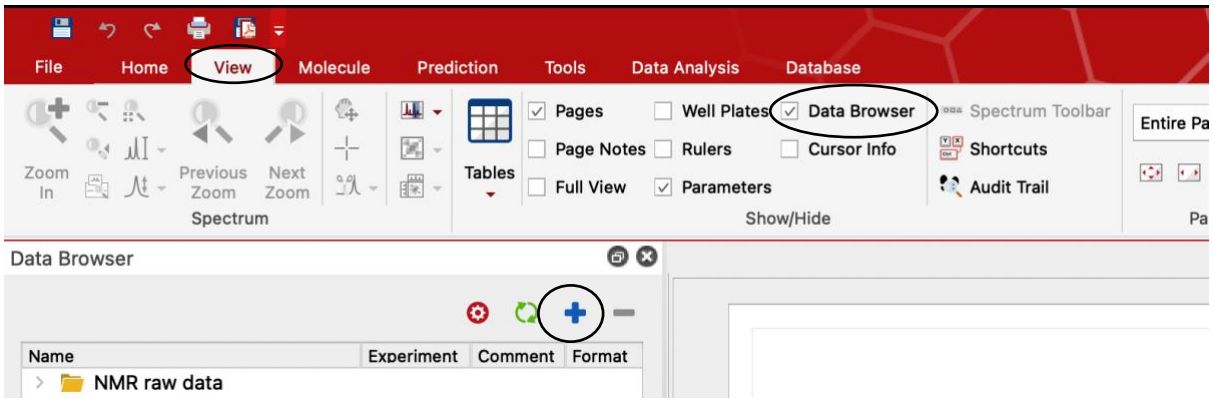
Instructions for using MestReNova

Hotkeys:

Z = zoom in (one click= zoom horizontally, two clicks= zoom vertically, three clicks= zoom all)
Shift+ Z = zoom out
F = Fullscreen
P = pan (to move around the spectrum)
K = Threshold peak picking
Ctrl + K = Manual peak picking
J = manual multiplet analysis
I = manual integration
H = fit intensity
Shift + I = Open integral manager
A = manual assignment
Esc = removes chosen command
L = Reference based on solvent (manual)
E = Expansion (makes a smaller zoomed in window of part of spectrum)
Ctrl + D = Export PDF

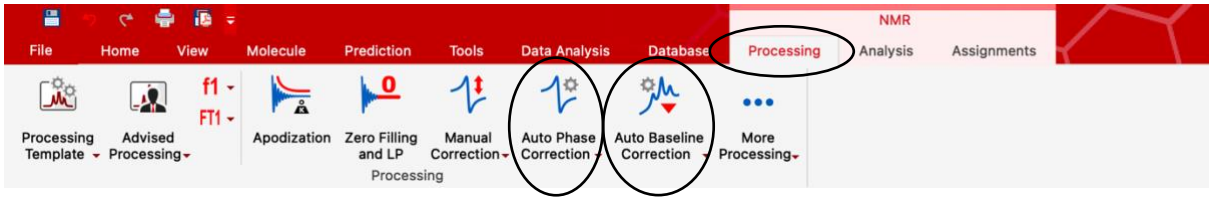
Access your files easily:

Go to View and check the Data Browser box, then choose the folder you want to have easy access to by pressing the blue plus-sign. Now the folder will be there every time you open the program.



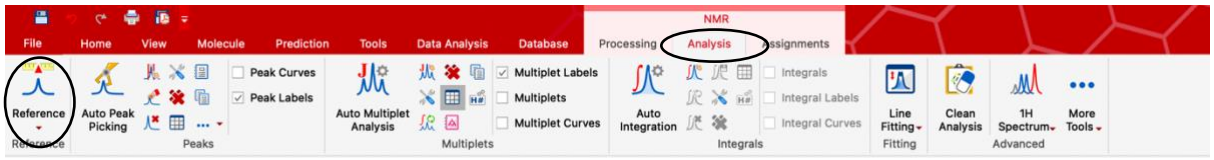
Processing your specter:

Start by doing a phase and baseline correction. This is done by going to the processing window and pressing Auto Phase Correction and Auto Baseline Correction.



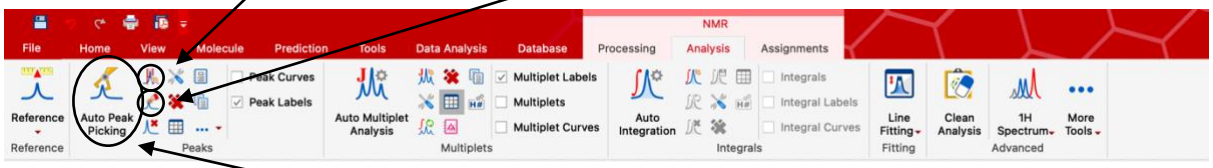
Calibrate your spectrum:

Go to the analysis window and press the Reference button (L) and find the peak that corresponds to your solvent signal.



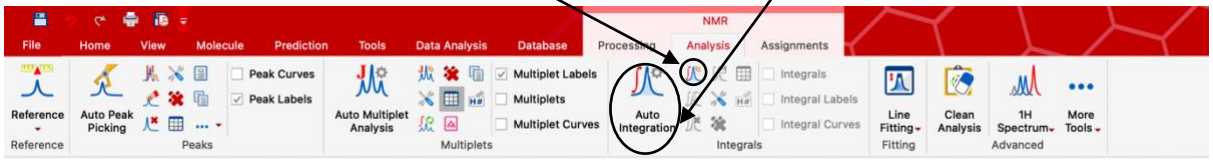
Analyze the spectrum:

The first thing you do is to mark the different peaks (this labels them with their corresponding ppm), this is done by either picking the peaks one by one (Ctrl + K) or by picking all the peaks in a threshold (K).

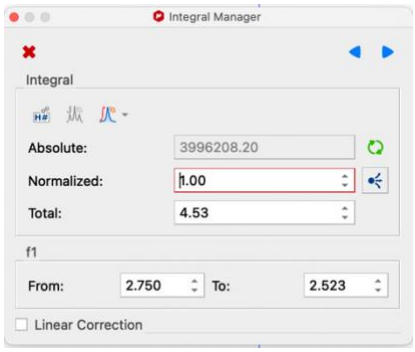


You can also choose the Auto Peak Picking function that does this automatically.

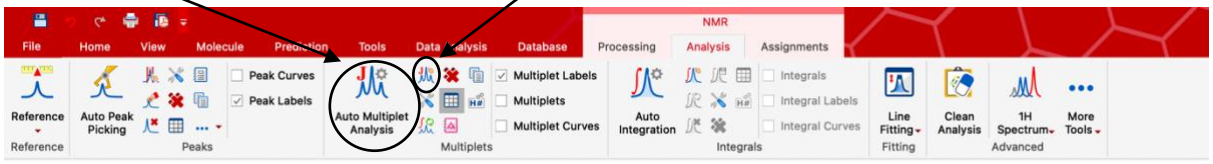
Then you need to integrate the signals. This can be done by pressing the Integration button (I) and integrating each peak or by pressing the Auto Integration button.



Next you need to scale the integrals either based on the total amount of protons (Total) or by setting the integral of a peak with a known number of protons (Normalized). This is done by right-clicking on one of the integrals and clicking “Edit integral” to open Integral Manager.



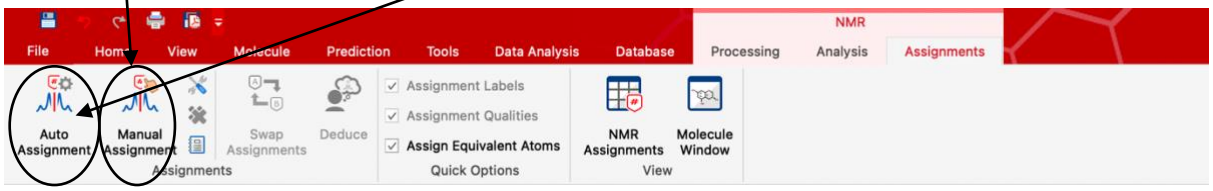
To analyze the multiplets you can press the Manual Multiplet analysis button and hold the cursor over a peak until it is marked in red, you can also use the Auto Multiplet Analysis function.



Assignment:

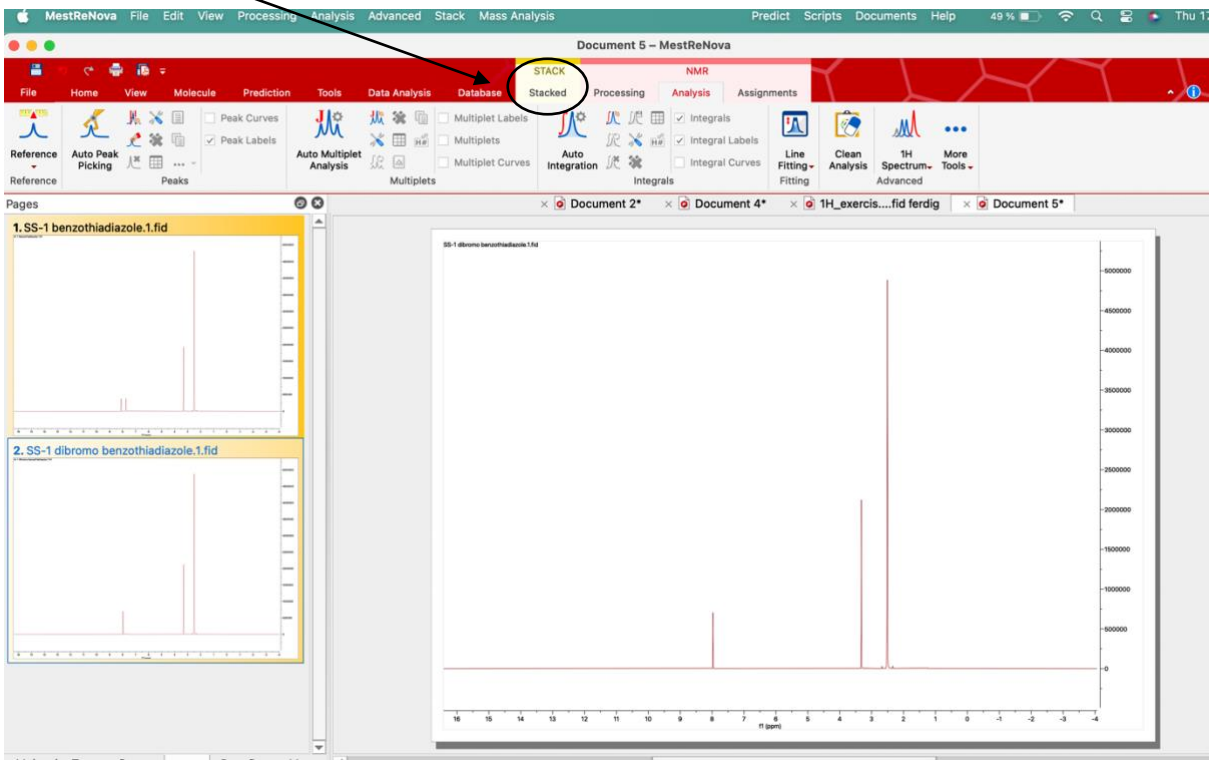
After you have analyzed the data in the spectrum you can assign the peaks to the protons in a molecule. The molecule can be drawn using MestReNova (using the functions in the Molecule window) or you can copy the structure from ChemDraw.

To assign the signals to the protons in your molecule you can use the Manual Assignment by clicking on the proton you want to assign and then the peak you want to assign it to. You can also use the Auto Assignment function.

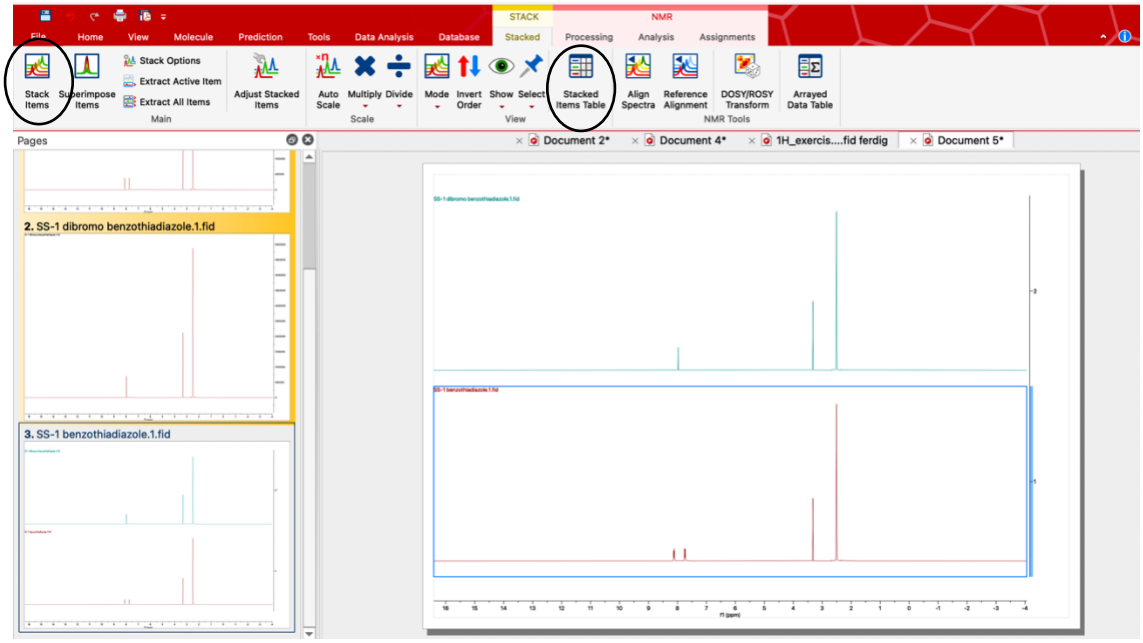


Stacking multiple spectra:

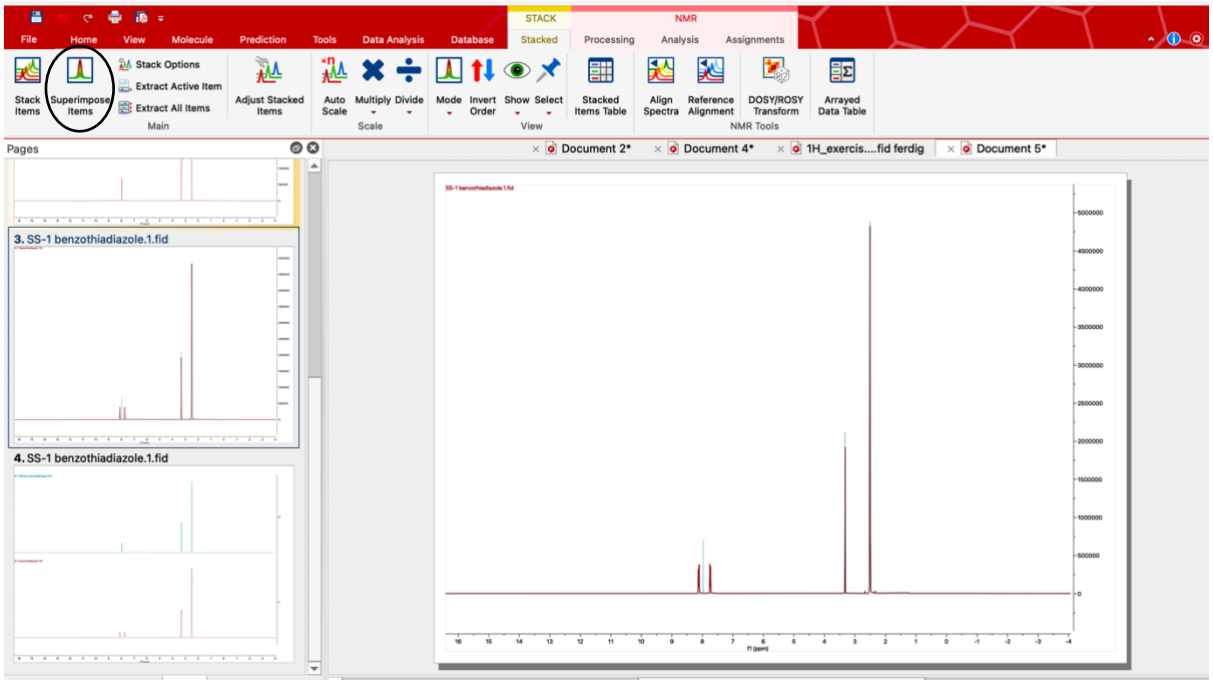
If you want to compare different spectra this can be done by stacking your spectra either on top of each other or above each other. This is done by marking the spectra you want to compare (mark one and then hold shift while marking the others) then the Stacked window will appear.



You can stack them above each other by using the Stack Items function (remember to calibrate the spectra!) When you zoom in on one of them you zoom in on both, this is useful to compare spectra. You can change the order in Stacked Items Table



You can also stack the spectra on top of each other using the Superimpose Items function. (Remember to calibrate the spectra)



How to Make Templates in MestReNova

1. Open a new file and upload a spectrum of desired kind (e.g. ^{1}H)
2. Make room for and add box for parameters.
3. Make room for image of molecule (or paste molecule directly from ChemDraw).
4. Process the spectrum: auto phase and baseline correction. Reference solvent peak.
5. Perform auto peak picking, integration and multiplet analysis (skip if you prefer to do it manually).
6. Make desired adjustments (e.g. number of decimals in peaks or integrals, removing file title from upper left corner, removing frame around spectrum etc). Before saving the template, it should look how you want your final NMR spectra to look like.
7. Save the templateby going to View>Layout Templates>Create Layout Template Document. The only page in the file should be the processed spectrum.
8. Repeat the process with each kind of spectrum (^{13}C, COSY, HSQC, HMBC). You should end up with 5 different templates.
9. To ensure that the size of the box for the spectrum, parameters and molecular structure is consistent for all templates, you can right click each box and go to Properties>Geometry and adjust the position and size.

How to Use Templates in MestReNova

- For applying processing (corrections, integrals, peak picking etc): go to View>Layout Templates>Layout Template Options. Make sure «Apply Processing Template» is ticked off.
- There are (at least) two ways to use the template:
  - Open the spectrum in MestReNova. Go to View>Layout Templates. A list of template files should appear. Choose the correct one.
  - Open the template file in MestReNova. From Data Browser, drag the spectrum over the template page.
- After applying template, you still need to:
  - Control integration, peak picking and multiplet analysis (or perform if you do it manually). Control solvent peak reference.
  - Adjust font size of parameters
  - Adjust height of baseline
- If you want to change something later, open the template over a spectrum and make desired changes. Save the template again.
- Note: any manual processing should be performed **after** applying template, or else it may disappear when the template is added.