



Assignments

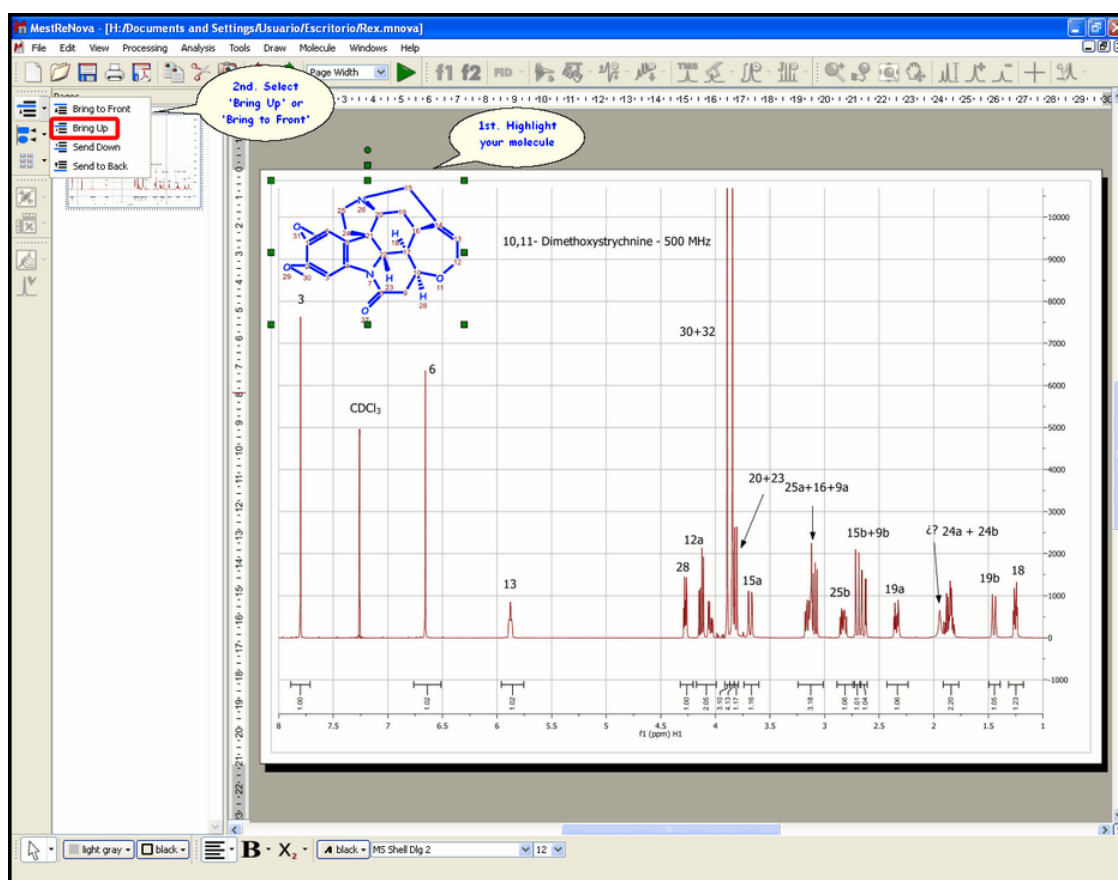
MestReNova: NMR plugin

Pablo Monje

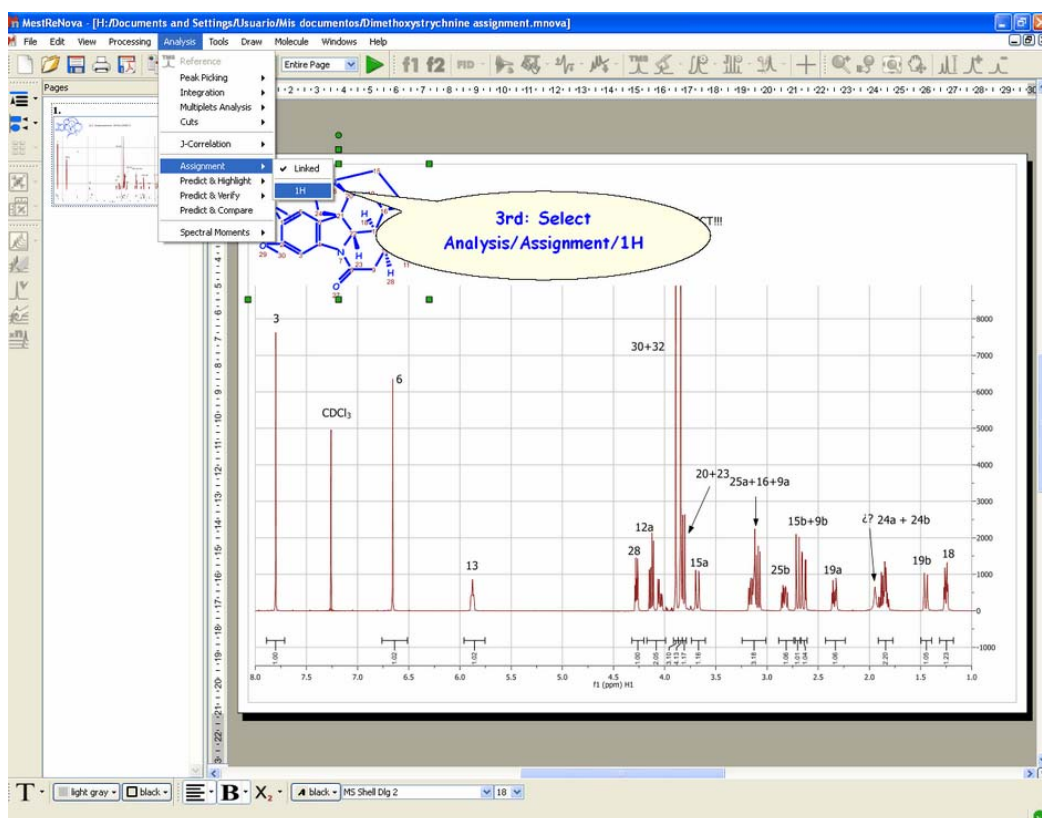
www.mestrelab.com

It is now possible within Mnova to carry out atom to peak assignments, both to 1D and 2D spectra **(Please note that this feature is not completely finished in this version and that it will be greatly enhanced in the oncoming release versions)**

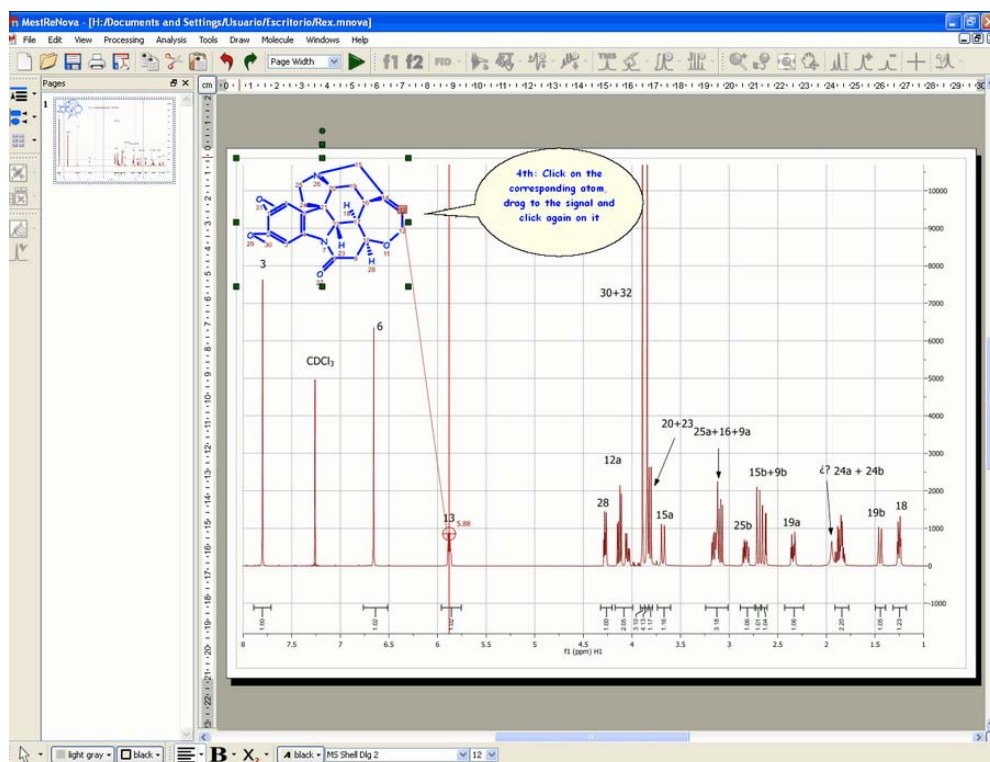
Mnova provides a very simple interface to assign your molecule. Just highlight the molecule and be sure that it is over your spectrum, (if the molecule is under the spectrum, click on 'Bring Up').



After that, please follow the menu 'Analysis/Assignment' to select the corresponding assignment. The option **'Linked'** will keep the assignment connected to the molecular structure (useful for example, to copy the assignments of the molecular structure to another page, in order to compare a real spectrum with a simulated one).

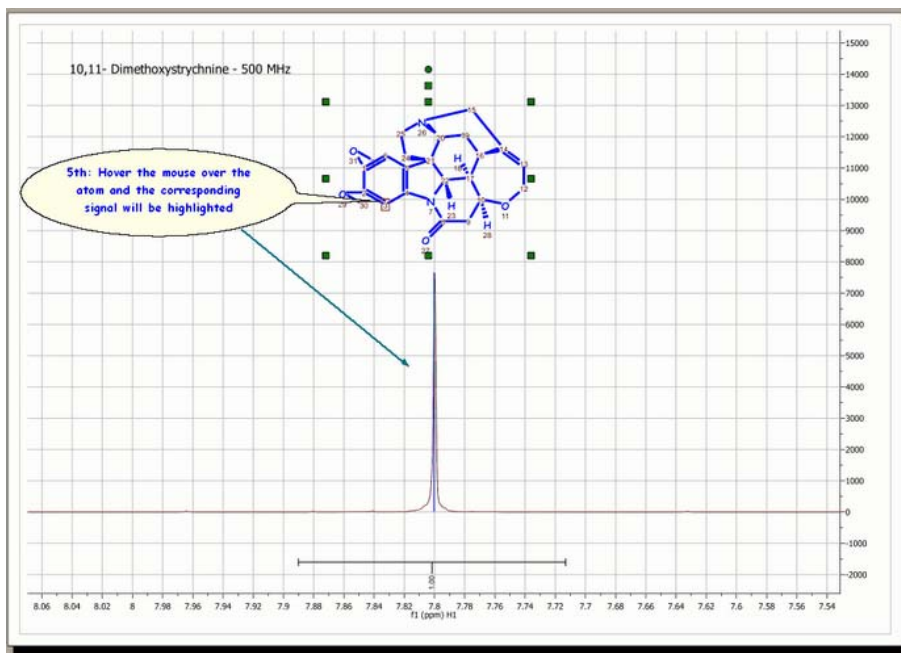


Finally, left click on the desired atom, so that it becomes highlighted in a red box and then release the mouse and drag it to your desired peak. Once your desired peak is highlighted on the spectrum, click on it to assign it.

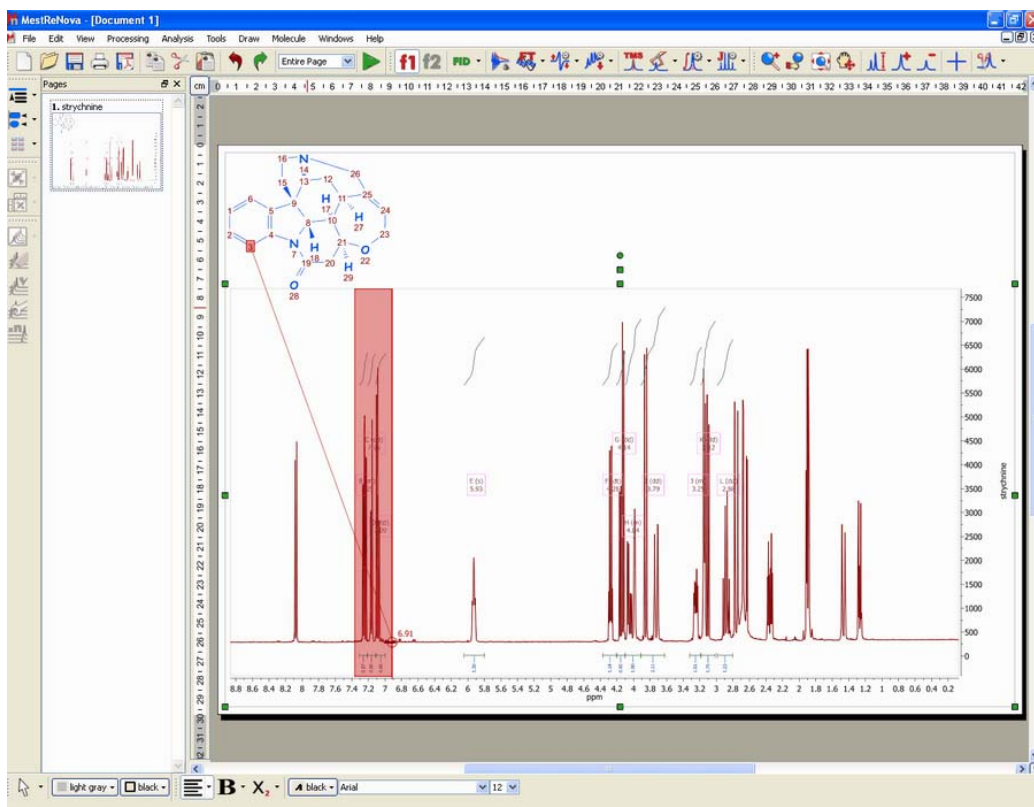




This peak will now be assigned to the atom. Once the assignment has been made, hovering the mouse over the atom will highlight the corresponding peak in the spectrum, and hovering the mouse over the peak will highlight the corresponding atom on the molecular structure.

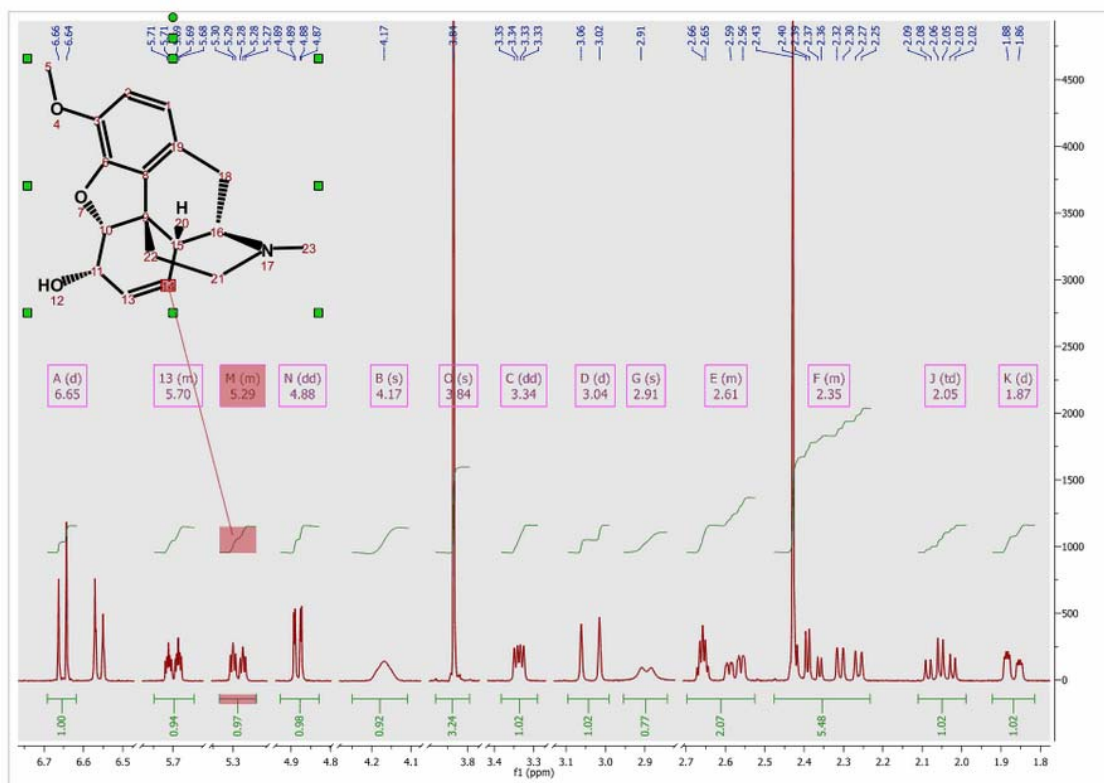


The user can also assign a multiplet, by clicking, dragging and releasing the mouse over the desired multiplet.

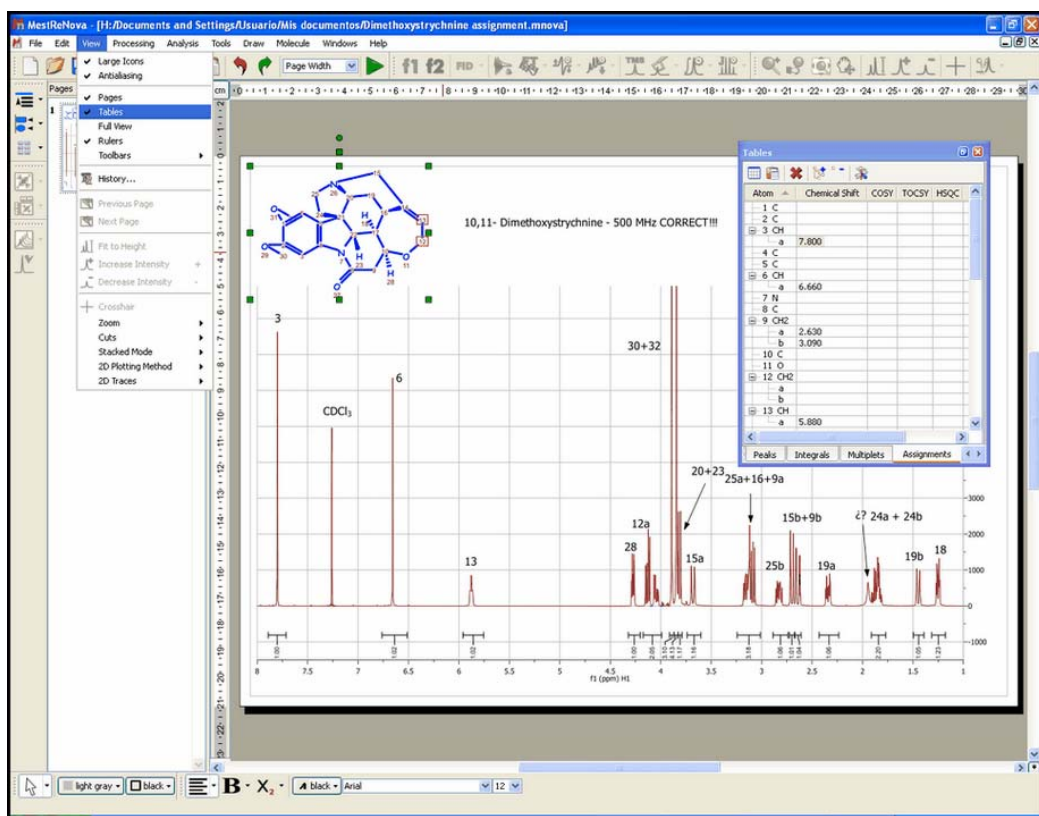




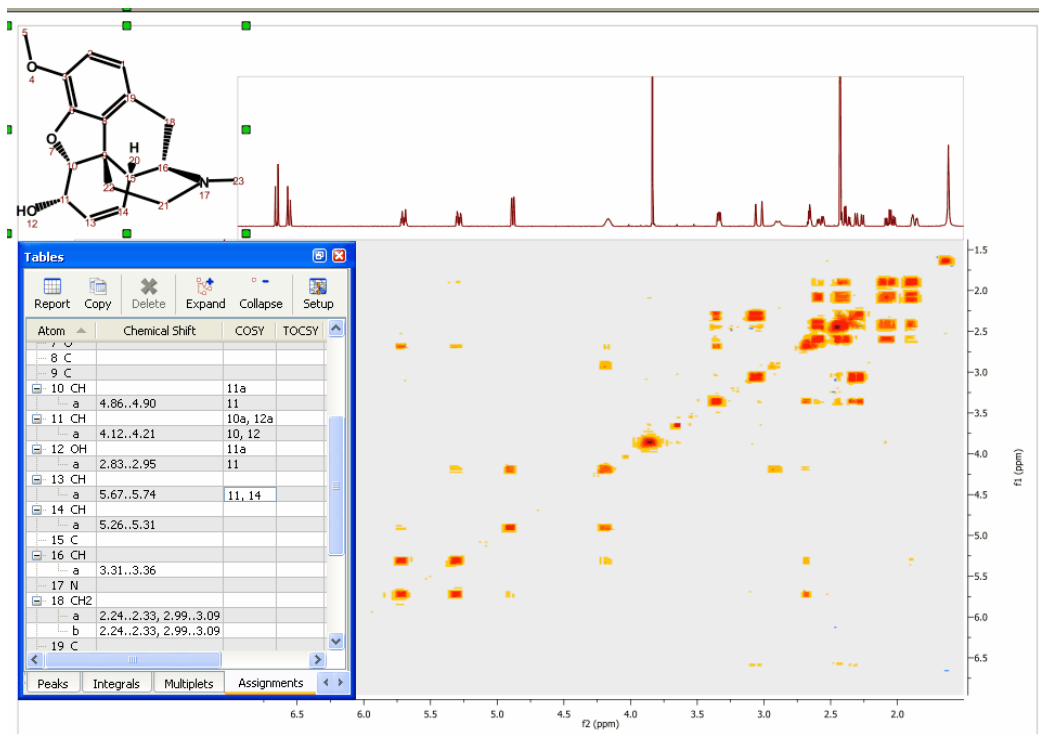
It is also possible to assign a multiplet by dragging the mouse to the **'multiplet box'** or the **'integral curve'**, as you can see in the picture below:



Once you have finished with the assignment, you can visualize the assignment list by following the menu 'View/Tables/Assignments' (with the spectrum highlighted) where you will also be able to edit any entry by double clicking on it and overwriting the new value. Bear in mind that you are also able to carry out the peak assignment directly from this table by typing the corresponding chemical shift in the edit box.



Currently, it is only possible to carry out assignments to 2D spectra by typing the corresponding number of the atom in the 'Assignments Table' :





A few notes on Molecular Structure Assignment

- ✓ The current release version of Mnova allows visualization or exporting of assignments in a table. The reporting functionality will be available in the forthcoming versions of Mnova.
- ✓ We plan for the oncoming releases of Mnova to also implement the functionality to carry assignments through different data sets in different pages (thus, for example, it would be possible to assign a 2D spectrum and for those assignments to be applied automatically to the corresponding 1D spectra).