



How to simulate a spectrum with NMRPredict Desktop?

MestReNova: NMR plugin

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Carrying out of predictions in Mnova with the **NMRPredict Desktop** plugin is very easy and intuitive.

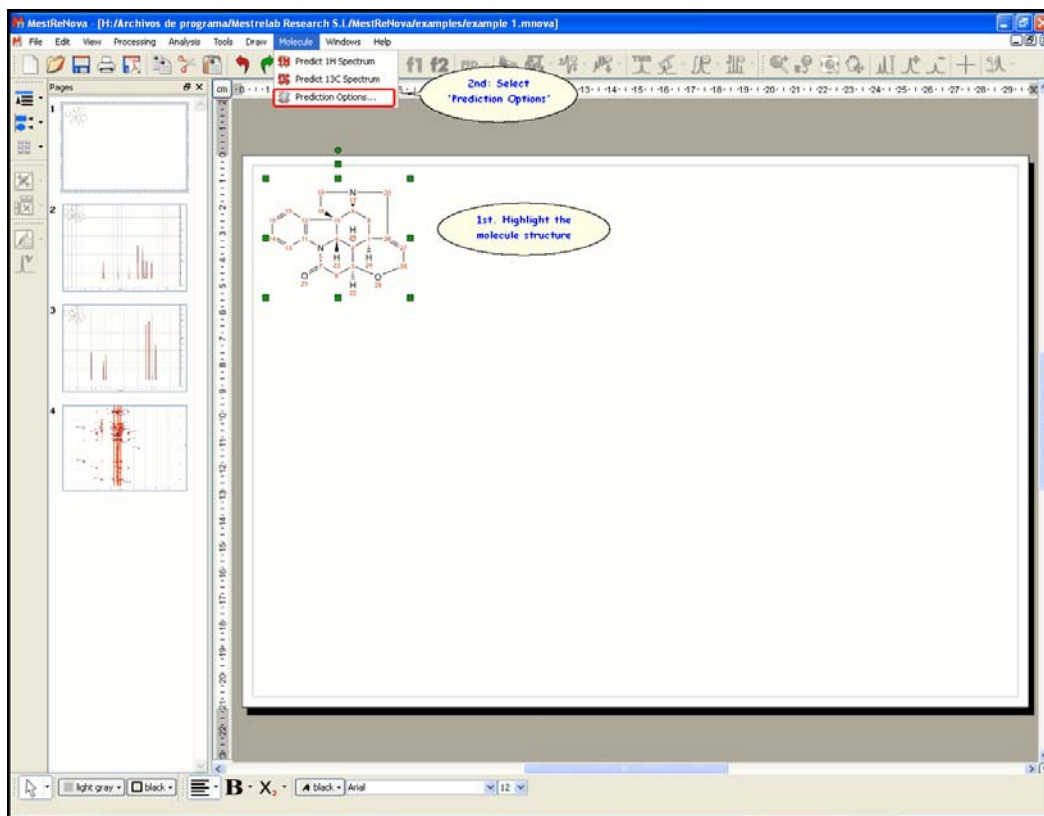
1. Just, import a molecular structure. Currently, molecular structures can be imported as a **.mol** file by simply using the Open command exactly in the same way as this would be applied to a spectrum. Bear in mind, that you are currently able to copy&paste **.cdx** structures from **ChemDraw** and **.mol** from **IsisDraw** but not drag&drop them. Support to 'drag & drop' operations are currently limited to **ChemSketch**.



ATTENTION

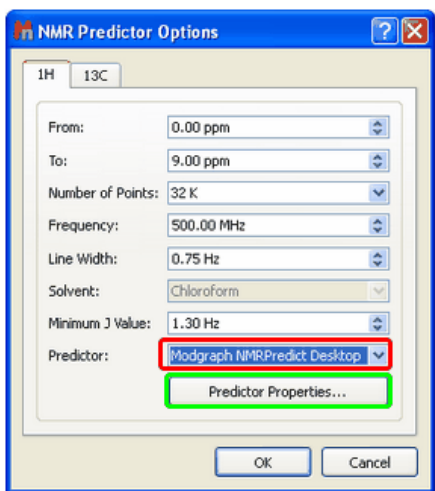
Bear in mind that, in terms of stereochemistry, drawing a structure as a chair or as a boat means nothing to the .mol file and the computer. In those cases the user must draw all the corresponding bonds to show the stereochemistry of the molecule, i.e., you must explicitly draw up and down bonds using wedges.

2. Highlight the molecule structure in the active page of Mnova and select 'Prediction Options' in the 'Molecule' menu .

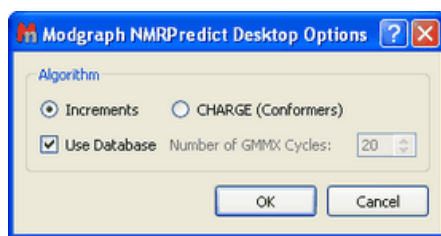




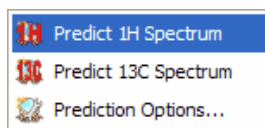
3. This will open the 'NMR Predictor Options' dialog box where you will have to select 'Modgraph NMRPredict Desktop' in the Predictor edit box (red square in the figure below).



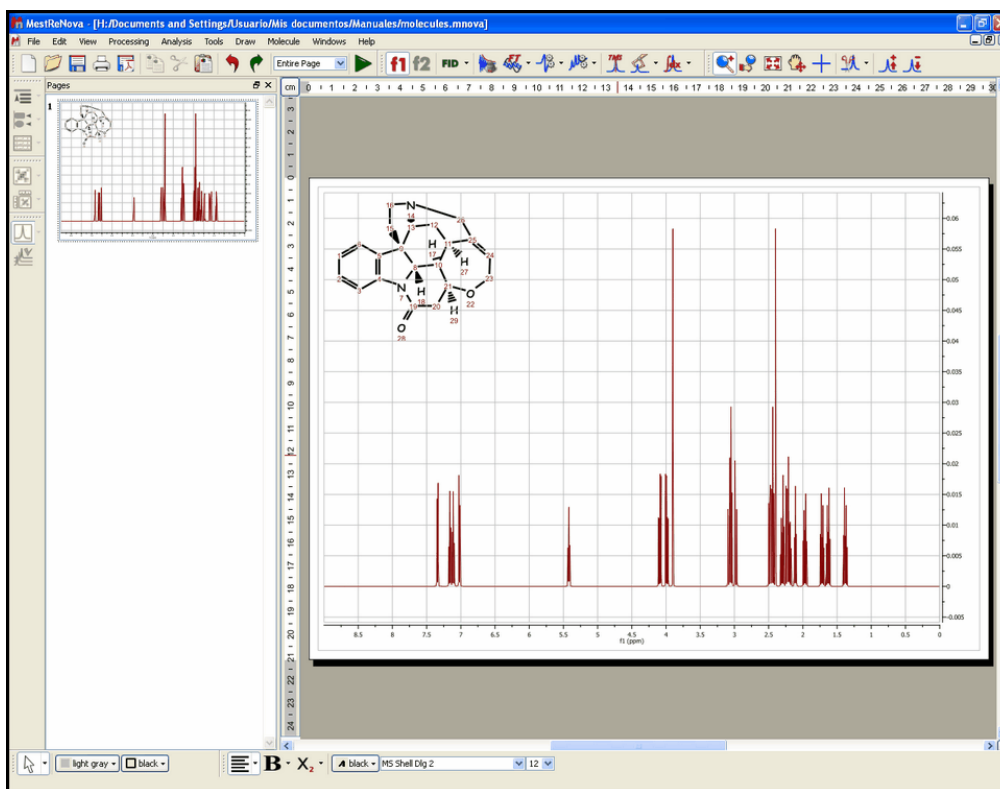
4. In this dialog box, the user is able to select the chemical shift limits of the spectral window, as well as other parameters, such as number of points, frequency, Line Width, solvent and minimum coupling constant value). If you are going to predict a ^1H -NMR spectrum, you can also select the prediction algorithm (Increments or Charge) by clicking on the 'Predictor Properties' button (in the green square in the figure above). After that, the '**NMRPredict Desktop Options**' dialog box will be displayed and you will be able to select the desired prediction algorithm (Increments or Charge). If you use the Increments methodology, you will have the option to use or not use the Database, whereas if you use the CHARGE algorithm you can set the 'number of GMMX cycles', as you can see in the picture below:



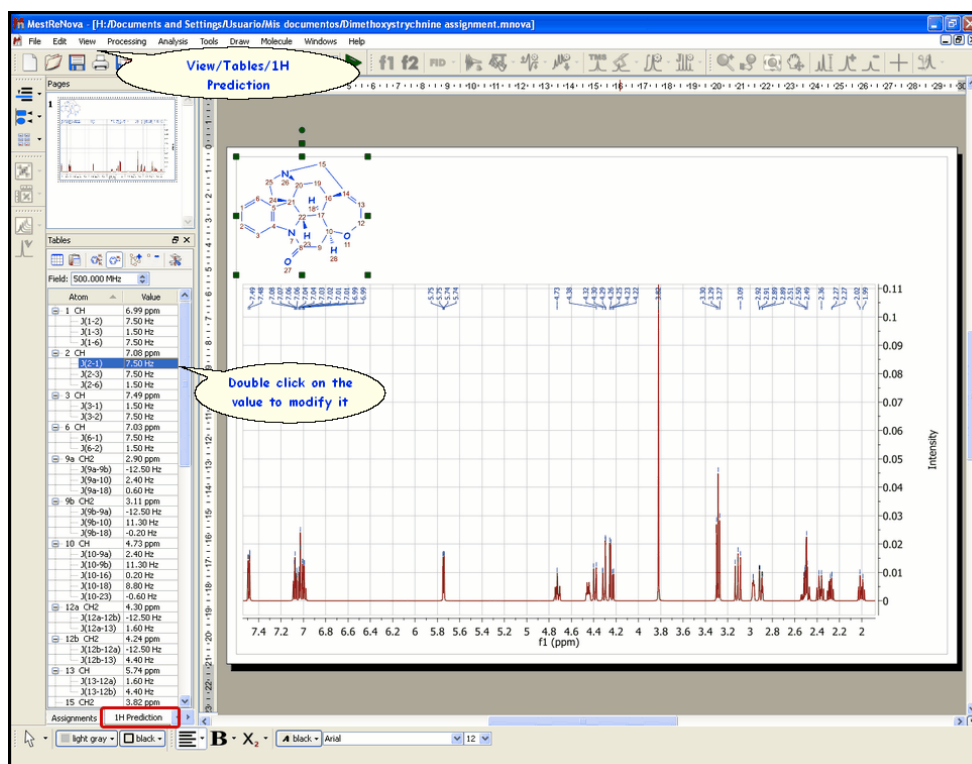
5. Click 'OK' and back again to the 'Molecule' menu to select 'Predict 1H Spectrum':



6. After that, you will obtain the desired predicted ^1H -NMR spectrum. This predicted spectrum can be analyzed as a real one (e.g. it can be integrated, peak picking, etc).



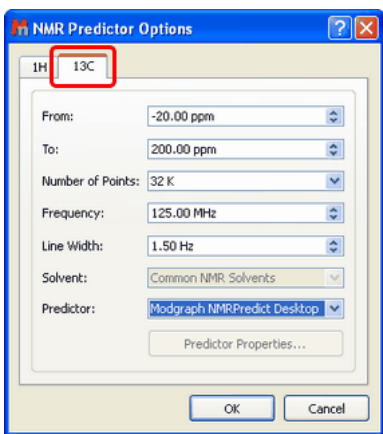
You can also modify the chemical shift and the coupling constant values from the table of the predicted spectrum. Just, highlighted the spectrum, follow the menu 'View/Tables/1HPrediction' and then double click on the value that you want to edit. The changes made on the table will take effect automatically in the simulated spectrum.





Finally, if you want to know the "predicted assignment", just hover the mouse over the desired atom, (so that it becomes highlighted in a red box) and the corresponding signal in the spectrum will automatically highlight in blue (increasing slightly its intensity); or vice versa (hovering the mouse over the peak will highlight the corresponding atom on the molecular structure).

If you need the ^{13}C -NMR predicted spectrum, follow the same procedure but selecting the options for '13C' (be sure that you select the correct tab for 13C in the 'NMR Predictor Box' dialog, red square in the figure below). As you can see in the 'NMR Predictor Option' dialog box below, you can select the limits, the number of points, the frequency and the line width of the spectrum.



Of course you will be able to change the appearance of your simulated spectra as you prefer. Here you are a sample:

