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# Mnova Training– Advanced

*For Mnova v16.0*

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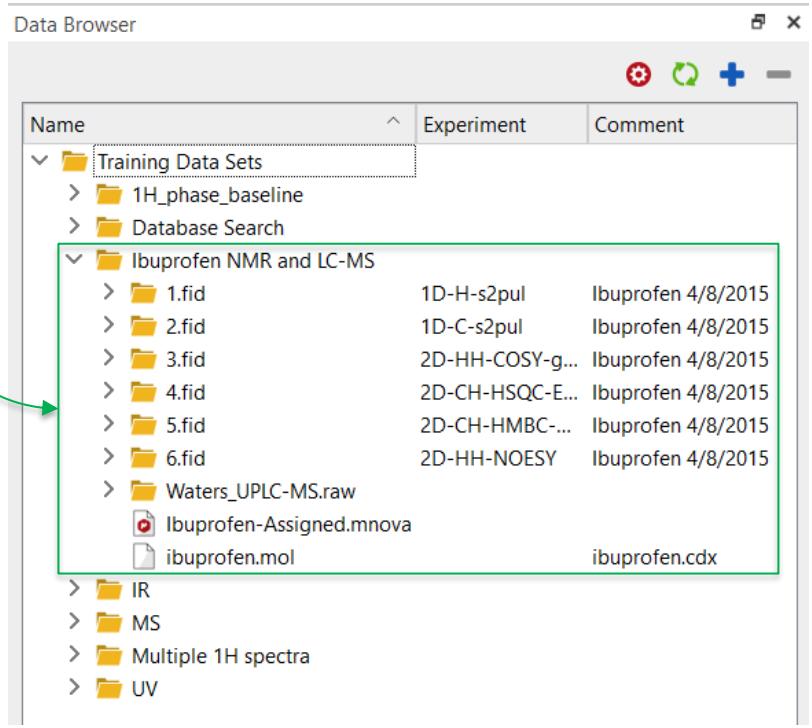
# Main Topics

- Opening and processing 2D NMR
- Assigning peaks to atoms
- Reporting assignment results
- Analyzing arrayed spectra for reaction monitoring

*Note: This tutorial covers the NMR, NMRPredict, MSChrom, and ElVis*

# Processing 1D & 2D NMR Spectra Together

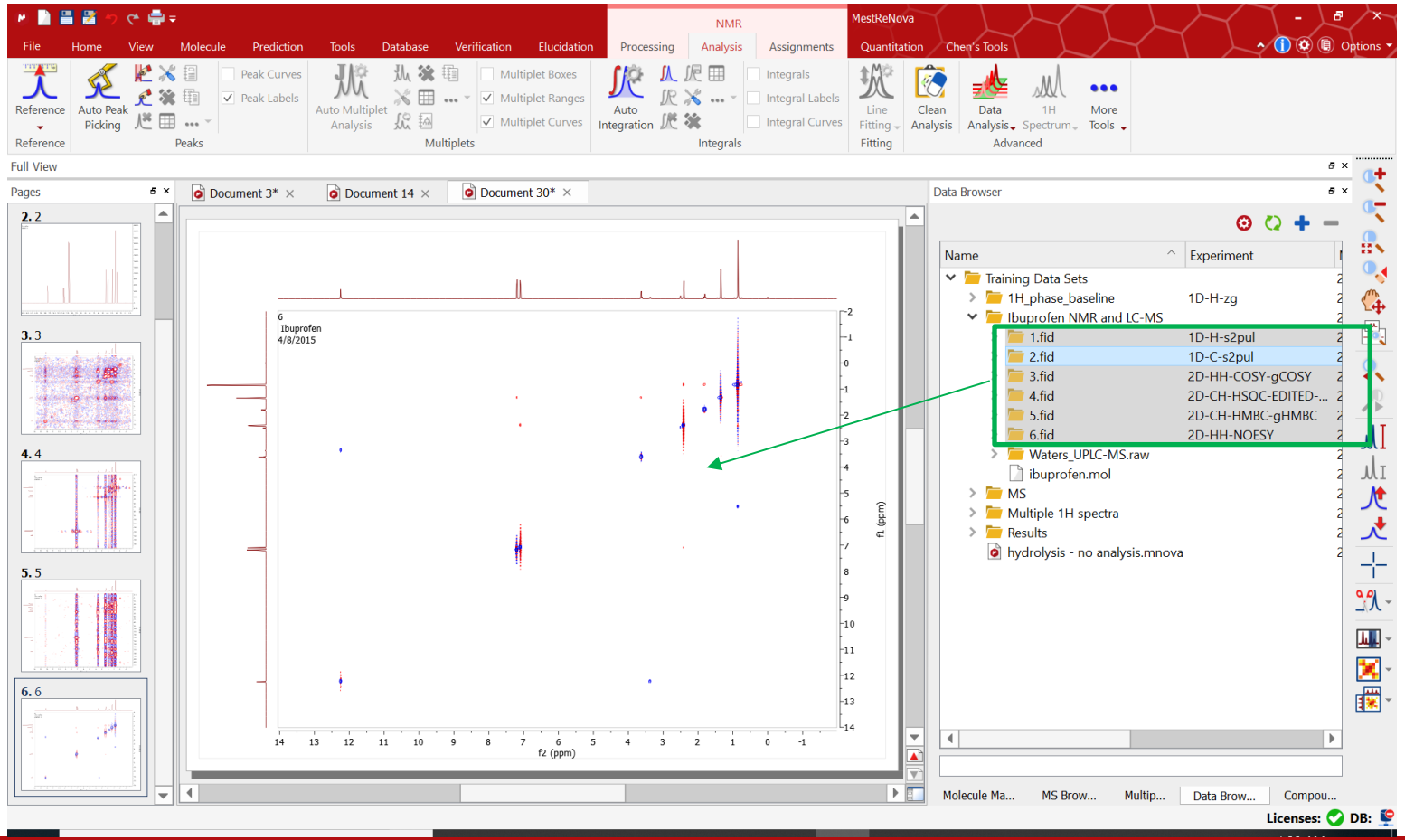
Sample data



PROCESSING

# Open a 1D and 2D spectra of Ibuprofen

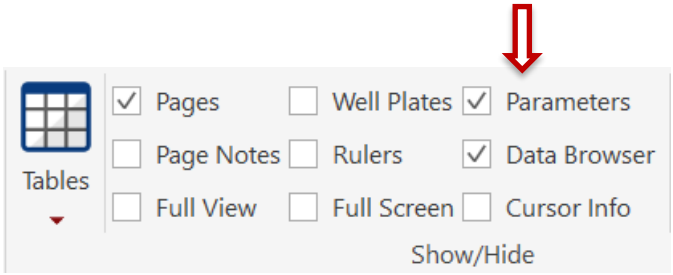
- Choose File > New to open a new blank document.
- In Data Browser, choose the 1D H/C, 2D HSQC, HMBC, COSY, and NOESY spectra and drag all of them to the main window.
- Re-process and analyze the H-1 and C-13 spectra according to the Basic Tutorial.

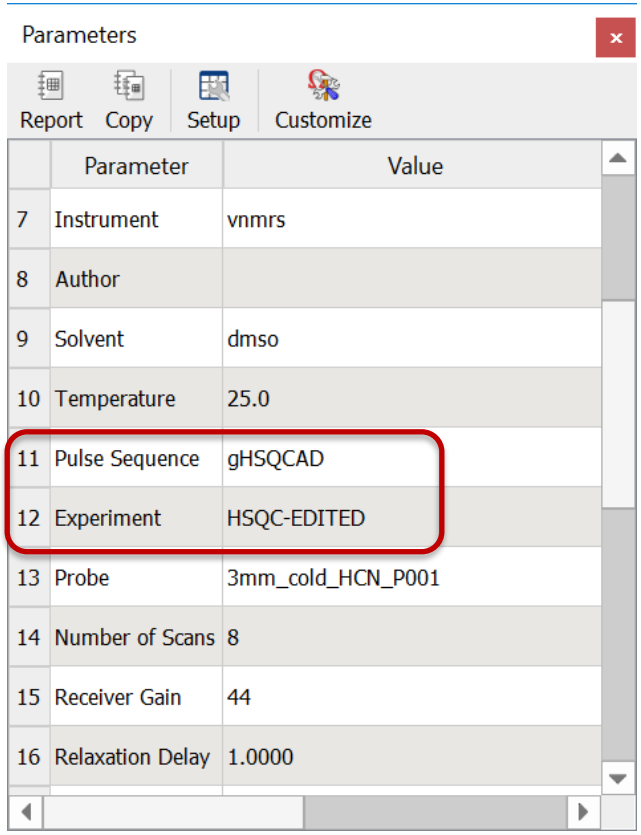


PARAMETERS

# 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



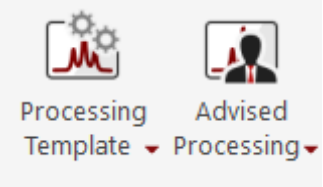

| | Parameter | Value |
|---|---|---|
| 7 | Instrument | vnmrs |
| 8 | Author | |
| 9 | Solvent | dmso |
| 10 | Temperature | 25.0 |
| 11 | Pulse Sequence | gHSQCAD |
| 12 | Experiment | HSQC-EDITED |
| 13 | Probe | 3mm_cold_HCN_P001 |
| 14 | Number of Scans | 8 |
| 15 | Receiver Gain | 44 |
| 16 | Relaxation 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*), using the parameters from the instrument.

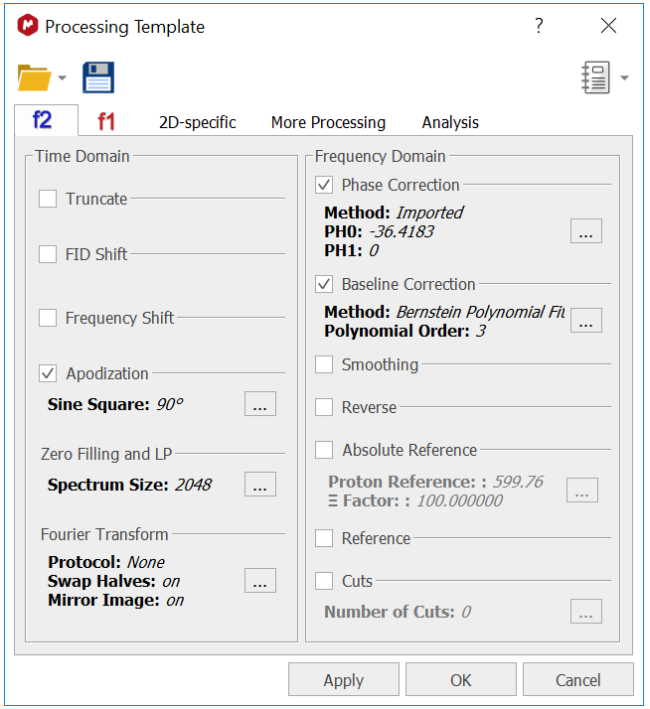
➢ The used parameters can be displayed using the processing Template tool



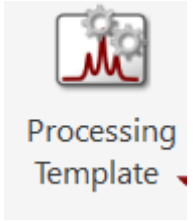

If the automated processed spectrum is not satisfactory to you, you will need to adjust some of the processing parameters to improve it.

➢ The first tool you can try is the Advised Processing, which applies parameters suggested by Mnova and reprocesses the spectrum.

➢ If the results is still not satisfactory, follow the next pages to adjust the parameters manually.

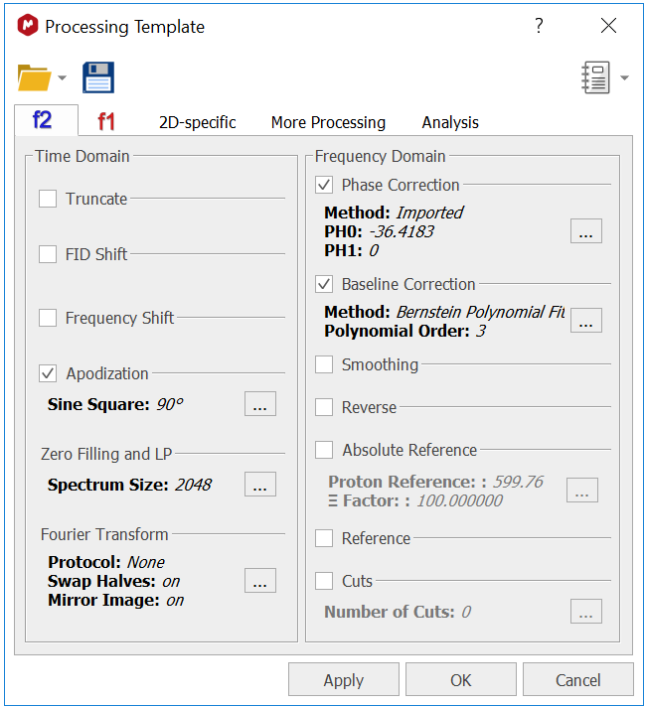


# Rules of thumb for 2D processing

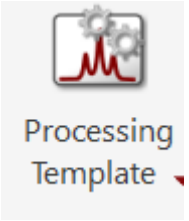



The following processing parameters are usually closed related the quality of the processed spectrum:

- 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, 512 or 1024
  - 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

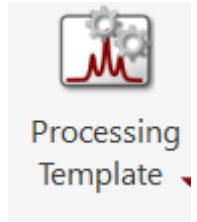



The 2D processing parameters that you may want to adjust and their recommended values*

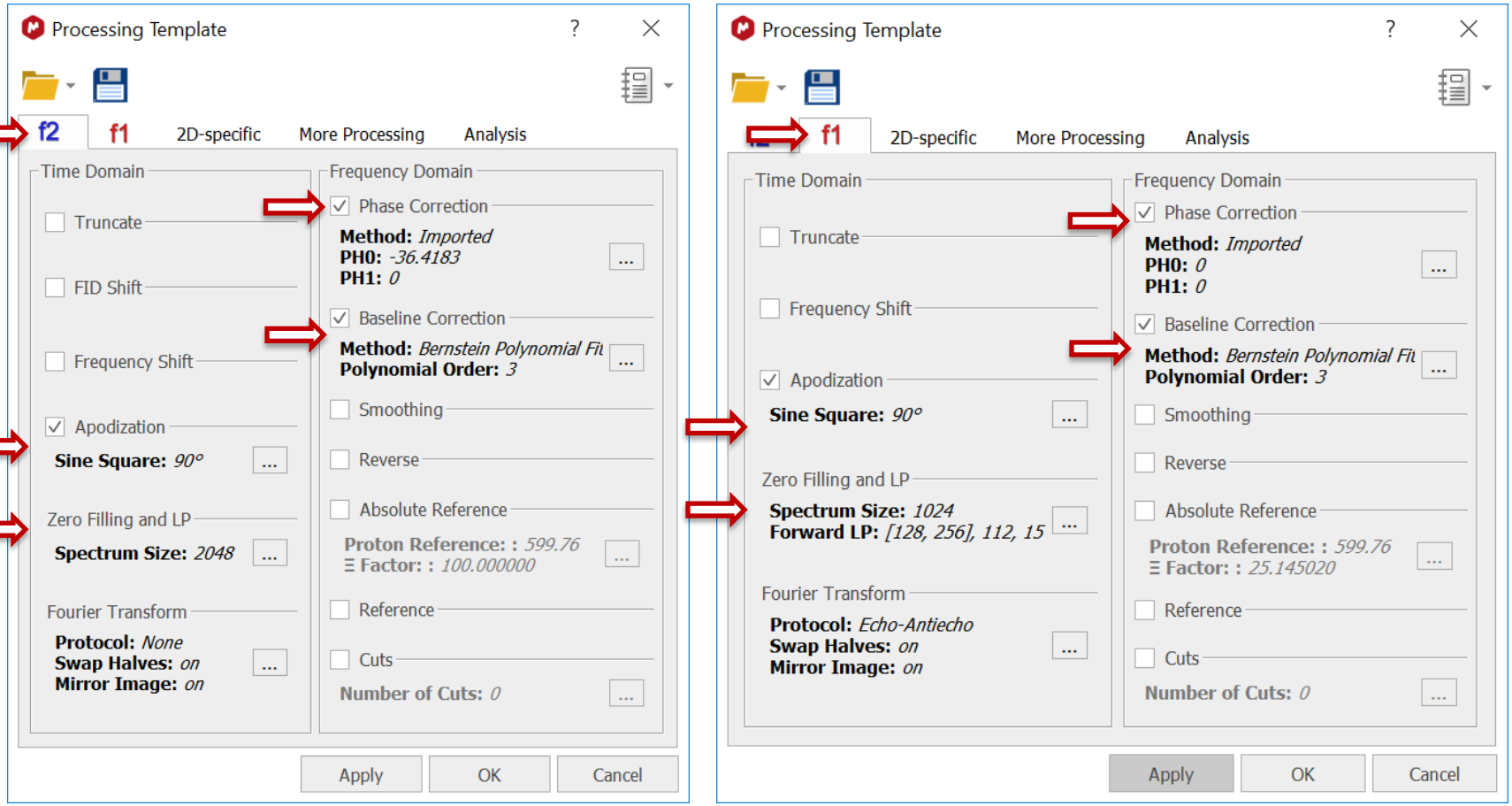
| | Apodi -zation | Zero-fill & Linear Prediction | Phase Correction | Baseline Correction | Others |
|---|---|---|---|---|---|
| **COSY** | Sine square 0 on both F2 and F1 | At least double to 2K or 4K on F2; or 512 or 1K on F1. Do linear prediction on F1 if # of increments < 128 | Use imported parameters 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



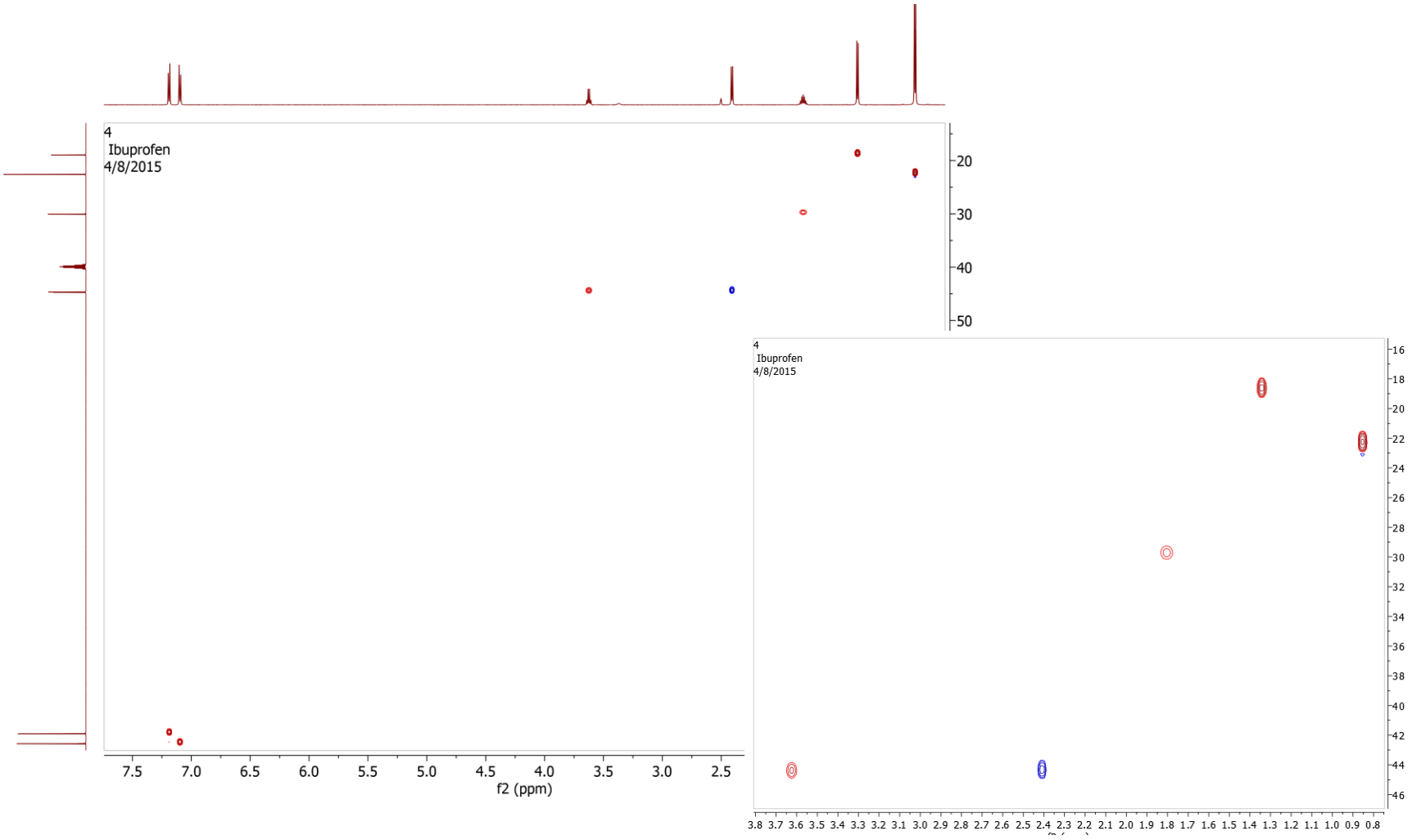

- Reprocess the HSQC spectrum as shown below.
- Note the apodization functions for F2 and F1
- Note the forward linear prediction for F1 applied here



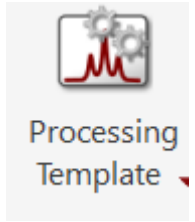

*Note: The Fourier Transform method is automatically set and normally you don't need to change it.*

# Re-process HSQC spectrum

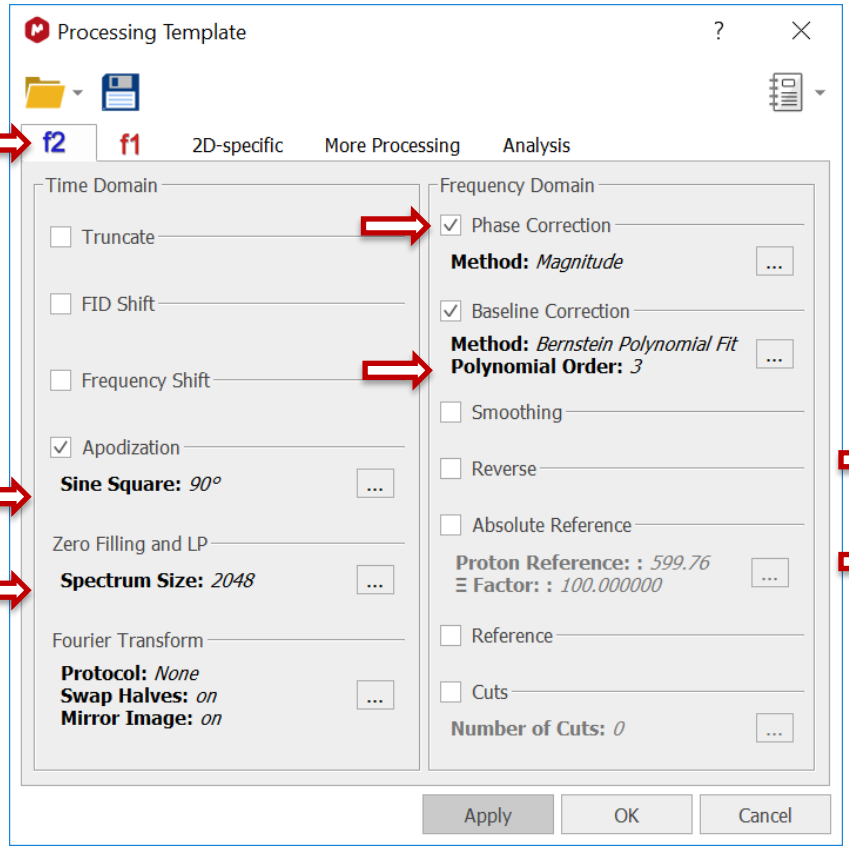
- The re-processed HSQC spectrum shows better line shape, and higher resolution on the F1 dimension

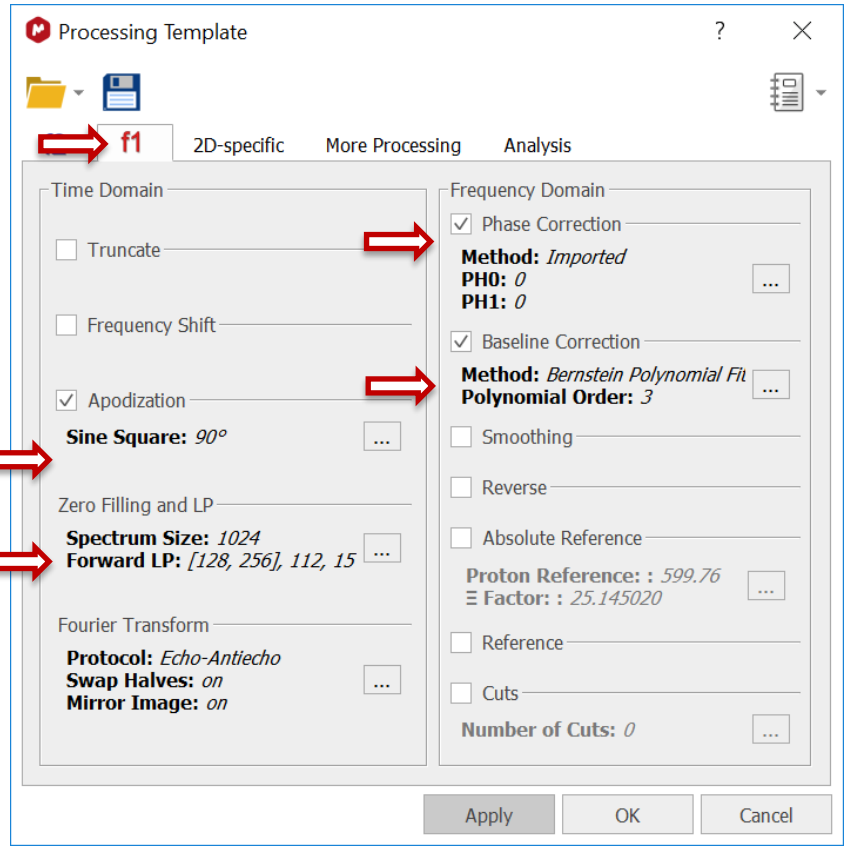


# Re-process HMBC spectrum




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

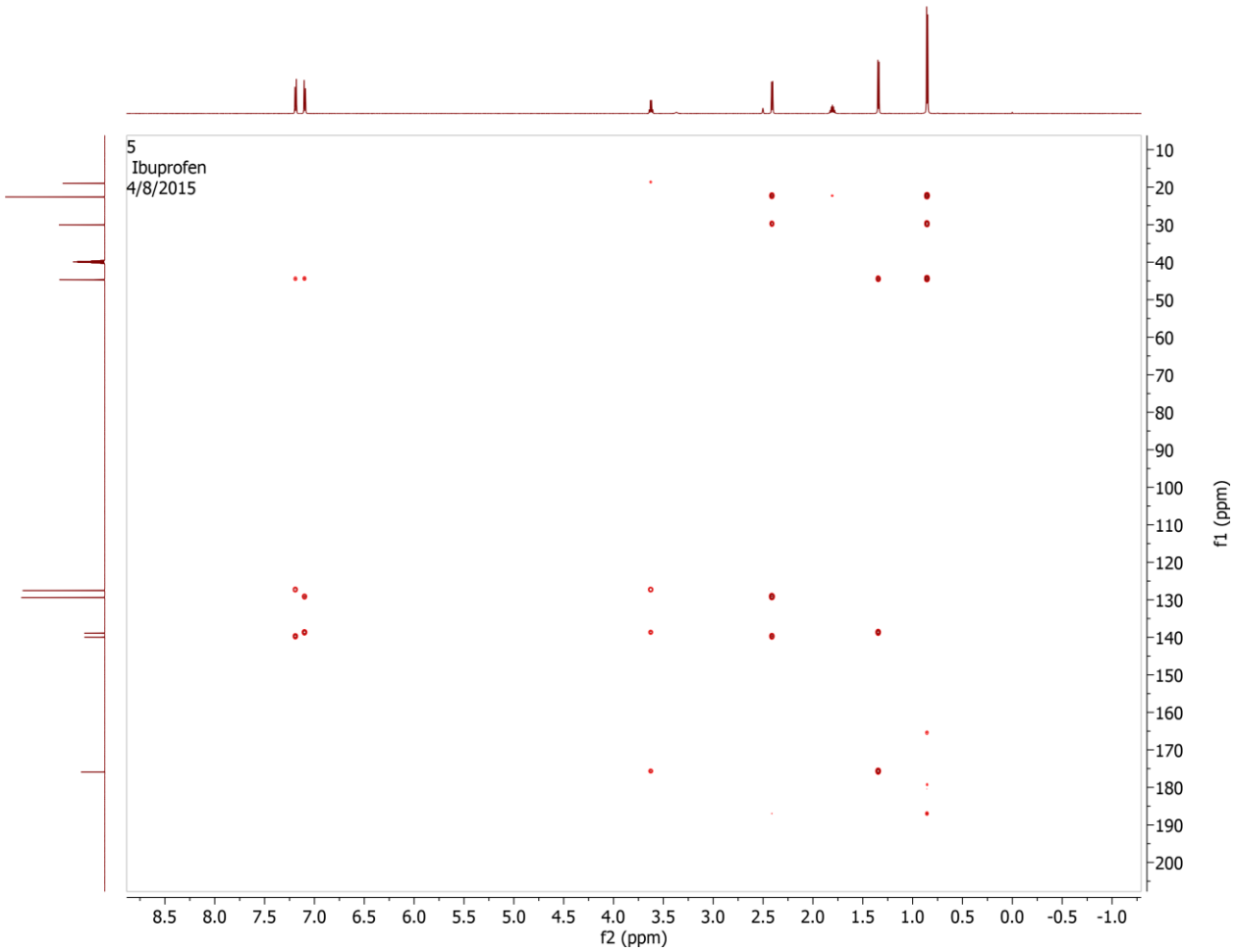



*Note: The Fourier Transform method is automatically set and normally you don't need to change it.*

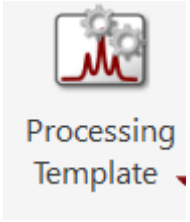
# Re-process HMBC spectrum

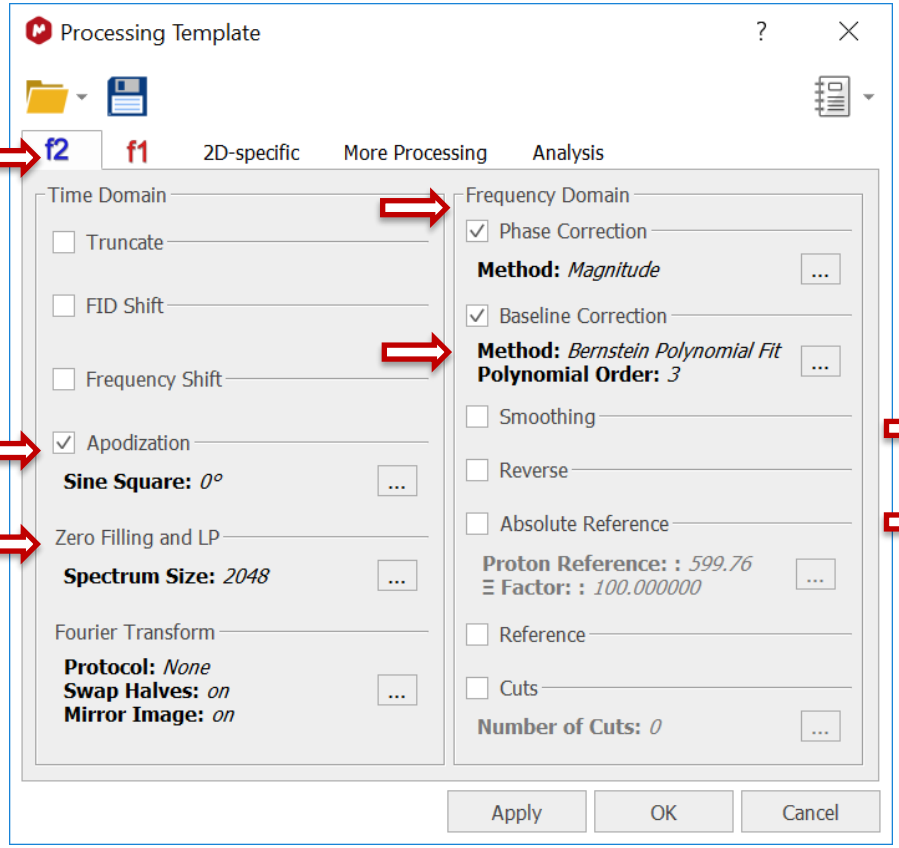
- The re-processed HSQC spectrum shows better line shape, and higher resolution on the F1 dimension

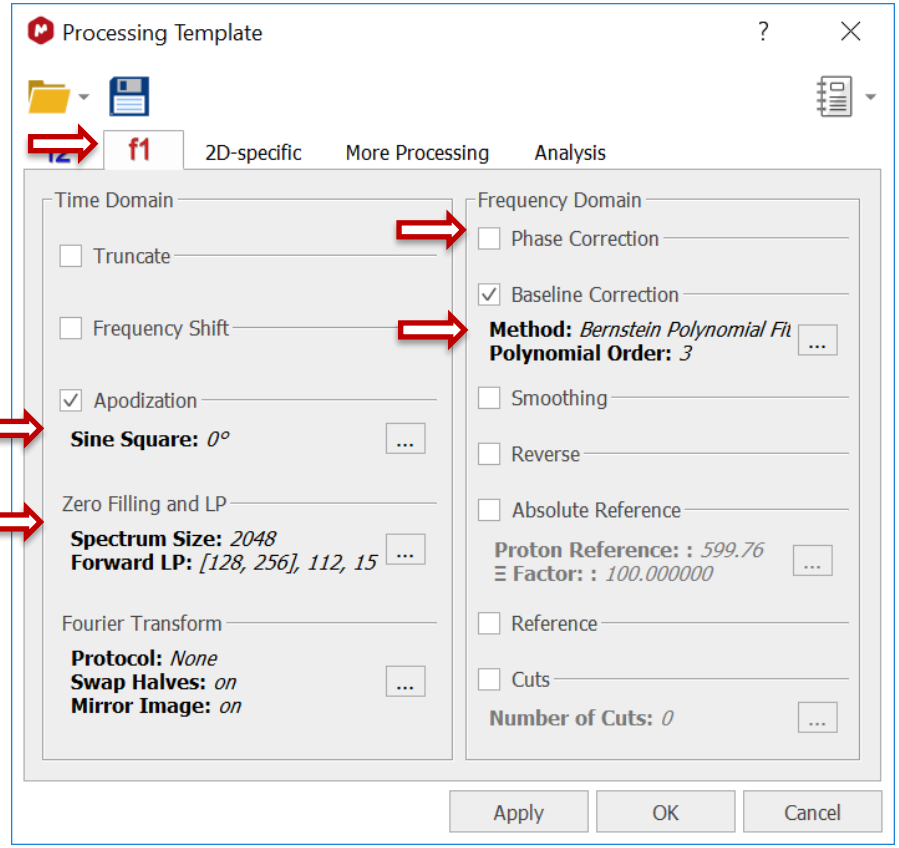


# Re-process COSY spectrum

- 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



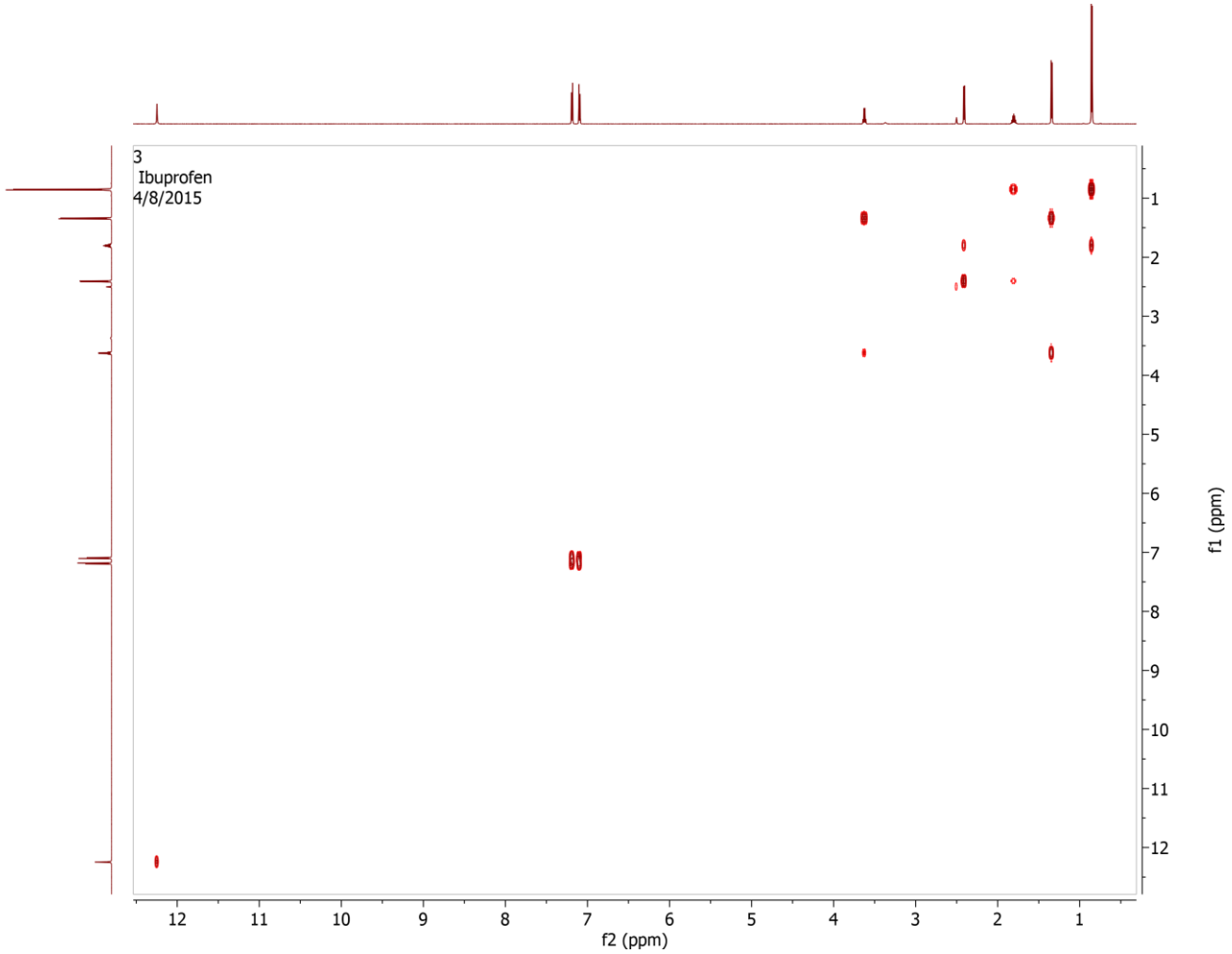



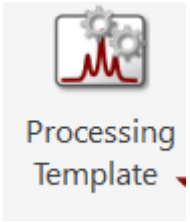

*Note: The Fourier Transform method is automatically set and normally you don't need to change it.*

# Re-process COSY spectrum

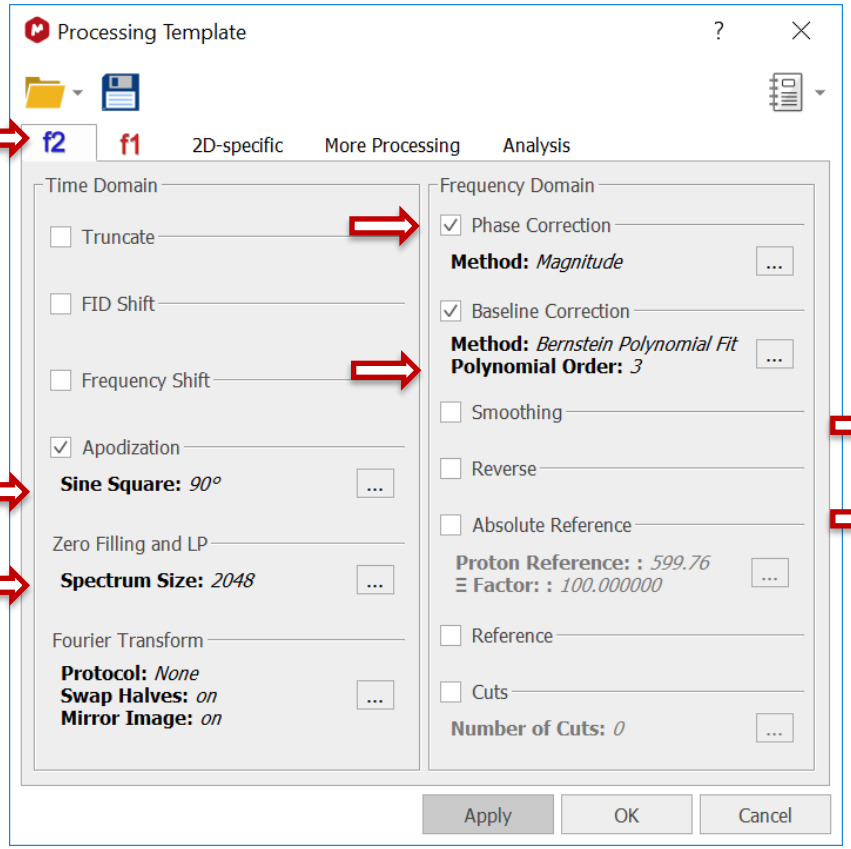
- The re-processed COSY spectrum shows better line shape, and higher resolution on the F1 dimension

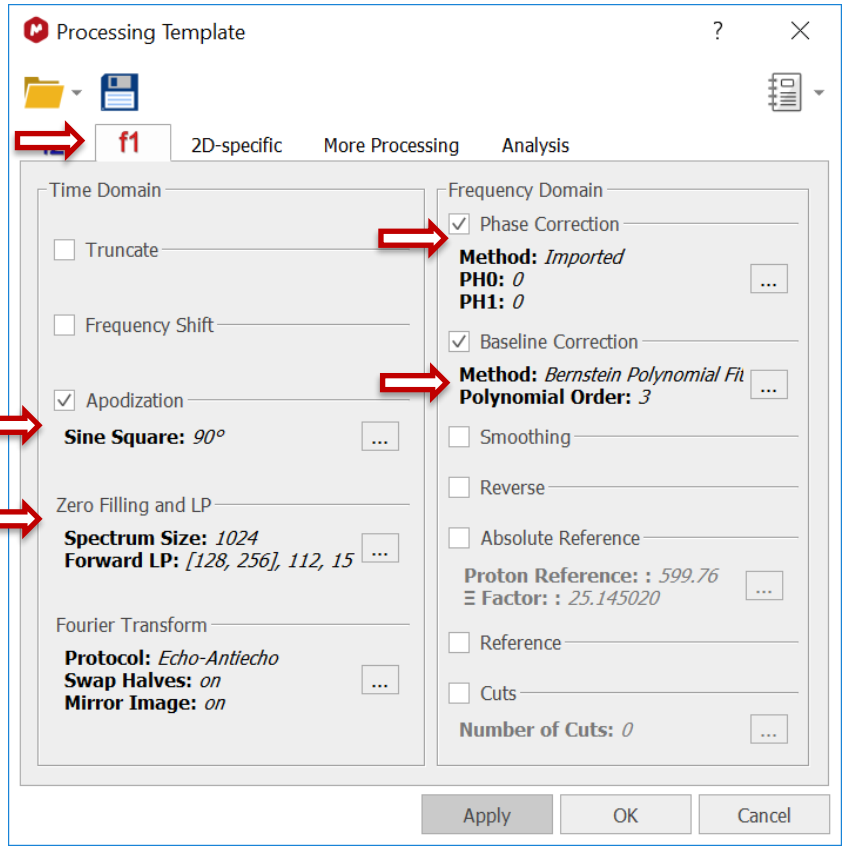


# Re-process NOESY spectrum




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

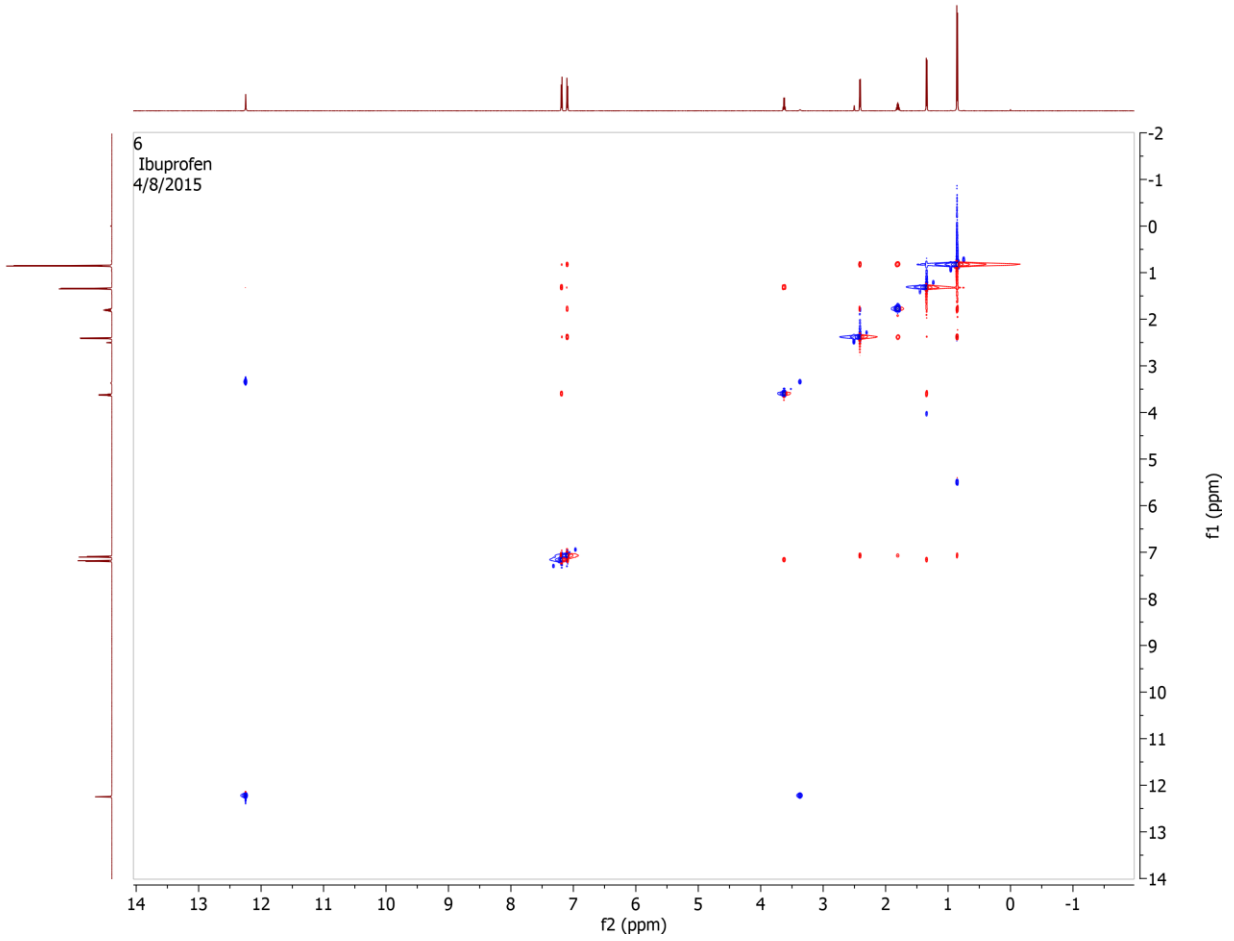



*Note: The Fourier Transform method is automatically set and normally you don't need to change it.*

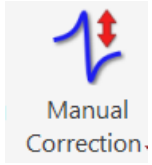
# Re-process NOESY spectrum

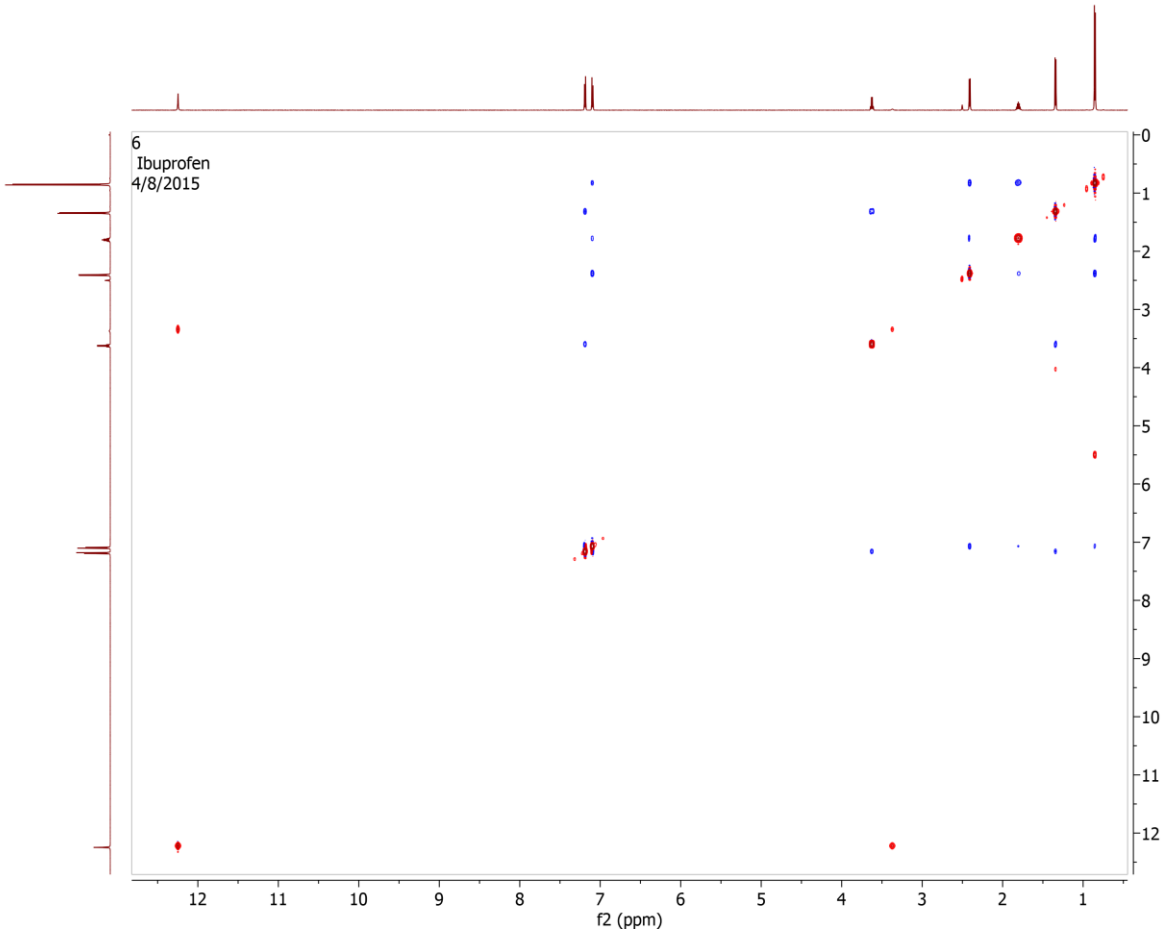
- The re-processed NOESY spectrum shows better line shape, and higher resolution on the F1 dimension, though there still some phase errors

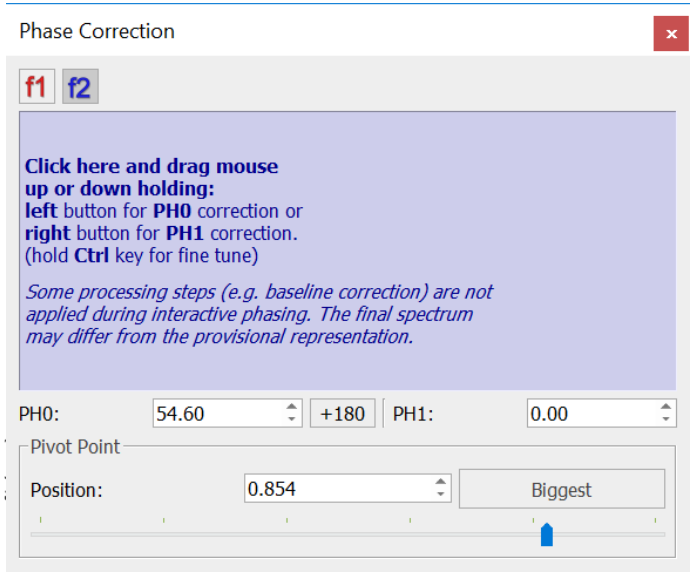


# Phase correction for NOESY spectrum

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



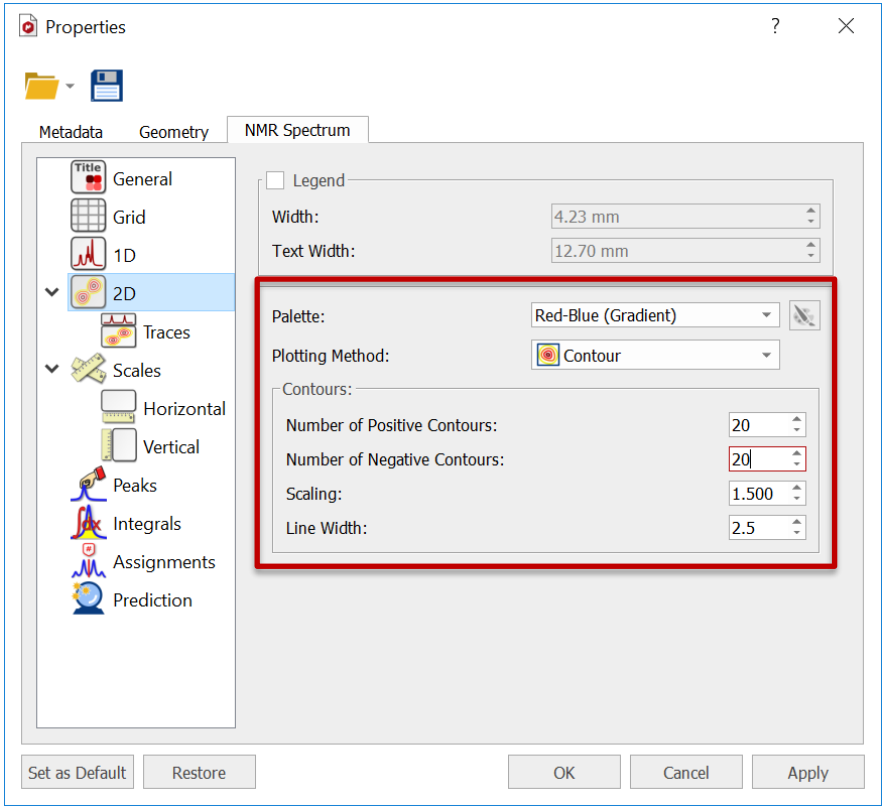



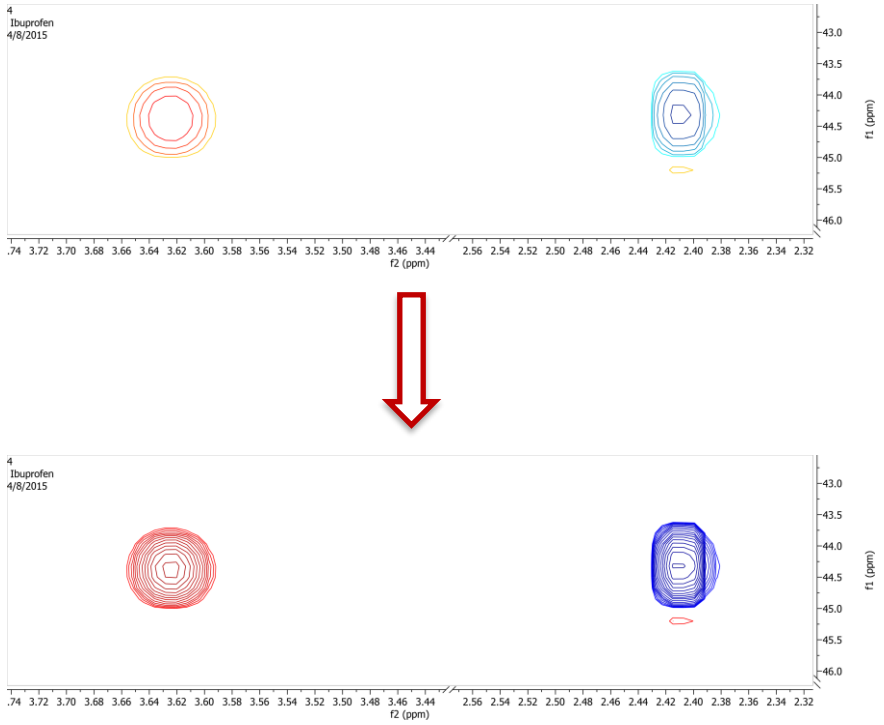



# Change the Display Properties



- 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

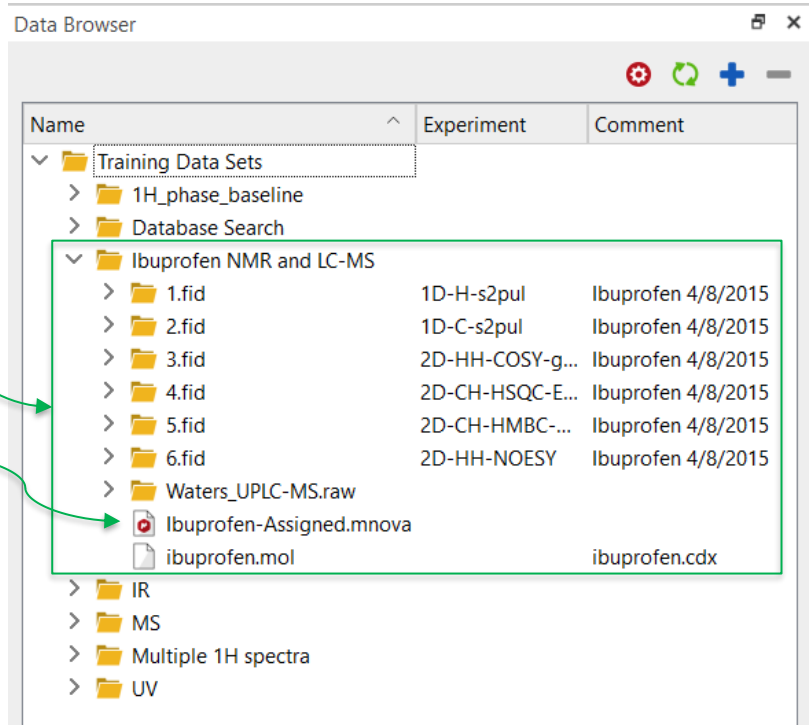


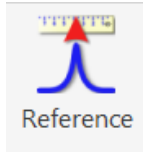
# Peak Assignment Using 1D & 2D NMR Spectra Together

Sample data

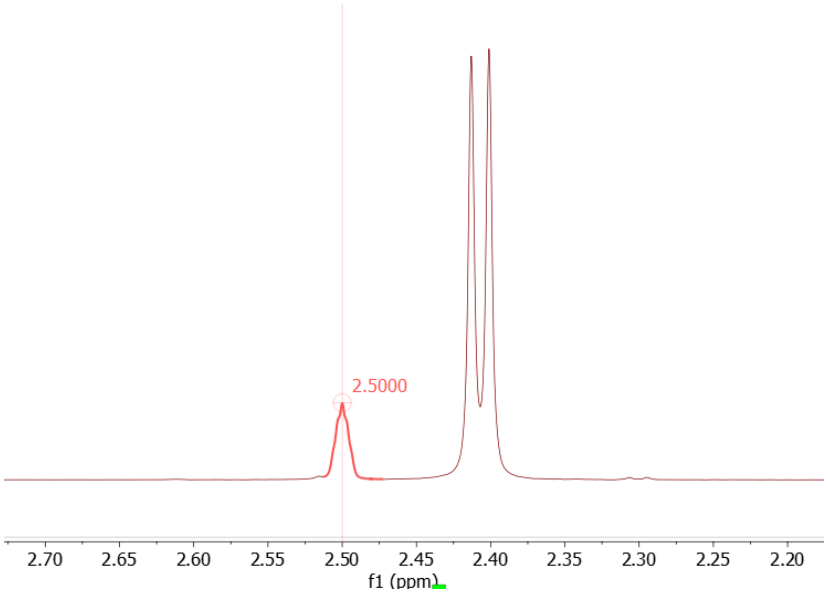
*This .mnova document has all 1D and 2D spectral peaks assigned to the atoms in Ibuprofen.*

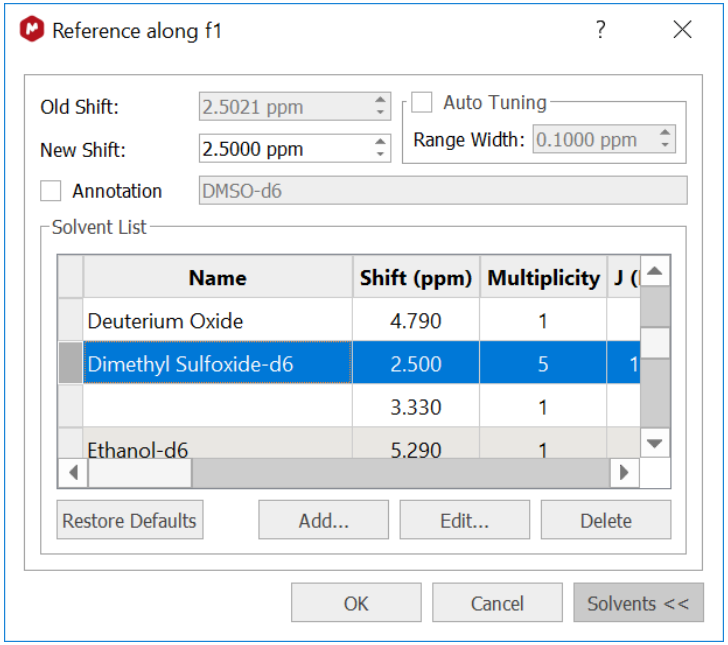


# Chemical shift referencing for H-1



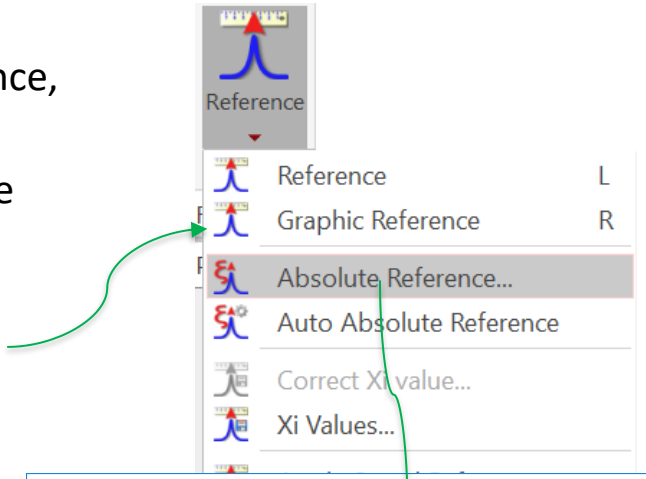

- This spectrum uses DMSO-d6 as the solvent. We can reference the chemical shifts by setting its middle peak to 2.5 ppm.
- Zoom to the DMSO peak at around 2.5 ppm. Choose Analysis > Reference, and click on the top of the middle peak.
- Set it to 2.5 ppm either manually or from the Solvent List.

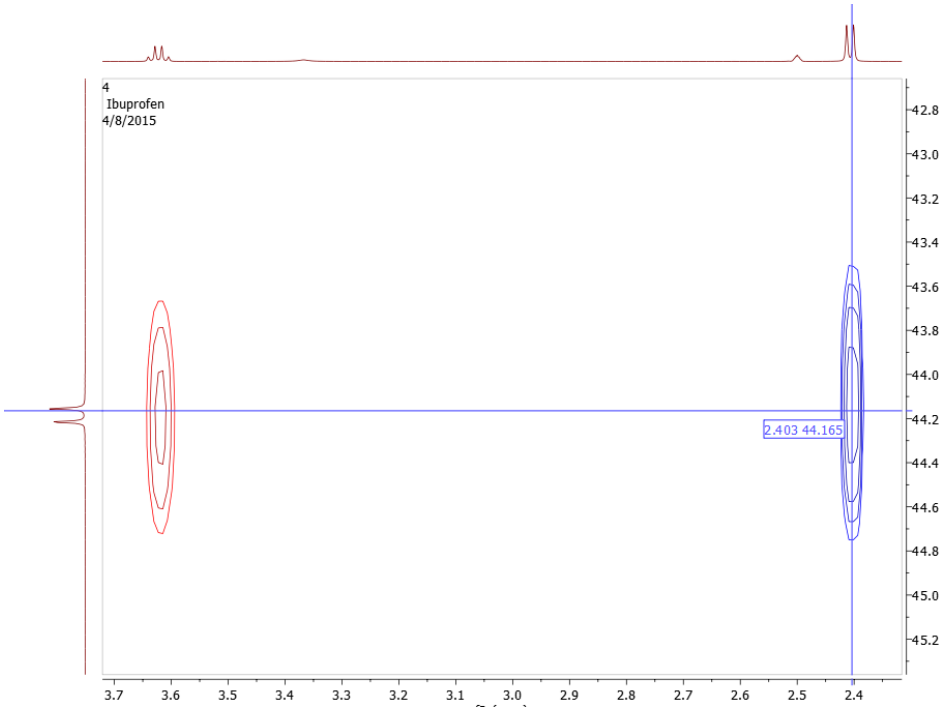


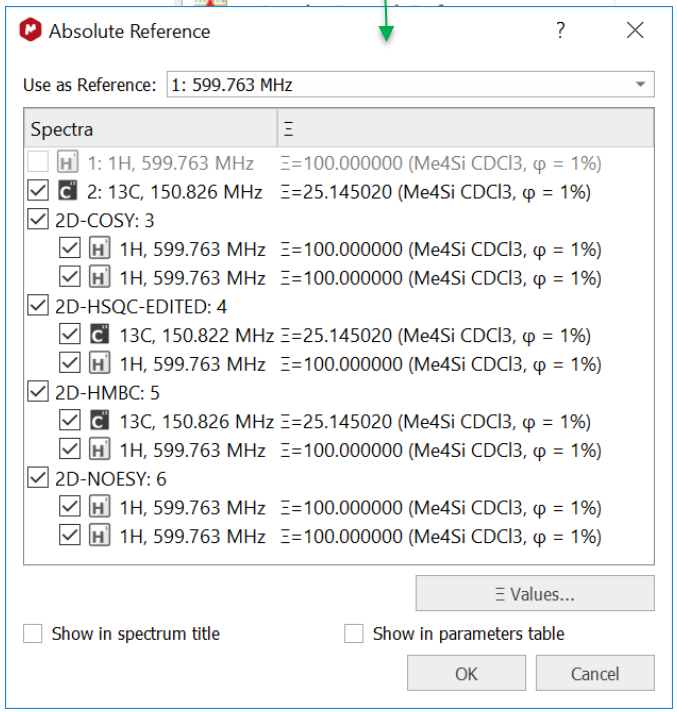



# Chemical shift referencing for other spectra

- 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.

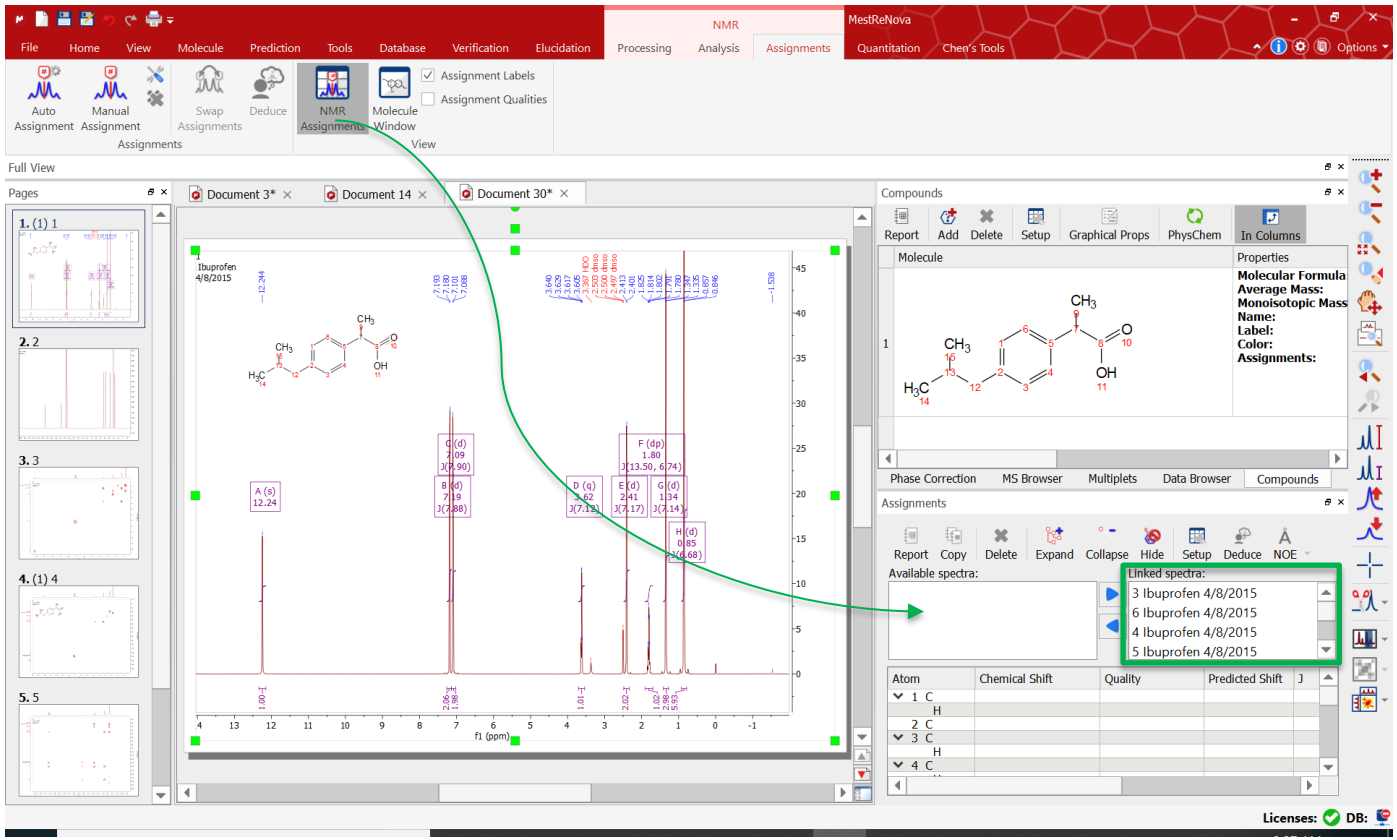


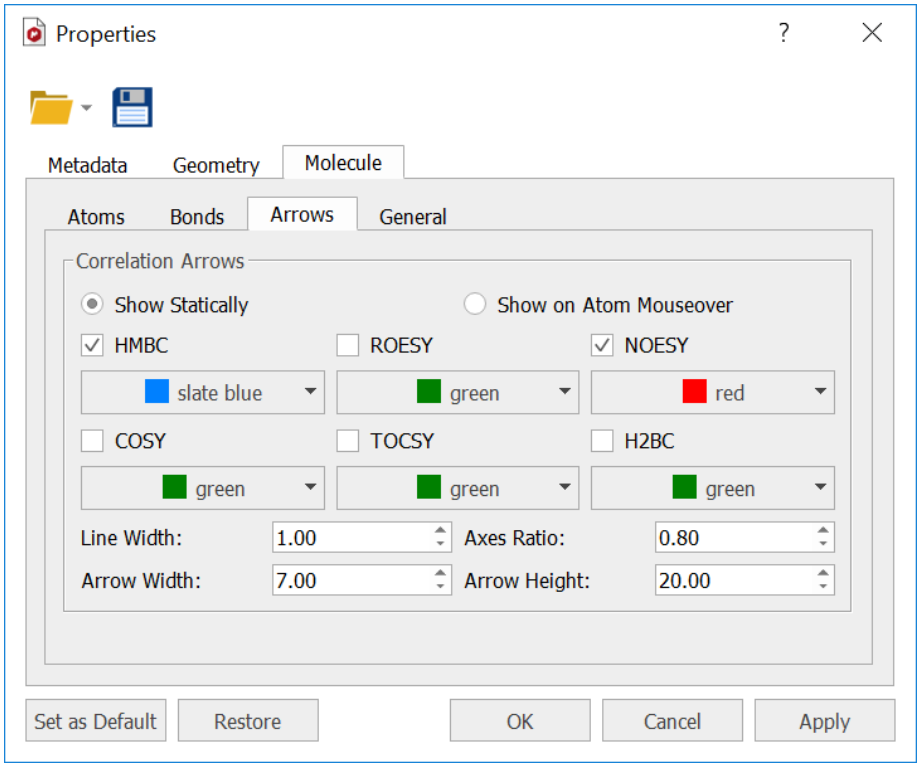
# Open the structure for peak assignment

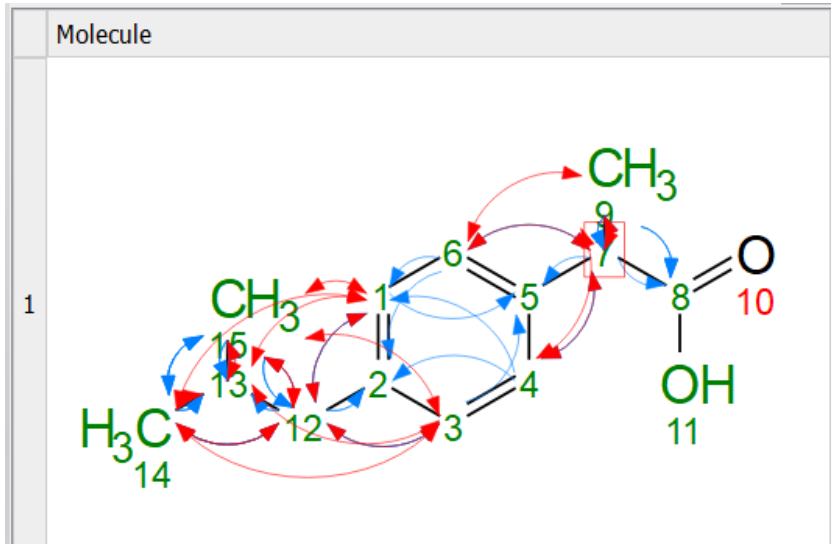
- Open the Ibuprofen.mol file from the Data Browser.
- Choose Molecule > Compound Table to show the structure on the side.
- Note: Open the same molecule only once. If needed, use Report on the Compound Table to report the structure to other pages. Do not open the same structure multiple times.
- Display 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



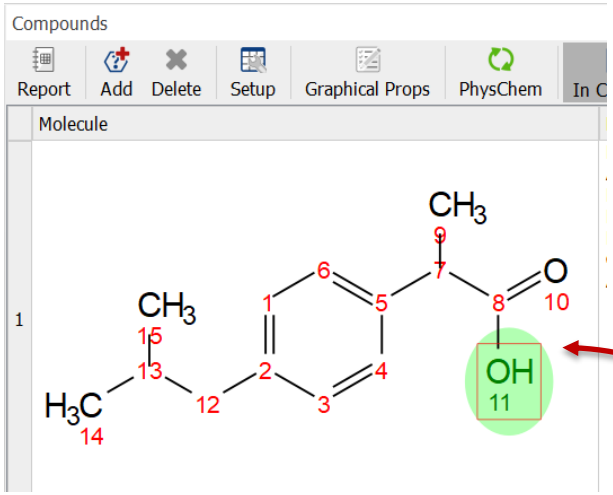



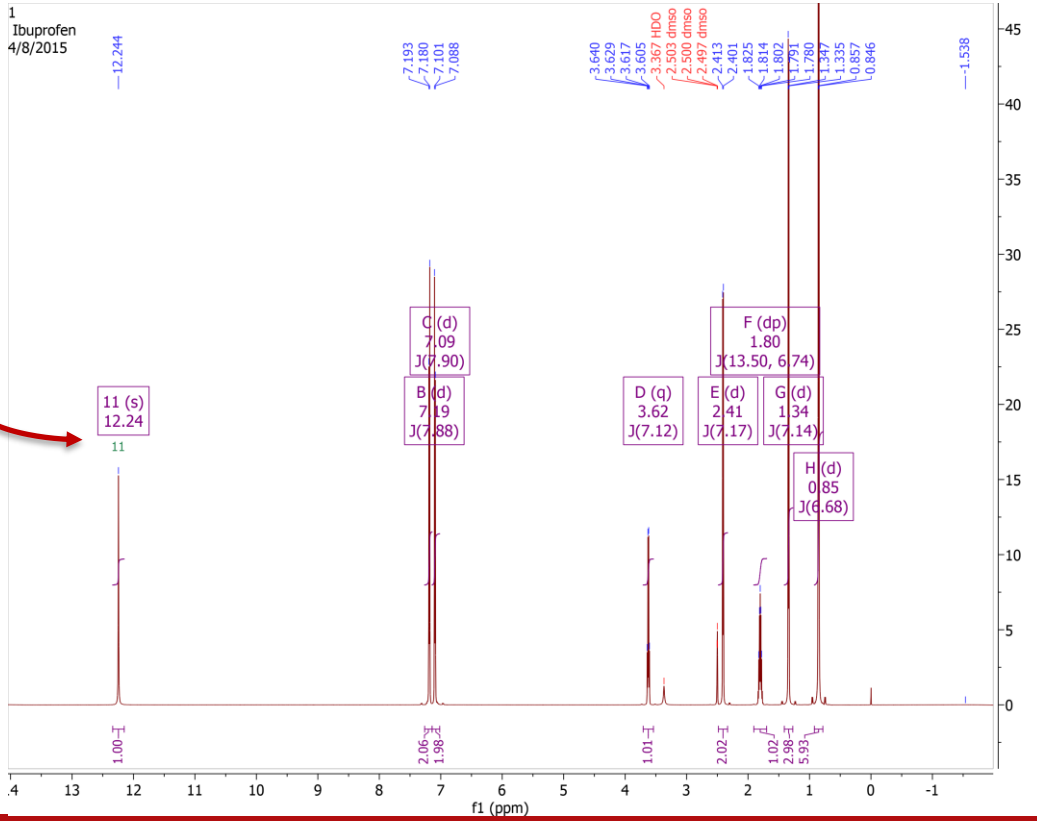

*Tip: Click Save as Default button to save the settings*

# Assign H-1 multiplets


Shortcut = A

- 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




**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

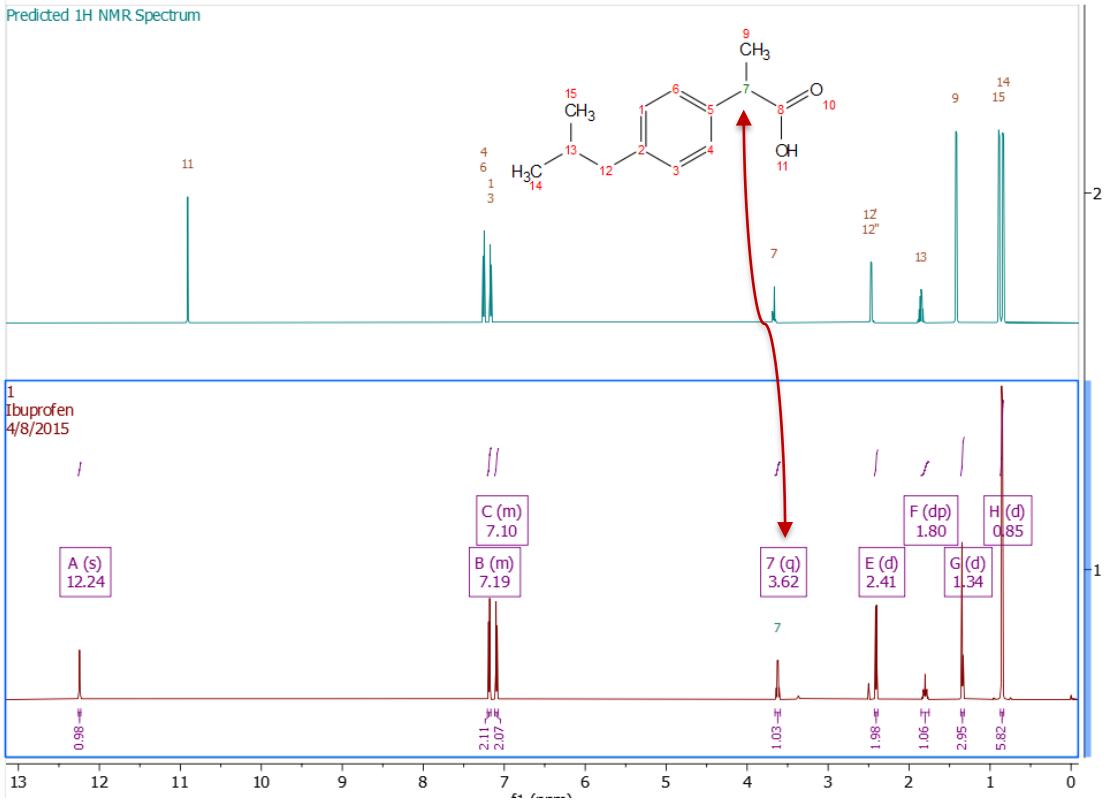
- Optionally, you can choose Predict > Predict and Compare to have a predicted H-1 spectrum stacked above the experimental one to guide your assignment of some peaks
- For example, the predicted quartet for H-7 is very close to the quartet observed at around 3.62ppm, so we can assign that observed quartet 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.


Shortcut = A

*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*

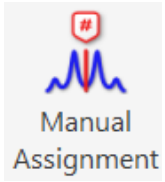
*If you need a copy of the structure in a page, click the structure in the Compounds Table and click Report.*

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

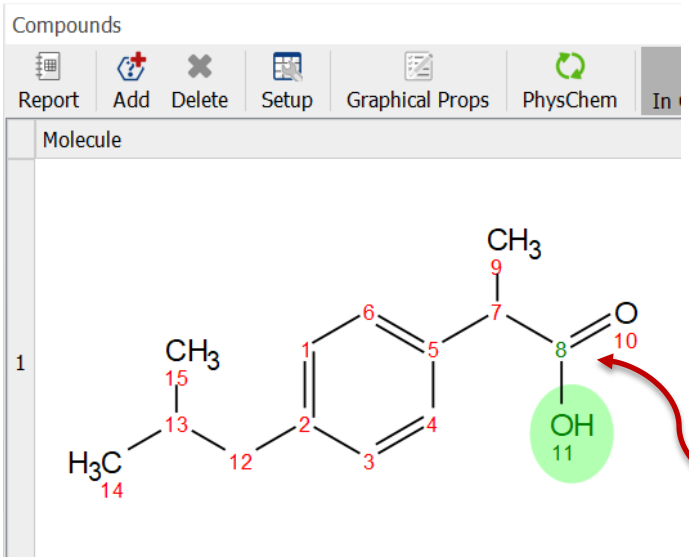


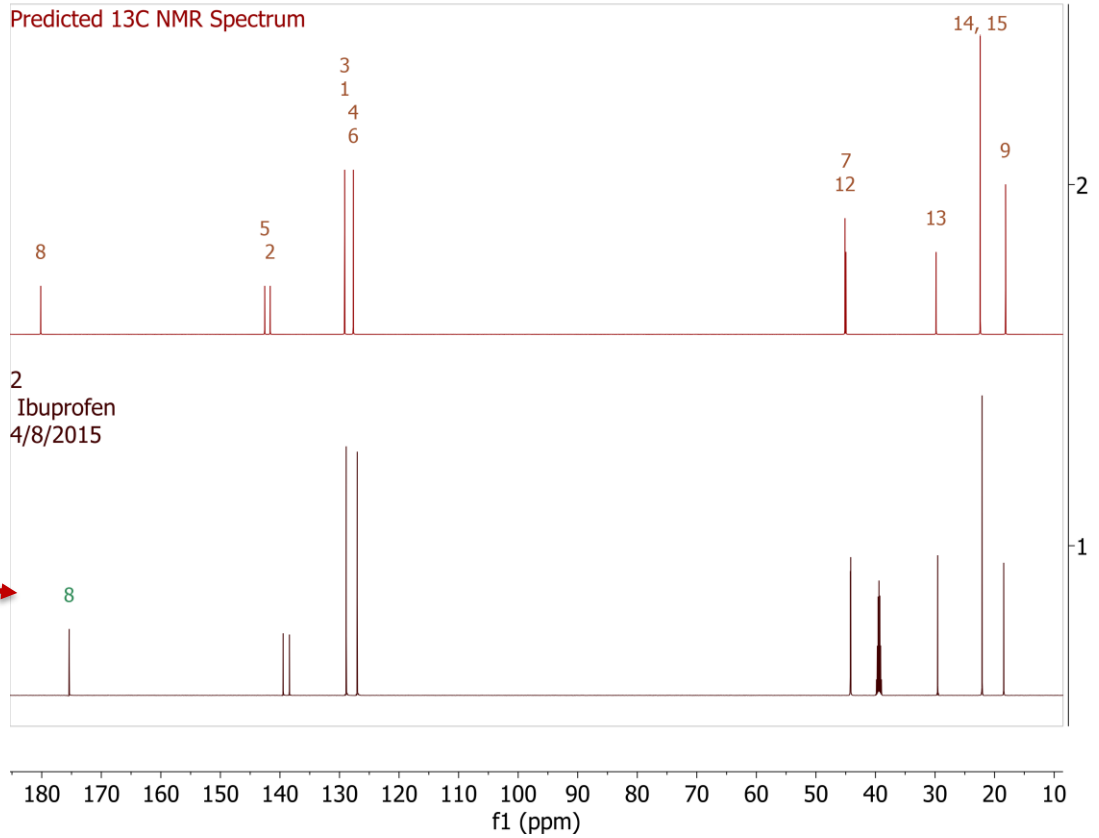
# Assign C-13 peaks

- 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



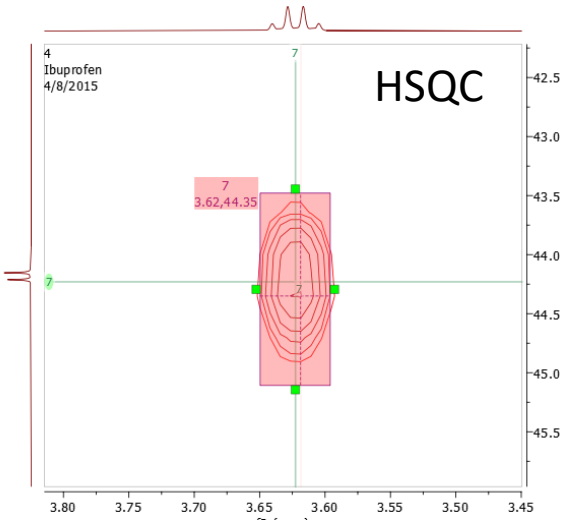

Shortcut = A



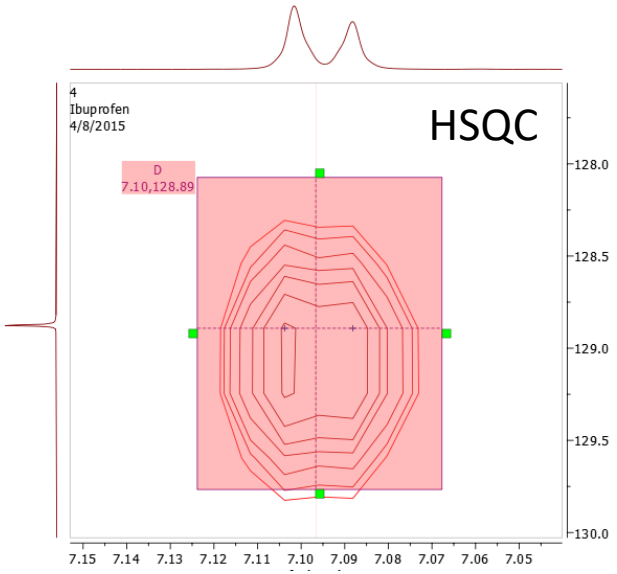



# General guidance for assigning 2D spectra

- 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

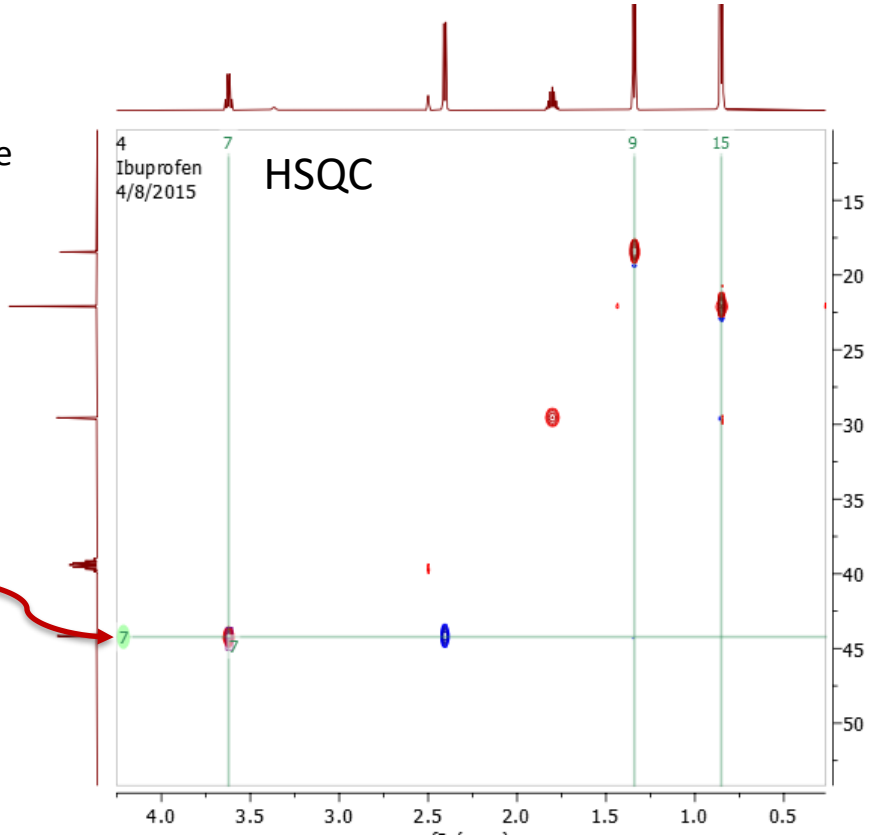
*Tip: For better visualization of the assignment results on a 2D spectrum, it is better to suppress the display of the 2D peaks and 2D multiplet labels. Right click on the spectrum and choose Properties, and turn off those options.*

# 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.

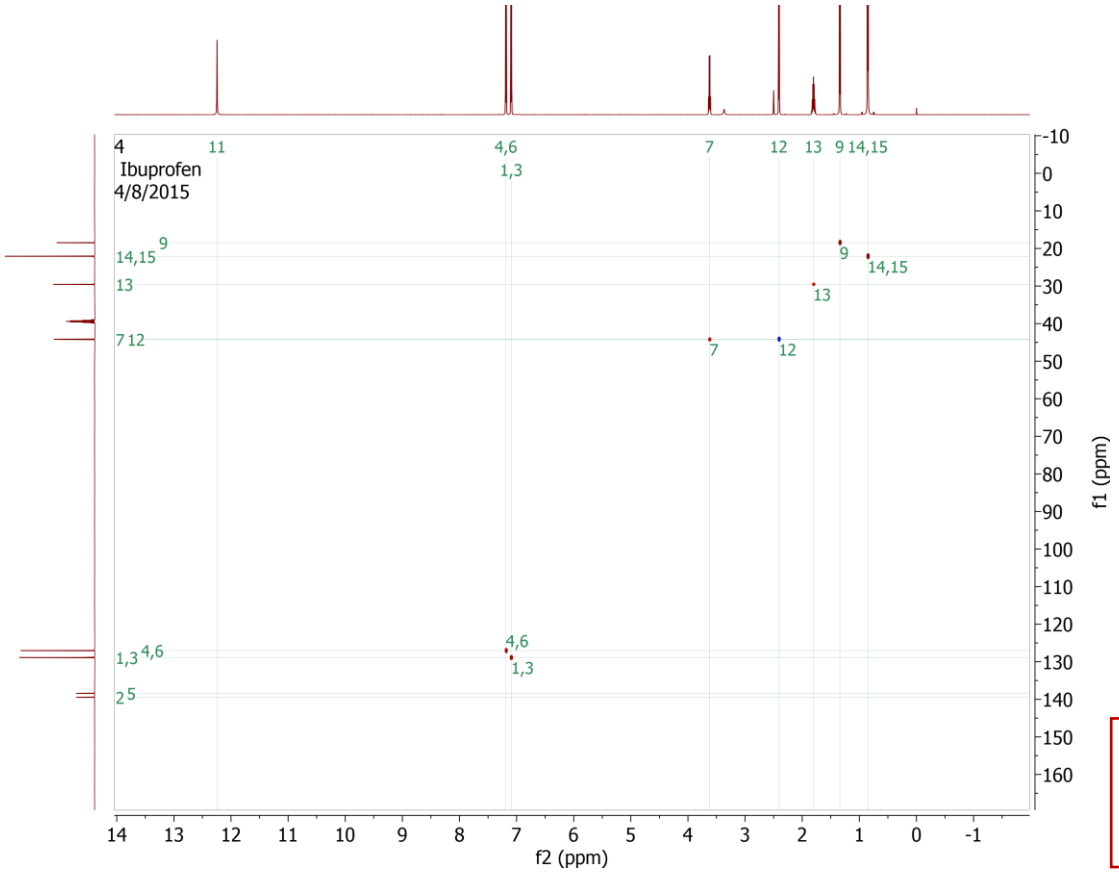

Shortcut = A

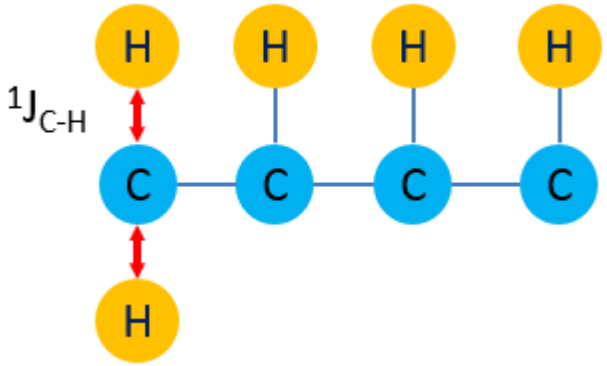
*Tip: Click and drag the number ("7") to adjust the chemical shift value of this assigned peak in the C-13 dimension. The change will be reflected in all other spectra, as well as in the Assignment Table. You can do this on 1D spectra too.*

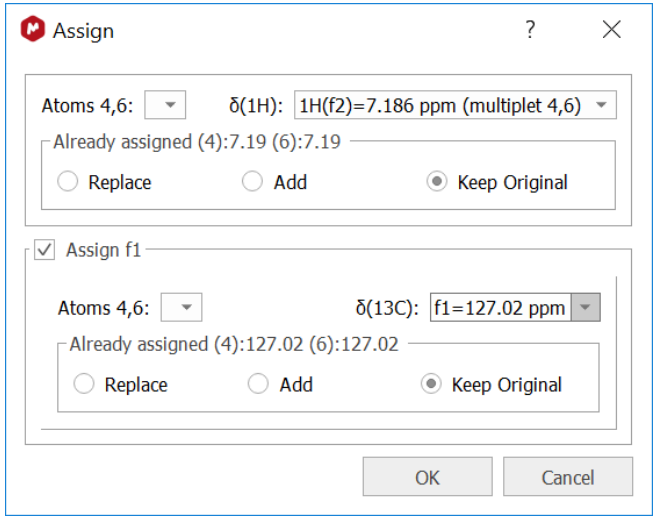


# Assign HSQC peaks

- 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*



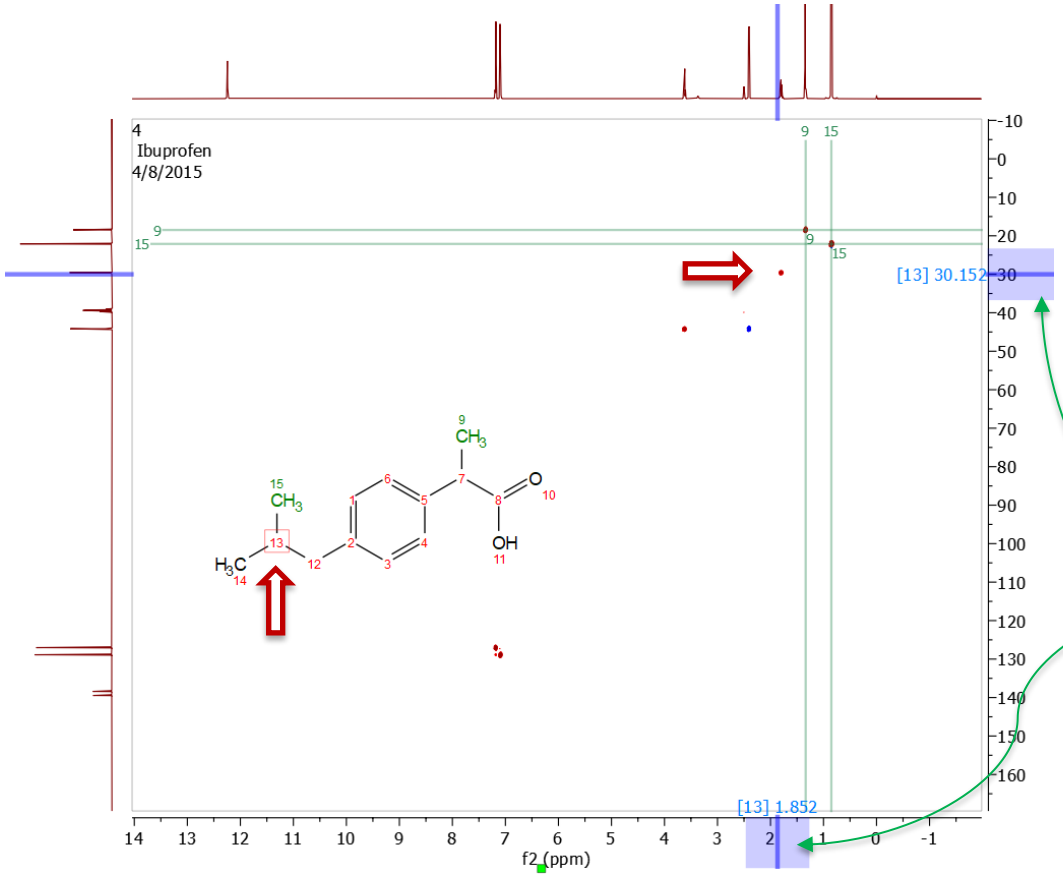




*The assigned chemical shifts can be from 1D or 2D peaks. Since a 1D spectrum typically has higher resolution, it is recommended to use those from 1D. Note you can also fine tune the chemical shift by moving the atom number on an assignment line.*

# Use Predict & Highlight to help assigning HSQC peaks

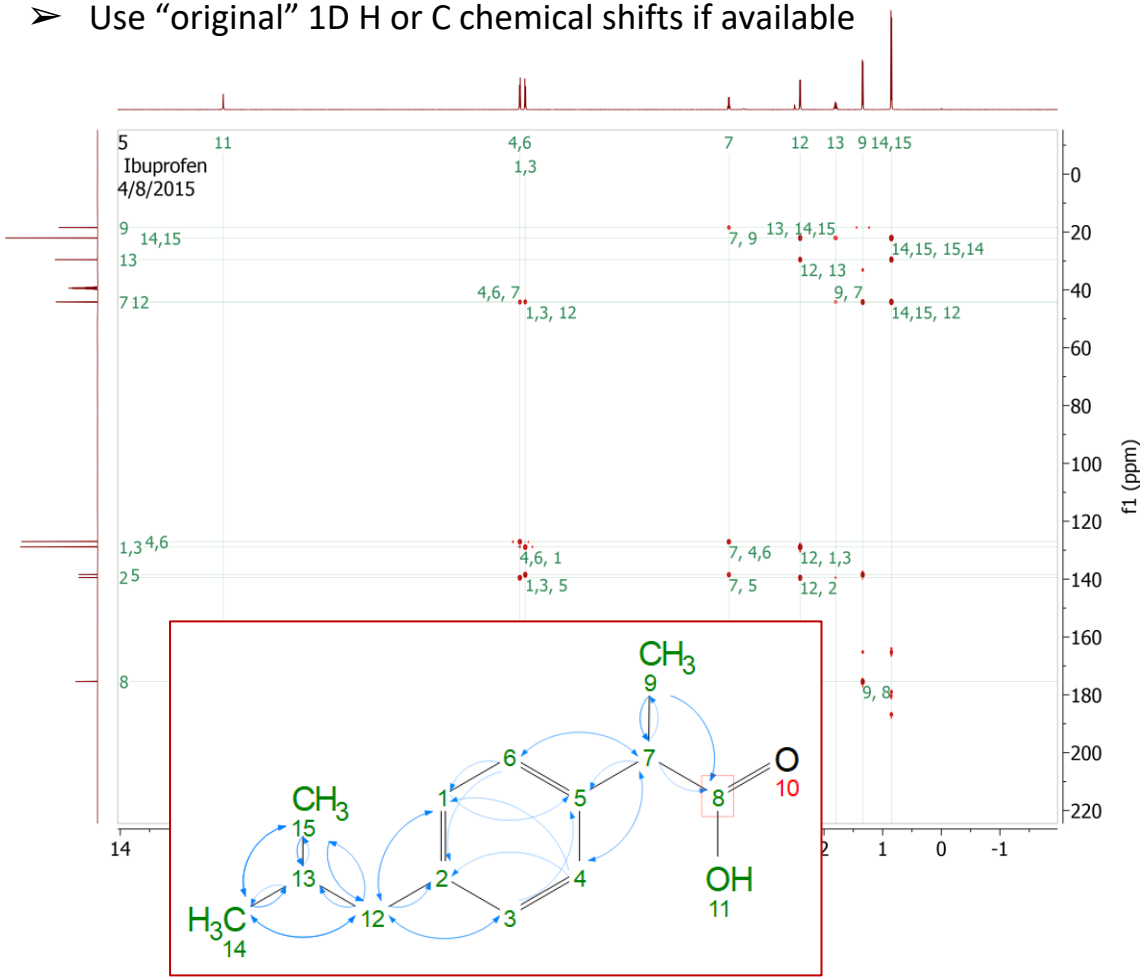
- Optionally, you can choose Predict > Predict and Highlight to display the predicted range of HSQC peaks for CH groups. The ranges can be helpful for assigning HSQC peaks to their corresponding CH groups

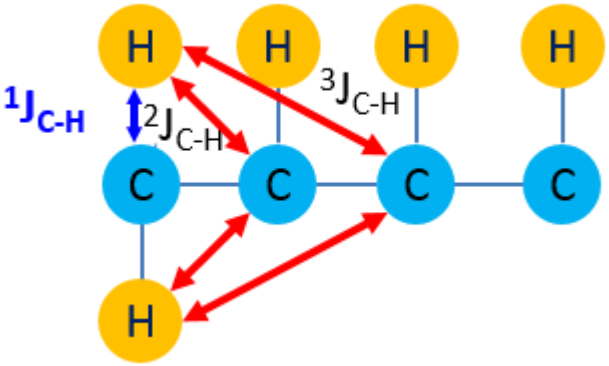


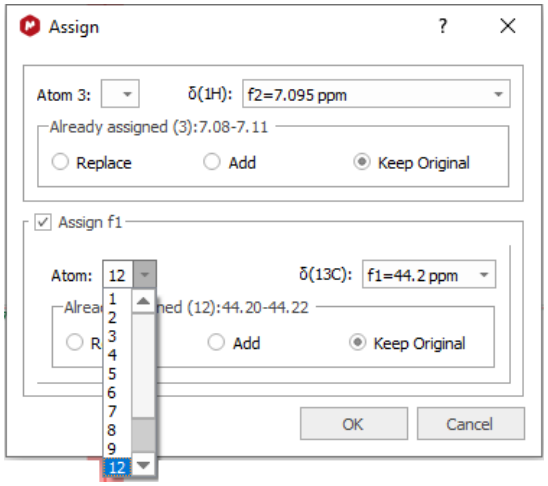

**Click on CH(13), it shows the value and error range of its predicted C-13 and H-1 shifts. This gives you an idea where to look for the cross peak to assign to this CH group.*

# 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

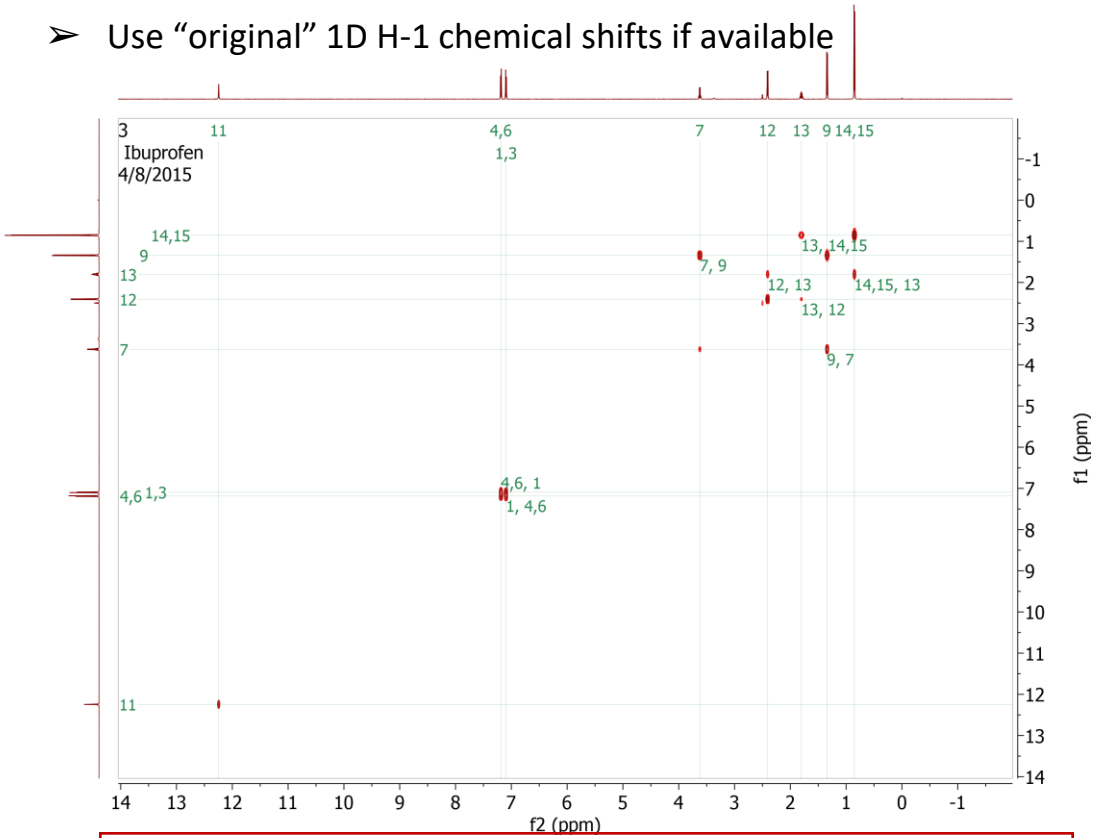


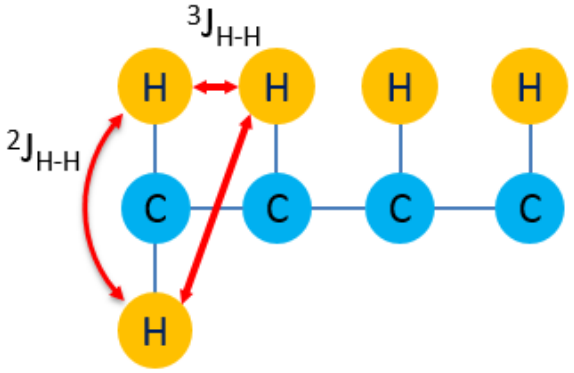



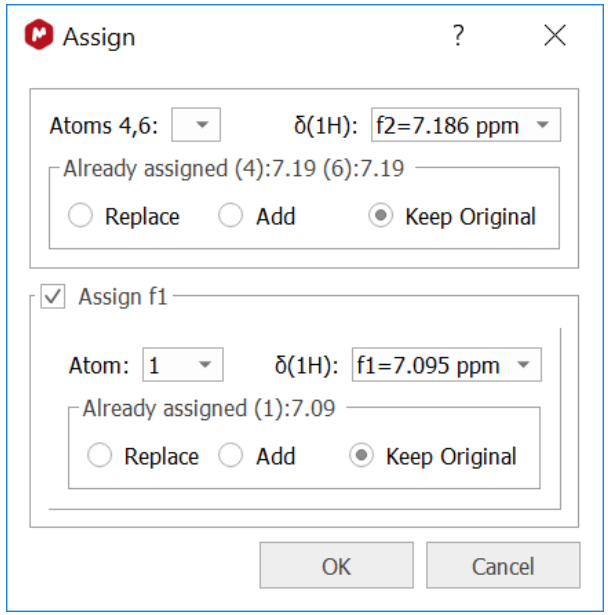



# Assign COSY peaks

- 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



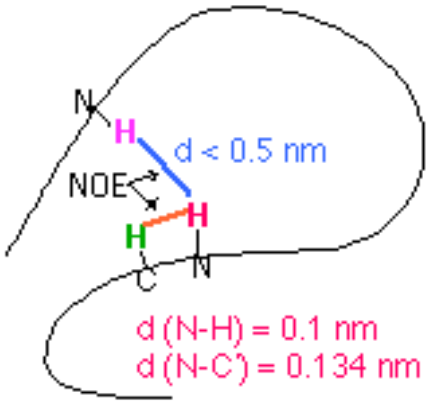



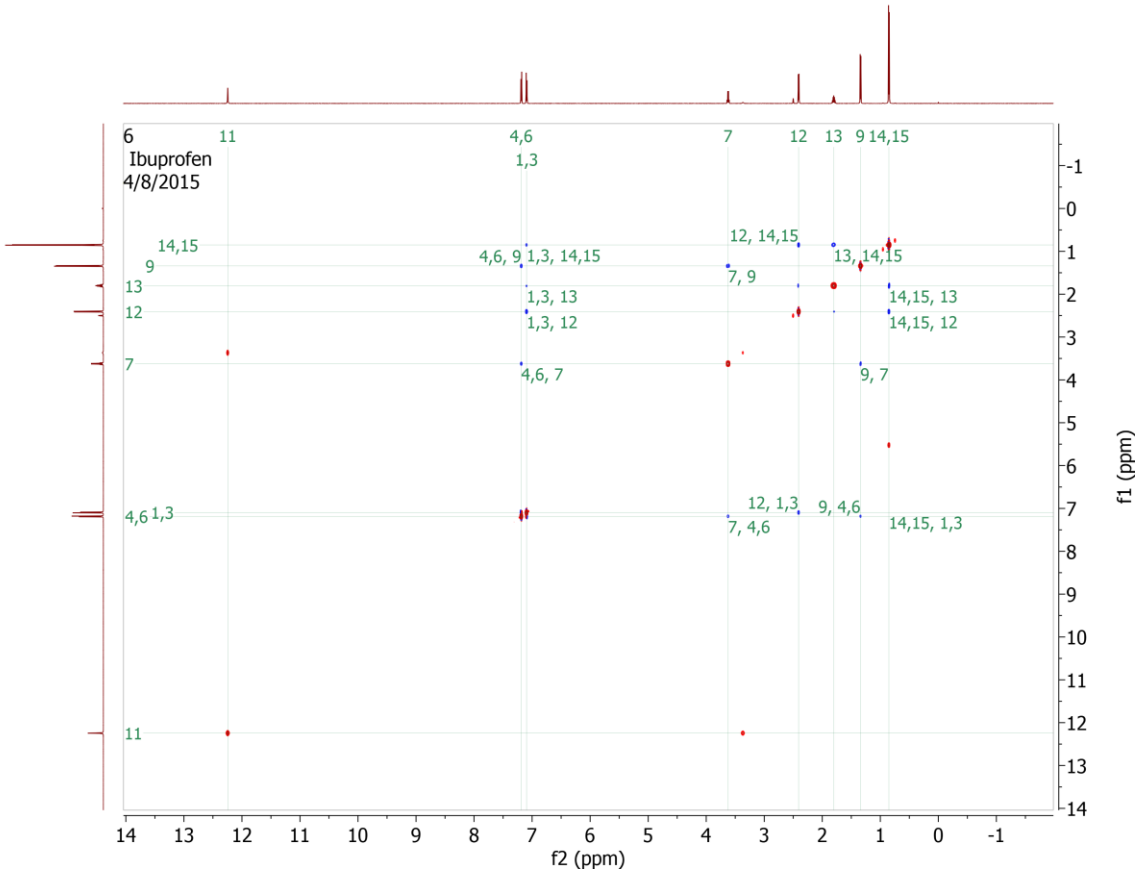



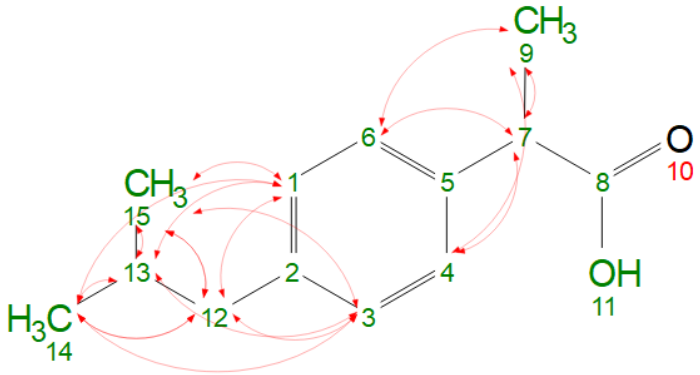

*Tip: Displaying the diagonal line can be helpful to distinguish cross peaks and diagonal ones. To do that, right click and open the Properties Dialog, and check Grids > Show Diagonal.*

# 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.



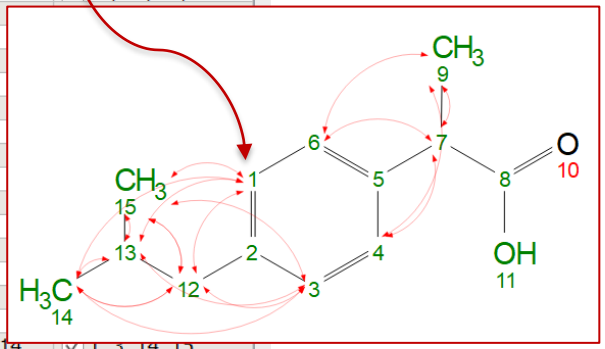
# Assignments table

- 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

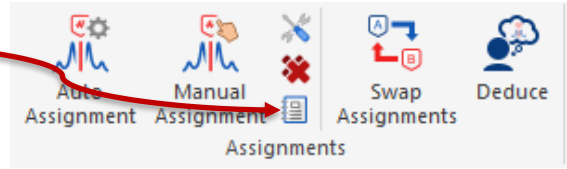
Report Copy Delete Expand Collapse Hide Setup Deduce NOE

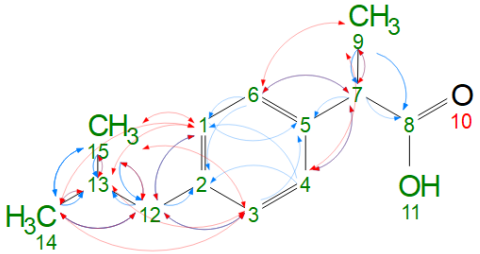
| Atom | Chemical Shift | Quality | Predicted Shift | J | NOE | COSY | HSQC | HMBC | NOESY |
|---|---|---|---|---|---|---|---|---|---|
| 1 C | 128.88 | | 129.12 | | | | 1 | ✓ 4, 6, 12 | |
| H | 7.09 | 0.71 | | | | ✓ 4, 6 | 1 | ✓ 5, 12 | ✓ 12, 13, 14, 15 |
| 2 C | 139.46 | | 141.62 | | | | | ✓ 4, 6, 12 | |
| 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 |



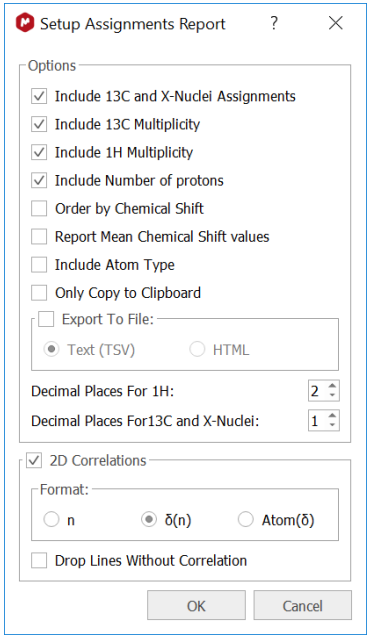
# Report assignments

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



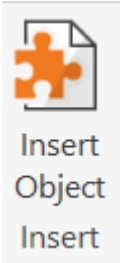



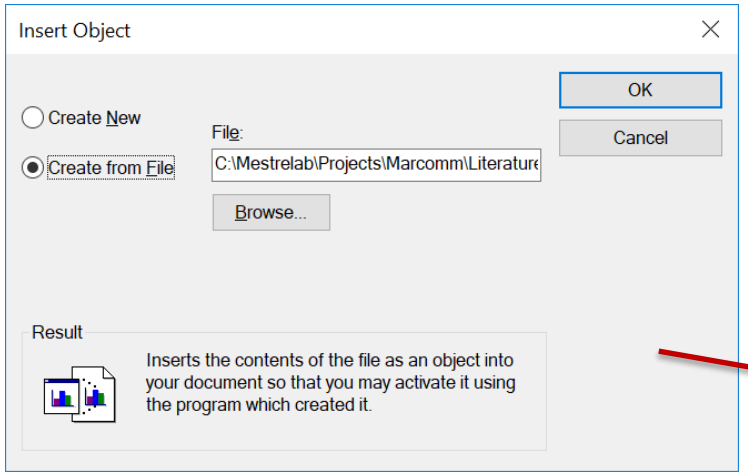

| No | δ H (Multiplicity, J) | δ C | HSQC-EDITED | HMBC | COSY | NOESY |
|---|---|---|---|---|---|---|
| 1 | 7.09 (d, 7.9 Hz) | 128.9 | 128.9(1) | 44.2(12),128.9(1), 128.9(3), 138.4(5) | 7.19(6) | 0.85(14), 0.85(15), 1.80(13),2.41(12) |
| 2 | - | 139.5 | - | 2.41(12),7.19(6) | - | - |
| 3 | 7.09 (d,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

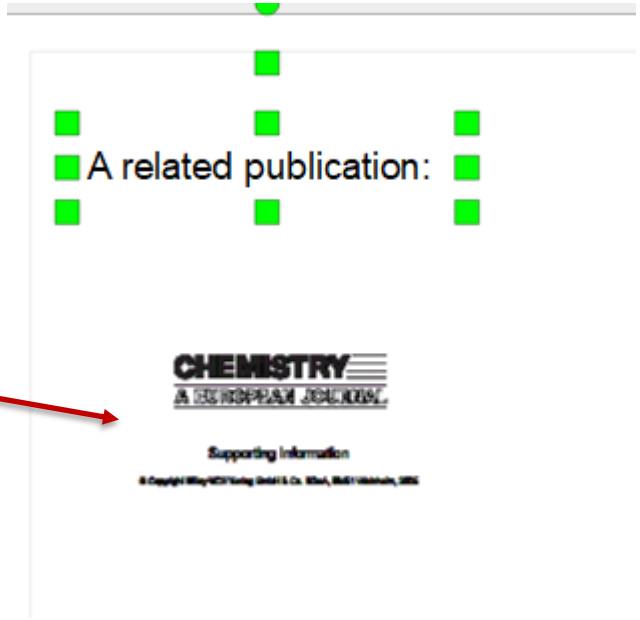


# Insert a PDF to the document

- 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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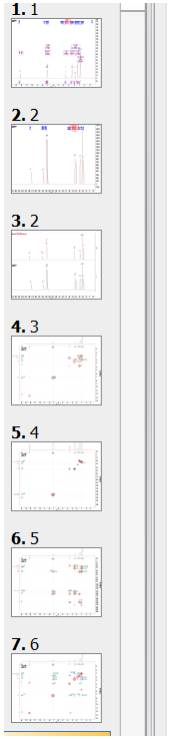
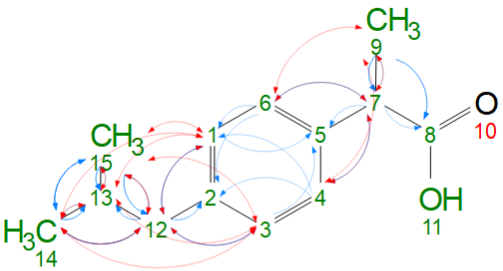
REPORT

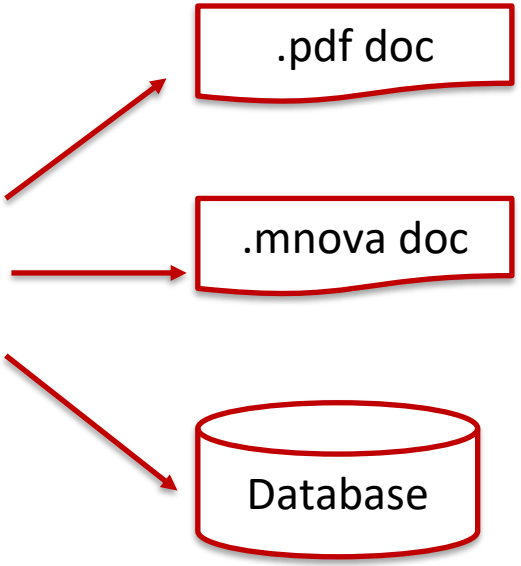
# Save the results

- 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.



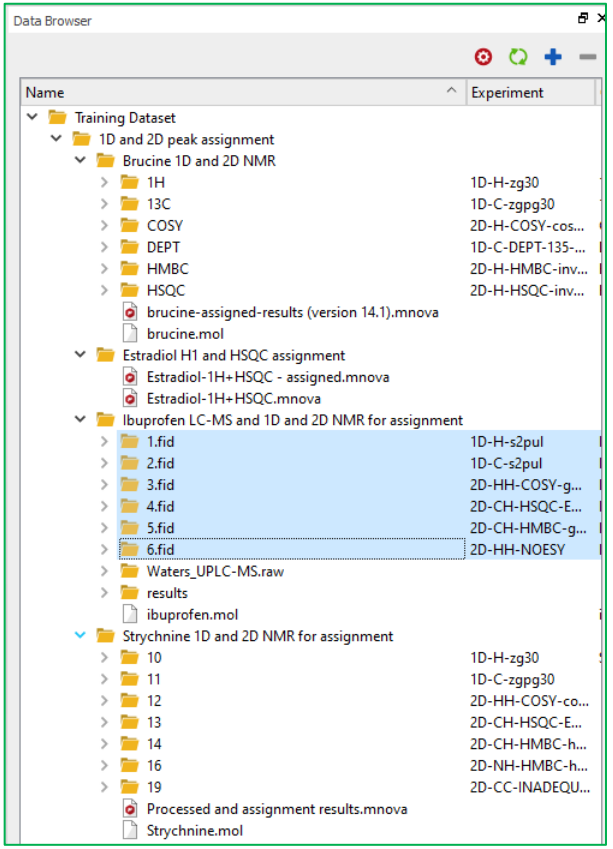




| No | δ H (Multiplicity, J, nH) | δ C (Multiplicity, J) | HSQC-EDITED | HMBC | COSY | NOESY |
|---|---|---|---|---|---|---|
| 1 | 7.09 (d, 7.9 Hz, 1H) | 128.9(s) | 128.9(1) | 44.2(12),138.4(5) | 7.19(4), 7.19(6) | 0.85(14), 0.85(15), 1.80(13),2.41(12) |
| 2 | - | 139.5(s) | - | - | - | - |
| 3 | 7.09 (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) |



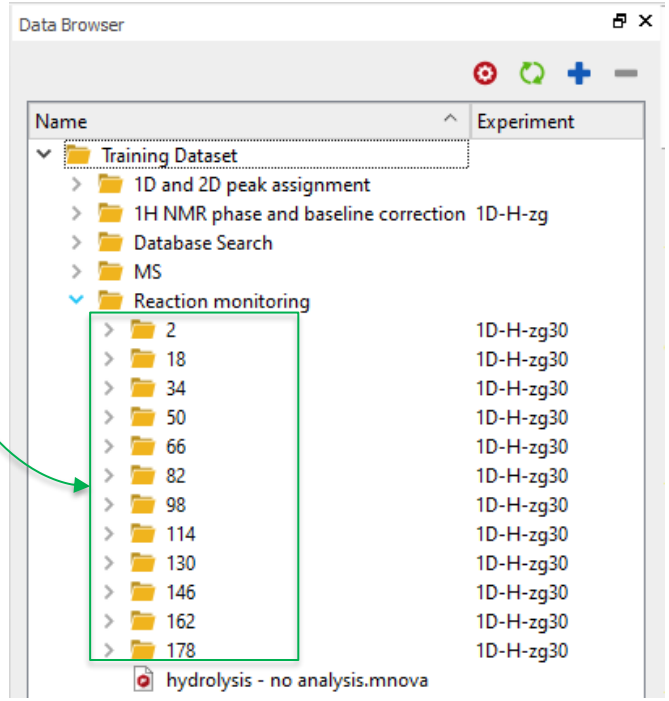
# More about peak assignment

- 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.



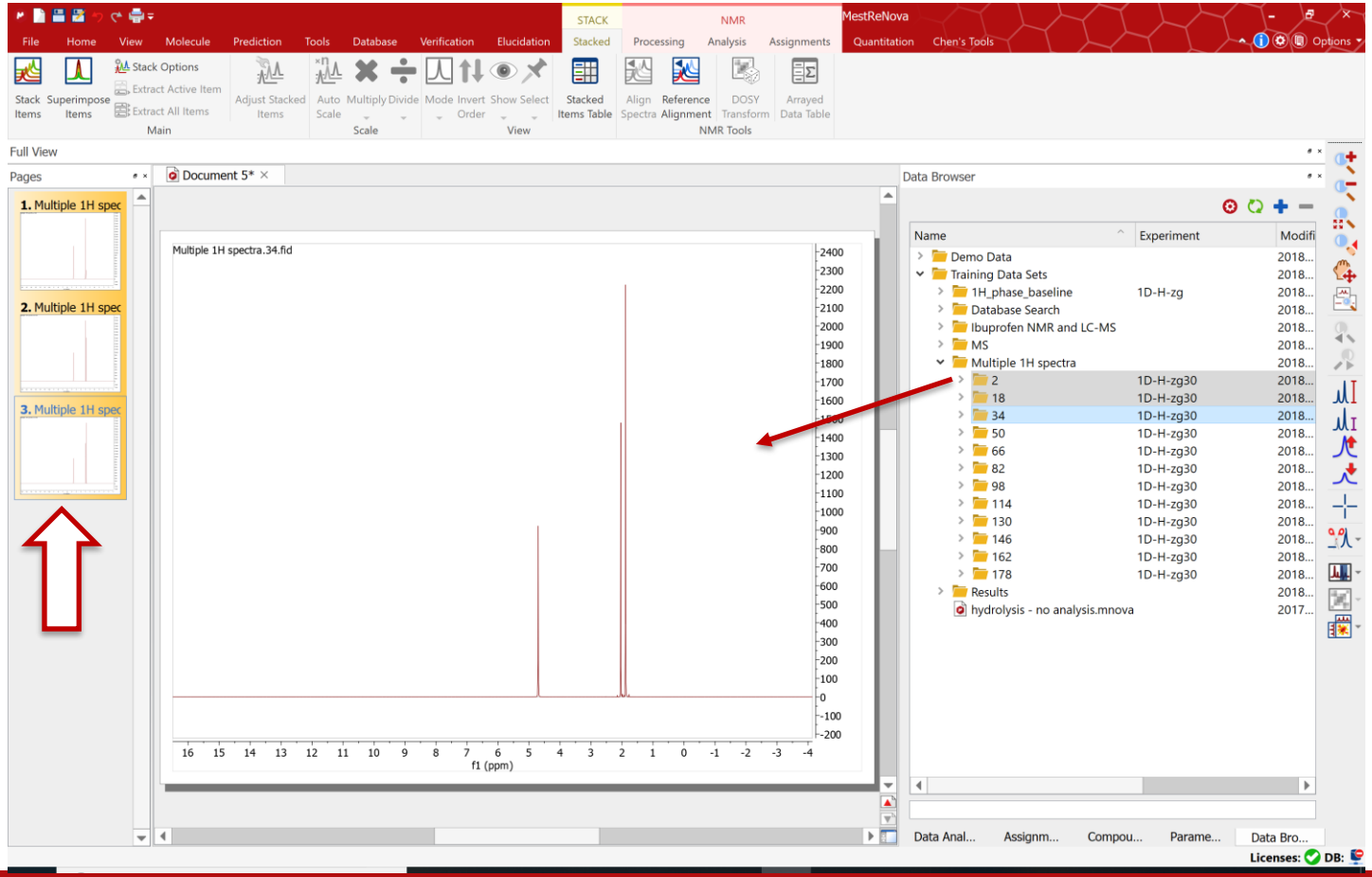
# Processing Arrayed Spectra for Reaction Monitoring etc.

Sample data

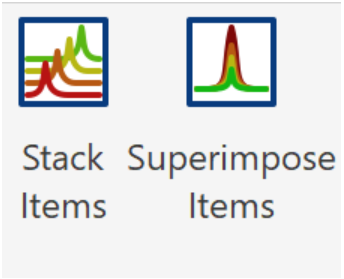


# Stack a few spectra

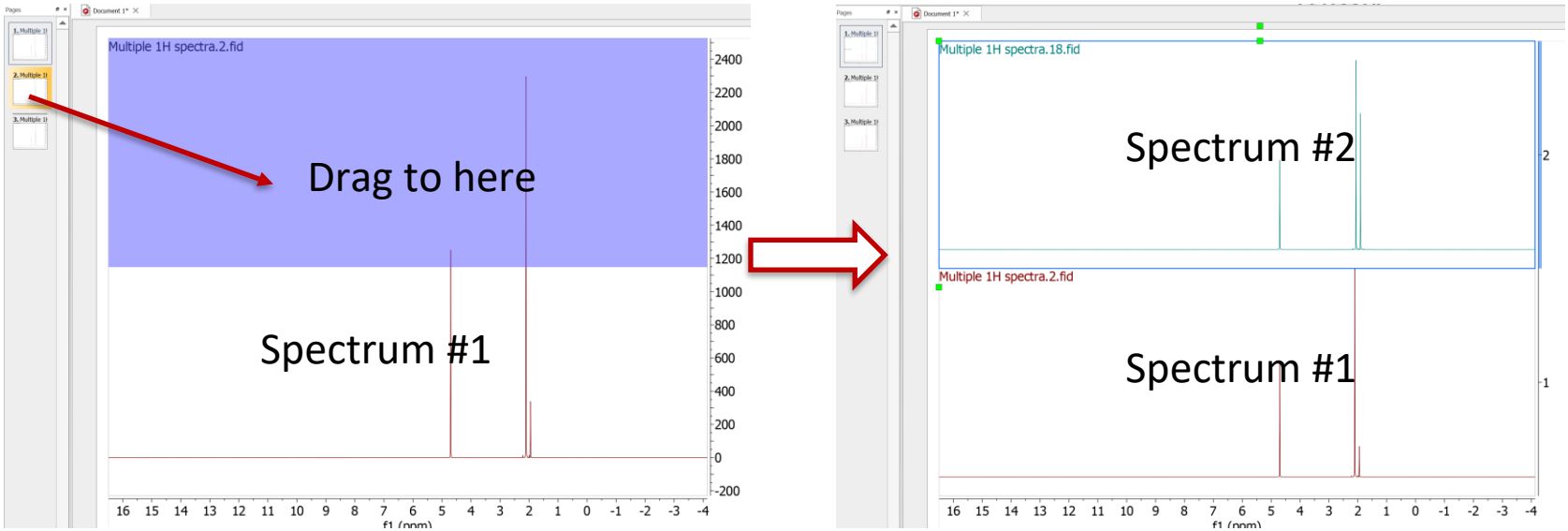
- Open the first 3 spectra from the Multiple 1H spectra folder in Data Browser
- The Stacked Ribbon is visible if you highlight multiple spectra in the Pages View



# Stack a few spectra

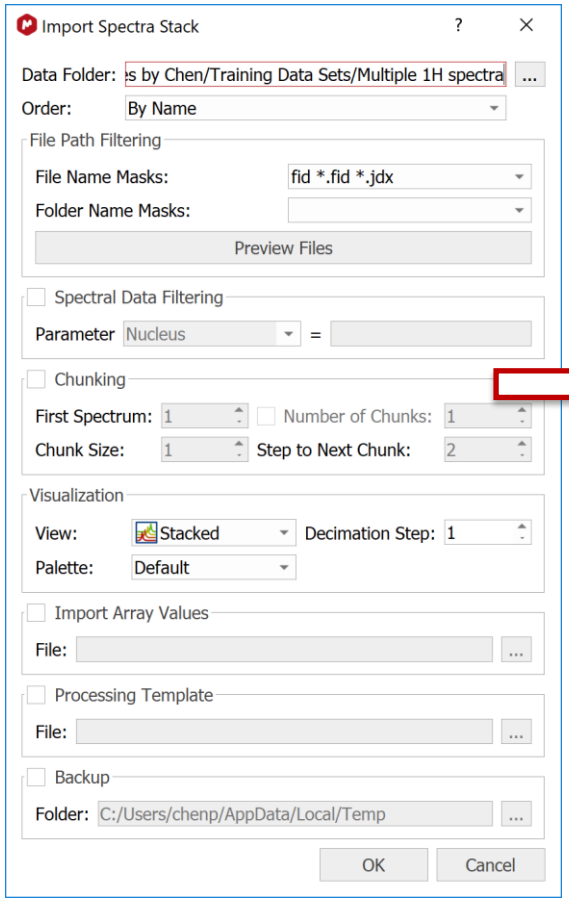


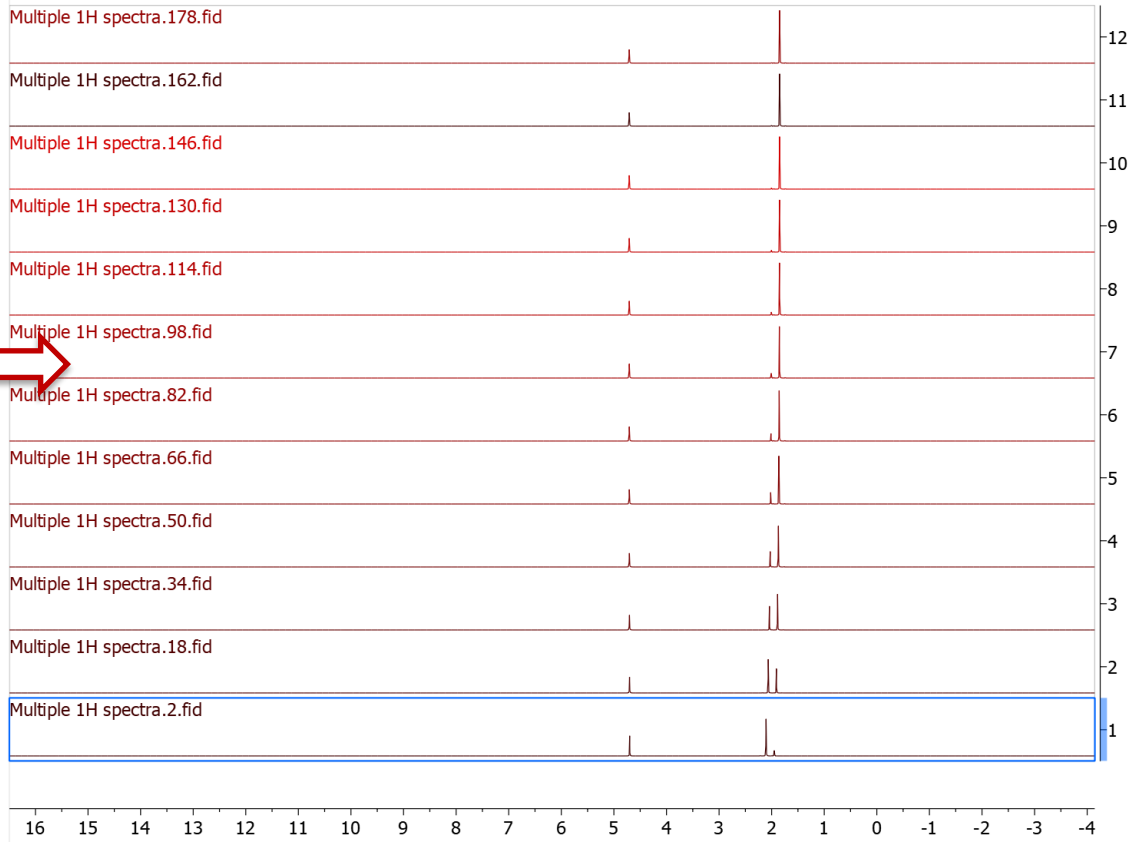

- You can use the Stack Items or Superimpose Items tools to stack or superimpose the highlighted spectra in the Pages View, or:
- Drag the thumbnail of another spectra from the Pages View to the current spectrum to stack them in desired way.
- Continue to drag the 3rd spectrum to the stack. Note you 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

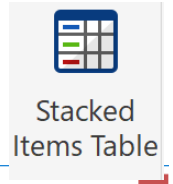
➢ Choose Tools > Loaded Scripts > Directory Spectra Stack, navigate to the directory "Multiple H-1 Spectra" in the training dataset. Click OK to import and stack all of them.

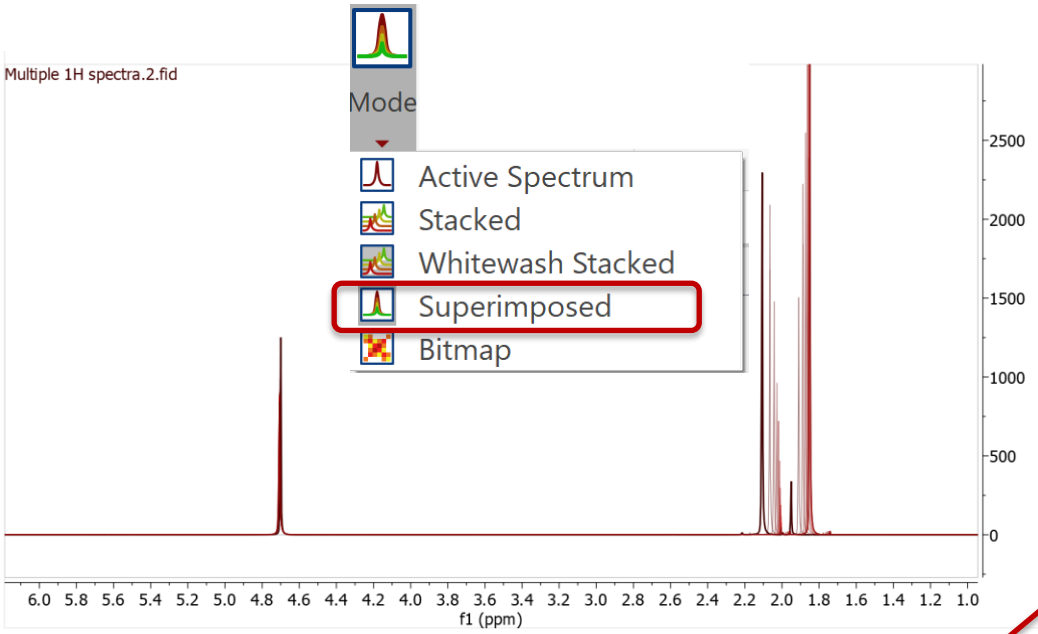


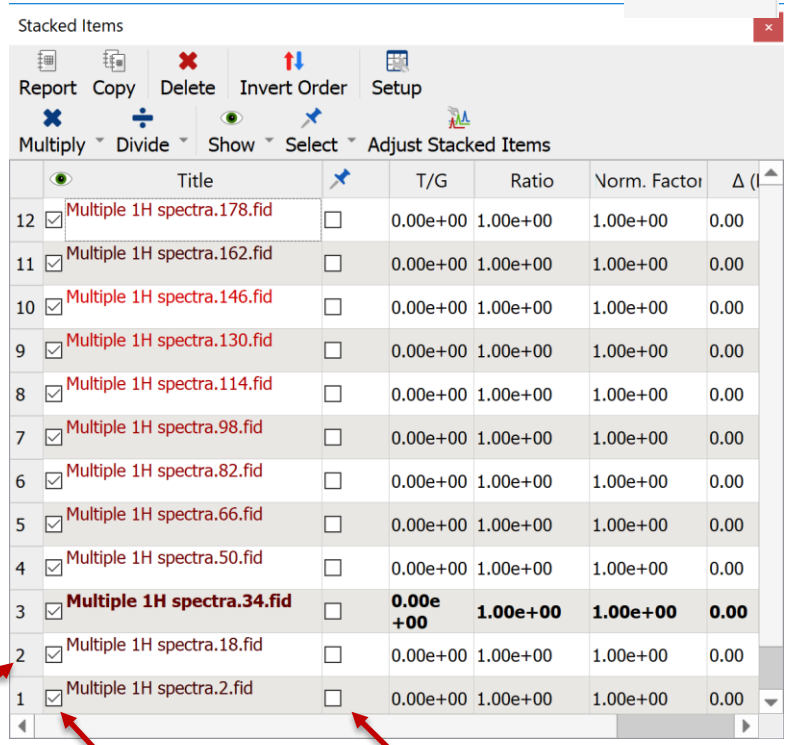



# Stacking mode and Stacked Items Table

- 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



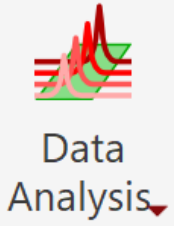




Click and drag here to change the order

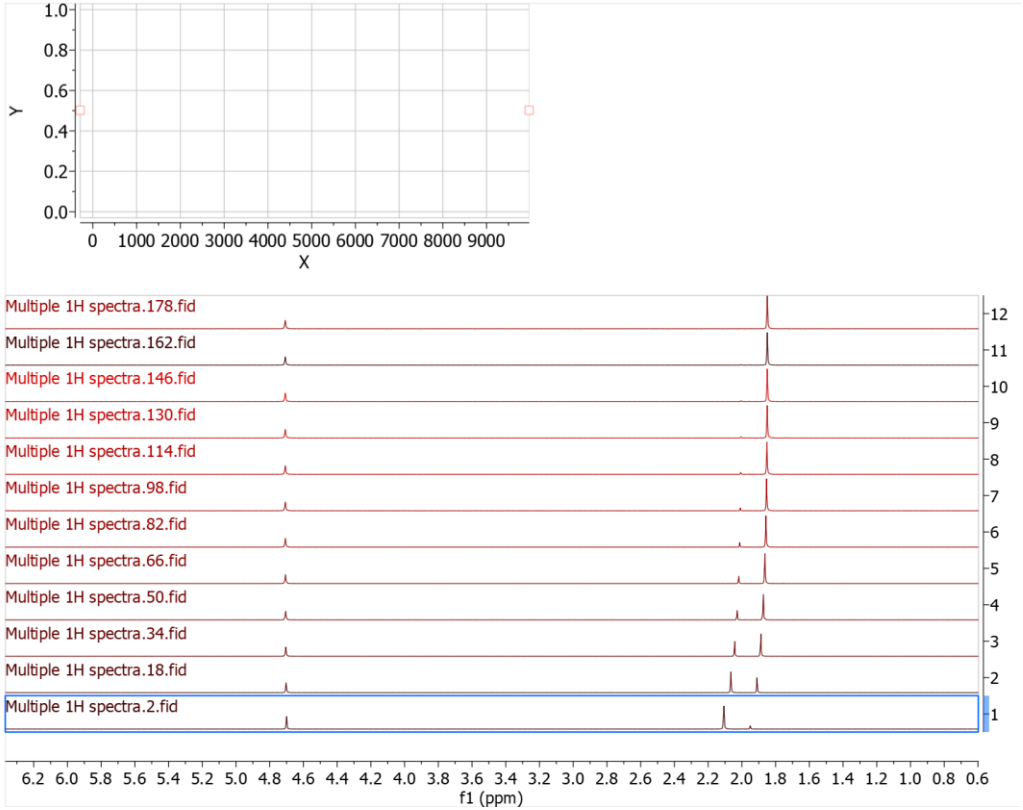
Check/uncheck these to show/hide spectra

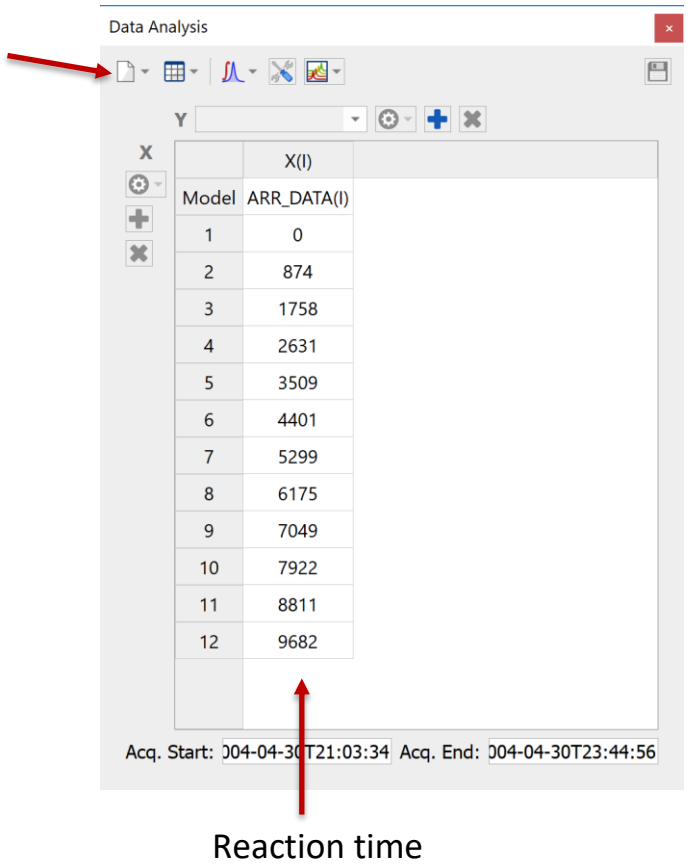
Check these to choose spectra to change

# Analyze arrayed spectra

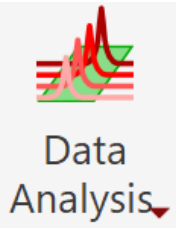



- Choose Analysis > Data Analysis > Show Table to display the Data Analysis Table.
- Click on the Empty Graph to import the X values (reaction time in this case) and display an empty XY graph.

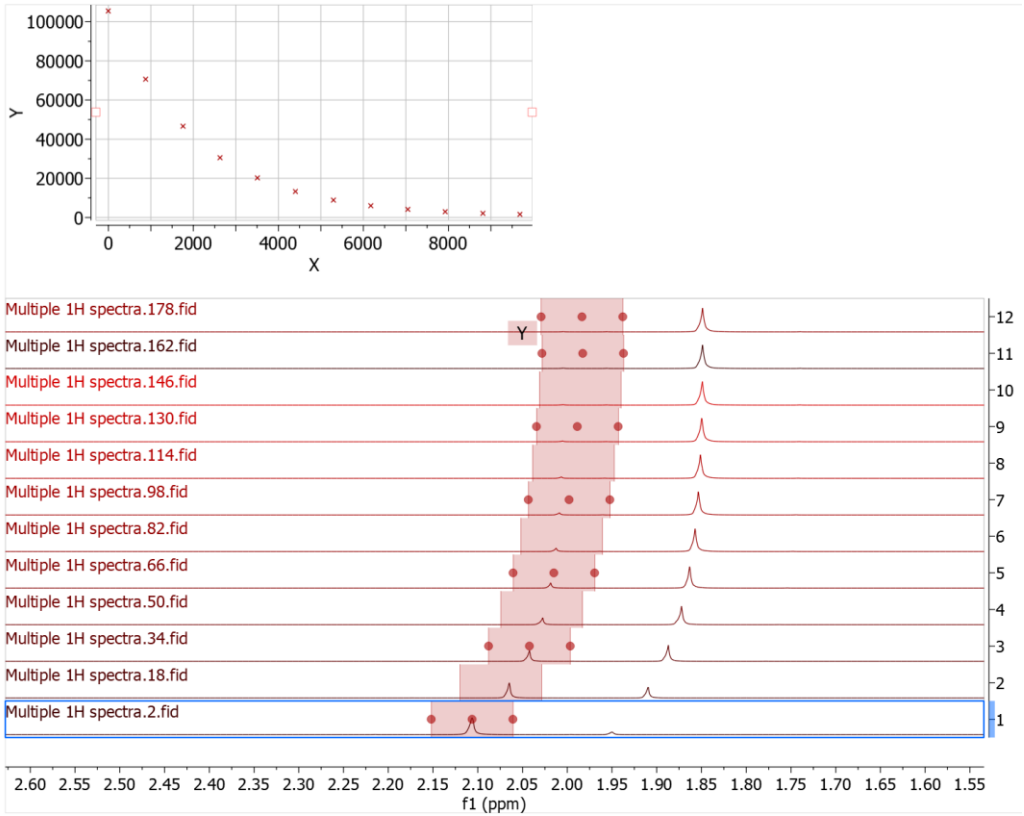


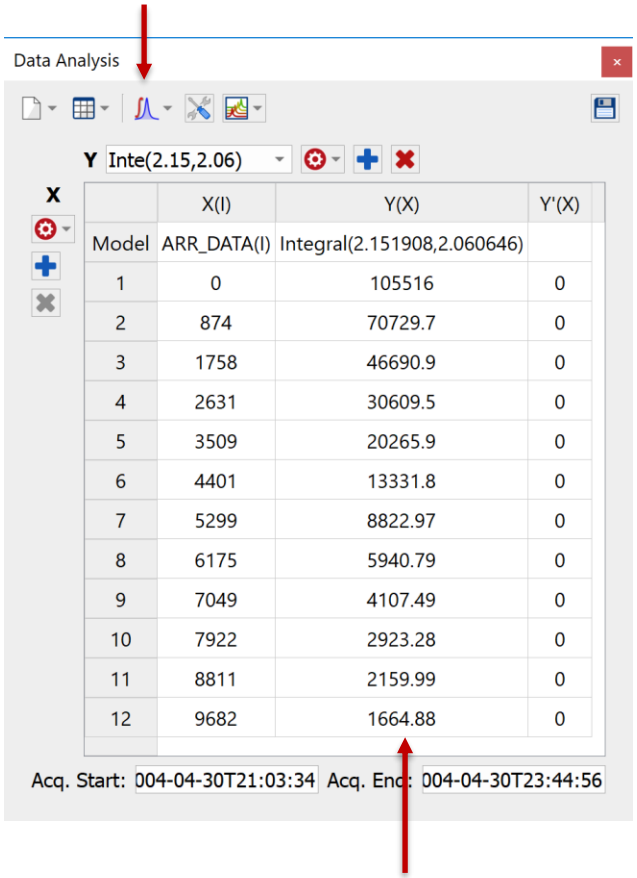



# Integrate arrayed spectra




- 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.

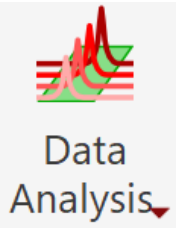



Integrals

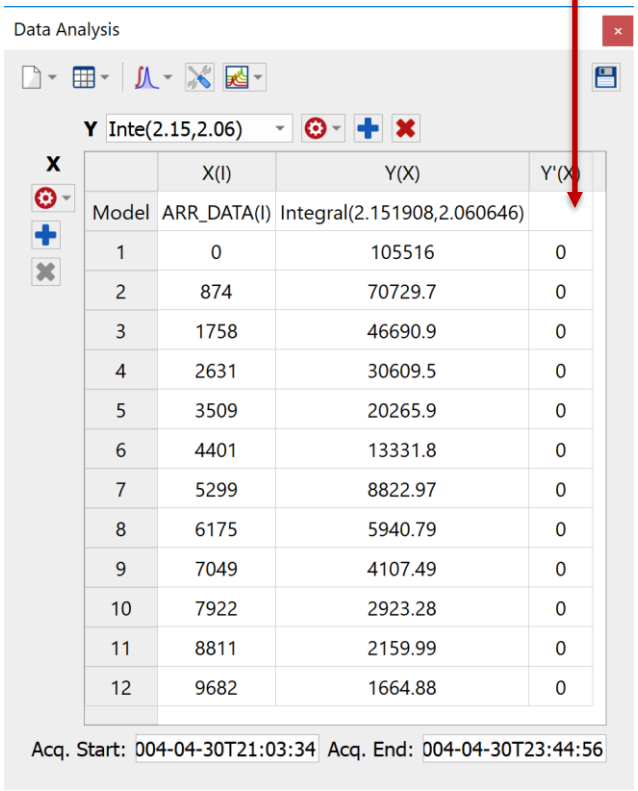
**Use Sum Method (default) for integration unless you are integrating overlapped peaks. Click Options for Integration in the Analysis Ribbon to verify. ** You can increase the # of handlers by using the Edit Model Option Tool.*

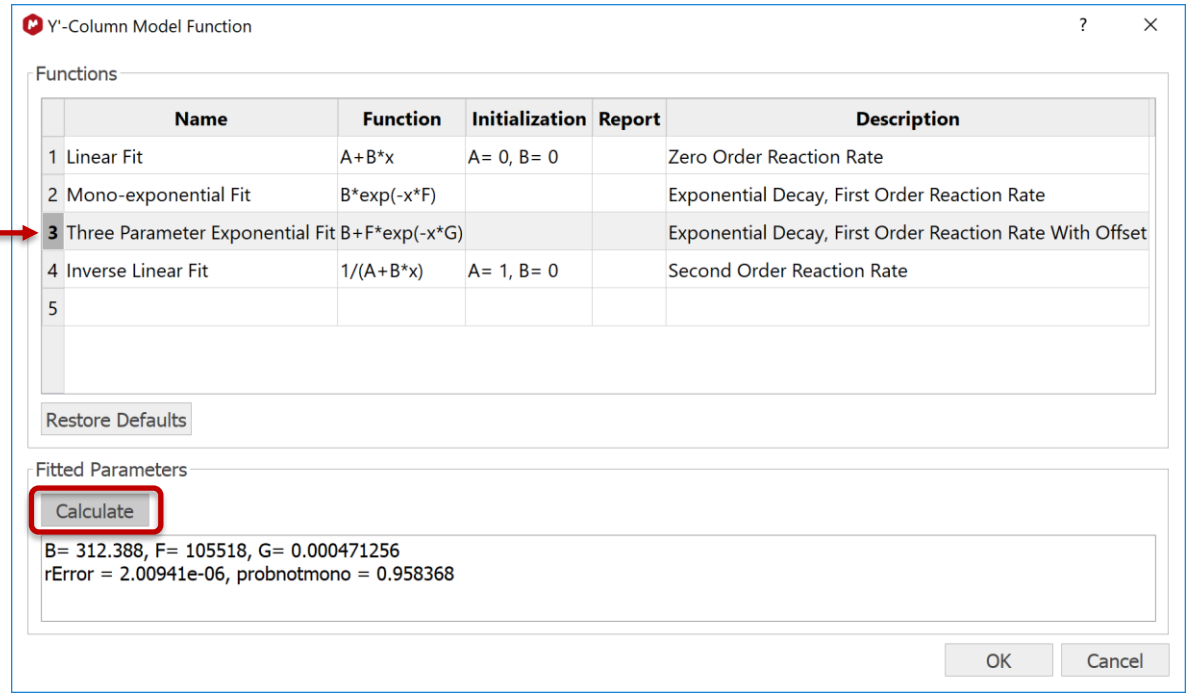
# Fit XY to a function



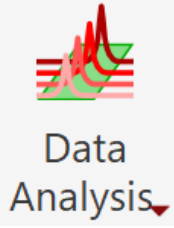

- Click the Model cell under Y'(X) in Data Analysis.
- Choose the 3rd function, and click Calculate to fit the XY values to a first order reaction (with offset)

Double click here

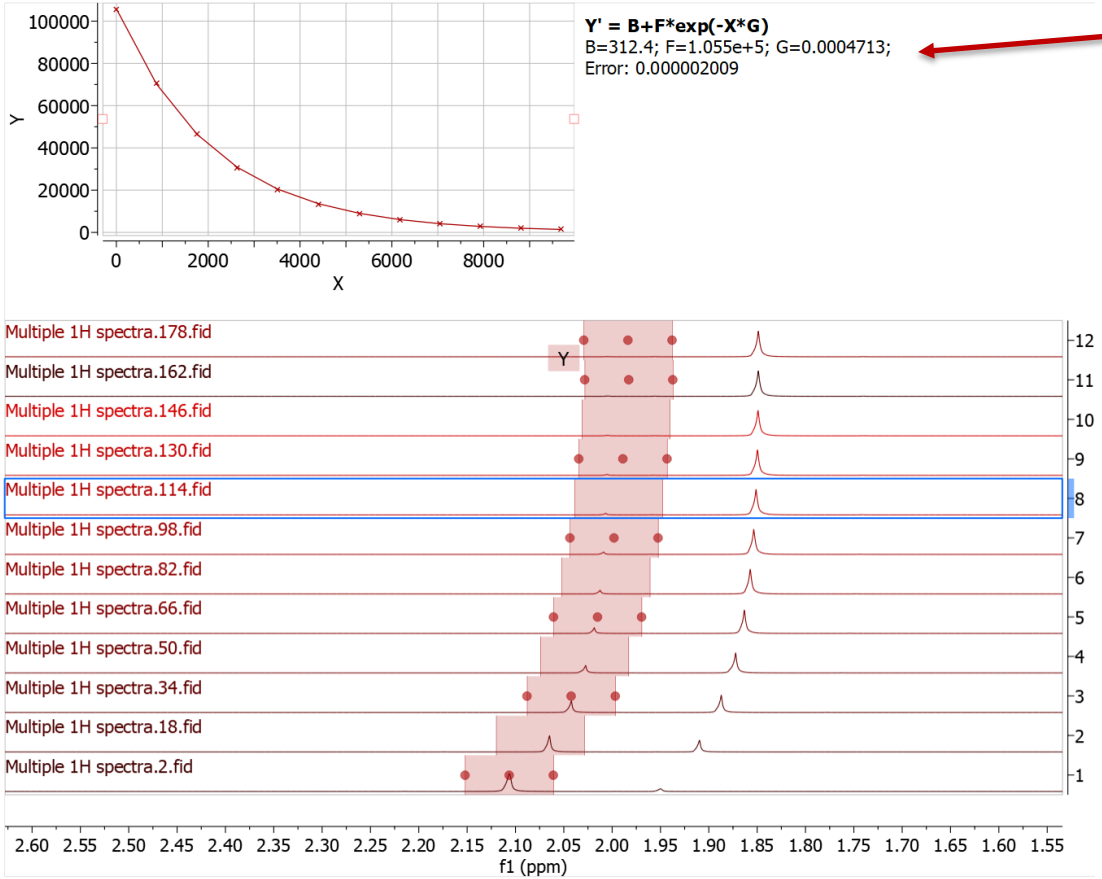


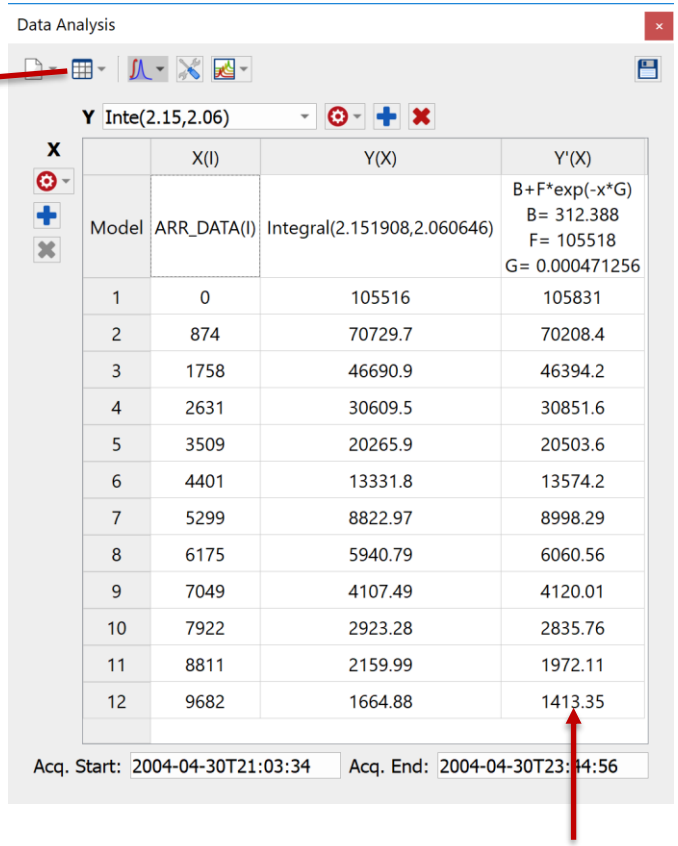



# Report kinetic parameters




- 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) |
|---|---|---|---|
| 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