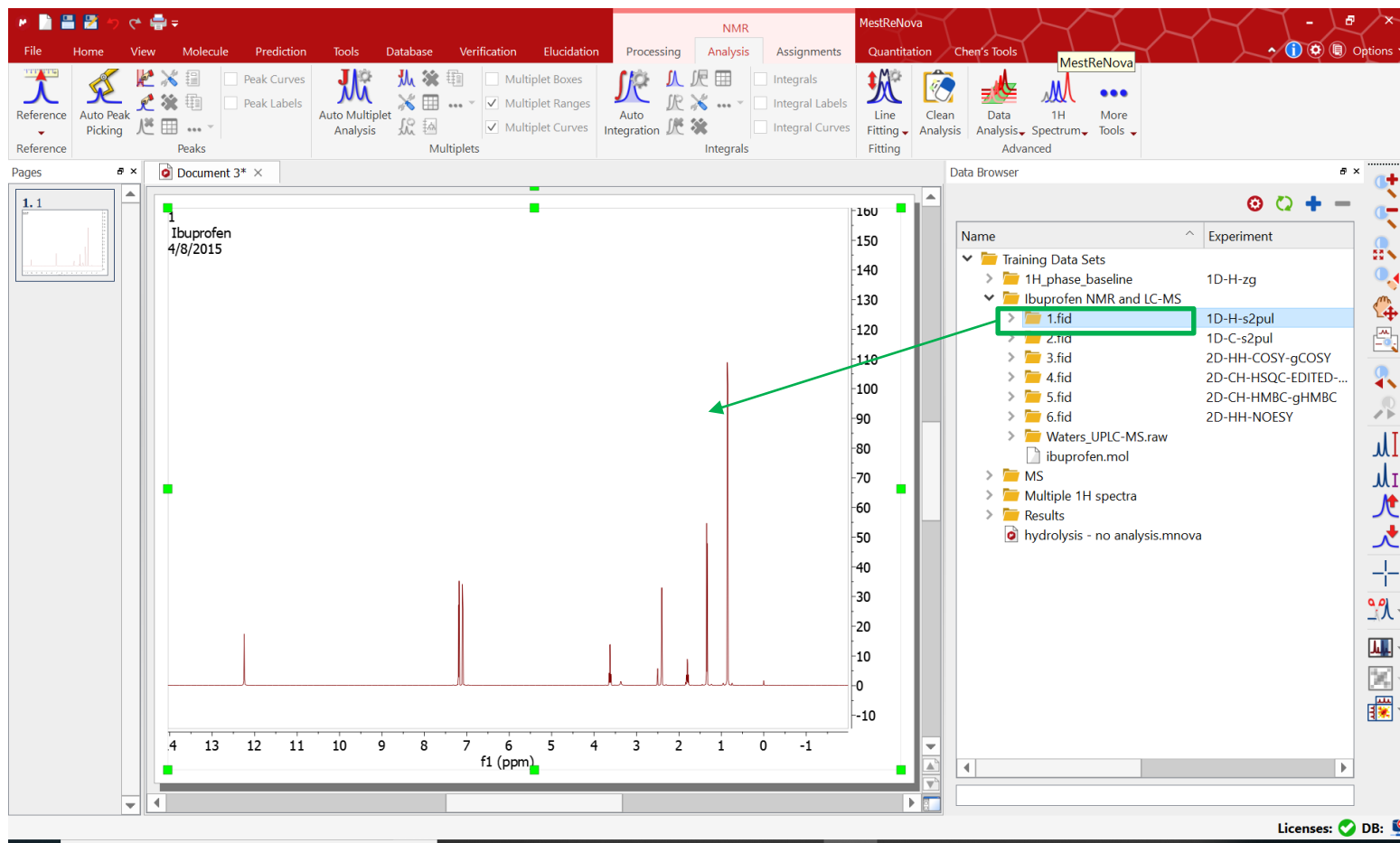
^1H processing and analysis: general procedure



Open a H-1 spectrum

PROCESSING

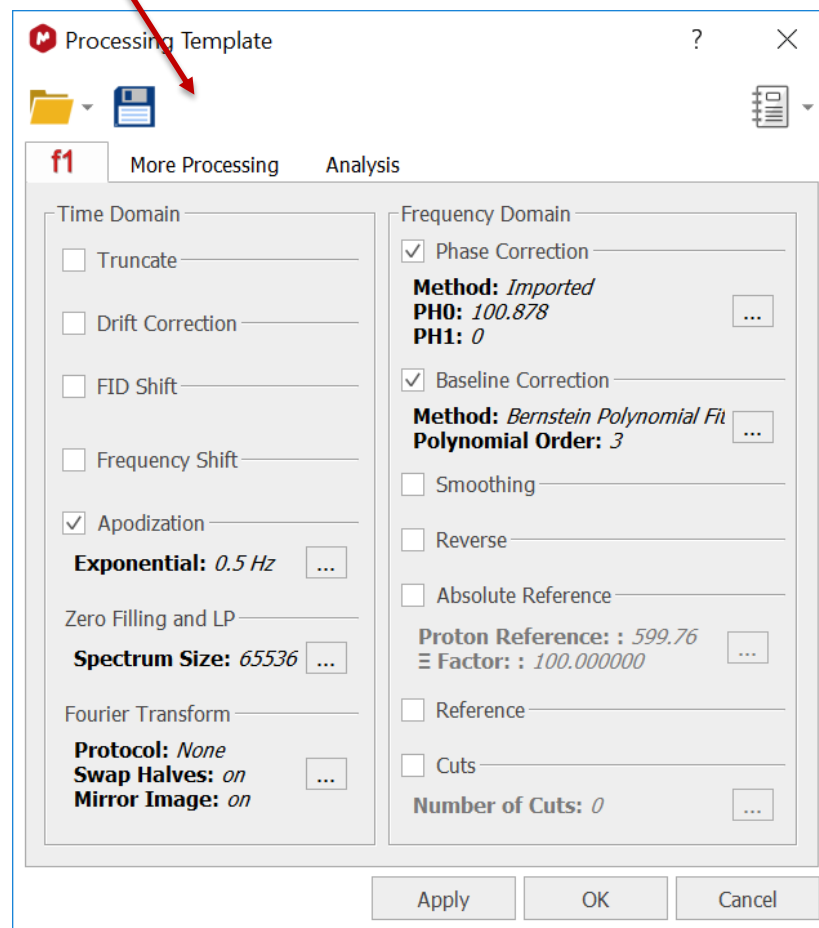
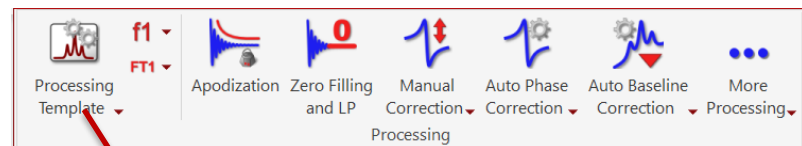
- In Data Browser, expand the folders Training Data Sets > Ibuprofen NMR and LC-MS, and drag the “1.fid” folder (1D H-1 spectrum) to the main window.
- Notice the H-1 spectrum is automatically processed and displayed.



PROCESSING

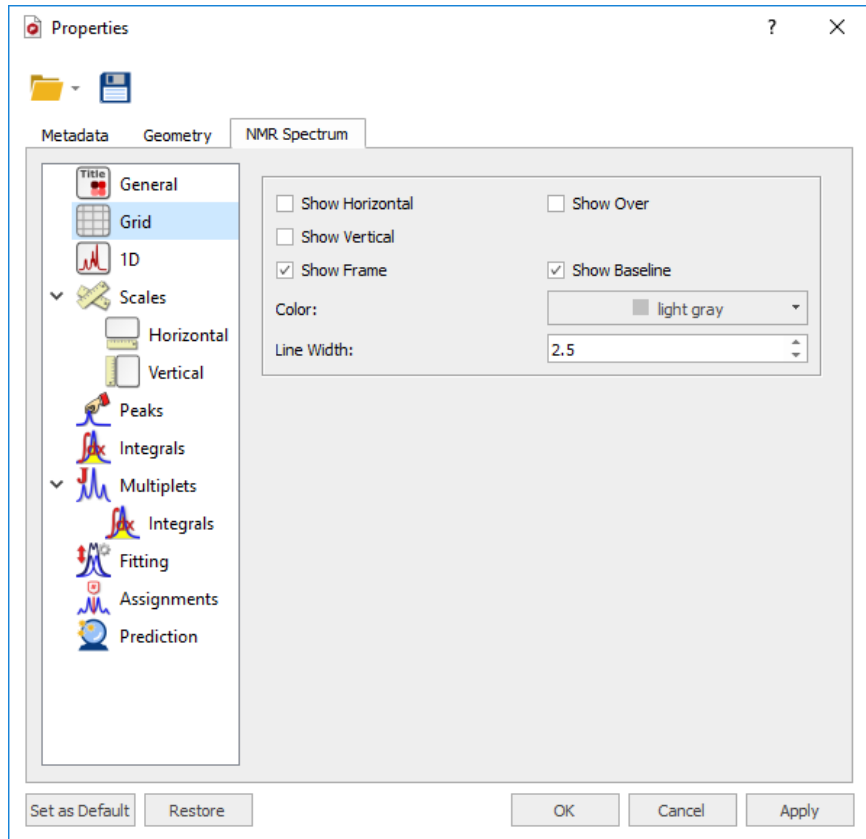
- In most cases, Mnova processes the spectrum automatically using the parameters from the instrument. The spectrum should be well-processed if the original processing parameters were well set. The Processing Tab is for you to re-process the spectrum when needed.
- Choose Processing > Processing Template 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



Change the Display Properties

- Double click on the spectrum 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



Navigate in the H-1 Spectrum
















VISUALIZATION

- 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)

The screenshot displays the MestReNova software interface. The top ribbon contains several toolbars: File, Home, View, Molecule, Prediction, Tools, Database, Verification, Elucidation, Processing, Analysis, Assignments, Quantitation, and Chen's Tools. The 'Spectrum Toolbar' is highlighted with a red arrow. The main plot area shows an H-1 NMR spectrum of Ibuprofen, with the x-axis labeled 'f1 (ppm)' ranging from 4.2 to 0.4 and the y-axis ranging from -5 to 60. The plot is titled 'Ibuprofen 4/8/2015'. On the right side, the 'Data Browser' panel shows a tree view of the project files, including '1H_phase_baseline', 'Ibuprofen NMR and LC-MS', and 'hydrolysis - no analysis.mnova'. A red box highlights the 'Full View' toolbar on the right side of the plot area, which contains icons for zooming in/out, panning, and changing the Y scale.

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

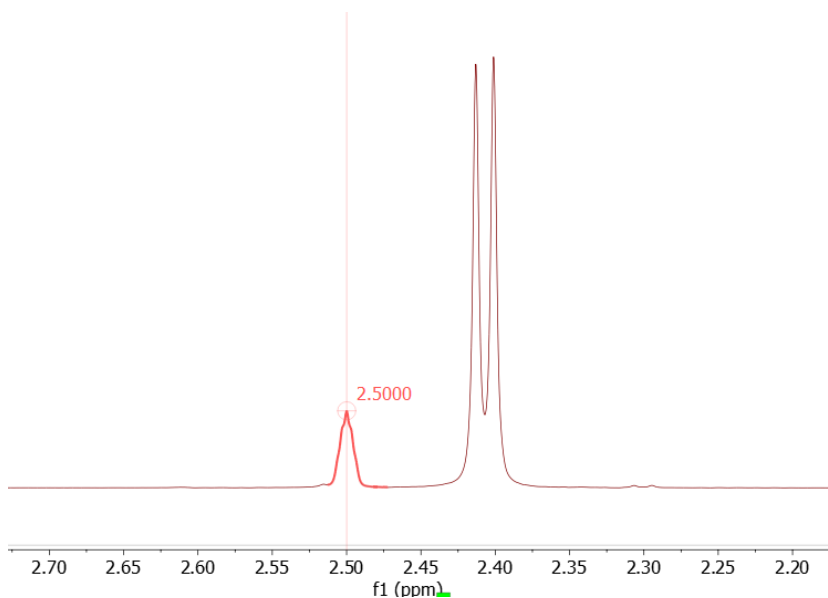
	Command	Shortcut
42	View > Full Screen	F11
43	View > Intensity > Decrease	-
44	View > Intensity > Fit to Highest Intensity	H
45	View > Intensity > Increase	+
46	View > Pages	Ctrl+F2
47	View > Pan	P
48	View > Zoom > Full Spectrum	F
49	View > Zoom > Manual Zoom	M
50	View > Zoom > Next Zoom	Shift+Right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

New Shift: 2.5000 ppm Range Width: 0.1000 ppm

Annotation DMSO-d6


Solvent List

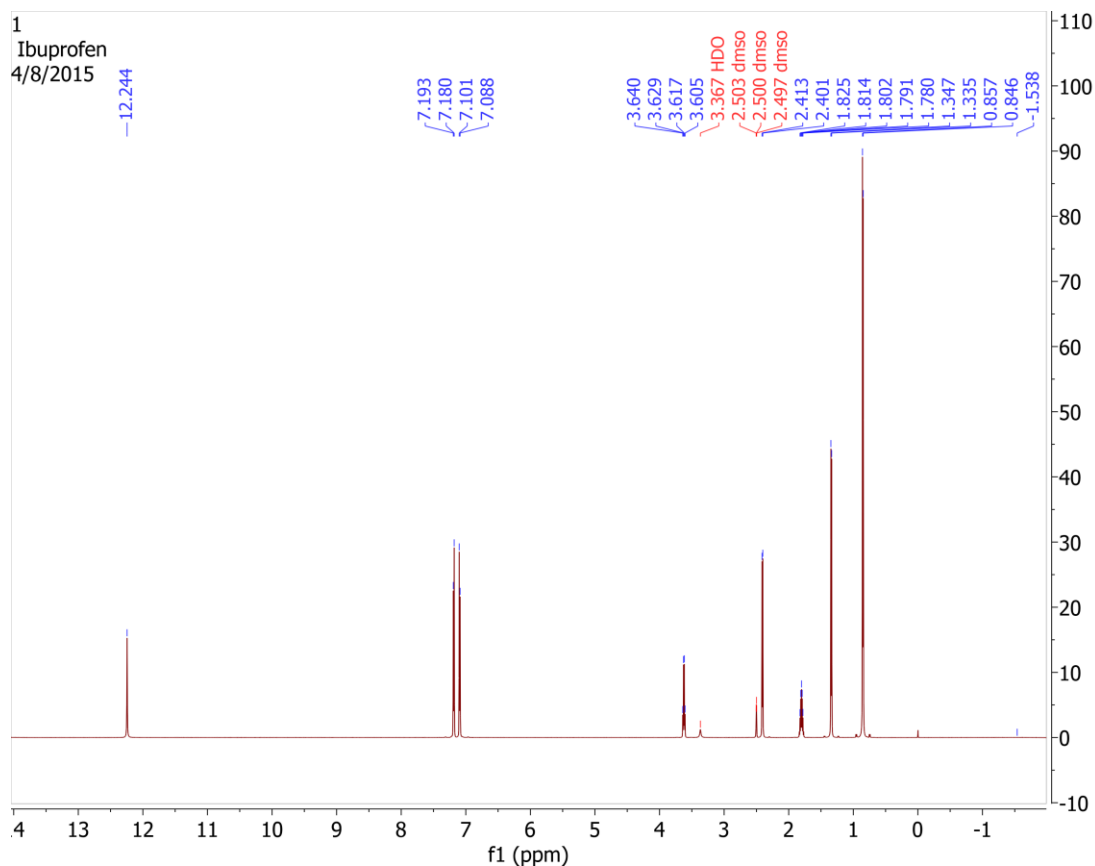
Name	Shift (ppm)	Multiplicity	J (
Deuterium Oxide	4.790	1	
Dimethyl Sulfoxide-d6	2.500	5	1
	3.330	1	
Ethanol-d6	5.290	1	

Restore Defaults Add... Edit... Delete

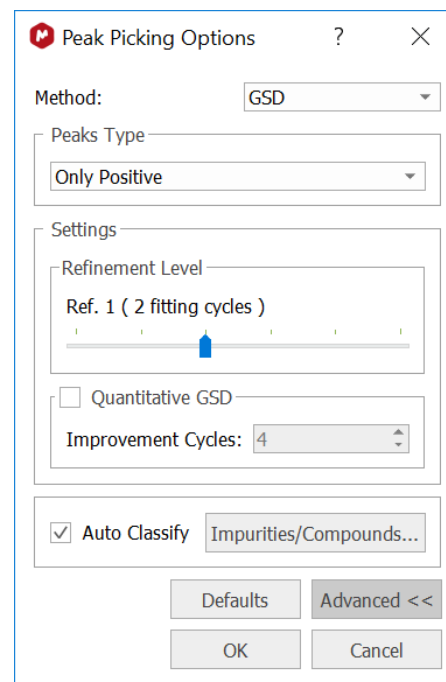
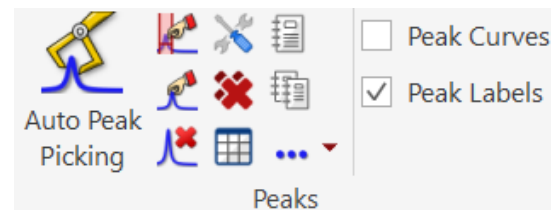
OK Cancel Solvents <<

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.



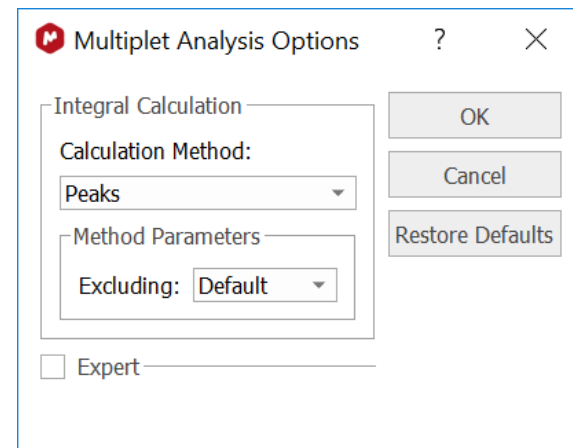
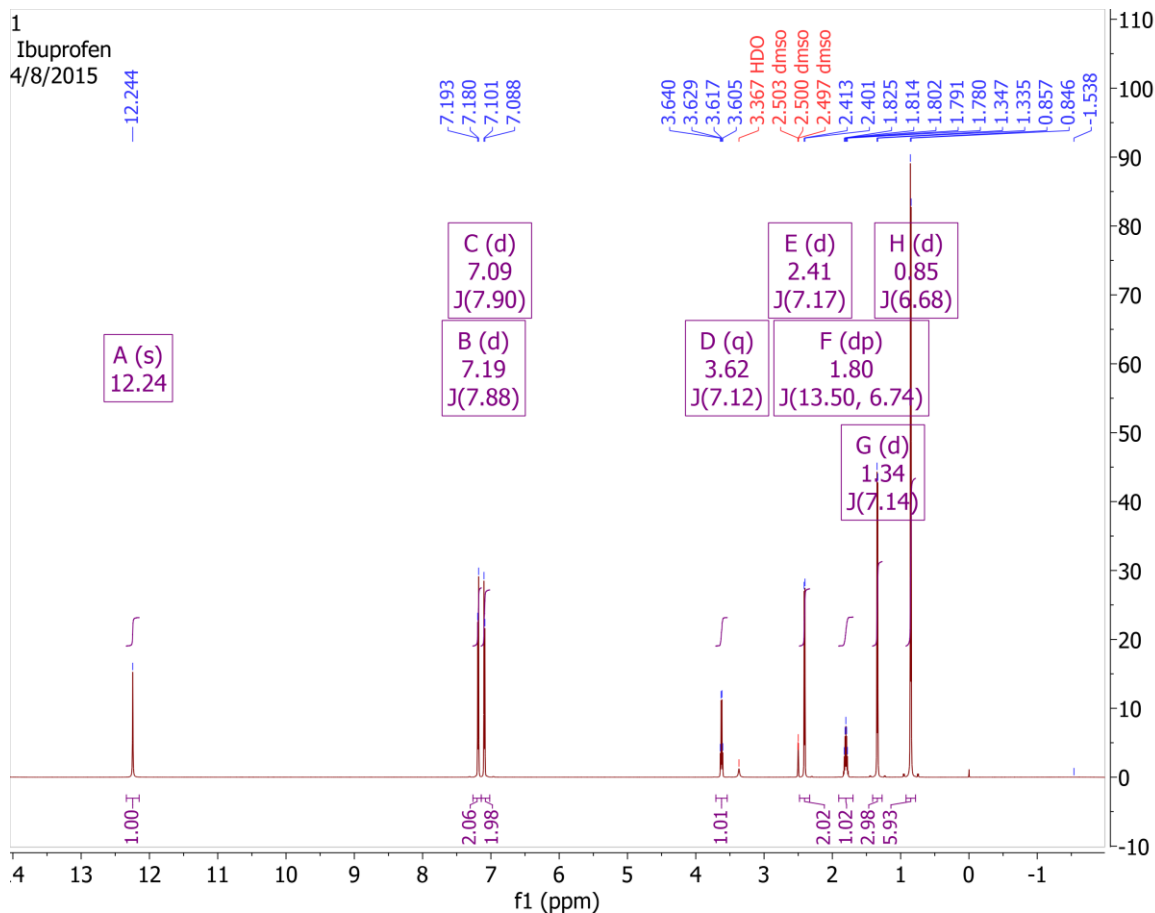
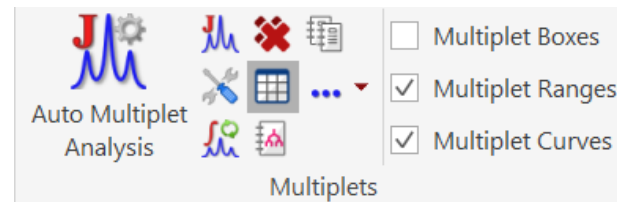
Peak picking



ANALYSIS

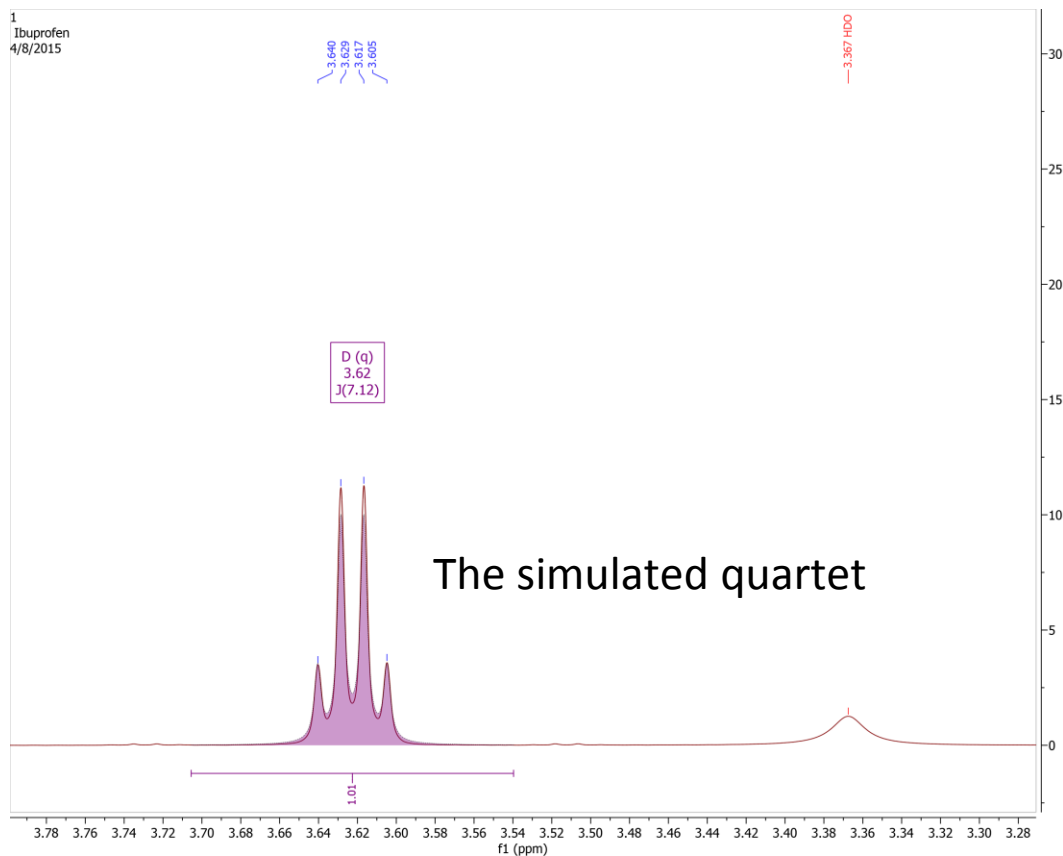
- Click the Multiplets > Options  to verify the multiplet analysis options. Default settings are used here as shown to the right.
- Click the Auto Multiplet Analysis tool to do the multiplet analysis based on the picked peaks

Multiplet analysis



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 ✕

✕

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

Name: Class:

δ: Middle

J-List: ←

Discard Peaks

Color:

Total Nuclides = 18

Nuclides:

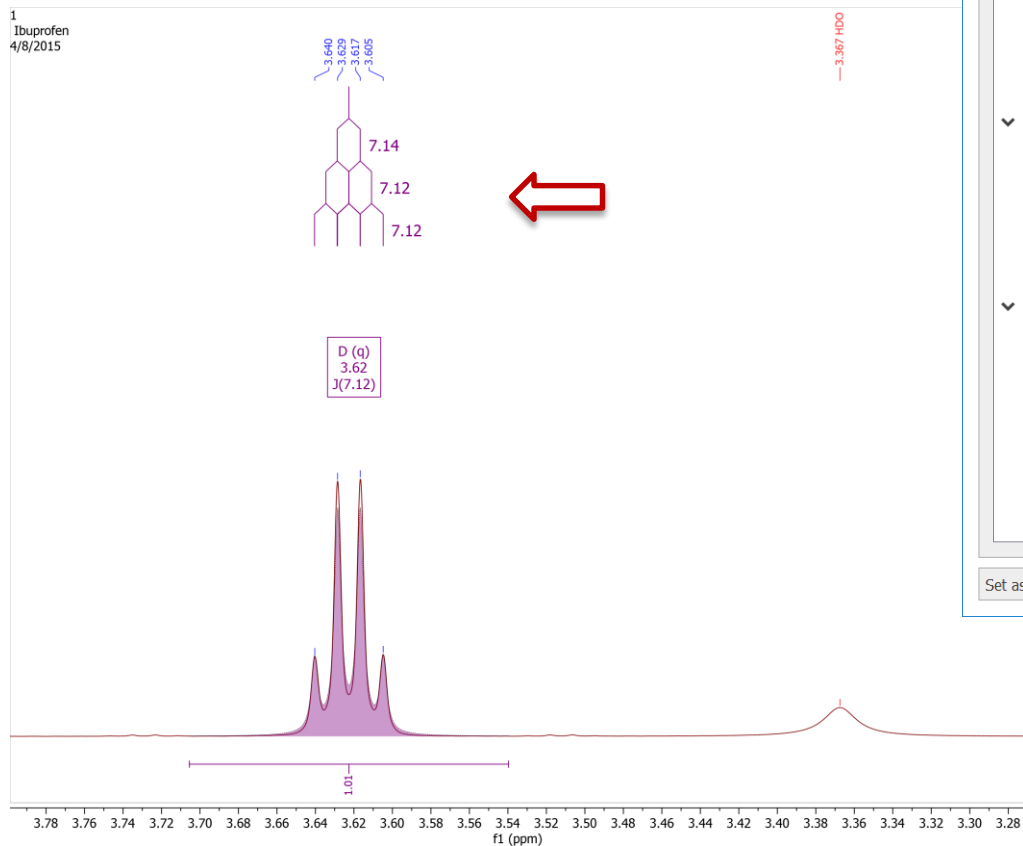
Integral:

Absolute:

From: To:

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

Properties

Metadata Geometry **NMR Spectrum**

General
Grid
1D
Scales
Horizontal
Vertical
Peaks
Integrals
Multiplets
Integrals
Fitting
Assignments
Prediction

Multiplets Labels

Font: MS Shell Dlg 2

Line Width: 2.5

Label: Name (Category) / Shift / J's

Shift Decimals: 2

Js Decimals: 2

Margin: 55 %

Follow Peak Visibility Rules Show Label Box

J's Tree

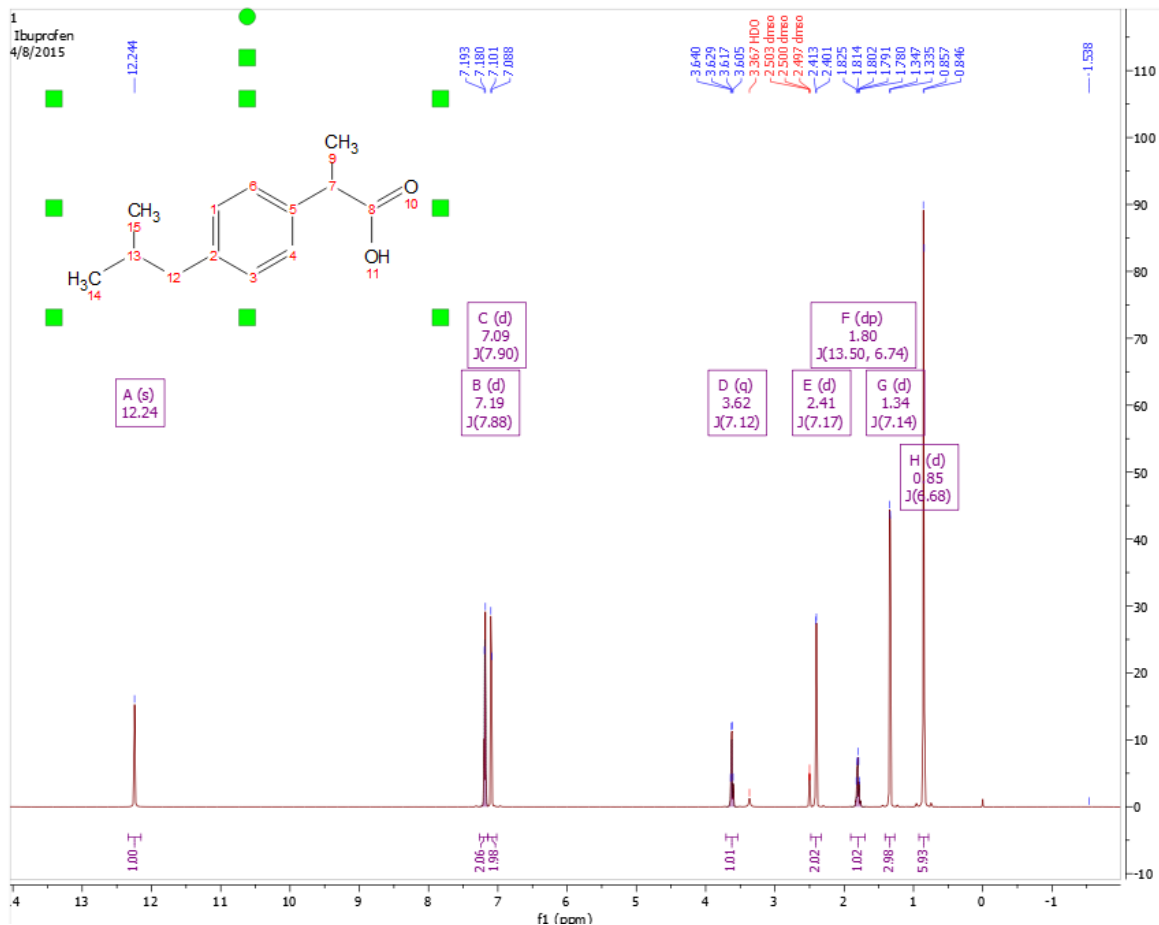
Show Label

Set as Default Restore OK Cancel Apply

Verify the number of Hs

ANALYSIS

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



Multiplet Manager

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

Name: D Class: q

δ: 3.623 ppm Middle

J-List: 7.14, 7.12, 7.12 Discard Peaks

Color: Purple

Total Nuclides = 18 (18 in molecule) ←

Nuclides: 1 Auto

Integral: 1.01

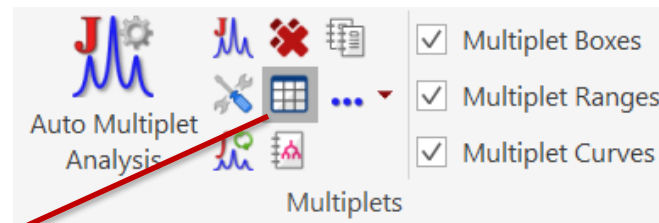
Absolute: 687.448

From: 3.705 To: 3.540

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

Report the multiplets

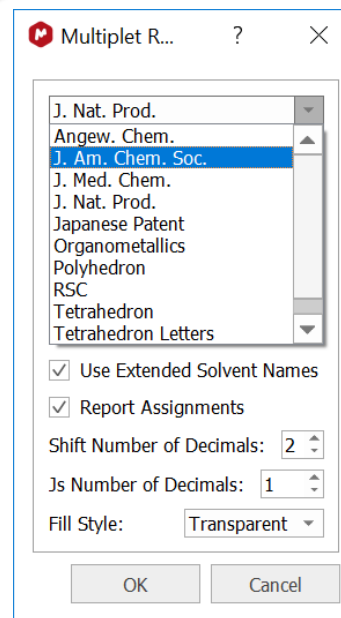


Multiplets

Report Multiplets Copy Multiplets Setup Report Delete

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)

	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	

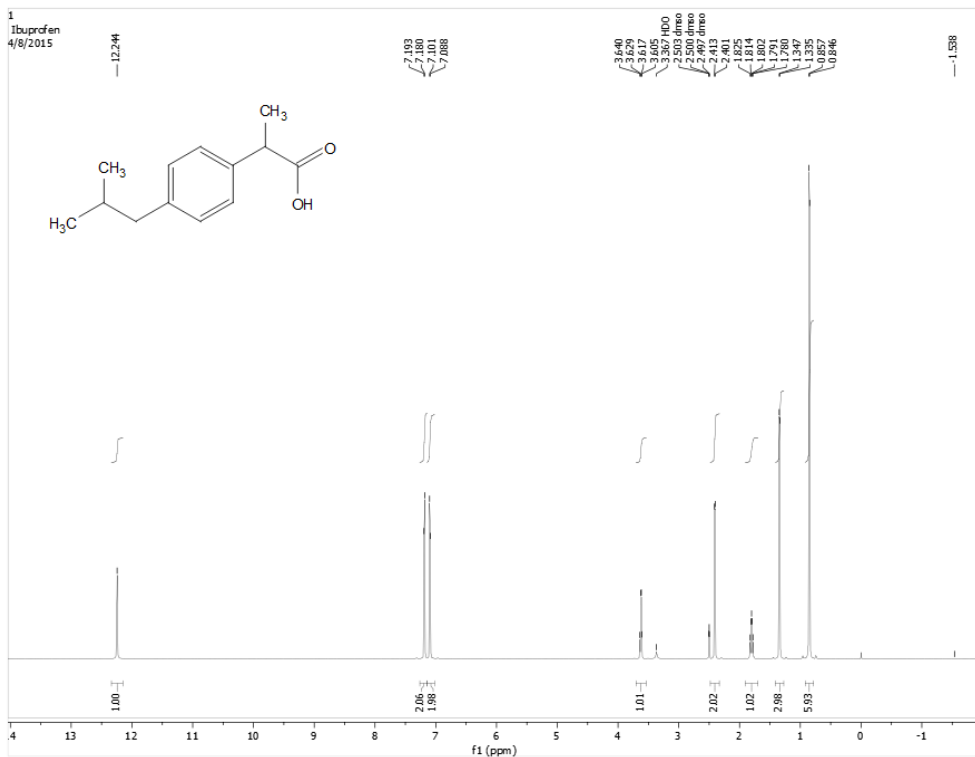


¹H NMR (DMSO-*d*₆, 600 MHz) δ 12.24 (1H, s), 7.19 (2H, d, *J*=7.9 Hz), 7.09 (2H, d, *J*=7.9 Hz), 3.62 (1H, q, *J*=7.1 Hz), 2.41 (2H, d, *J*=7.2 Hz), 1.80 (1H, dp, *J*=13.5, 6.7 Hz), 1.34 (3H, d, *J*=7.1 Hz), 0.85 (6H, d, *J*=6.7 Hz)

PUBLISHING

- 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



Properties

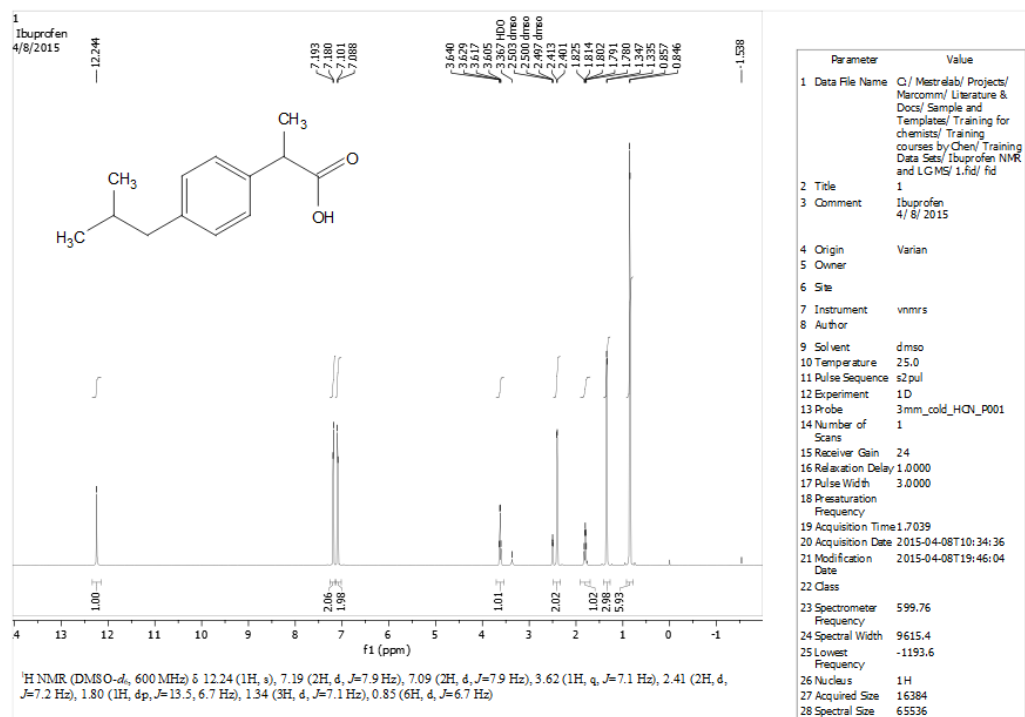
Metadata Geometry **NMR Spectrum**

General
Grid
1D
Scales
Horizontal
Vertical
Peaks
Integrals
Multiplets
Integrals
Fitting
Assignments
Prediction

Style: Line
Color: black
Line Width: 1.0

Set as Default Restore OK Cancel Apply

- 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.

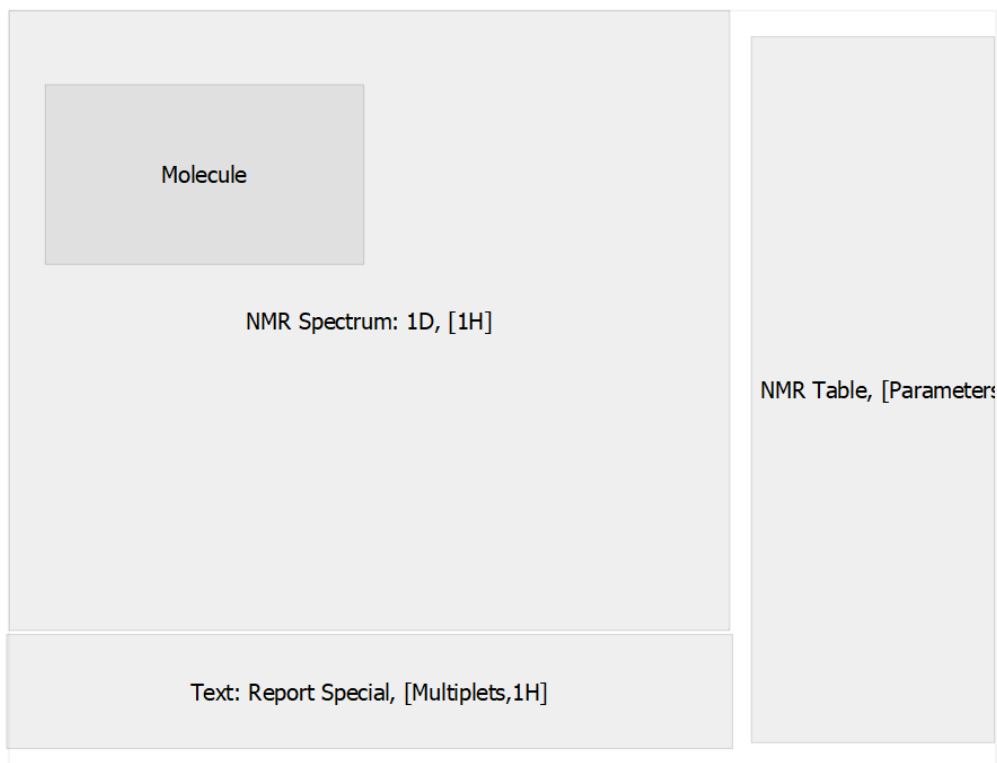


Display the parameters

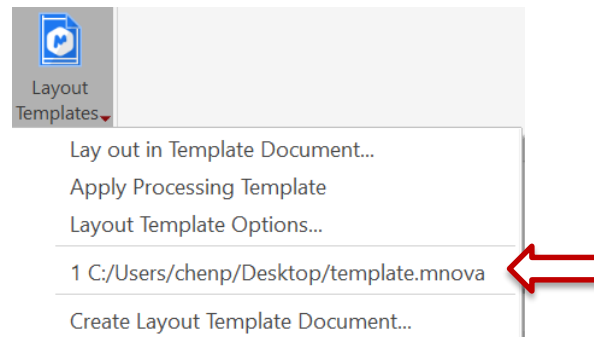
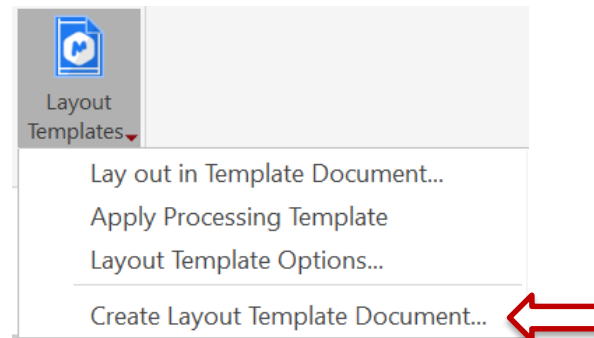
Parameters		
Parameter	Value	
1 Data File Name	C:/Mestrelab/Projects/Marcomm/Liter...	
2 Title	1	
3 Comment	Ibuprofen 4/8/2015	
4 Origin	Varian	
5 Owner		
6 Site		
7 Instrument	vnmrs	
8 Author		
9 Solvent	dms0	
10 Temperature	25.0	
11 Pulse Sequence	s2pul	
12 Experiment	1D	
13 Probe	3mm_cold_HCN_P001	
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



Open a C-13 spectrum

PROCESSING

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

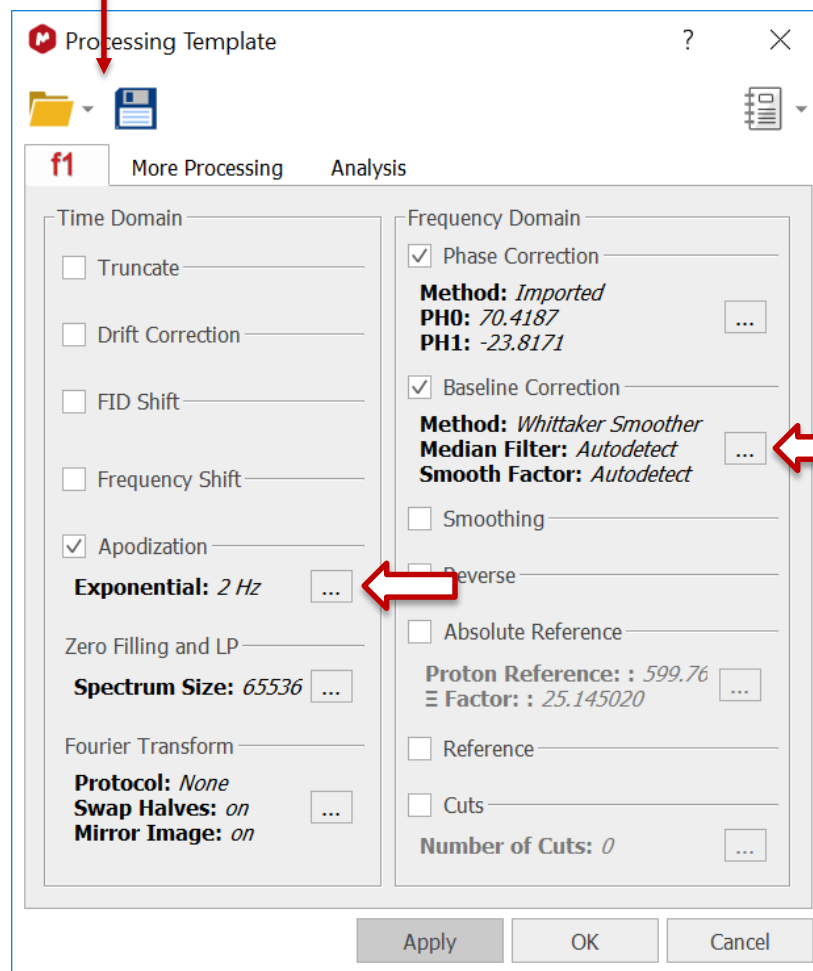
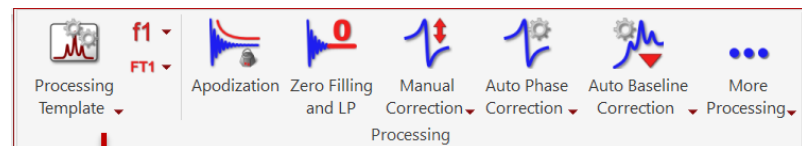
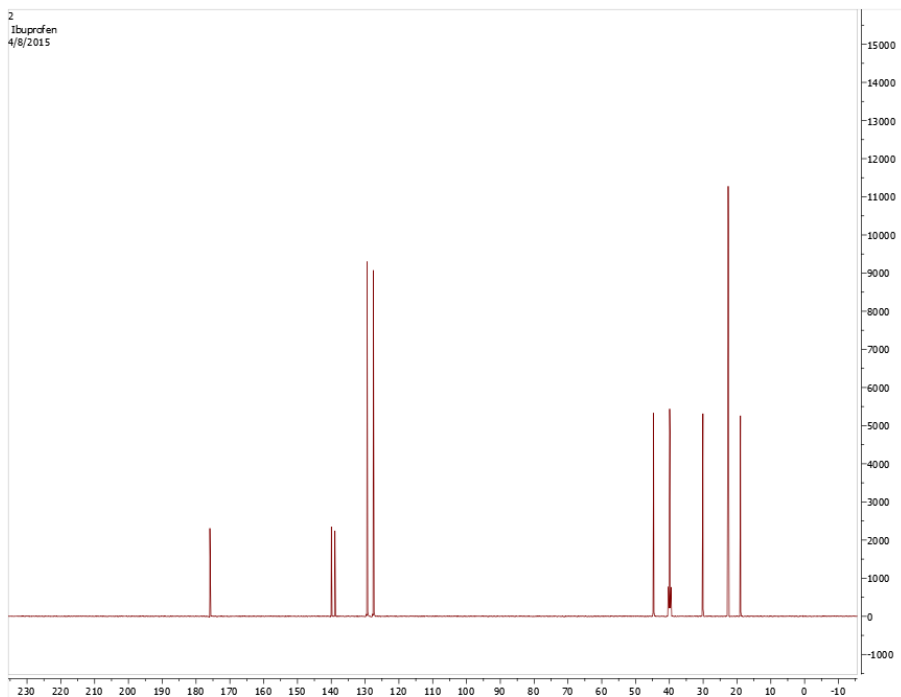
The screenshot shows the MestReNova software interface. The top menu bar includes File, Home, View, Molecule, Prediction, Tools, Database, Verification, Elucidation, Processing, Analysis, Assignments, Quantitation, and Chen's Tools. The Processing and Analysis tabs are active. The main window displays a C-13 NMR spectrum of Ibuprofen, with the x-axis labeled 'f1 (ppm)' ranging from 230 to -10. The spectrum shows several peaks, with the most prominent ones at approximately 170, 135, 130, 35, 30, and 20 ppm. The Data Browser on the right shows a tree view of files, with '2.fid' highlighted in a green box. A green arrow points from the '2.fid' file to the corresponding peak in the spectrum.

Name	Experiment	M
Training Data Sets		20
1H_phase_baseline	1D-H-zg	20
Ibuprofen NMR and LC-MS		20
1.fid	1D-H-s2pul	20
2.fid	D-C-s2pul	20
3.fid	2D-HH-COSY-gCOSY	20
4.fid	2D-CH-HSQC-EDITED...	20
5.fid	2D-CH-HMBC-gHMBC	20
6.fid	2D-HH-NOESY	20
Waters_UPLC-MS.raw		20
ibuprofen.mol		20
MS		20
Multiple 1H spectra		20
Results		20
hydrolysis - no analysis.mnova		20

PROCESSING

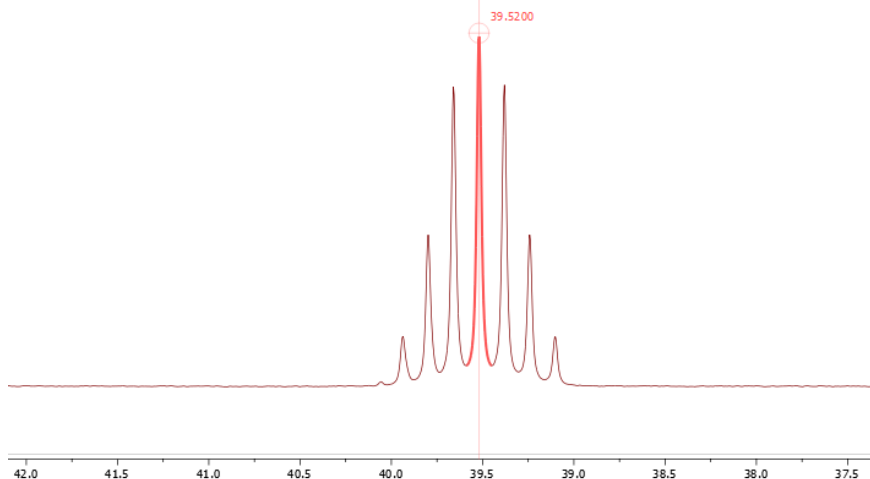
- Choose Processing > Processing Template, and set the parameters similar to the ones shown to the right.
- Click OK or Apply to re-process the spectrum.

Verify the processing parameters



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 Auto Tuning

New Shift: 39.5200 ppm 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

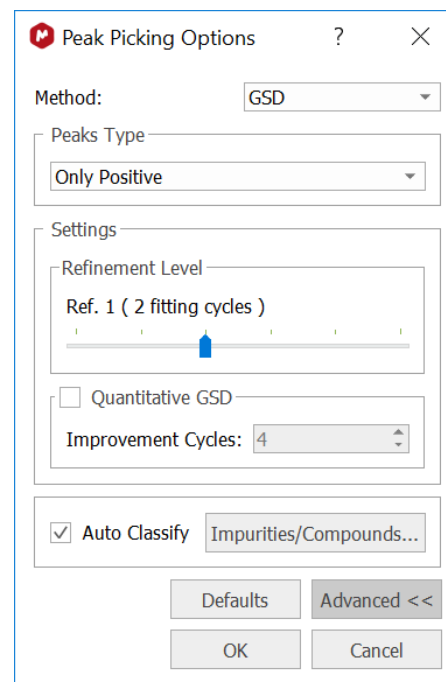
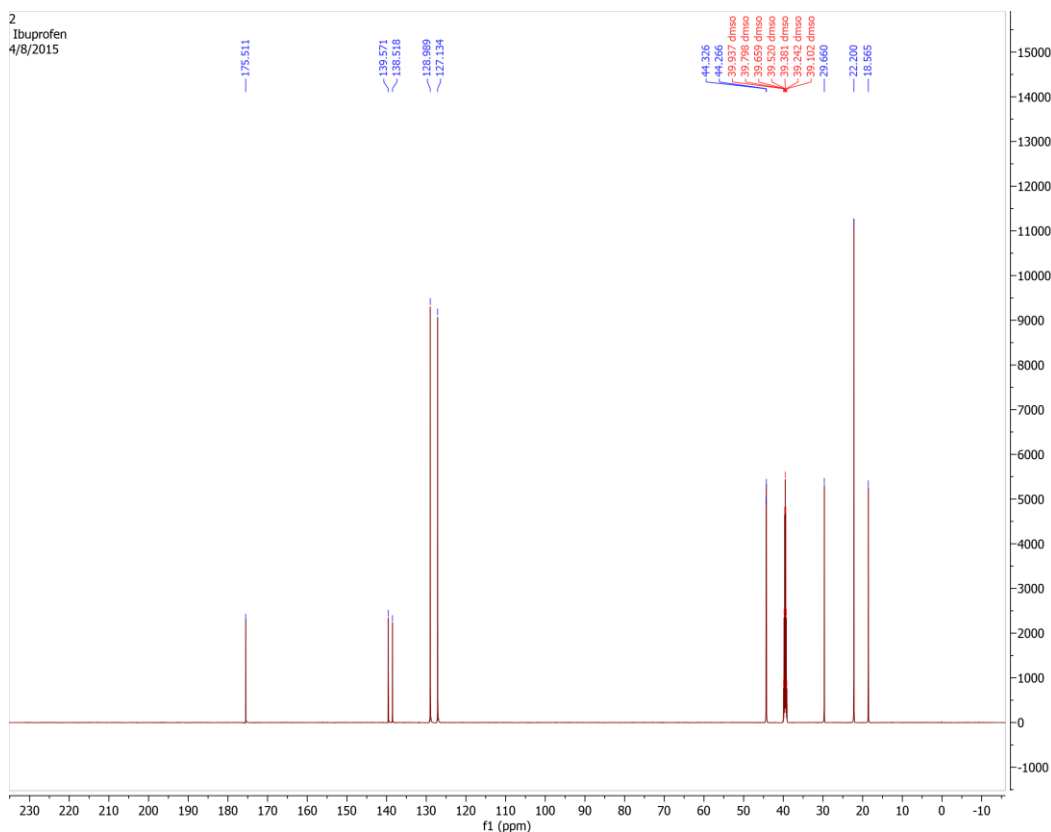
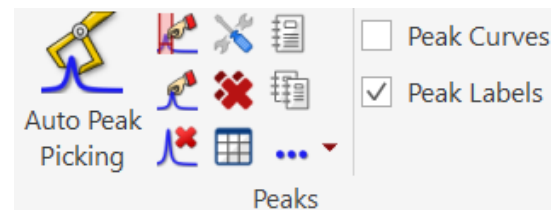
Restore Defaults Add... Edit... Delete

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.

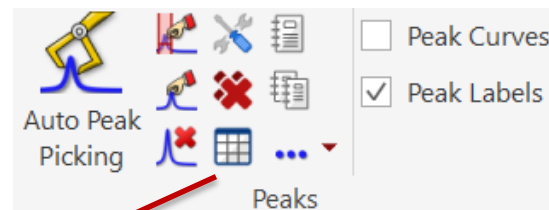
Peak picking



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

¹³C NMR (151 MHz, dmso) δ 175.5, 139.6, 138.5, 129.0, 127.1, 44.3, 44.3, 39.9, 39.8, 39.7, 39.5, 39.4, 39.2, 39.1, 29.7, 22.2, 18.6.

	ppm	intensity	Width	Area	Type	Flags	ty/Corr	inotati
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		

Setup Peak R... ?

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

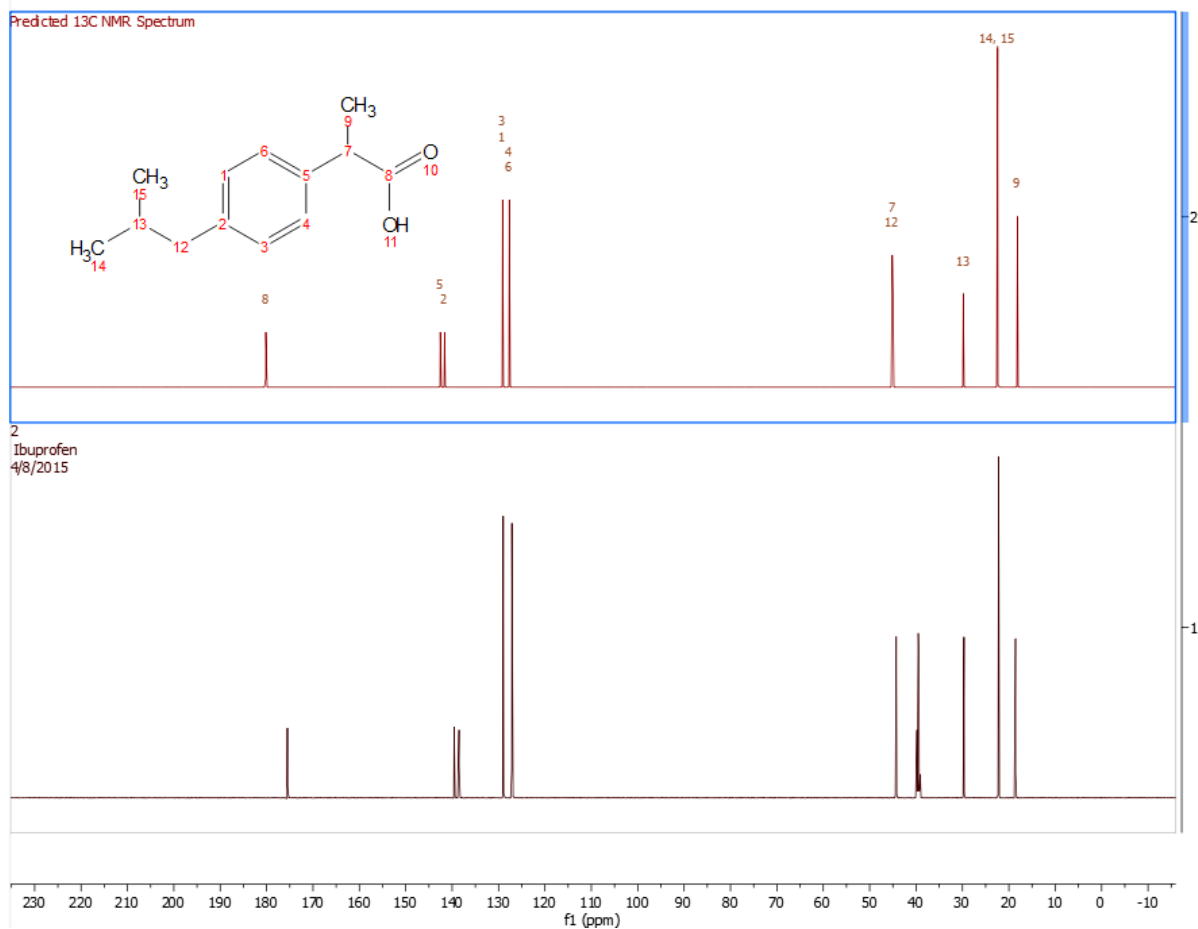
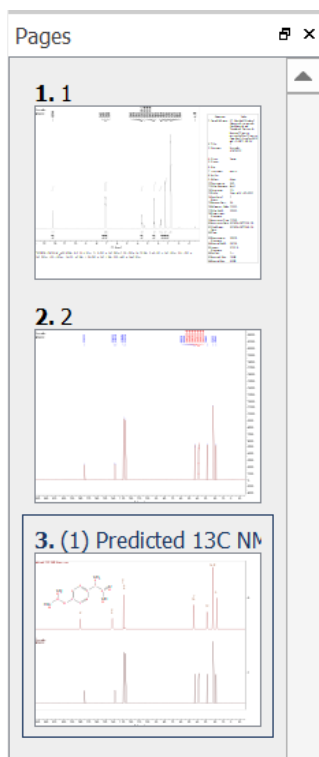
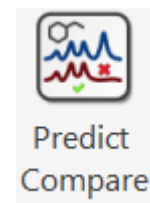
OK Cancel

¹³C NMR (151 MHz, DMSO-d₆) δ 175.5, 139.6, 138.5, 129.0, 127.1, 44.3, 44.3, 29.7, 22.2, 18.6.

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.



Open the LC-MS data

LC-MS

- In Data Browser, open the LC-MS data Ibuprofen (low resolution data acquired on Waters).

H-1
C-13
MS

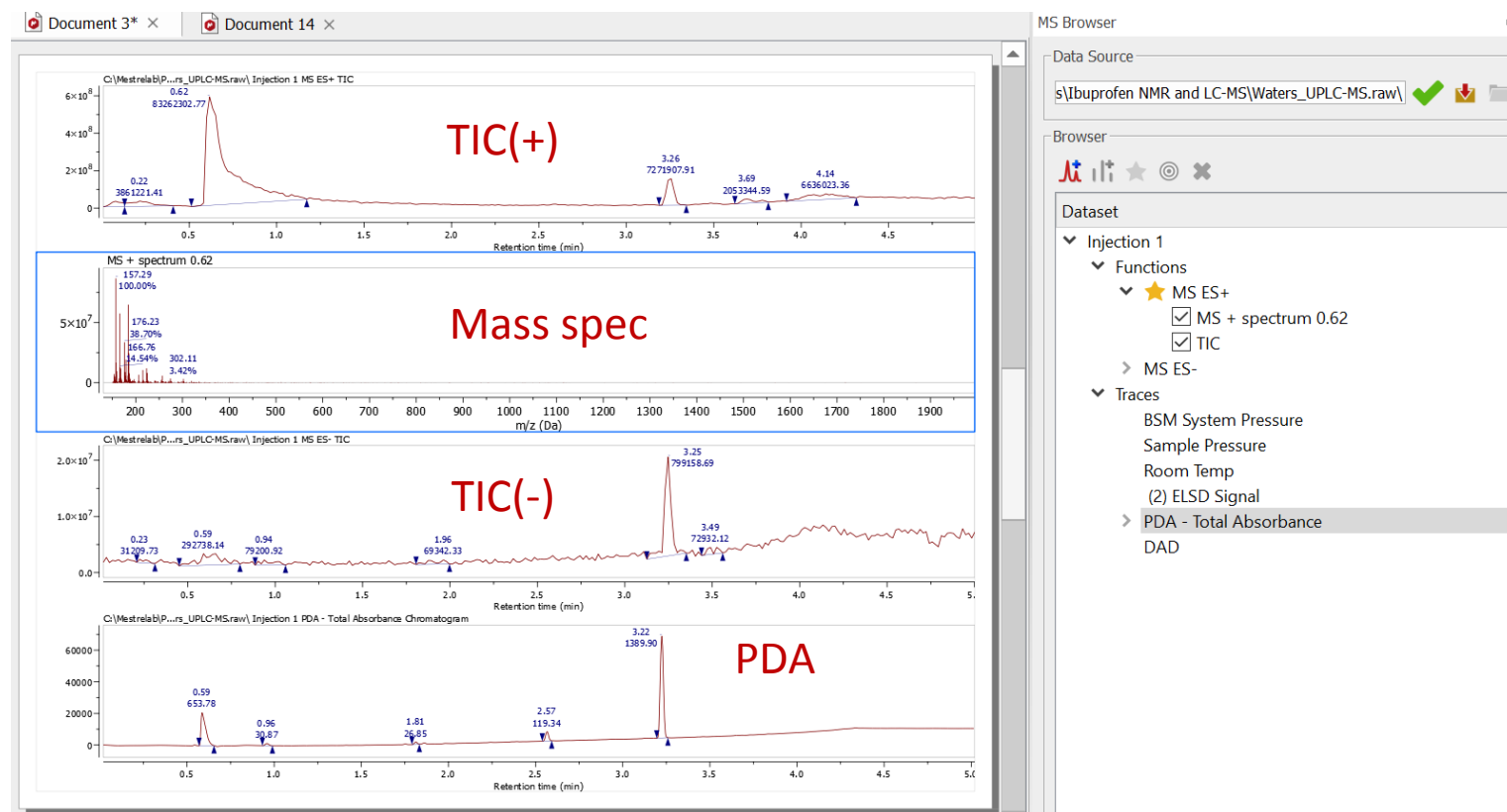
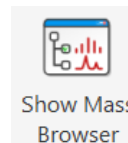
The screenshot shows the MestReNova software interface. The top menu bar includes File, Home, View, Molecule, Prediction, Tools, Database, Verification, Elucidation, Analysis, MASS, MestReNova, Quantitation, and Chen's Tools. The main workspace is divided into several panels:

- Pages:** Document 3* and Document 14.
- Full View:** Contains three sub-panels:
 - 1.1: A small chromatogram plot.
 - 2.2: A small mass spectrum plot.
 - 3. C:\Mestrelab\P...rs_t: A larger mass spectrum plot.
- Main Plot:** A large Total Ion Chromatogram (TIC) showing a major peak at 0.62 minutes. Below it is a mass spectrum for the peak at 0.62 minutes, showing a base peak at m/z 184.19 (74.78%) and other significant peaks at 176.23, 185.11, 166.76, and 274.14.
- Data Browser:** A file tree on the right side of the interface. The file 'Waters_UPLC-MS.raw' is highlighted with a green box. A green arrow points from this file to the mass spectrum plot in the main workspace.

At the bottom of the interface, there are buttons for 'Multiplet Manager', 'Multiplets', 'Data Browser', and 'Compounds'. The status bar at the very bottom indicates 'Licenses: DB:'. On the far right, there is a vertical toolbar with various icons for data manipulation and visualization.

VISUALIZATION

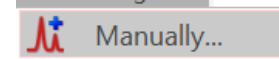
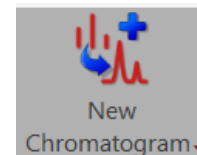
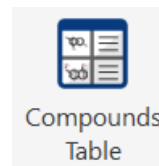
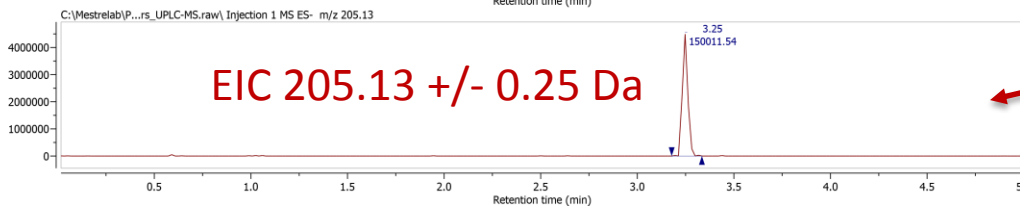
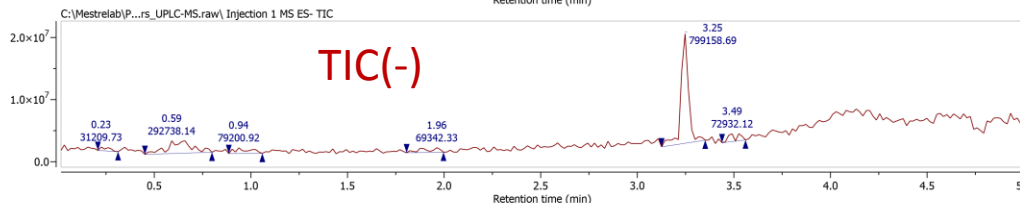
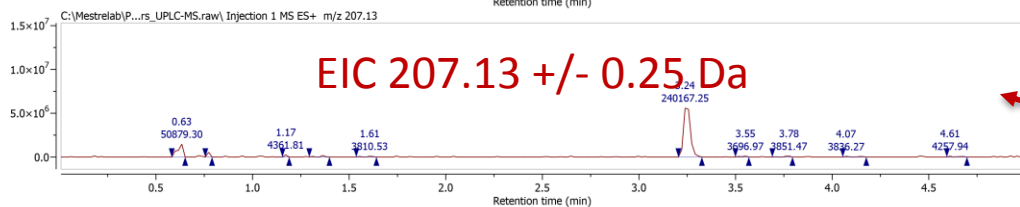
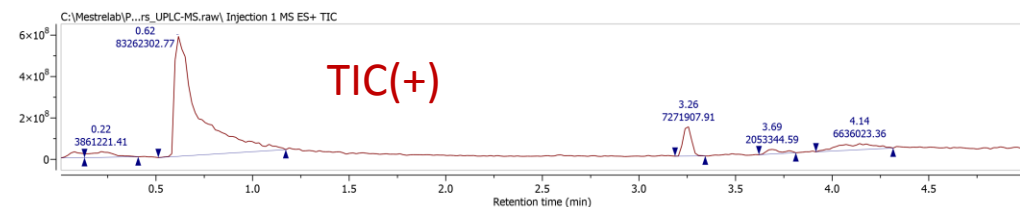
- Choose MASS Analysis > Show Mass Browser to display the Mass Browser.
- Open the negative polarization TIC
- Open the PDA Total Absorbance Chromatogram



Verify the structure

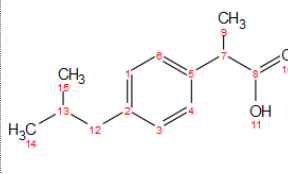
ANALYSIS

- 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

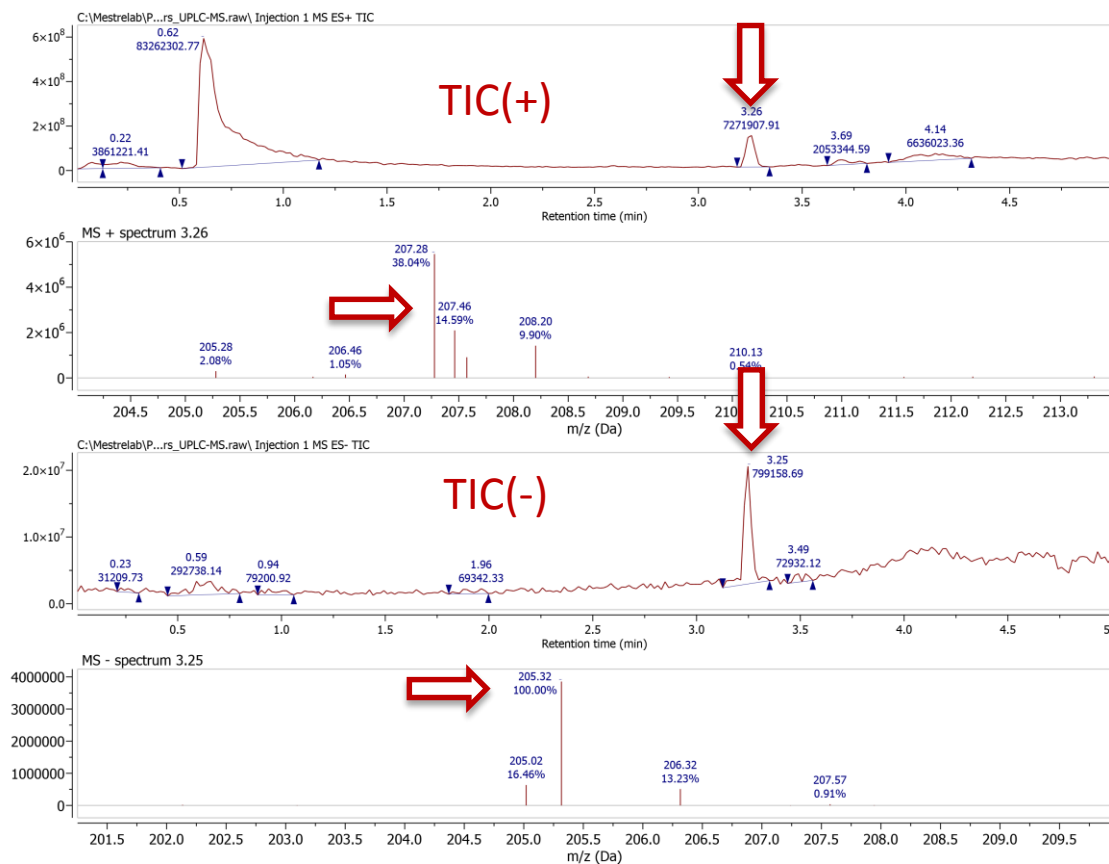
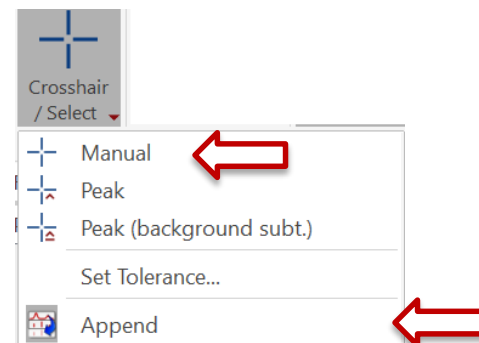
Tolerance: 0.250 Da

OK Cancel

Find the molecule ion peaks

ANALYSIS

- 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.

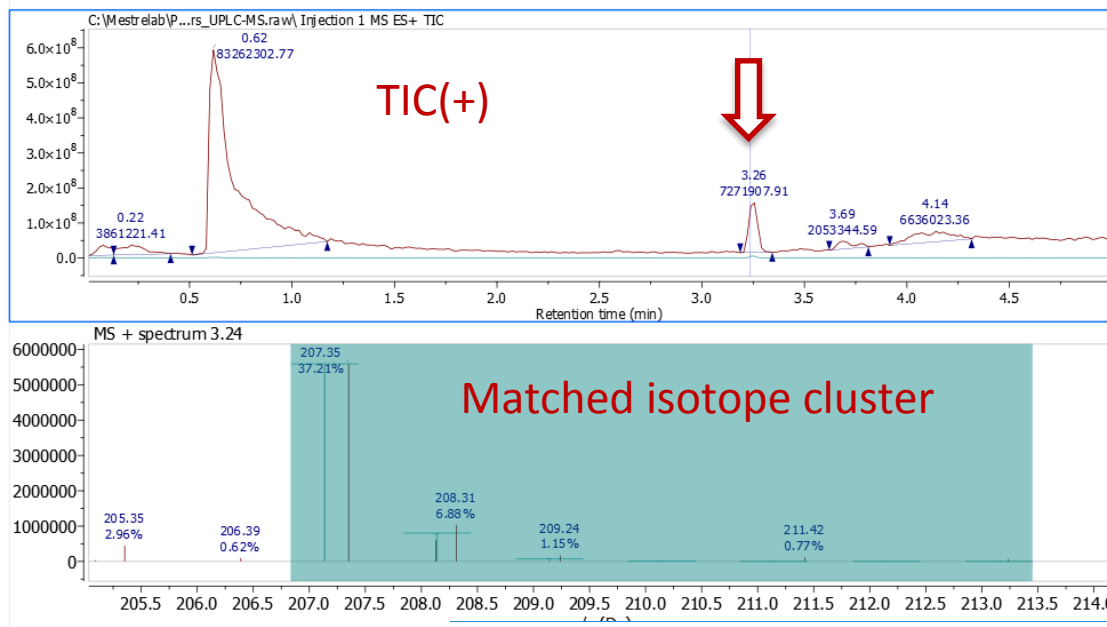
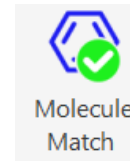


Tip: Use the Mass Browser to hide or delete unwanted plots. Right-click on a plot and choose Move up/Move Down etc. to re-order of the plots

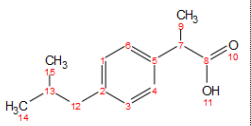
Use Mol Match to verify the elemental composition

ANALYSIS

- 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



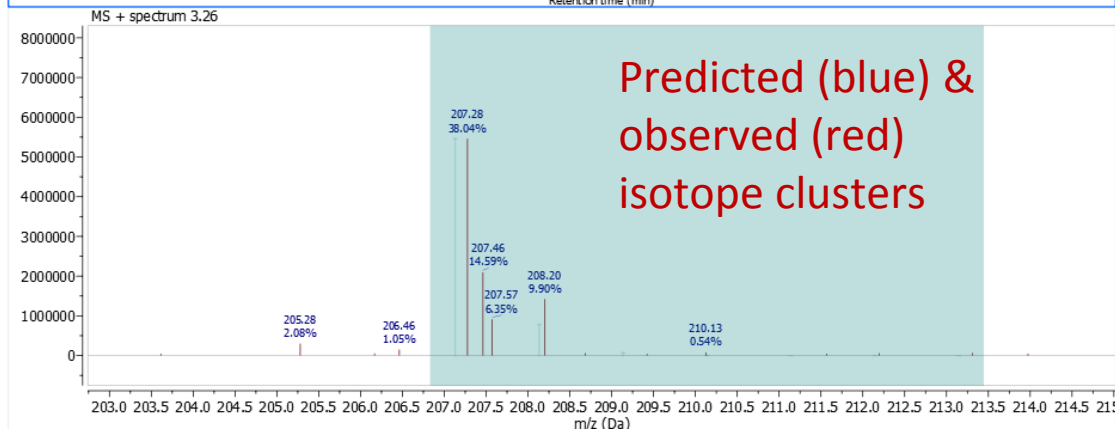
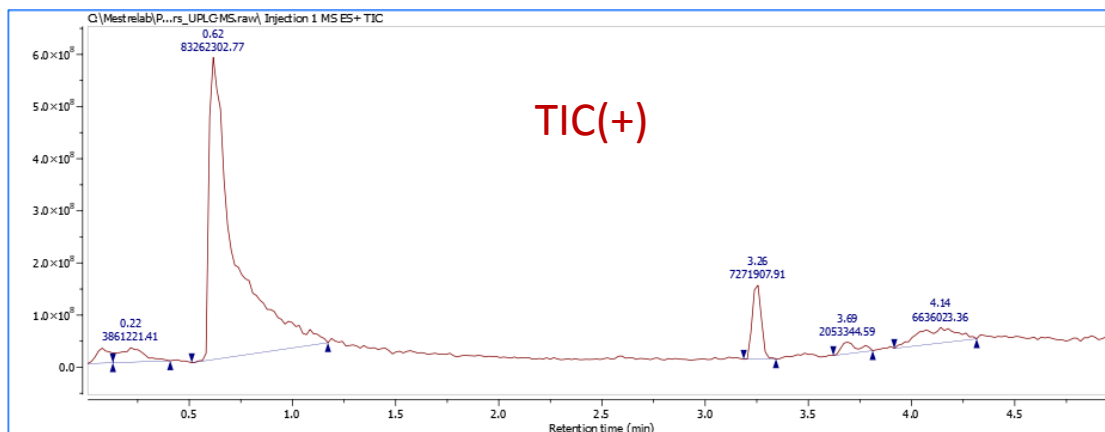
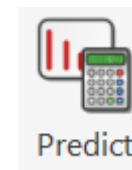
Molecule Match

Report	Molecule Match	View	Settings	Setup	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+ / -	

Predict and verify the molecule ion peaks

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.



Molecular Formula ? X

Molecular Formula:

Recent

- C₁₃H₁₈O₂
- C₂₇H₃₃NO₂Cl
- C₁₉H₃₈N₂O₂

Compounds

	Formula	Weight
1	C ₁₃ H ₁₈ O ₂	206.1307

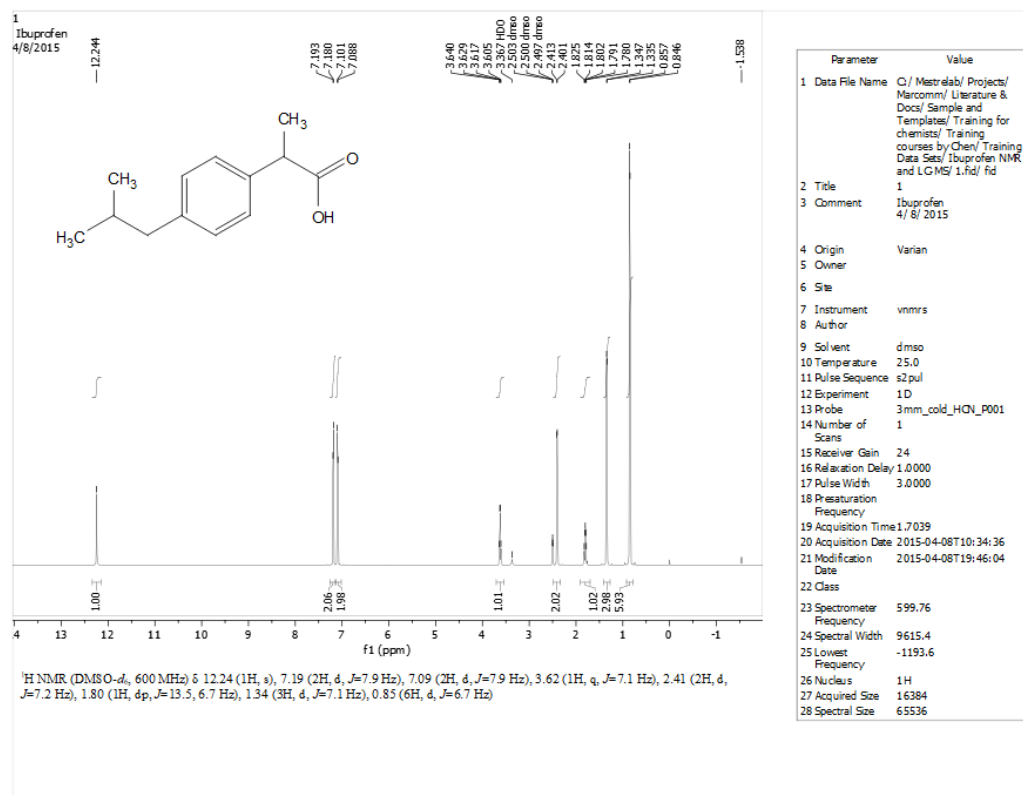
Mass Prediction X

Report Copy Highlight Export Delete Clear Setup

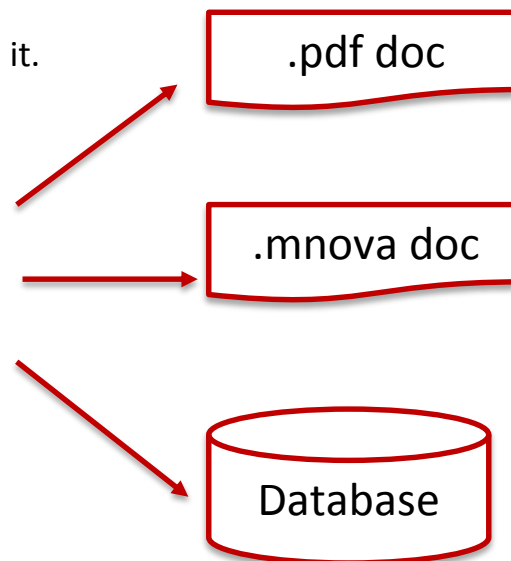
	Formula	Adduct / Loss	rgc SI	m/z	Status
1	C ₁₃ H ₁₈ O ₂	H ⁺ / —	+1	207.13796	✓
2	C ₁₃ H ₁₈ O ₂	Na ⁺ / —	+1	229.11990	✓
3	C ₁₃ H ₁₈ O ₂	K ⁺ / —	+1	245.09384	✓
4	C ₁₃ H ₁₈ O ₂	CH ₃ OHH ⁺ / —	+1	239.16417	✓
5	C ₁₃ H ₁₈ O ₂	NH ₄ ⁺ / —	+1	224.16451	✓
6	C ₁₃ H ₁₈ O ₂	— / H ⁺	-1	205.12340	✓
7	C ₁₃ H ₁₈ O ₂	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	✓

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



Save the results



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 menu is visible with various options. A red arrow points to the 'Help' option in this menu. The main window shows the 'Help' section with a 'MestReNova Manual' browser window open. The manual's table of contents is visible, with 'Using GSD for multiplets analysis' highlighted. To the right, a red banner reads 'Using GSD for multiplets analysis' and the text below explains that Mnova uses Global Spectral Deconvolution (GSD) for peak picking and multiplet analysis. Below the text, a graph shows a peak with a red line and a label '-3.46'.

Help

- Help: Get help using Mnova
- License Manager: Get licenses information like...
- Request Licenses: Buy or request evaluation lice...
- Check for Updates: Check if you are using the late...

MestReNova Manual

Contents Index Search Favorites

- Introduction
 - Installation Guide
 - Mnova 12
 - Fast Visual Guide to process rou...
 - Fast Visual Guide to process rou...
- The Mnova interface
 - Graphics and Annotations
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- Analysis Tools
 - Chemical Shift Referencing
 - Peak Picking
 - Integration
- Multiplets analysis
 - Multiplet Manager
 - Using GSD for multiplets an...
 - Setting multiplets
 - How to resolve overlapped
 - Multiplets Table and Report
 - Multiplet Analysis options
 - Multiplets Properties

Using GSD for multiplets analysis

Exploiting the power of GSD for an improved Multipl...

By default Mnova uses Global Spectral Deconvolution (GS...
picking and multiplet analysis.

Multiplet Analysis benefit directly from the exploitation of G...
automatic analysis, with the enhanced peak picking capabilitie...
automatic multiplicity identification and labeling.

Here you can see an example of a triplet which is hidden unde...

PHOTON
extended

-3.51 -3.48 -3.46 -3.43

-3.46

3.49 3.49

N



Mestrelab Research

chemistry software solutions

Mnova Training - Advanced

Version 12.0.3

Oct. 23, 2018

Chen Peng, PhD,

VP of Business Development, North America & Asia

Mestrelab Research SL

chen.peng@mestrelab.com

858.736.4563

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



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>.

Open a 1D and 2D spectra of Ibuprofen

PROCESSING

- 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.

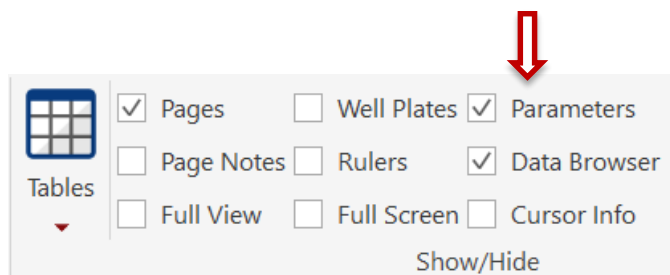
The screenshot shows the MestReNova software interface. The main window displays a 2D HSQC NMR spectrum of Ibuprofen, with the title '6 Ibuprofen 4/8/2015'. The x-axis is labeled 'f2 (ppm)' and ranges from 14 to -1. The y-axis is labeled 'f1 (ppm)' and ranges from -2 to -14. The Data Browser on the right shows a list of files, with a green box highlighting the 1D and 2D spectra files (1.fid to 6.fid) and a green arrow pointing to the main spectrum window.

Name	Experiment
1.fid	1D-H-s2pul
2.fid	1D-C-s2pul
3.fid	2D-HH-COSY-gCOSY
4.fid	2D-CH-HSQC-EDITED-...
5.fid	2D-CH-HMBC-gHMBC
6.fid	2D-HH-NOESY

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



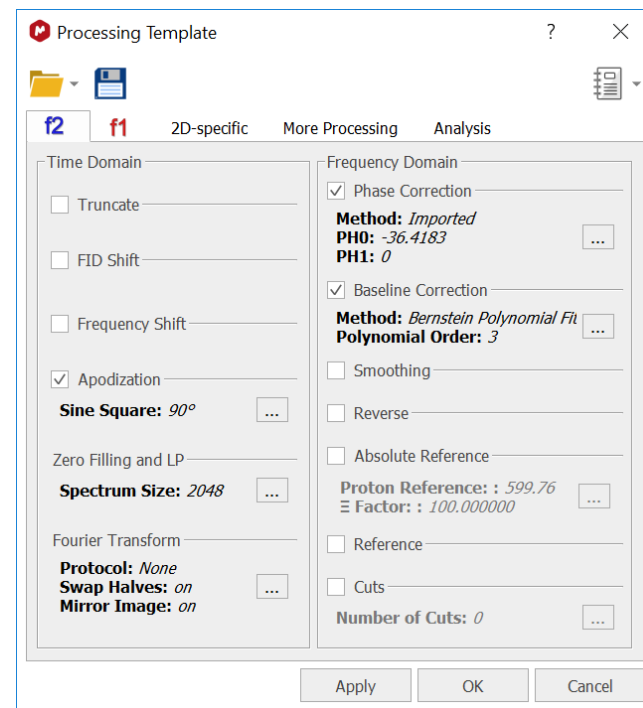
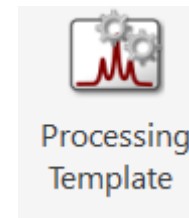
The image shows a 'Parameters' dialog box with a table of parameters. The 'Pulse Sequence' and 'Experiment' rows are highlighted with a red box.

	Parameter	Value
7	Instrument	nmrs
8	Author	
9	Solvent	dms
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

- Apodization: To improve the line shape, resolution and S/N ratio
 - COSY: Use Sine Square 0 for F2 & F1
 - Others: Use Sine 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.



PROCESSING

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

Re-process HSQC spectrum



Processing
Template

Processing Template

f2 f1 2D-specific More Processing Analysis

Time Domain

Truncate

FID Shift

Frequency Shift

Apodization
Sine Square: 90°

Zero Filling and LP
Spectrum Size: 2048

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

Frequency Domain

Phase Correction
Method: Imported
PH0: -36.4183
PH1: 0

Baseline Correction
Method: Bernstein Polynomial Fit
Polynomial Order: 3

Smoothing

Reverse

Absolute Reference
Proton Reference: : 599.76
Factor: : 100.000000

Reference

Cuts
Number of Cuts: 0

Apply OK Cancel

Processing Template

f2 f1 2D-specific More Processing Analysis

Time Domain

Truncate

Frequency Shift

Apodization
Sine Square: 90°

Zero Filling and LP
Spectrum Size: 1024
Forward LP: [128, 256], 112, 15

Fourier Transform
Protocol: Echo-Antiecho
Swap Halves: on
Mirror Image: on

Frequency Domain

Phase Correction
Method: Imported
PH0: 0
PH1: 0

Baseline Correction
Method: Bernstein Polynomial Fit
Polynomial Order: 3

Smoothing

Reverse

Absolute Reference
Proton Reference: : 599.76
Factor: : 25.145020

Reference

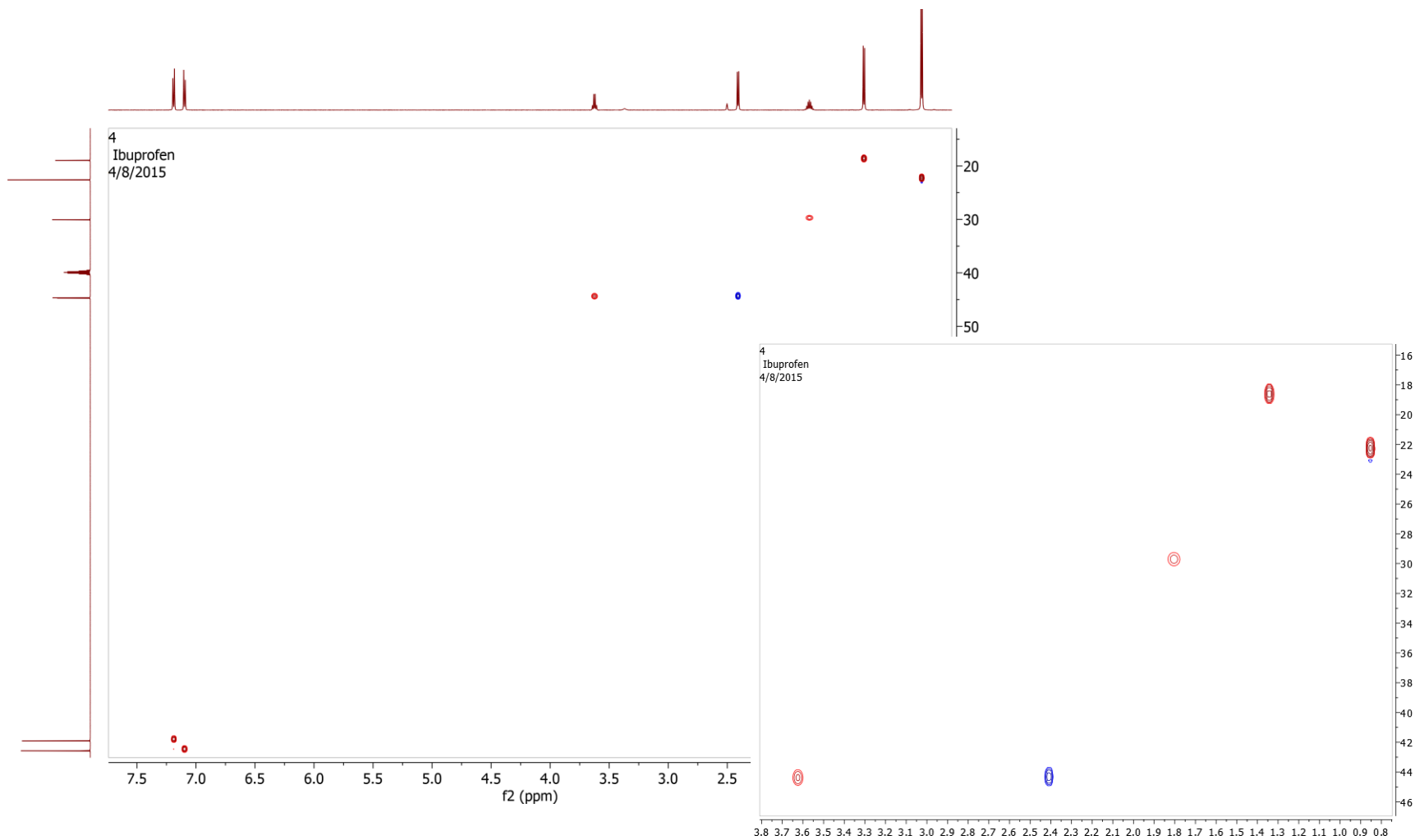
Cuts
Number of Cuts: 0

Apply OK Cancel

PROCESSING

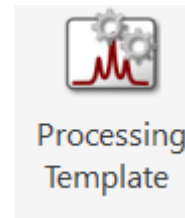
Re-process HSQC spectrum

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



PROCESSING

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

Processing Template

f2 f1 2D-specific More Processing Analysis

Time Domain

Truncate

FID Shift

Frequency Shift

Apodization
Sine Square: 90°

Zero Filling and LP
Spectrum Size: 2048

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

Frequency Domain

Phase Correction
Method: Magnitude

Baseline Correction
Method: Bernstein Polynomial Fit
Polynomial Order: 3

Smoothing

Reverse

Absolute Reference
Proton Reference: : 599.76
Factor: : 100.000000

Reference

Cuts
Number of Cuts: 0

Apply OK Cancel

Processing Template

f2 f1 2D-specific More Processing Analysis

Time Domain

Truncate

Frequency Shift

Apodization
Sine Square: 90°

Zero Filling and LP
Spectrum Size: 1024
Forward LP: [128, 256], 112, 15

Fourier Transform
Protocol: Echo-Antiecho
Swap Halves: on
Mirror Image: on

Frequency Domain

Phase Correction
Method: Imported
PH0: 0
PH1: 0

Baseline Correction
Method: Bernstein Polynomial Fit
Polynomial Order: 3

Smoothing

Reverse

Absolute Reference
Proton Reference: : 599.76
Factor: : 25.145020

Reference

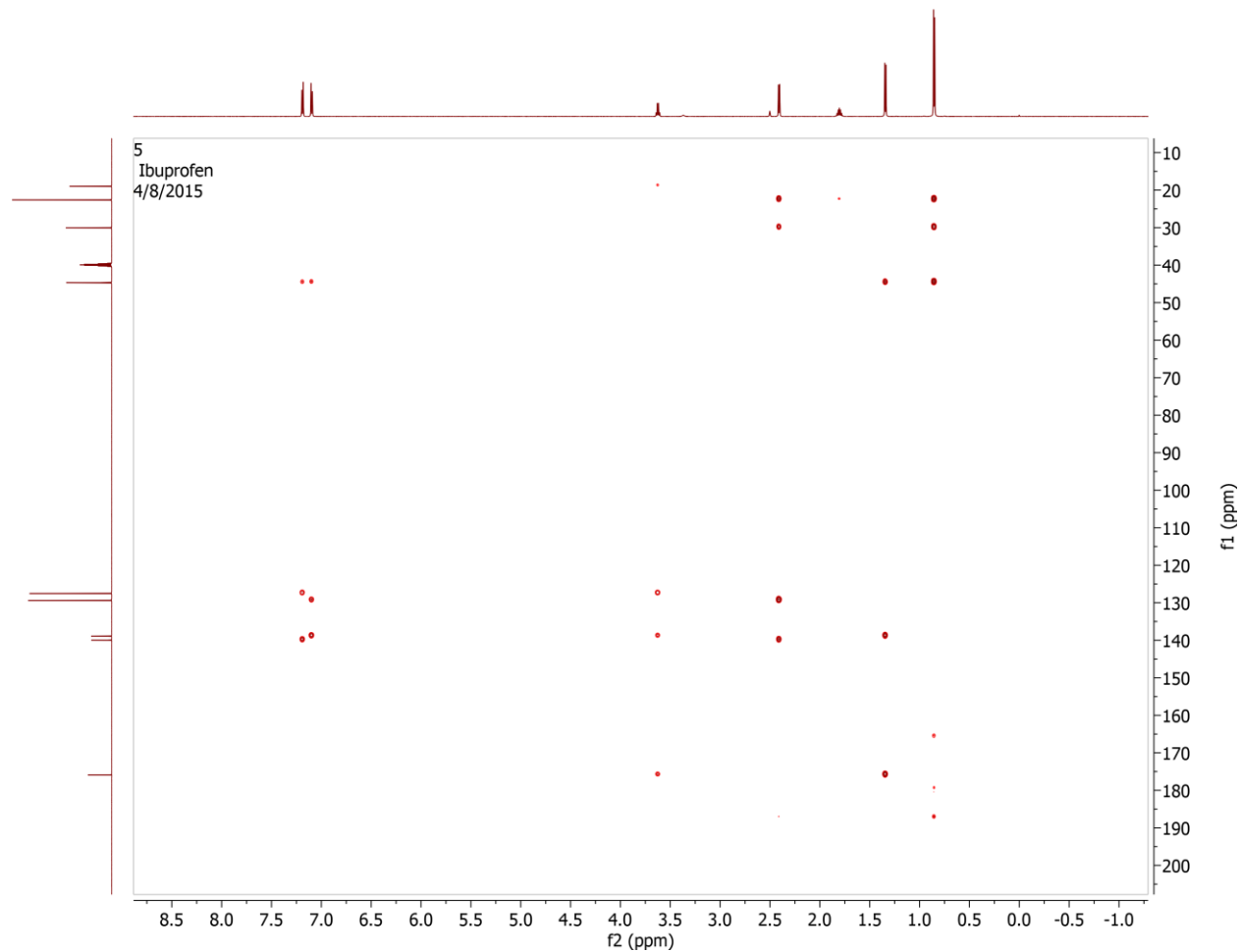
Cuts
Number of Cuts: 0

Apply OK Cancel

Re-process HMBC spectrum

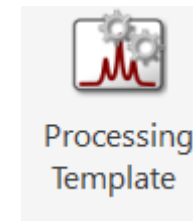
PROCESSING

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



PROCESSING

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

Processing Template

f2 f1 2D-specific More Processing Analysis

Time Domain

Truncate

FID Shift

Frequency Shift

Apodization

Sine Square: 0°

Zero Filling and LP

Spectrum Size: 2048

Fourier Transform

Protocol: None

Swap Halves: on

Mirror Image: on

Frequency Domain

Phase Correction

Method: Magnitude

Baseline Correction

Method: Bernstein Polynomial Fit

Polynomial Order: 3

Smoothing

Reverse

Absolute Reference

Proton Reference: : 599.76

Factor: : 100.000000

Reference

Cuts

Number of Cuts: 0

Apply OK Cancel

Processing Template

f2 f1 2D-specific More Processing Analysis

Time Domain

Truncate

Frequency Shift

Apodization

Sine Square: 0°

Zero Filling and LP

Spectrum Size: 2048

Forward LP: [128, 256], 112, 15

Fourier Transform

Protocol: None

Swap Halves: on

Mirror Image: on

Frequency Domain

Phase Correction

Baseline Correction

Method: Bernstein Polynomial Fit

Polynomial Order: 3

Smoothing

Reverse

Absolute Reference

Proton Reference: : 599.76

Factor: : 100.000000

Reference

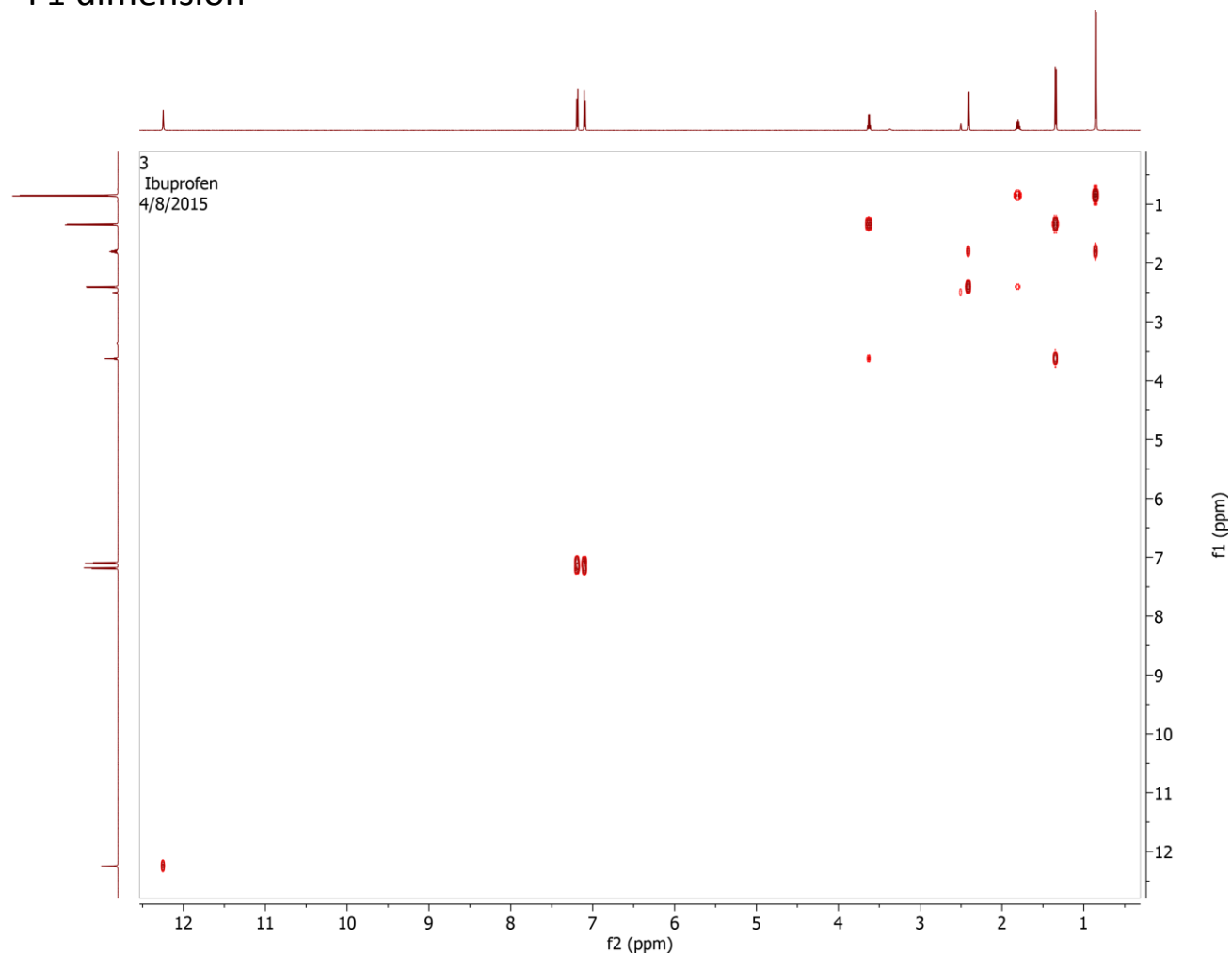
Cuts

Number of Cuts: 0

Apply OK Cancel

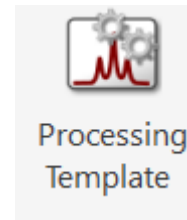
Re-process COSY spectrum

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



PROCESSING

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

Processing Template

f2 f1 2D-specific More Processing Analysis

Time Domain

Truncate

FID Shift

Frequency Shift

Apodization
Sine Square: 90°

Zero Filling and LP
Spectrum Size: 2048

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

Frequency Domain

Phase Correction
Method: Magnitude

Baseline Correction
Method: Bernstein Polynomial Fit
Polynomial Order: 3

Smoothing

Reverse

Absolute Reference
Proton Reference: : 599.76
Factor: : 100.000000

Reference

Cuts
Number of Cuts: 0

Apply OK Cancel

Processing Template

f2 f1 2D-specific More Processing Analysis

Time Domain

Truncate

Frequency Shift

Apodization
Sine Square: 90°

Zero Filling and LP
Spectrum Size: 1024
Forward LP: [128, 256], 112, 15

Fourier Transform
Protocol: Echo-Antiecho
Swap Halves: on
Mirror Image: on

Frequency Domain

Phase Correction
Method: Imported
PH0: 0
PH1: 0

Baseline Correction
Method: Bernstein Polynomial Fit
Polynomial Order: 3

Smoothing

Reverse

Absolute Reference
Proton Reference: : 599.76
Factor: : 25.145020

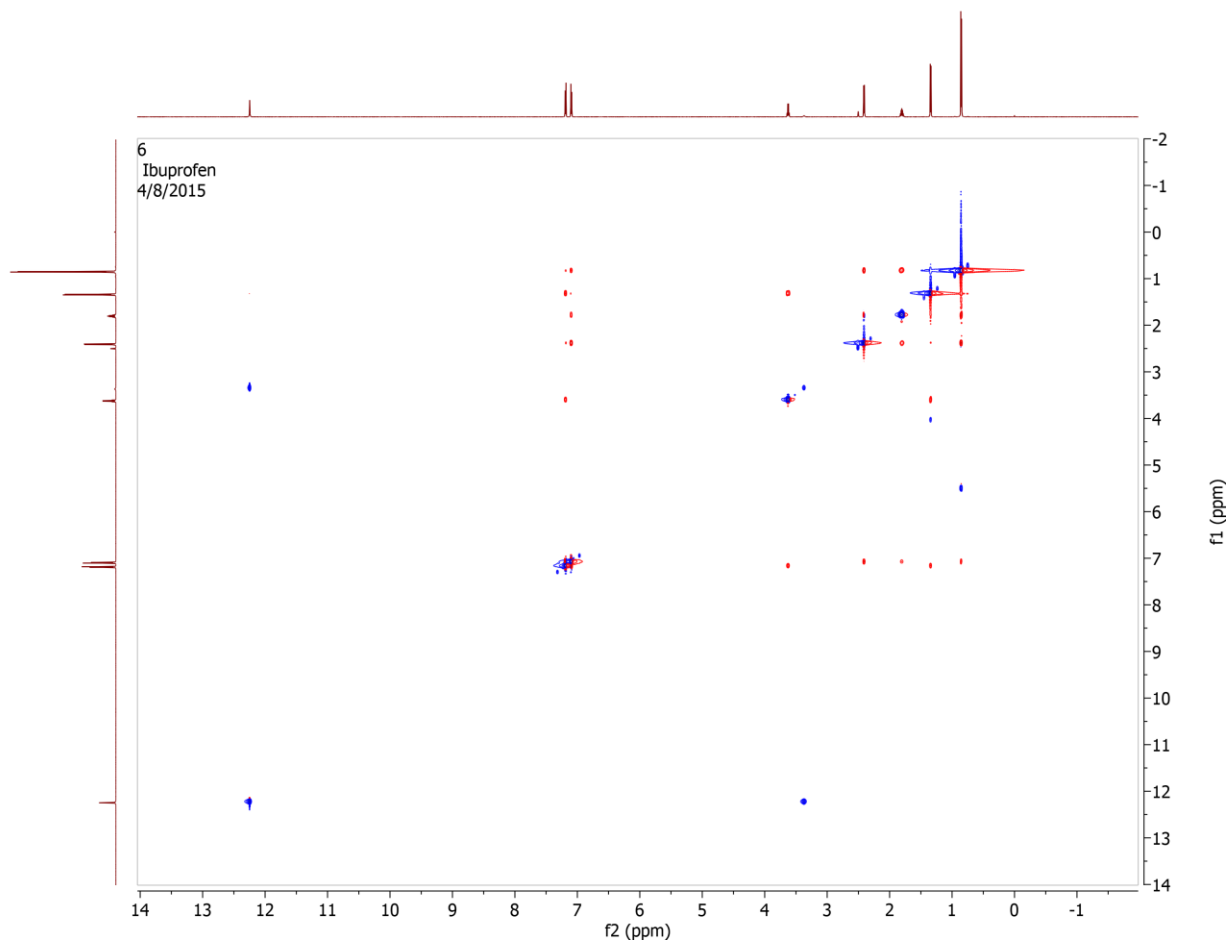
Reference

Cuts
Number of Cuts: 0

Apply OK Cancel

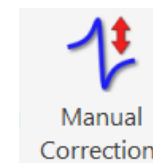
Re-process NOESY spectrum

- 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



Phase Correction

f1 f2

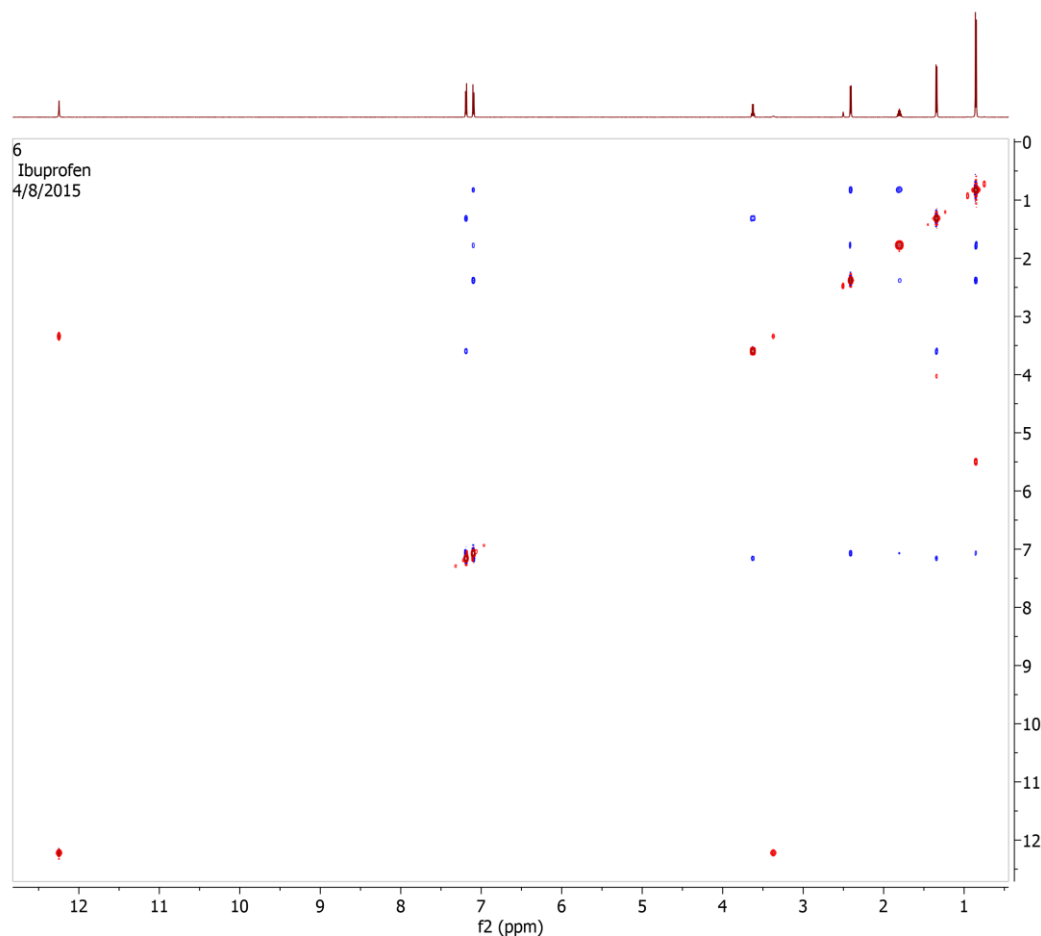
Click here and drag mouse up or down holding: left button for PH0 correction or right button for PH1 correction. (hold Ctrl key for fine tune)

Some processing steps (e.g. baseline correction) are not applied during interactive phasing. The final spectrum may differ from the provisional representation.

PH0: 54.60 +180 PH1: 0.00

Pivot Point

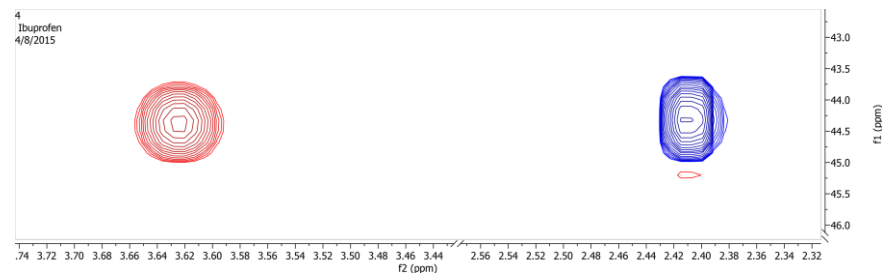
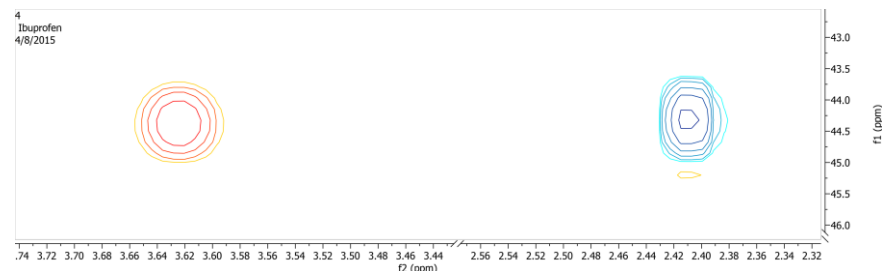
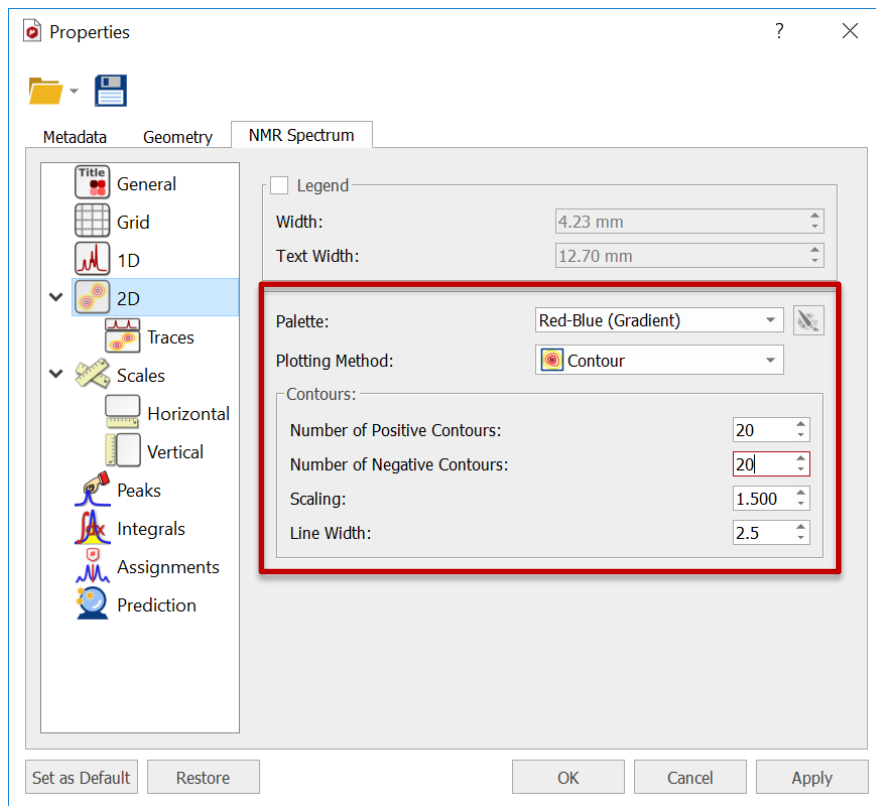
Position: 0.854 Biggest



PROCESSING

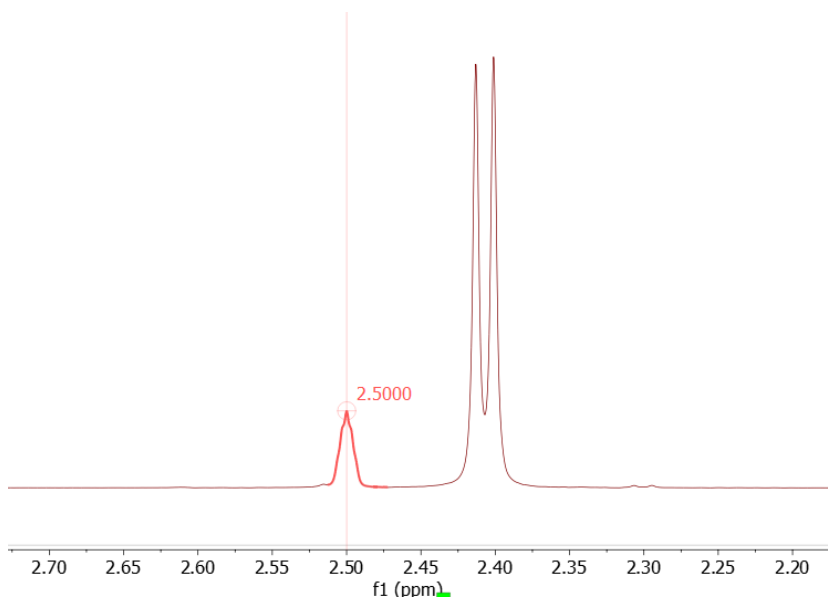
Change the Display Properties

- Double 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



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 for H-1



Reference along f1

Old Shift: 2.5021 ppm Auto Tuning

New Shift: 2.5000 ppm Range Width: 0.1000 ppm

Annotation: DMSO-d6

Solvent List

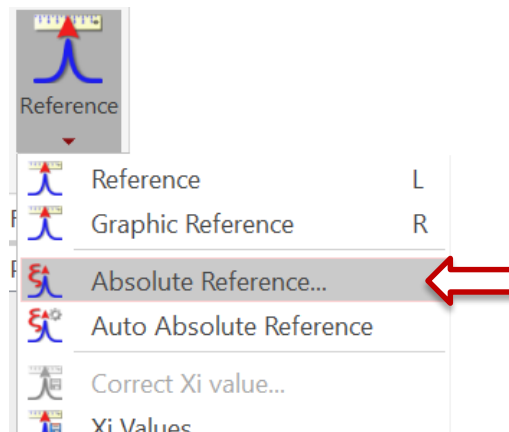
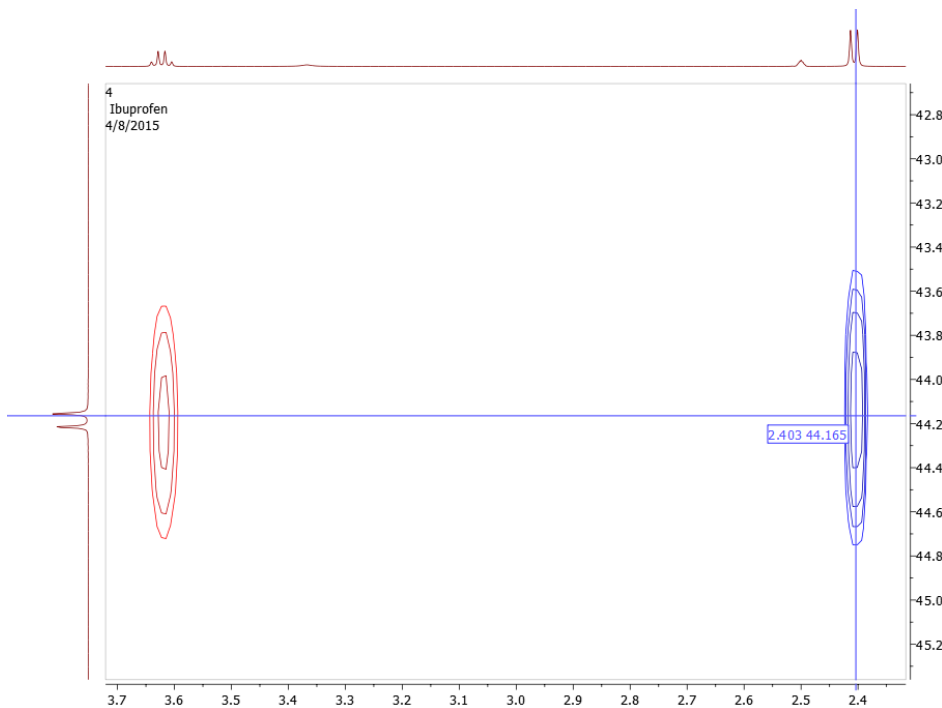
Name	Shift (ppm)	Multiplicity	J (Hz)
Deuterium Oxide	4.790	1	
Dimethyl Sulfoxide-d6	2.500	5	1
	3.330	1	
Ethanol-d6	5.290	1	

Restore Defaults Add... Edit... Delete

OK Cancel Solvents <<

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.
- Note this works only if the spectra were from the same sample acquired on the same instrument.



Absolute Reference ? X

Use as Reference: 1: 599.763 MHz

Spectra		
<input type="checkbox"/>	H 1: 1H, 599.763 MHz	$\Xi=100.000000$ (Me4Si CDCl3, $\phi = 1\%$)
<input checked="" type="checkbox"/>	C 2: 13C, 150.826 MHz	$\Xi=25.145020$ (Me4Si CDCl3, $\phi = 1\%$)
<input checked="" type="checkbox"/>	2D-COSY: 3	
<input checked="" type="checkbox"/>	H 1H, 599.763 MHz	$\Xi=100.000000$ (Me4Si CDCl3, $\phi = 1\%$)
<input checked="" type="checkbox"/>	H 1H, 599.763 MHz	$\Xi=100.000000$ (Me4Si CDCl3, $\phi = 1\%$)
<input checked="" type="checkbox"/>	2D-HSQC-EDITED: 4	
<input checked="" type="checkbox"/>	C 13C, 150.822 MHz	$\Xi=25.145020$ (Me4Si CDCl3, $\phi = 1\%$)
<input checked="" type="checkbox"/>	H 1H, 599.763 MHz	$\Xi=100.000000$ (Me4Si CDCl3, $\phi = 1\%$)
<input checked="" type="checkbox"/>	2D-HMBC: 5	
<input checked="" type="checkbox"/>	C 13C, 150.826 MHz	$\Xi=25.145020$ (Me4Si CDCl3, $\phi = 1\%$)
<input checked="" type="checkbox"/>	H 1H, 599.763 MHz	$\Xi=100.000000$ (Me4Si CDCl3, $\phi = 1\%$)
<input checked="" type="checkbox"/>	2D-NOESY: 6	
<input checked="" type="checkbox"/>	H 1H, 599.763 MHz	$\Xi=100.000000$ (Me4Si CDCl3, $\phi = 1\%$)
<input checked="" type="checkbox"/>	H 1H, 599.763 MHz	$\Xi=100.000000$ (Me4Si CDCl3, $\phi = 1\%$)

Show in spectrum title Show in parameters table

Open the structure for peak assignment

ANALYSIS

- 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.
- Choose View > Tables and check Assignment Table. Make sure all spectra are “linked” in it.

The screenshot displays the MestReNova software interface for NMR analysis. The main window shows a 1H NMR spectrum of Ibuprofen (4/8/2015) with the following peak assignments and integration values:

Assignment	Chemical Shift (ppm)	Integration
A (s)	12.24	1.00
B (d)	7.19	3(7.88)
D (q)	3.62	3(7.12)
E (d)	2.41	3(7.17)
G (d)	1.34	3(7.14)
H (d)	0.85	3(6.68)

The right panel shows the chemical structure of Ibuprofen with atoms numbered 1-14. The properties section includes:

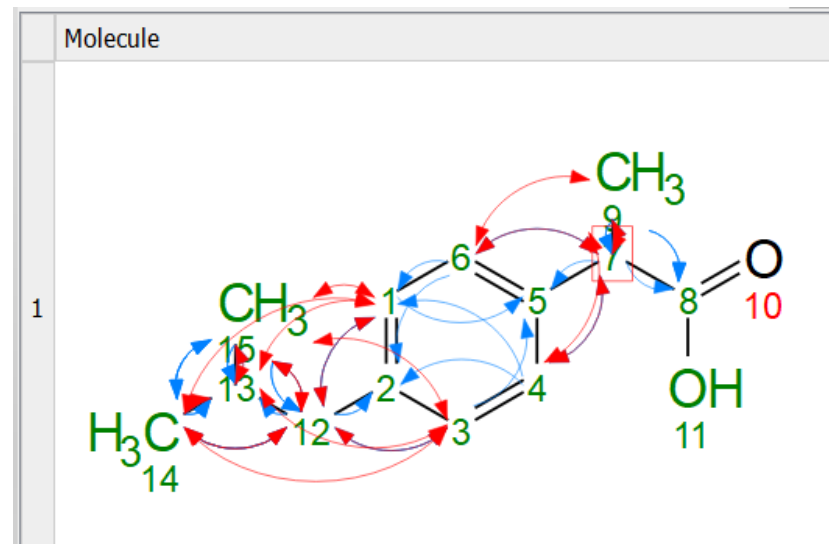
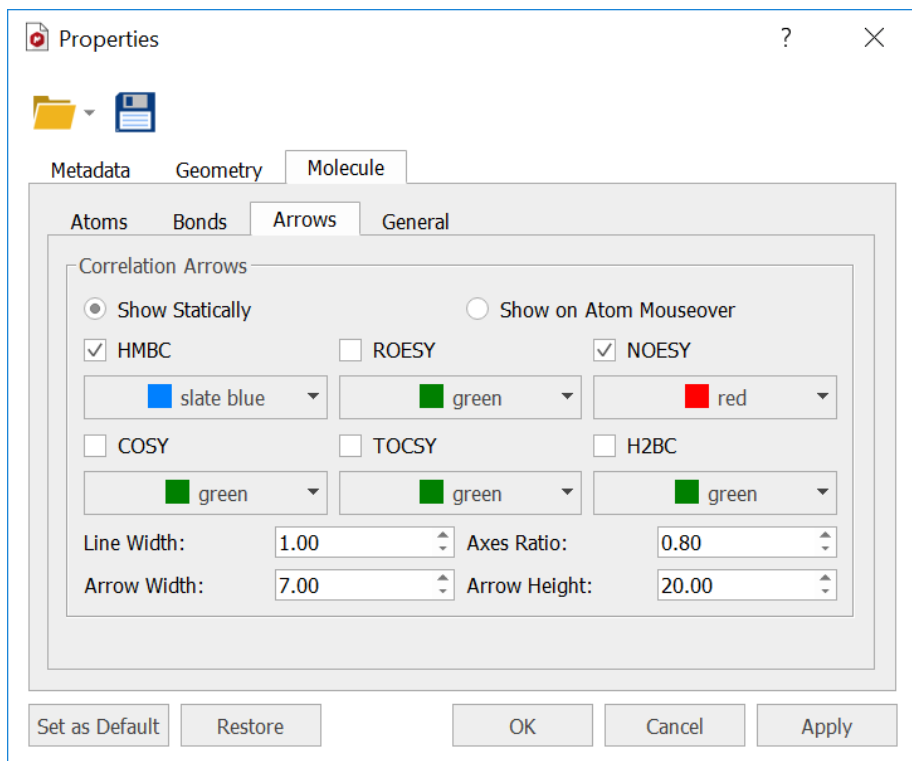
- Molecular Formula: C₁₃H₁₈O₂
- Average Mass: 226.29
- Monoisotopic Mass: 226.13
- Name: Ibuprofen
- Color: (empty)
- Assignments: (empty)

The bottom right panel shows the Assignment Table with columns for Atom, Chemical Shift, Quality, Predicted Shift, and J.

Atom	Chemical Shift	Quality	Predicted Shift	J
1 C				
2 C				
3 C				
4 C				

Show 2D correlation as arrows

- Double-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 as the assignments are added

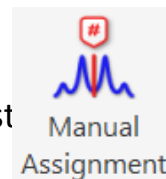


Tip: Click Save as Default button to save the settings

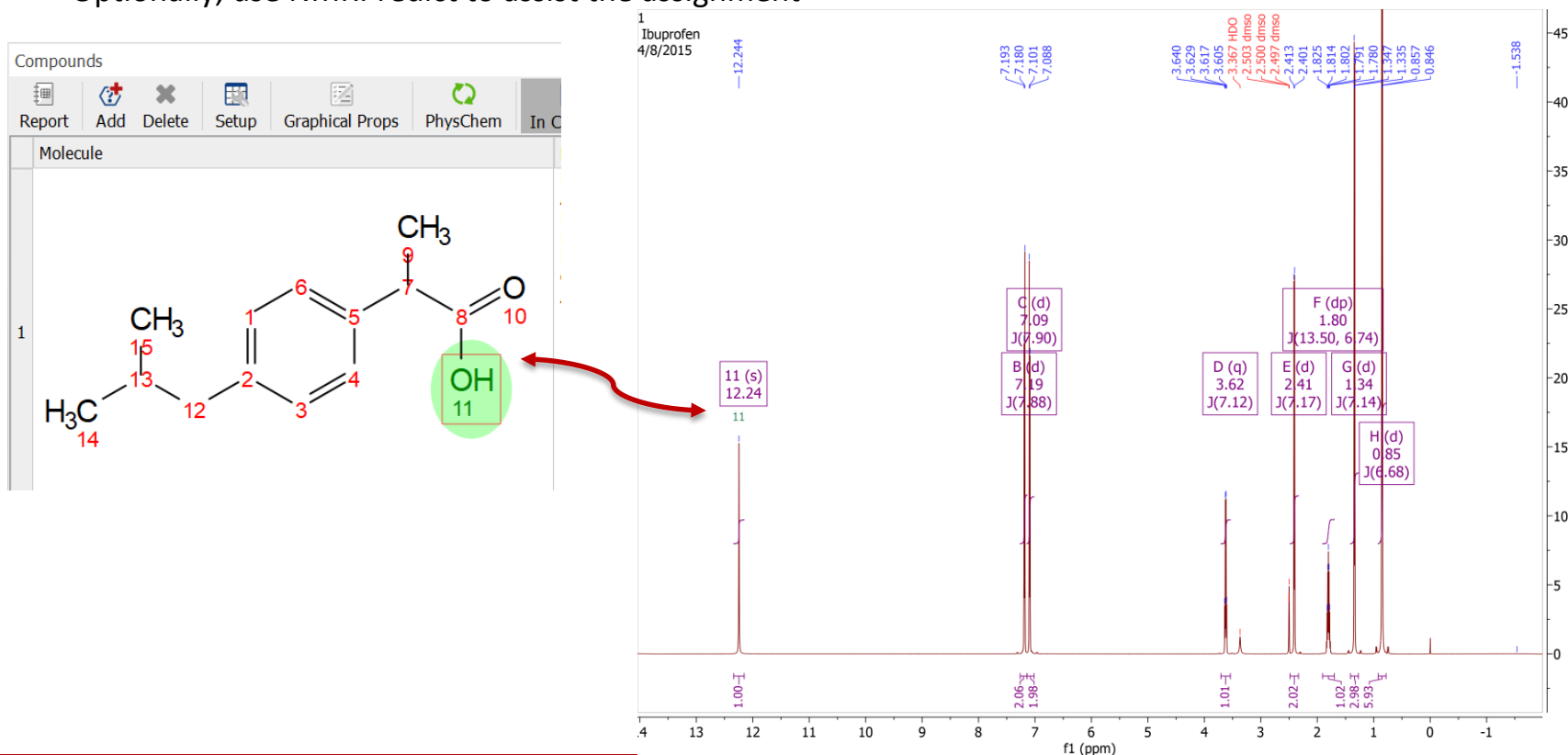
ANALYSIS

- 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
- Optionally, use NMRPredict to assist the assignment

Assign H-1 multiplets



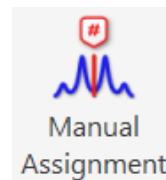
Shortcut = A



ANALYSIS

- 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

Assign C-13 peaks

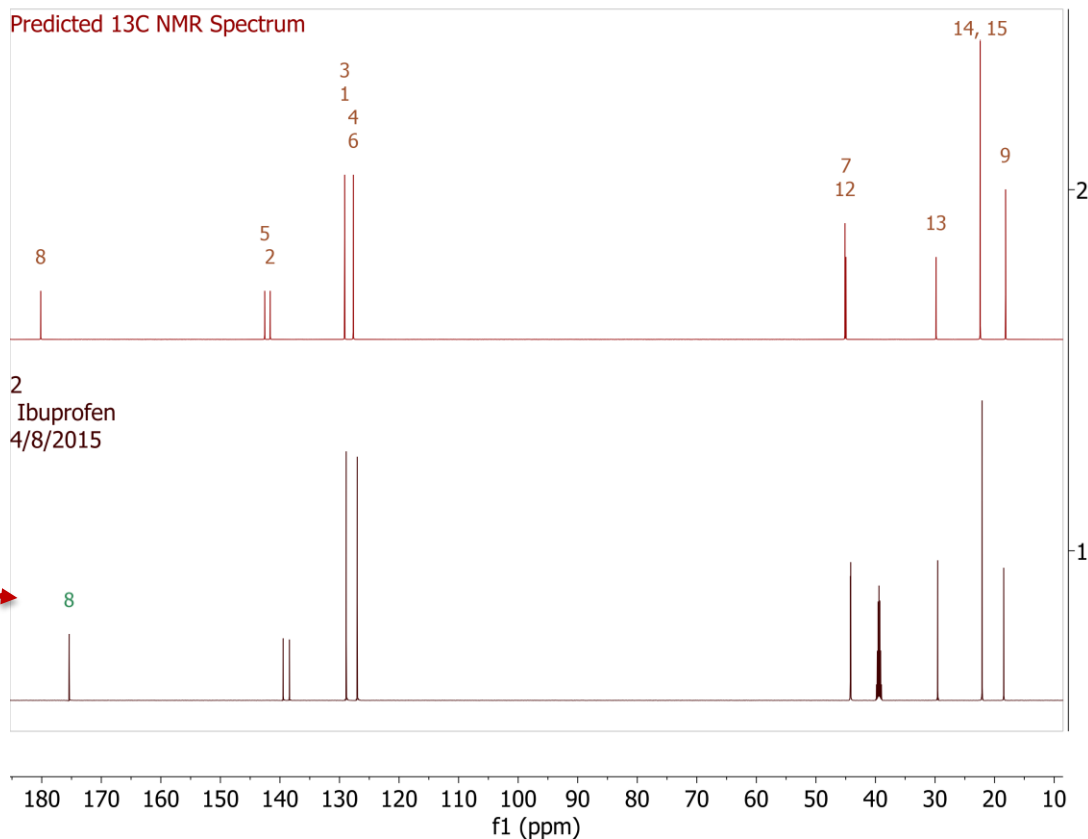
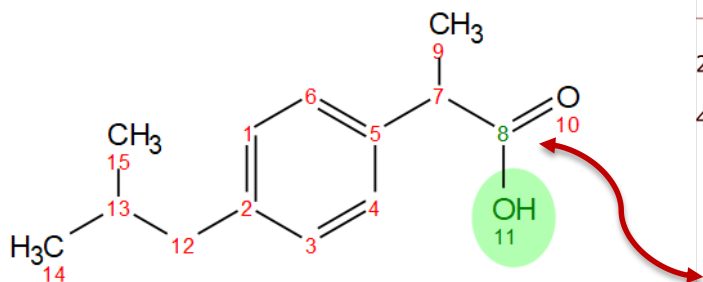


Shortcut = A

Compounds

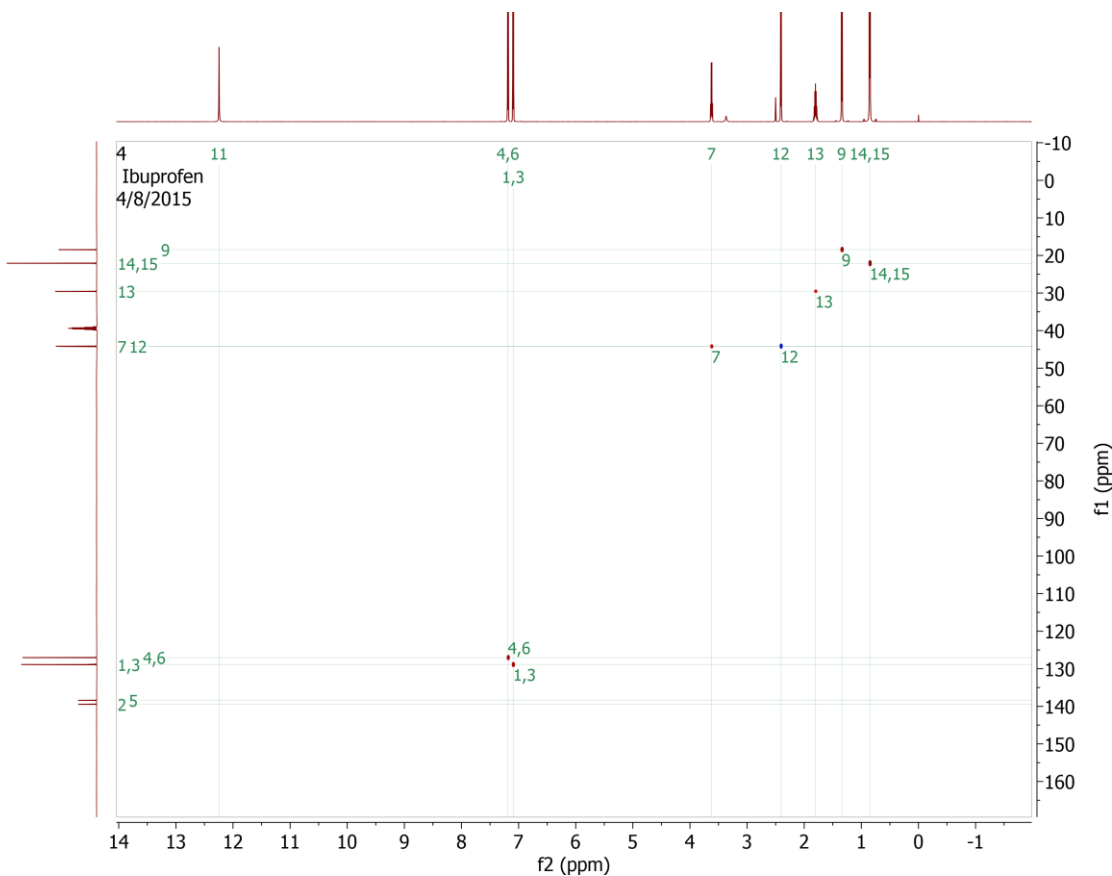
Report Add Delete Setup Graphical Props PhysChem In

Molecule

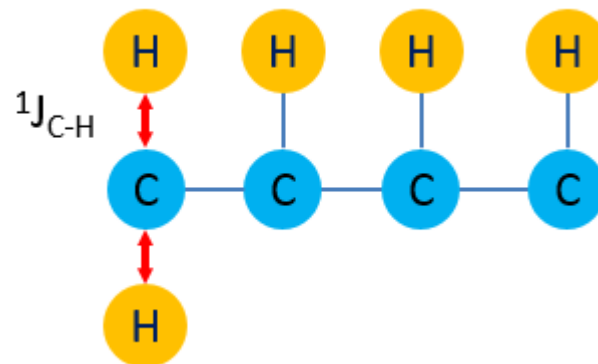


ANALYSIS

- Assign a cross peak to connected H-C atom pair
- Always start from F2 to F1
- Hold Alt key to display the Assign Dialog for more choices
- Always use "original" 1D H/C chemical shifts if available



Assign HSQC peaks



Assign ? ×

Atoms 4,6: 13 $\delta(1H)$: 1H(f2)=7.186 ppm (multiplet 4,6)

Already assigned (4):7.19 (6):7.19

Replace
 Add
 Keep Original

Assign f1

Atoms 4,6: 13 $\delta(13C)$: f1=127.02 ppm

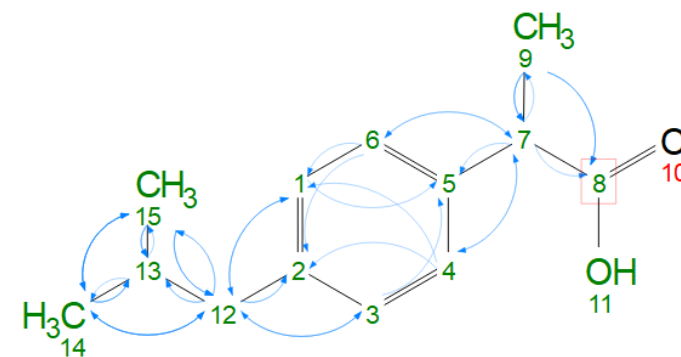
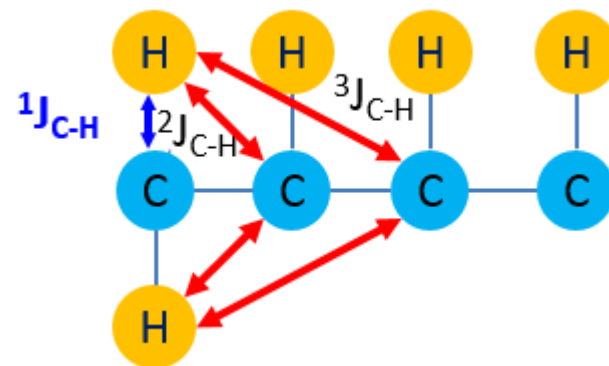
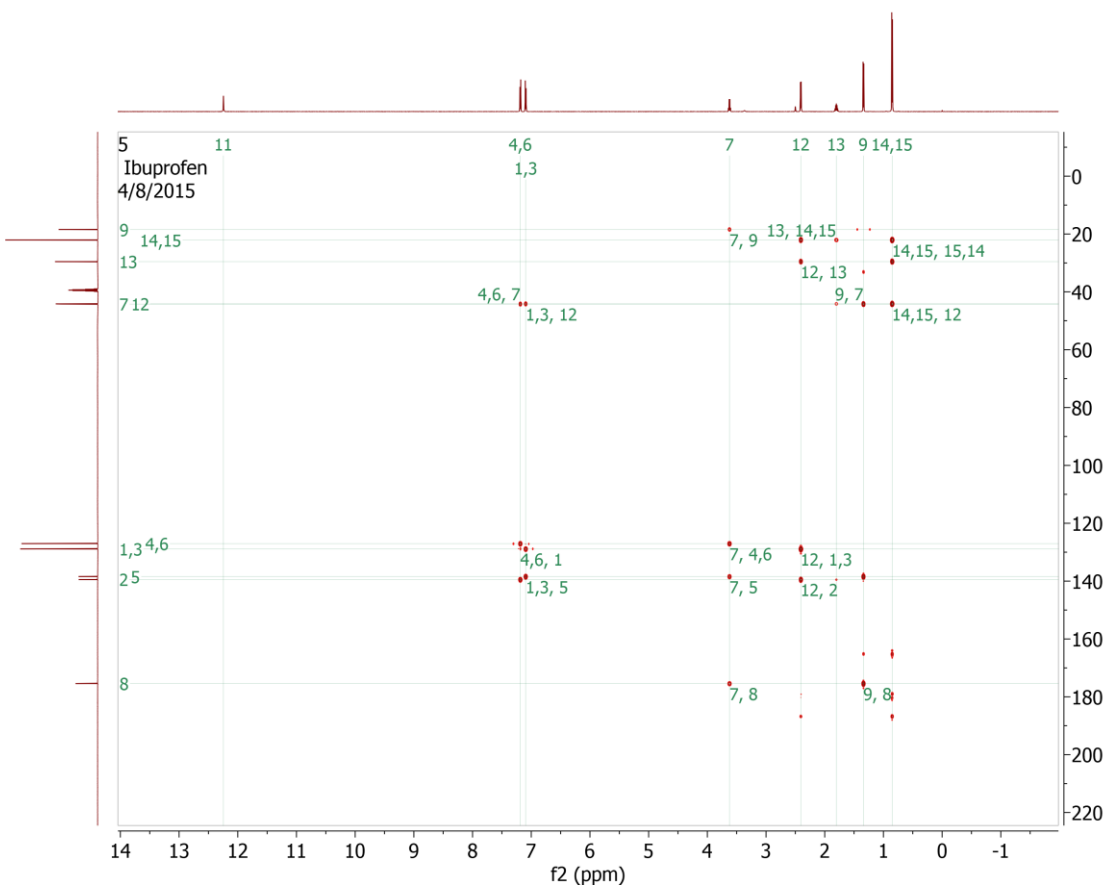
Already assigned (4):127.02 (6):127.02

Replace
 Add
 Keep Original

ANALYSIS

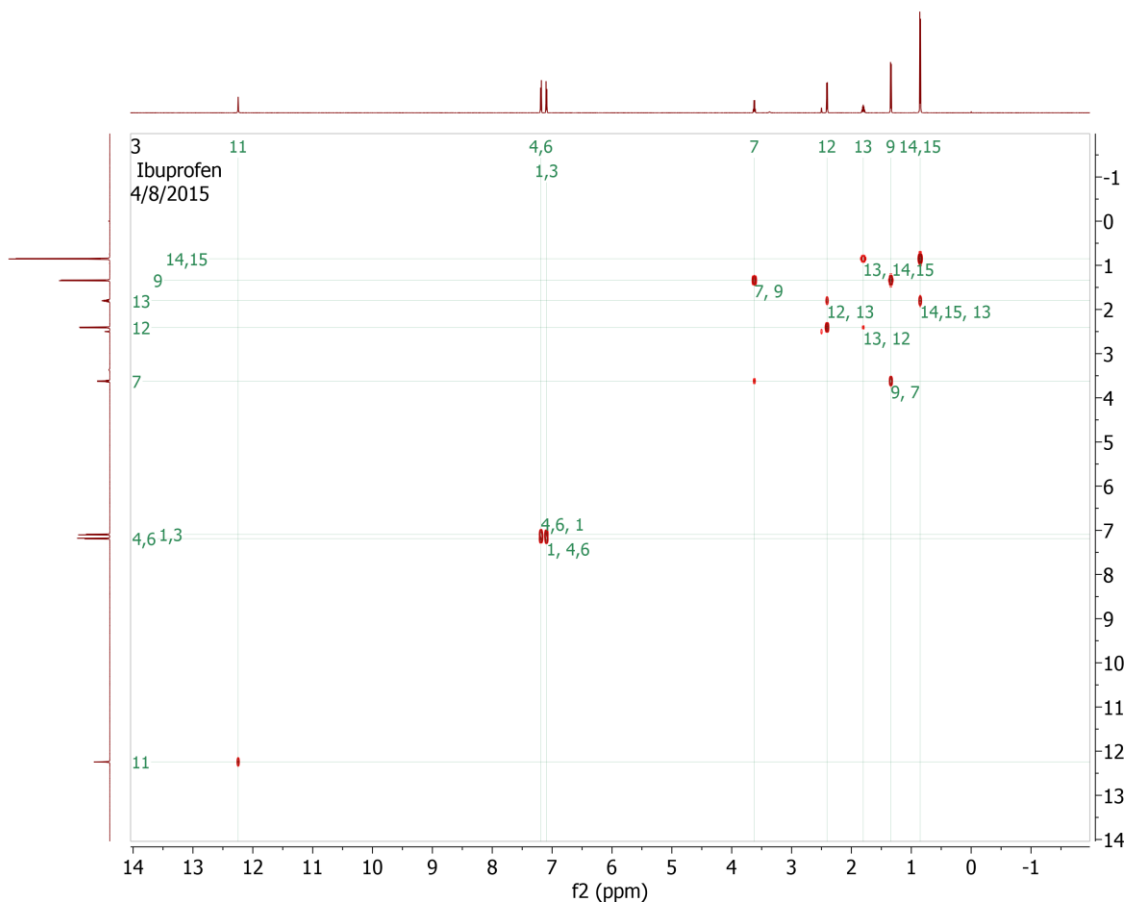
- Assign a cross peak to connected H-C with 2 or 3 bonds away
- Always start from F2 to F1
- Always use “original” 1D H/C chemical shifts if available

Assign HMBC peaks

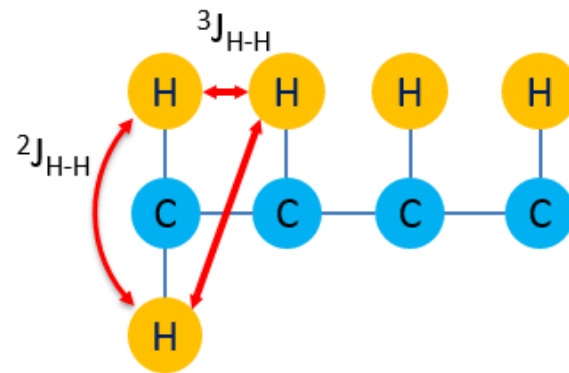


ANALYSIS

- Assign a cross peak to connected H-H pair with 2 or 3 bonds away. Weak couplings between 4-5 bonds is also possible
- Always start from F2 to F1
- Always use "original" 1D H-1 chemical shifts if available



Assign COSY peaks



M Assign ? X

Atoms 4,6: ▼ $\delta(1H)$: f2=7.186 ppm ▼

Already assigned (4):7.19 (6):7.19

Replace
 Add
 Keep Original

Assign f1

Atom: 1 ▼ $\delta(1H)$: f1=7.095 ppm ▼

Already assigned (1):7.09

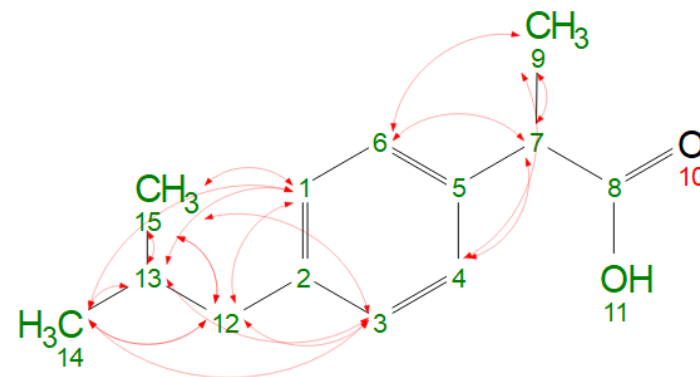
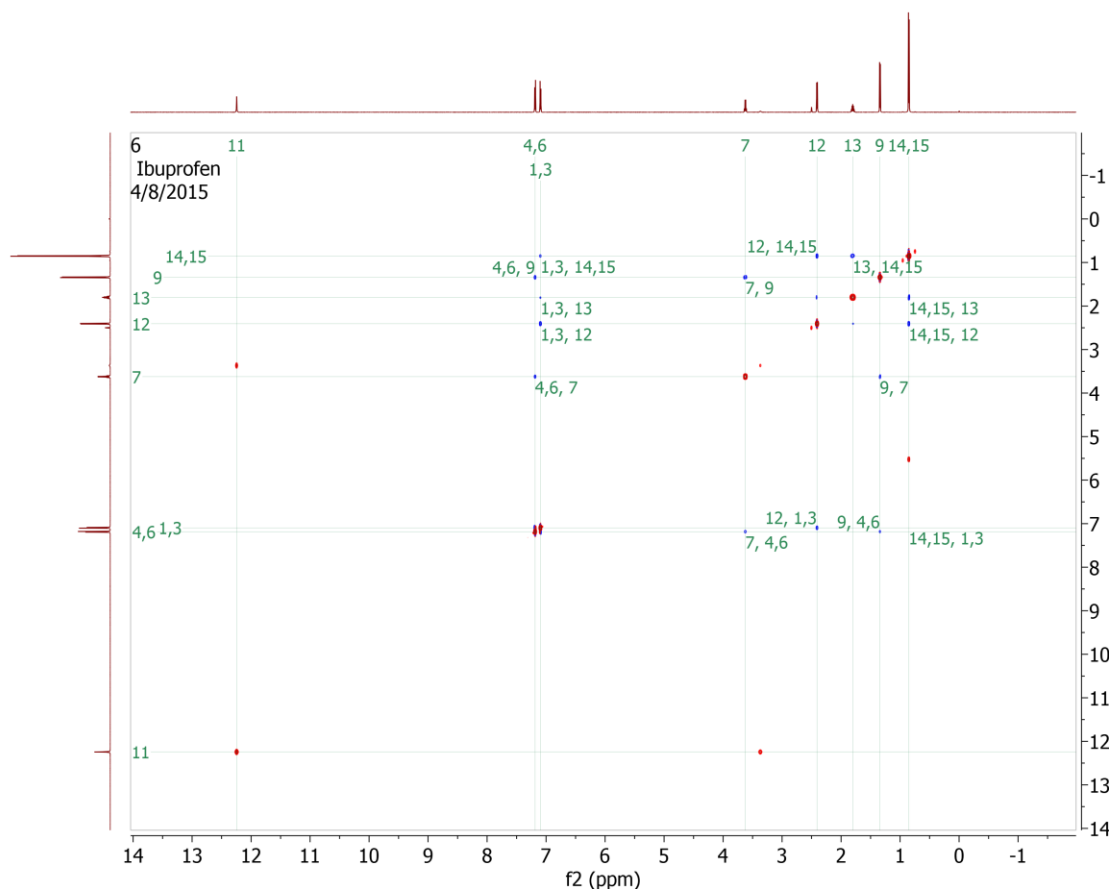
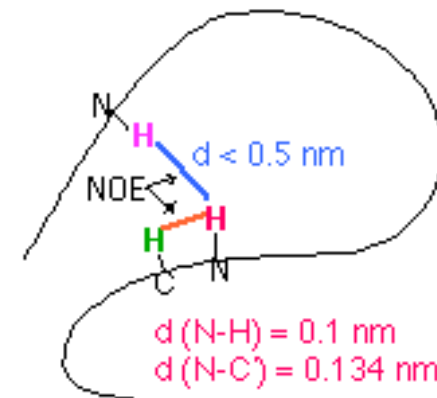
Replace
 Add
 Keep Original

OK
 Cancel

ANALYSIS

- Assign a cross peak to spatially approximate H-H pair (~5Å or less).
- For small molecules, NOE cross peaks are usually negative in phase. Positive one may be from J-couplings and should be ignored with caution.
- Always start from F2 to F1
- Always use "original" 1D H-1 chemical shifts if available

Assign NOESY peaks



Assignments table

REPORT

- 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 ×

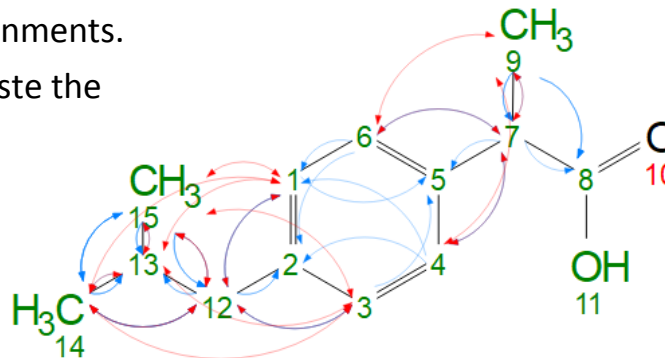
Report Copy Delete Expand Collapse Hide Setup Deduce NOE ▾

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	✓ 7, 9
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, 9
▼ 7 C	44.22		44.96				7	✓ 4, 6, 9	
H	3.62	0.71				✓ 9	7	✓ 4, 5, 6, 8, 9	✓ 4, 6, 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	✓ 4, 6, 7
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

REPORT

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

Report assignments



Setup Assignments Report ? X

Options

Include 13C and X-Nuclei Assignments

Include 13C Multiplicity

Include 1H Multiplicity

Include Number of protons

Order by Chemical Shift

Report Mean Chemical Shift values

Include Atom Type

Only Copy to Clipboard

Export To File:

Text (TSV) HTML

Decimal Places For 1H:

Decimal Places For 13C and X-Nuclei:

2D Correlations

Format:

n δ(n) Atom(δ)

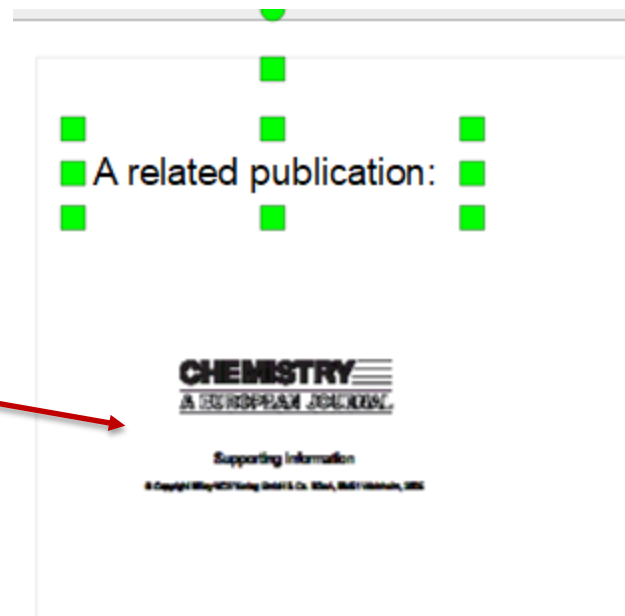
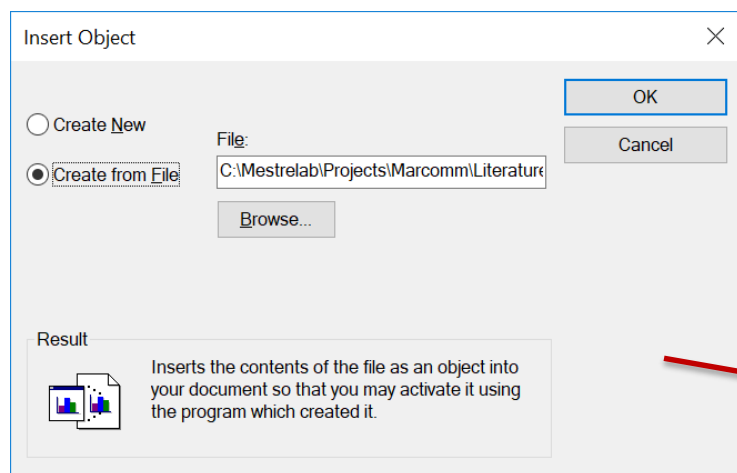
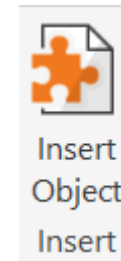
Drop Lines Without Correlation

OK Cancel

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)

Insert a PDF to the document

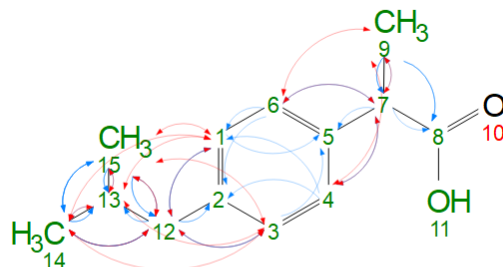
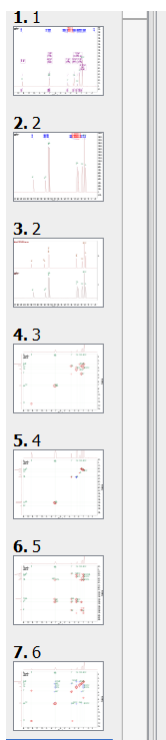
- Choose Home > Insert Object, choose Create from File, and insert a PDF to the document
- A preview logo of the document is displayed.
- Add a text box annotation to it
- You can double click on the preview to open it



Save the results

REPORT

- 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)	H SQC-EDITED	HMBC	COSY	NOE SY
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)

.pdf doc

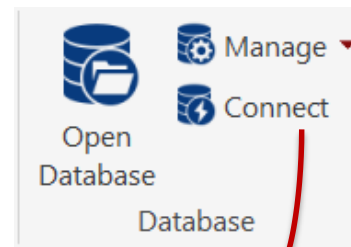
.mnova doc

Database

DATABASE

- 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)

Install MyData DB Server



Connection

Server: localhost

Port: 5504

User: Test

Password: database

Save Password Show Password

OK Cancel

**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.*

DATABASE

Save data to database



Save to Database ▾

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

Select Items

Select

None

All

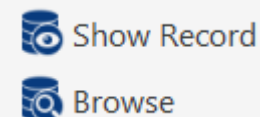
	Page	Type	Preview	Description
1	7	Molecule		
2	1	NMR Spectrum		1
3	2	NMR Spectrum		2
4	3	NMR Spectrum		3
5	4	NMR Spectrum		4
6	5	NMR Spectrum		5
7	6	NMR Spectrum		6
8	7	Text	A related publication:	A related publication:
9	7	Text	Chen Peng's assignment results	Chen Peng's assignment results
10	7	Text		Noδ H (Multiplicity...
11	7	OLE Object		

OK Cancel

Browse and download from database

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



Database - Record View

File Edit View Configure

Molecule Preview

Button Navigator

mndb://Test@localhost:5504/DB1/1 Molecule Molecule C13H18O2

NMR Preview

Mass Preview

Fields

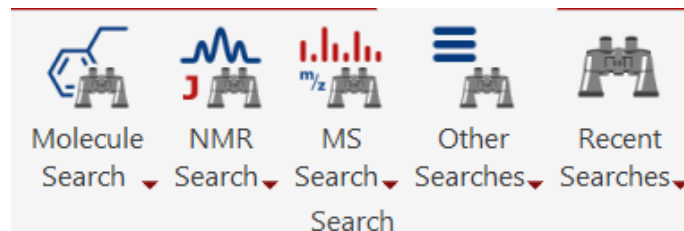
	Field	Content
1:0:8	Molecular Formula	C13H18O2
1:0:10	Monoisotopic Mass	206.13068
1:1:34	Title	1
1:1:38	Solvent	dmsO
		C:/Mestrelab/Projects/Marcomm/Literature & Docs/Sample and Templates/Training for

- Copy Ctrl+C
- Paste Item to Mnova
- Paste Record to Mnova
- Update 1H Prediction DB
- Update 13C Prediction DB

DATABASE

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

Search your own database



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

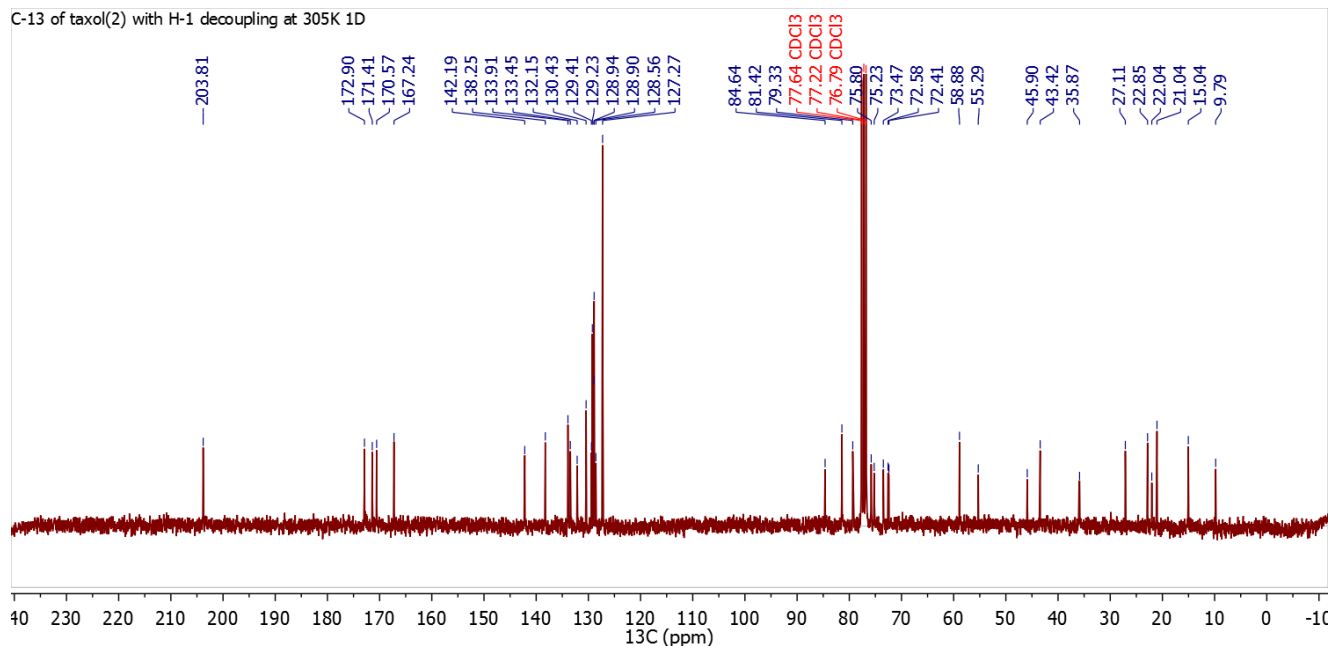
- 1H NMR Spectra: 157,000
- Structures: 157,000
- Compounds: 155,000
- Replicate Spectra: 2,000
- Collected and reviewed by Alexander Yarkov, with carefully reviewed peak assignments, and specific measurement and instrument parameters, where available.
- Using proprietary quality assurance measures developed 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



C-13 of taxol(2) with H-1 decoupling at 305K 1D



WILEY DB

Hit list, and preview of hits

The screenshot displays the 'Database - Search Results' window. It is divided into several panes:

- Molecule Preview:** Shows a chemical structure of a complex organic molecule, labeled 'Str.'.
- NMR Preview:** Shows a ^{13}C NMR spectrum with peaks labeled with their chemical shifts.
- Fields:** A table containing search parameters:

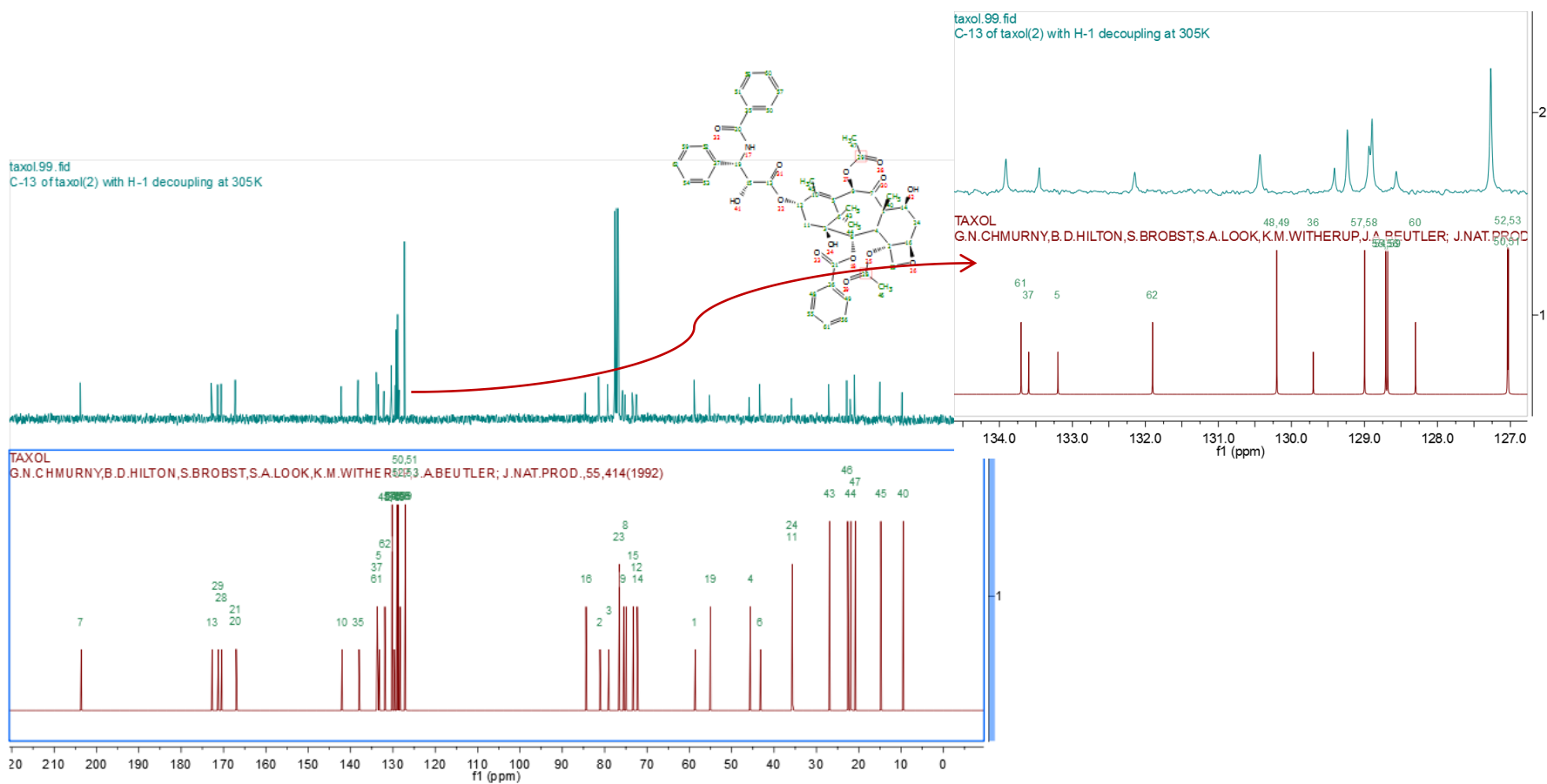
Field	Content
32923:1:34 Title	TAXOL
32923:1:35 Spectrum Comment	G.N.CHMURNY,B.D.HILTON,S.BROBST,S.A.LO...
32923:1:38 Solvent	CDCL3
32923:1:43 Data File Name	/home/michael/RefDB01/data/WileyCNMR/temp/CNMROC2_001_32922.dx
32923:1:45 Nucleus	^{13}C
32923:1:46 Acquisitio...	
32923:1:55 Spectrome...	500.0
32923:1:57 Spectral W...	125000.0
32923:1:58 Temperature	298.0
- Mass Preview:** A small window at the bottom showing mass spectral data.
- Scores:** A table listing 26 search results:

Record	Item Type	Item Number	Search Score
1	mndb... NMR S...	1	948
2	mndb... NMR S...	1	948
3	mndb... Molec...	0	923
4	mndb... Molec...	0	923
5	mndb... NMR S...	1	923
6	mndb... NMR S...	1	923
7	mndb... NMR S...	1	897
8	mndb... NMR S...	1	897
9	mndb... Molec...	0	897
10	mndb... NMR S...	1	897
11	mndb... NMR S...	1	897
12	mndb... Molec...	0	897
13	mndb... NMR S...	1	897
14	mndb... NMR S...	1	871
15	mndb... Molec...	0	871
16	mndb... NMR S...	1	871
17	mndb... Molec...	0	871
18	mndb... Molec...	0	871
19	mndb... NMR S...	1	871
20	mndb... NMR S...	1	846
21	mndb... Molec...	0	846
22	mndb... NMR S...	1	846
23	mndb... Molec...	0	846
24	mndb... NMR S...	1	846
25	mndb... NMR S...	1	846
26	mndb... Molec...	0	846

A red arrow points from the 'Hit list' table to the right, with the text 'Hit list' written next to it.

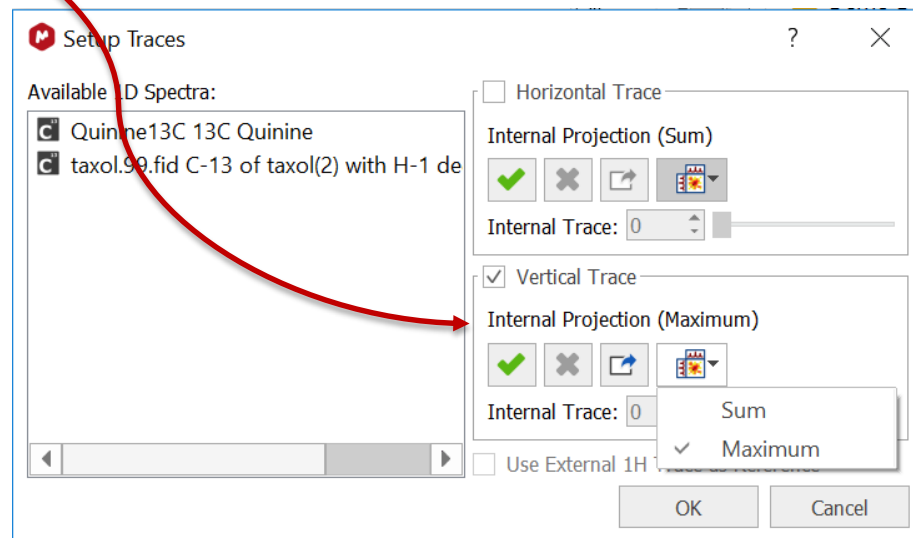
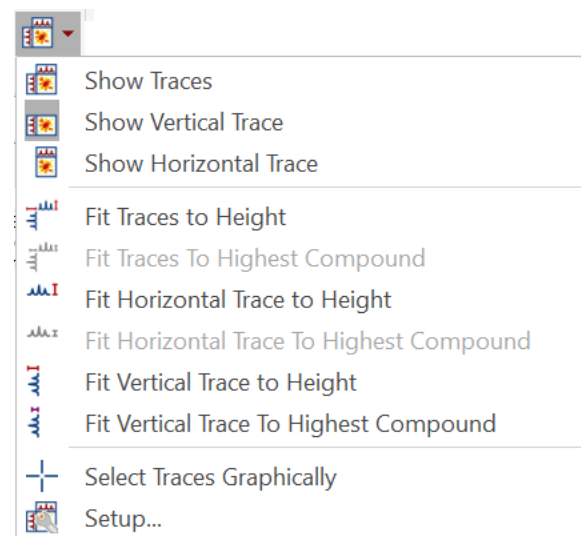
Search a C-13 spectrum

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



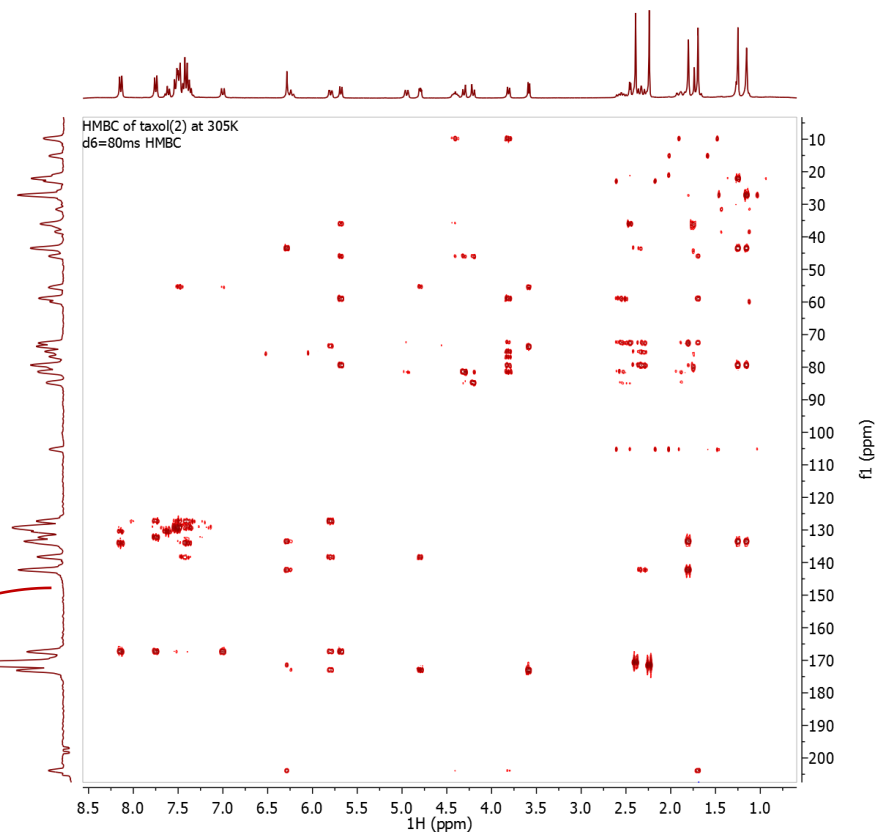
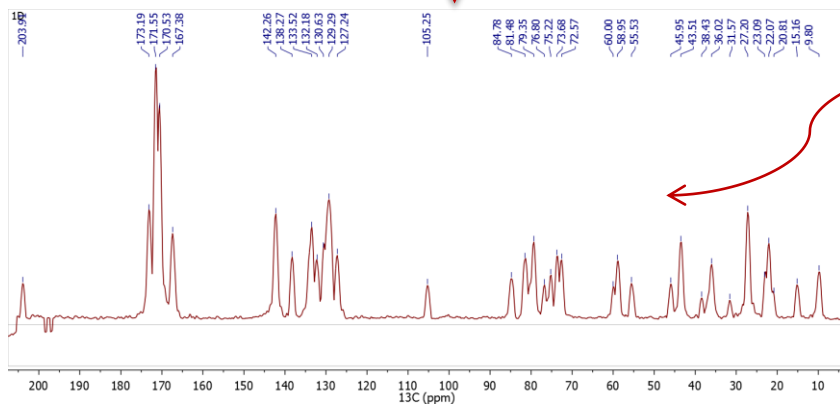
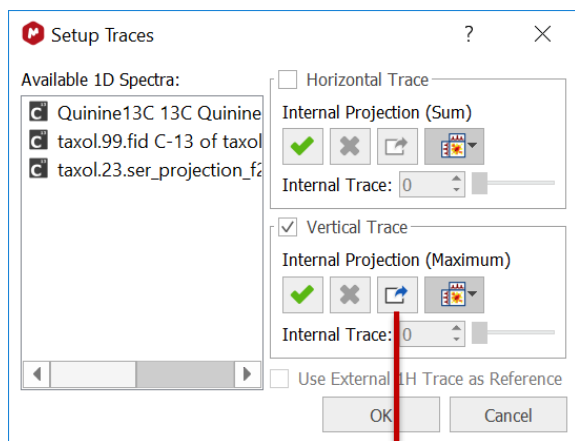
Search C-13 peaks from HMBC

- ❑ 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

WILEY DB

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

The screenshot displays the Mestrelab Research software interface with the following components:

- Molecule Preview:** Shows the chemical structure of Taxol.
- Fields:** A table with the following data:

Field	Content
32923:0:8 Molecular Formula	C47H51NO14
32923:0:10 Monoisotopic Mass	853.330959
32923:1:34 Title	TAXOL
32923:1:35 Spectrum Comment	G.N.CHMURNY,B.D.HILTON,S...
32923:1:38 Solvent	CDCL3
32923:1:43 Data File Name	/home/michael/RefDB01/data/WileyCNMR/temp/CNMROC2_001_32922.dx
- Query:** 1D Peaks Query: 34 Peaks
- NMR Preview:** A 13C NMR spectrum plot showing intensity versus chemical shift (ppm).
- Mass Preview:** A mass spectrum plot showing intensity versus m/z.
- Scores:** A table of search results:

Record	Item Type	Item Number	Search Score
1	mndb:...	NMR S...	882
2	mndb:...	NMR S...	882
3	mndb:...	Molec...	882
4	mndb:...	NMR S...	882
5	mndb:...	NMR S...	882
6	mndb:...	NMR S...	882
7	mndb:...	Molec...	852
8	mndb:...	NMR S...	852
9	mndb:...	Molec...	852
10	mndb:...	NMR S...	852
11	mndb:...	Molec...	852
12	mndb:...	NMR S...	852
13	mndb:...	NMR S...	852
14	mndb:...	NMR S...	852
15	mndb:...	Molec...	852
16	mndb:...	NMR S...	852
17	mndb:...	NMR S...	852
18	mndb:...	Molec...	823
19	mndb:...	NMR S...	823
20	mndb:...	Molec...	823

ARRAYED SPECTRA

- Open and stack multiple 1D spectra
- Re-process multiple spectra
- Analyze arrayed spectra together

Process arrayed spectra

Stack a few spectra

ARRAYED 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

The screenshot displays the MestReNova software interface. The top menu bar includes File, Home, View, Molecule, Prediction, Tools, Database, Verification, Elucidation, STACK, Processing, Analysis, Assignments, Quantitation, and Chen's Tools. The STACK ribbon is active, showing options like Stack Options, Extract Active Item, Adjust Stacked Items, Auto Scale, Multiply Divide, Mode Invert, Show Select, Stacked Items Table, Align Spectra, Reference Alignment, DOSY Transform, and Arrayed Data Table.

The main window shows a plot of 'Multiple 1H spectra.34.fid' with a y-axis from -2400 to -200 and an x-axis (f1) from 16 to -4 ppm. The plot displays two distinct peaks at approximately 4.7 ppm and 1.2 ppm. A red arrow points from the 'Multiple 1H spectra' folder in the Data Browser to the plot.

The Data Browser on the right shows a tree view of the file system. The 'Multiple 1H spectra' folder is expanded, showing a list of subfolders (2, 18, 34, 50, 66, 82, 98, 114, 130, 146, 162, 178) and their corresponding experiment names (1D-H-zg30). A red arrow points from the 'Multiple 1H spectra' folder in the Data Browser to the plot.

The Pages view on the left shows three thumbnails of 'Multiple 1H spec' spectra, with a red arrow pointing to the first one.

At the bottom right, there is a 'Licenses: DB:' status indicator.

ARRAYED SPECTRA

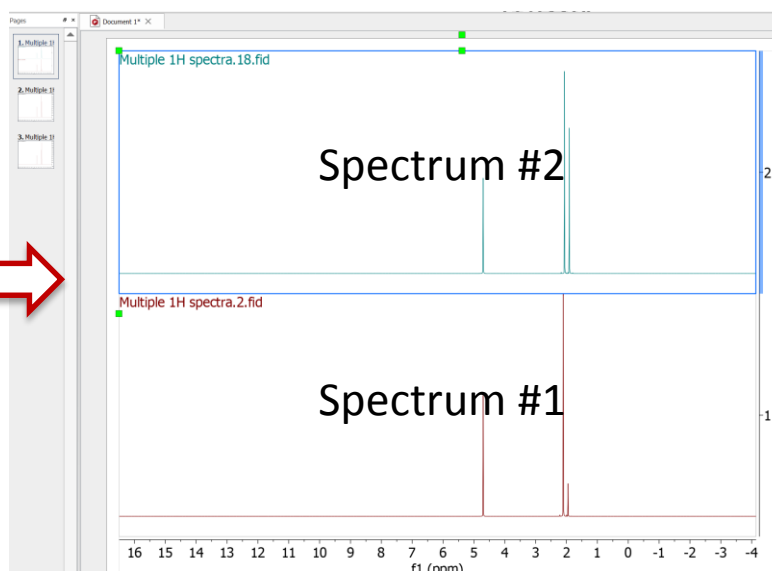
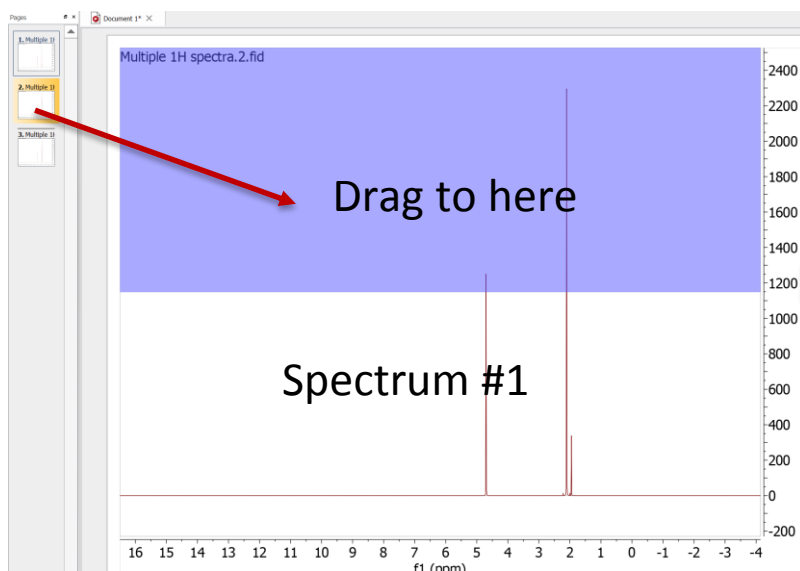
Stack a few spectra

- 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
Items

Superimpose
Items



ARRAYED SPECTRA

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.

Import Spectra Stack

Data Folder: s by Chen/Training Data Sets/Multiple 1H spectra ...

Order: By Name

File Path Filtering

File Name Masks: fid *.fid *.jdx

Folder Name Masks:

Preview Files

Spectral Data Filtering

Parameter Nucleus =

Chunking

First Spectrum: 1 Number of Chunks: 1

Chunk Size: 1 Step to Next Chunk: 2

Visualization

View: Stacked Decimation Step: 1

Palette: Default

Import Array Values

File: ...

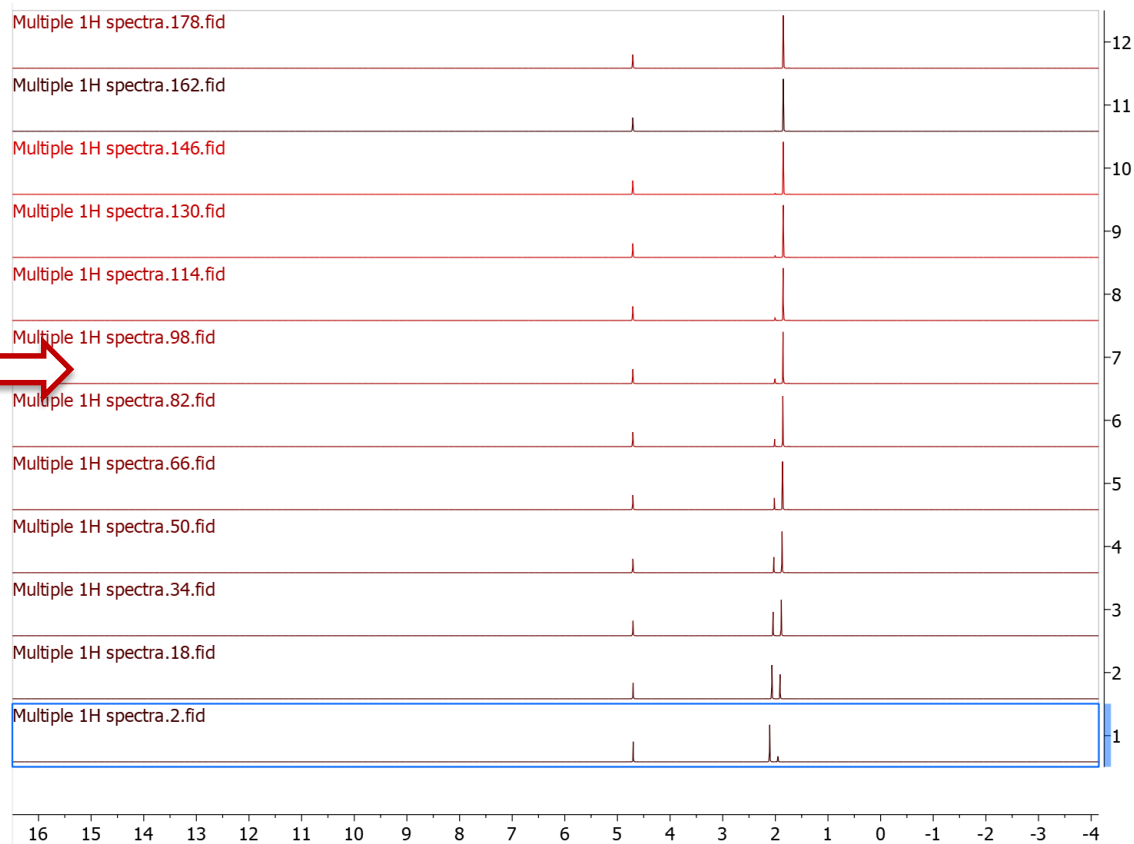
Processing Template

File: ...

Backup

Folder: C:/Users/chenp/AppData/Local/Temp ...

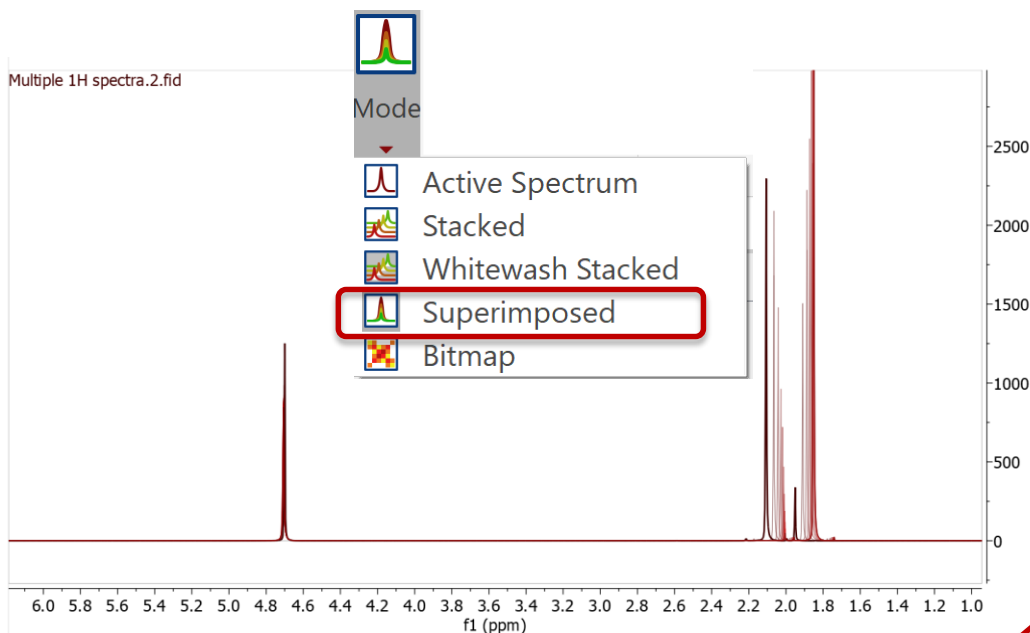
OK Cancel



Stacking mode and Stacked Items Table

ARRAYED SPECTRA

- 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



Stacked Items Table

Stacked Items

Report Copy Delete Invert Order Setup

Multiply Divide Show Select Adjust Stacked Items

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

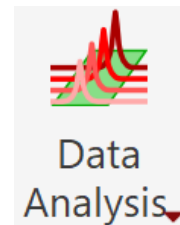
Click and drag here to change the order

Check/uncheck these to show/hide spectra

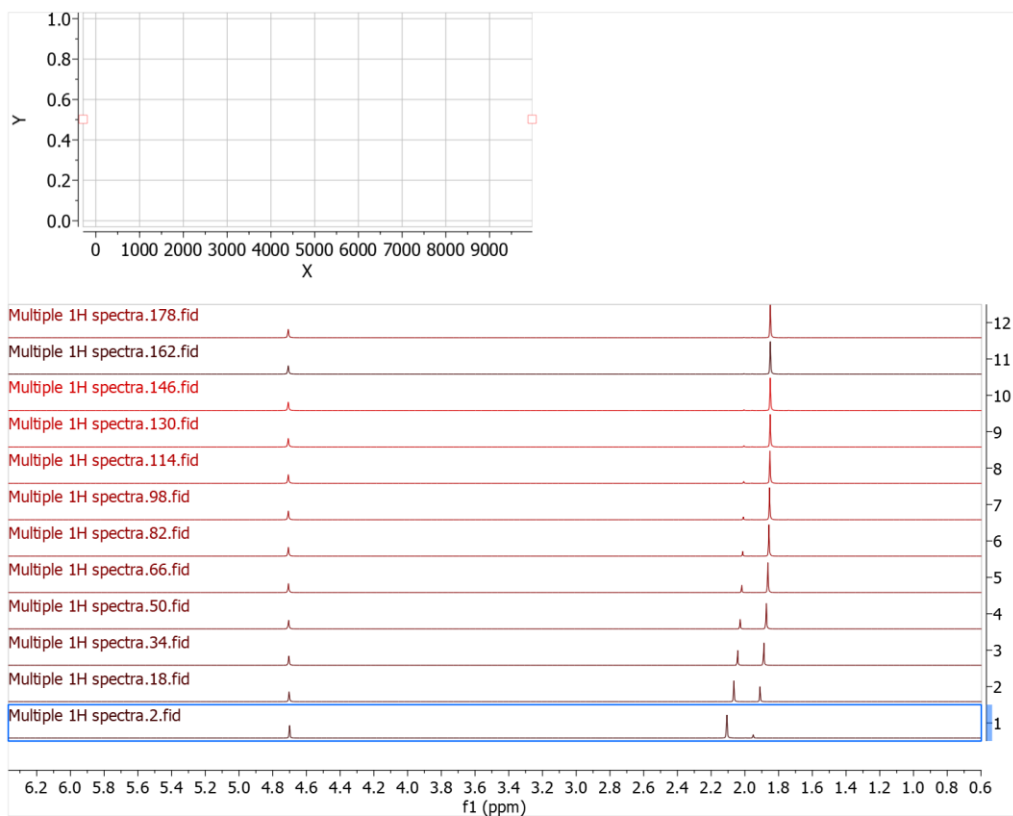
Check these to choose spectra to change

ARRAYED SPECTRA

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.



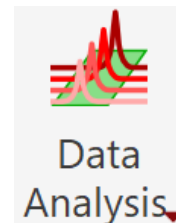
Model	X(I)
1	0
2	874
3	1758
4	2631
5	3509
6	4401
7	5299
8	6175
9	7049
10	7922
11	8811
12	9682

Acq. Start: 004-04-30T21:03:34 Acq. End: 004-04-30T23:44:56

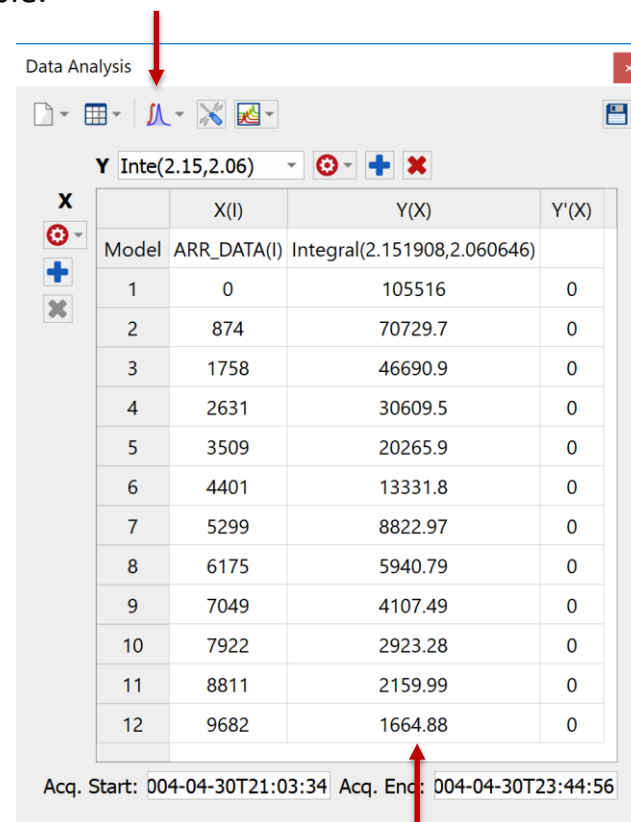
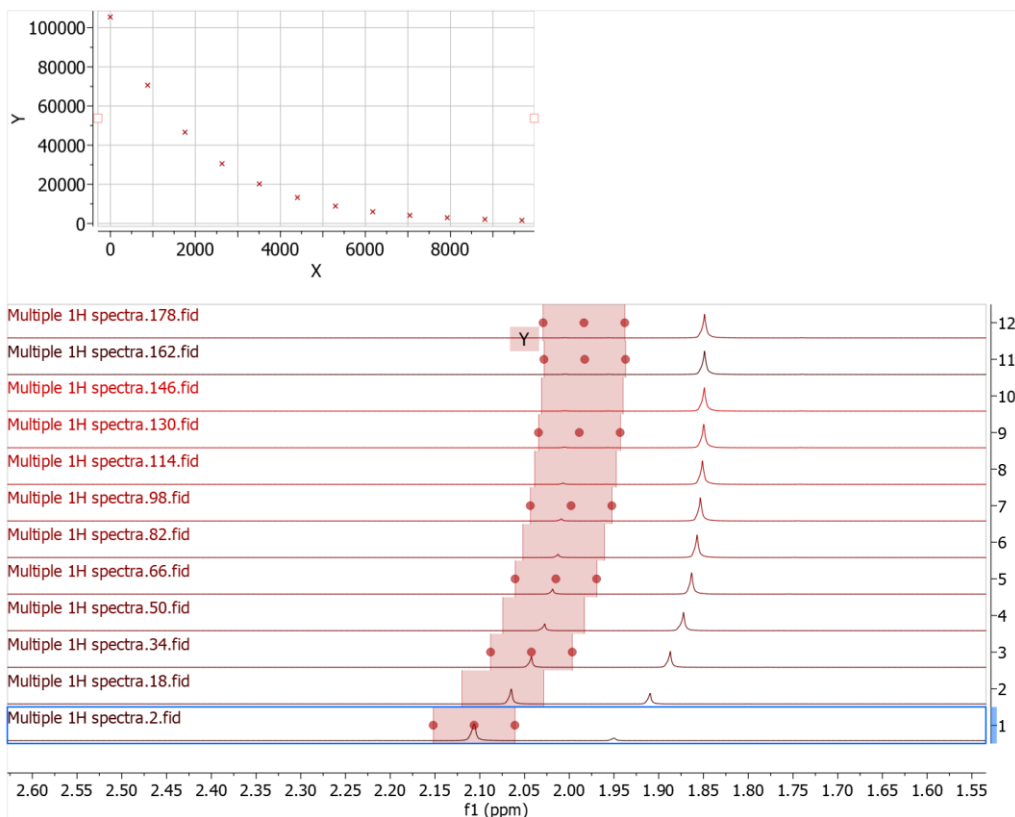
Reaction time

ARRAYED SPECTRA

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 for other spectra**
- The integrals are displayed on the XY graph and in the Data Analysis Table.

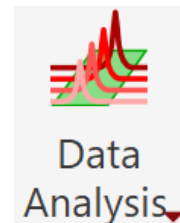


*Use Sum Method (default) for integration unless you are integrating overlapped peaks. Click Options for Integration in the Analysis Ribbon to verify. ** You can increase the # of handlers by using the Edit Model Option Tool.

Integrals

ARRAYED SPECTRA

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

Data Analysis

Y: **Inte(2.15,2.06)**

	X(I)	Y(X)	Y'(X)
Model	ARR_DATA(I)	Integral(2.151908,2.060646)	
1	0	105516	0
2	874	70729.7	0
3	1758	46690.9	0
4	2631	30609.5	0
5	3509	20265.9	0
6	4401	13331.8	0
7	5299	8822.97	0
8	6175	5940.79	0
9	7049	4107.49	0
10	7922	2923.28	0
11	8811	2159.99	0
12	9682	1664.88	0

Acq. Start: 004-04-30T21:03:34 Acq. End: 004-04-30T23:44:56

Y'-Column Model Function

	Name	Function	Initialization	Report	Description
1	Linear Fit	A+B*x	A= 0, B= 0		Zero Order Reaction Rate
2	Mono-exponential Fit	B*exp(-x*F)			Exponential Decay, First Order Reaction Rate
3	Three Parameter Exponential Fit	B+F*exp(-x*G)			Exponential Decay, First Order Reaction Rate With Offset
4	Inverse Linear Fit	1/(A+B*x)	A= 1, B= 0		Second Order Reaction Rate
5					

Restore Defaults

Fitted Parameters

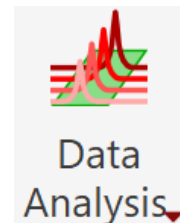
Calculate

B= 312.388, F= 105518, G= 0.000471256
rError = 2.00941e-06, probnotmono = 0.958368

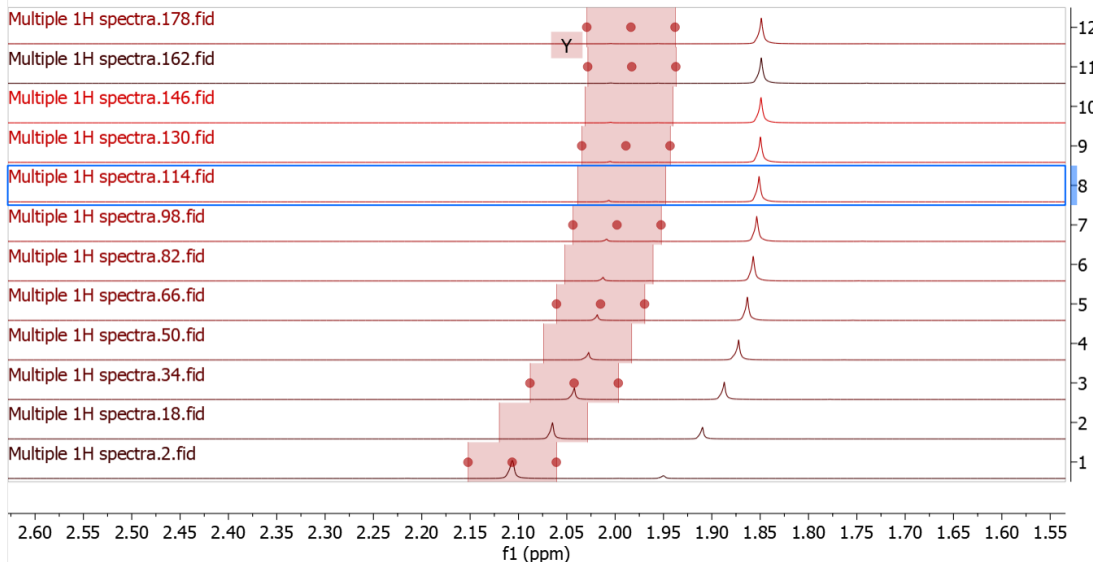
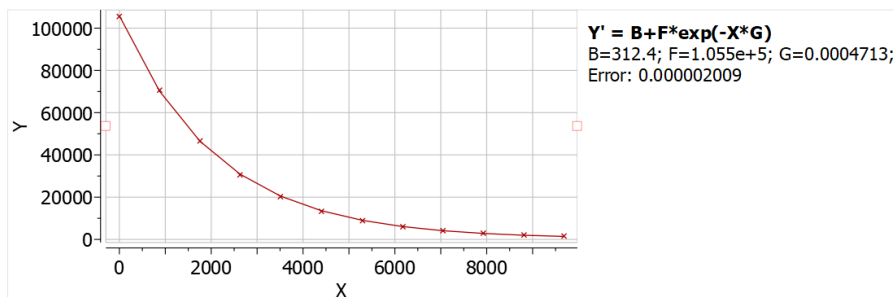
OK Cancel

ARRAYED SPECTRA

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.



Data Analysis

Y Inte(2.15,2.06)

X	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

Acq. Start: 2004-04-30T21:03:34 Acq. End: 2004-04-30T23:14:56

Fitting results

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 has tabs for 'Help' and 'About'. The 'Help' tab is active, showing a 'MestReNova Manual' window. The manual's table of contents is visible, with 'Using GSD for multiplets analysis' selected. A red banner at the top of the manual window reads 'Using GSD for multiplets analysis'. Below the banner, the text states: 'Exploiting the power of GSD for an improved Multiplet Analysis'. It explains that Mnova uses Global Spectral Deconvolution (GSD) for peak picking and multiplet analysis, and that multiplet analysis benefits from automatic analysis with enhanced peak picking capabilities. A graph at the bottom shows a peak at 3.49 ppm, with a red banner above it indicating 'Using GSD for multiplets analysis'.