



NMRPredict Online and NMRPredictDesktop

MestReNova: NMR plugin

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Mestrelab Research SL offers NMR Prediction in two flavours. One as a stand alone program (NMRPredict Online) and one which is fully integrated into Mnova (NMRPredict Desktop).

NMRPredict Online is designed for the NMR specialist who needs as much detail as possible about how and why each prediction has been arrived at and the ability to change prediction parameters.

NMRPredict Desktop is designed for the general chemist who uses NMR as one of many techniques and who needs fast accurate predictions which can be easily compared with their experimental spectra.

NMRPredict Online is a stand alone program where a large database of up to 424,000 ^{13}C and X-Nuclei spectra needs to be installed.

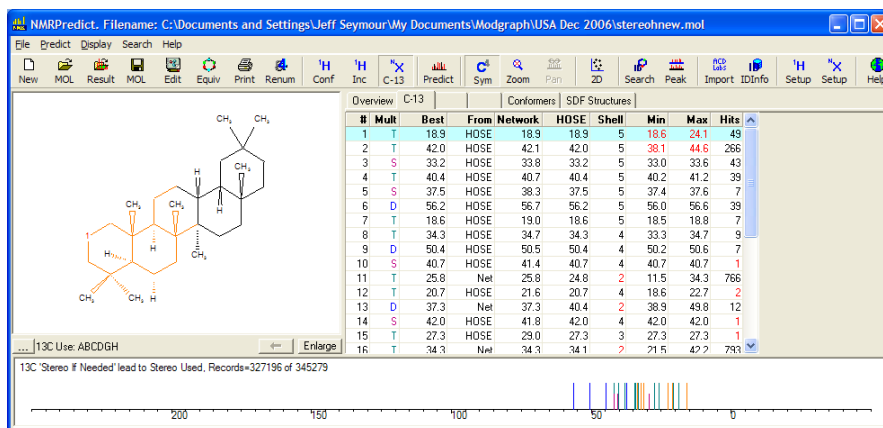
NMRPredict Desktop is a “plug-in” for Mnova which can easily be installed and activated with a licence from Mestrelab Research.

^{13}C NMR Prediction in NMRPredict Online

NMRPredict Online makes predictions using both a sophisticated Neural Network algorithm and a “HOSE code” database of up to 345,000 spectra. In simple terms, HOSE code predictions are more accurate when the query molecule is well represented in the underlying database, but are likely to be inaccurate when the query molecule is unlike any structure in the database. A Neural Network is more tolerant of such lack of representation in the training set, and gives a fairly high level of reliability in all cases.

NMRPredict Online gives the results from the Neural Network, the HOSE code and a “Best” prediction which is a combination of the two results.

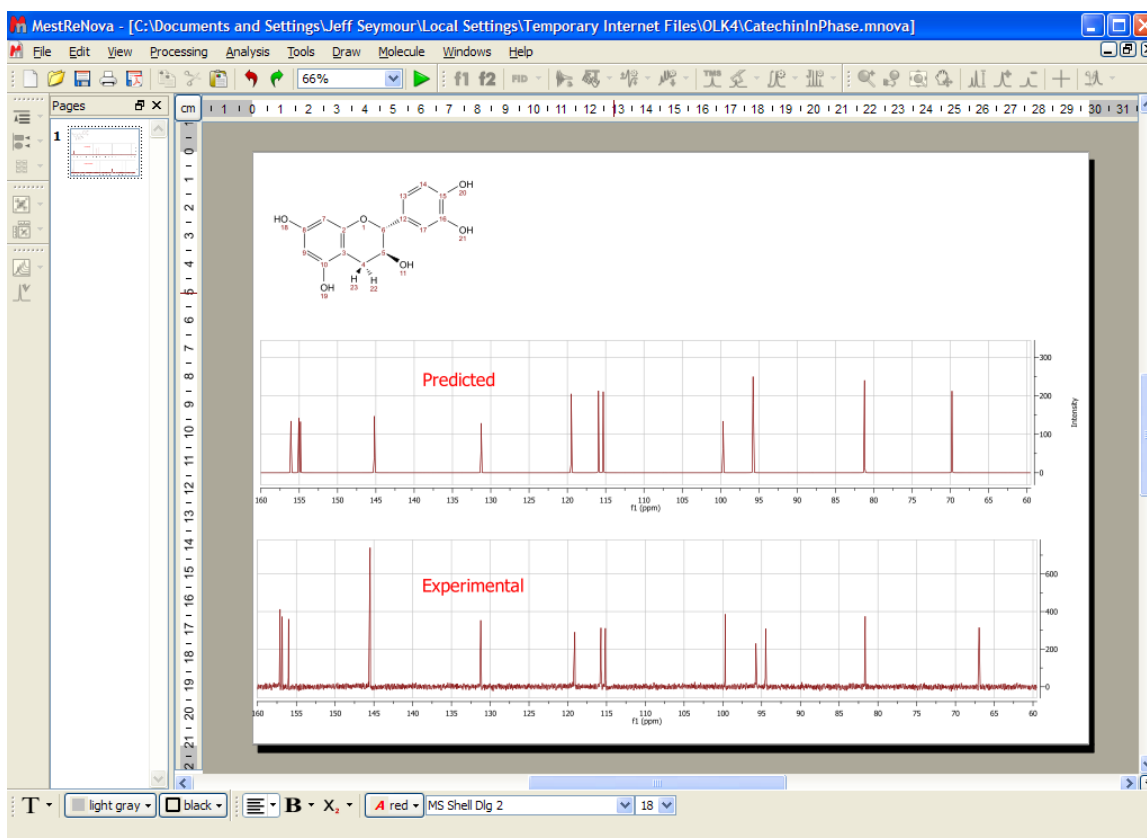
An example of a ^{13}C prediction from NMRPredict Online is shown below.





¹³C NMR Prediction in NMRPredict Desktop

¹³C NMR predictions in NMRPredict Desktop only use the Neural Network algorithm. Neural Network predictions are usually accurate to about 2.0 ppm which is probably adequate for all users. An important feature of NMRPredict Desktop is that experimental and predicted spectra can be compared. An example of a ¹³C prediction from NMRPredict Desktop is shown below:

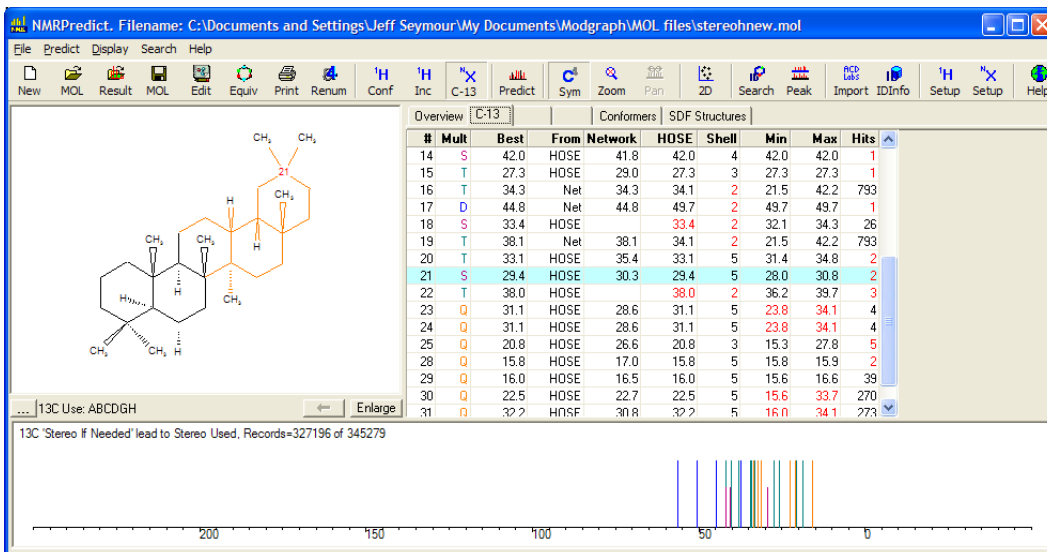


Note that it is possible for users to build their own ¹³C NMR databases within NMRPredict Online. This means that users can then make predictions using both external and internal databases. Accurately built user databases will always help to improve predictions. Of course, since NMRPredict Desktop only uses the Neural Network prediction algorithm, user databases cannot be used.

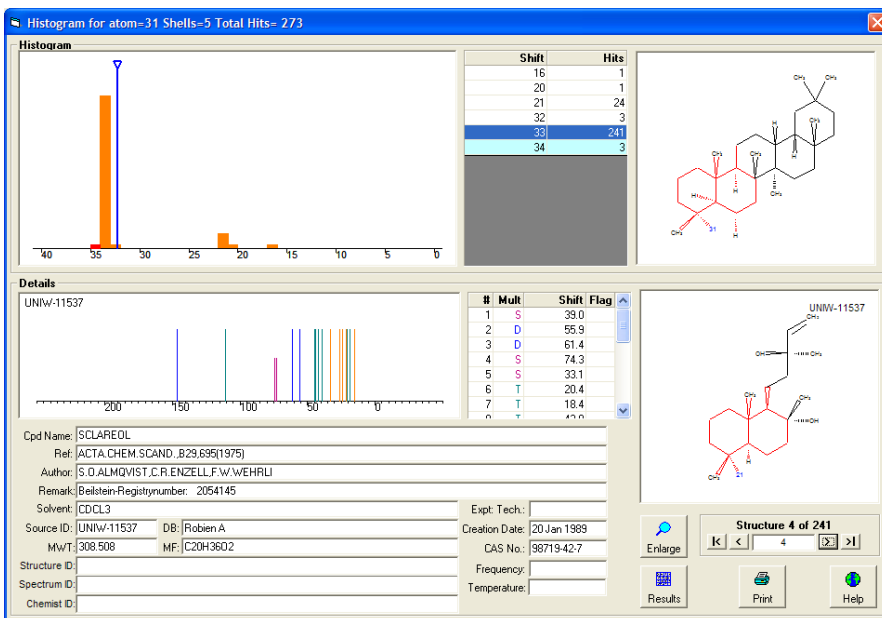
Detail available in ¹³C prediction in NMRPredict Online

One of the main differences between NMRPredict Online and NMRPredict Desktop is the amount of detail which is available behind a prediction. It is possible to see how many “shells” could be reached for each predicted atom by the HOSE code system (5 being the maximum and 3 or more shells usually being reliable), how many database records were used to arrive at the prediction and the minimum and maximum values found in the database records.

An example is shown below:

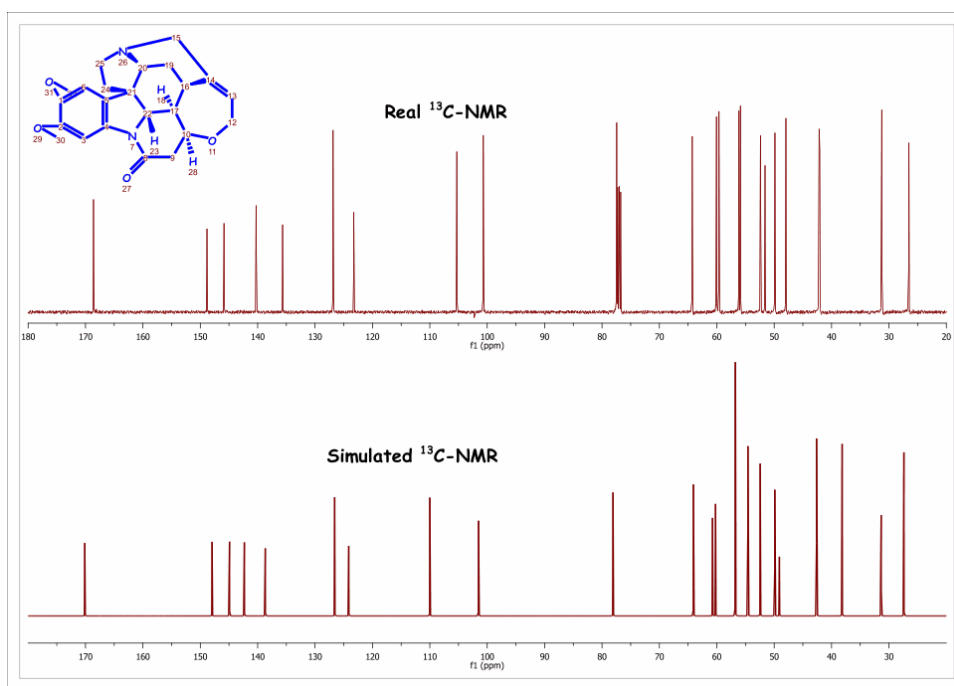


It is then possible to “drill down” and examine exactly which database records were used for each prediction. This gives the specialist an opportunity to look closely at what should be similar reference molecules to their query molecule. An example is shown below:



Detail available in ^{13}C prediction in NMRPredict Desktop

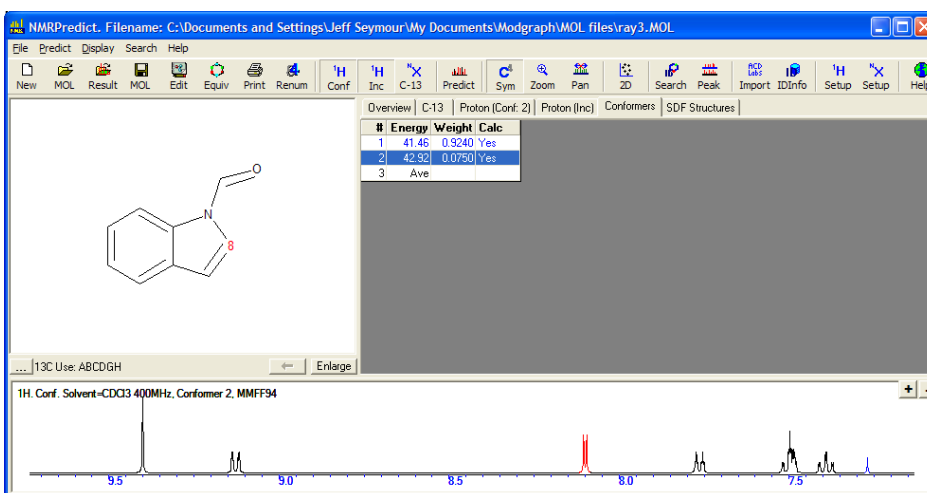
NMRPredict Desktop obviously does not allow users to “drill down” into the data behind a prediction – because there is no data as such. However, the general chemist is not usually interested in such detail. Their interest is in comparing the predicted with their own experimental data – which is exactly what is possible within NMRPredict Desktop.

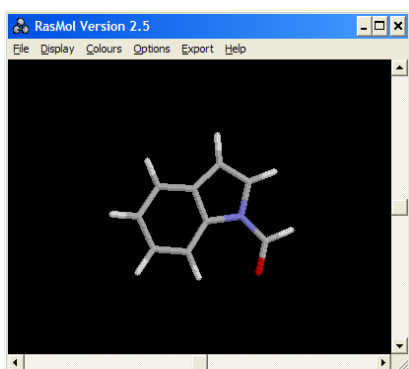


Detail available in proton prediction in NMRPredict Online

In NMRPredict Online a proton spectrum is predicted for each conformer found plus a weighted average spectrum is generated. In addition, it is possible to inspect the 3D structure of each conformer.

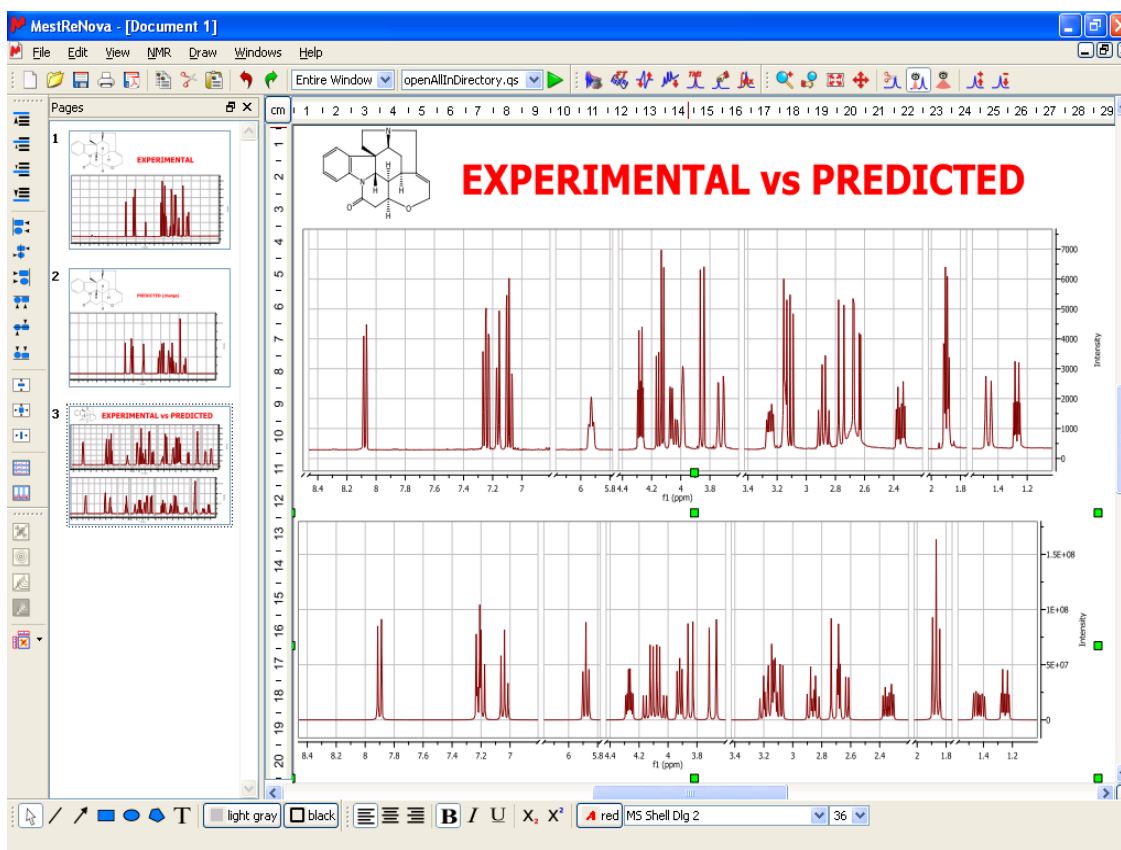
An example is shown below:





Detail available in proton prediction in NMRPredict Desktop

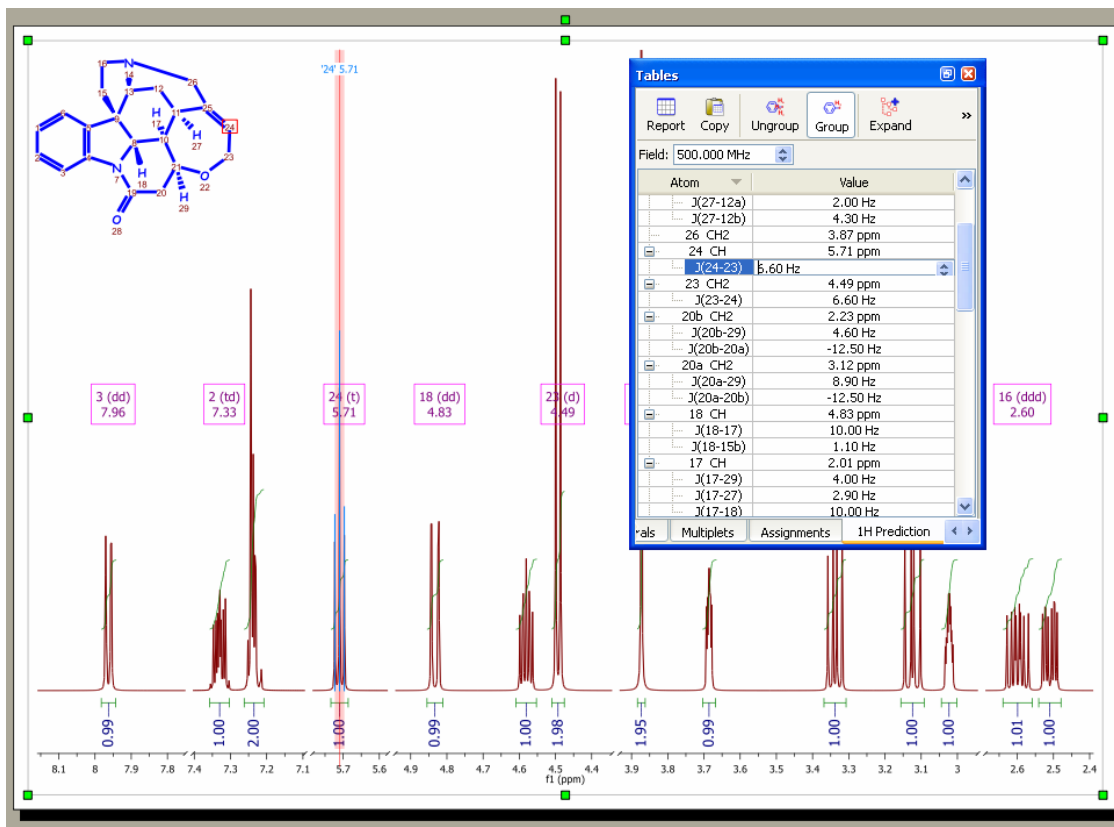
In NMRPredict Desktop only the weighted average spectrum is shown but, as with carbon prediction, it is possible to compare the predicted with the experimental spectrum:



This predicted spectrum can be analyzed as a real one (e.g. it can be integrated, etc). The user can also visualize and edit the chemical shift and coupling constants values from the tables of the predicted spectrum by following the menu 'View/Tables'.

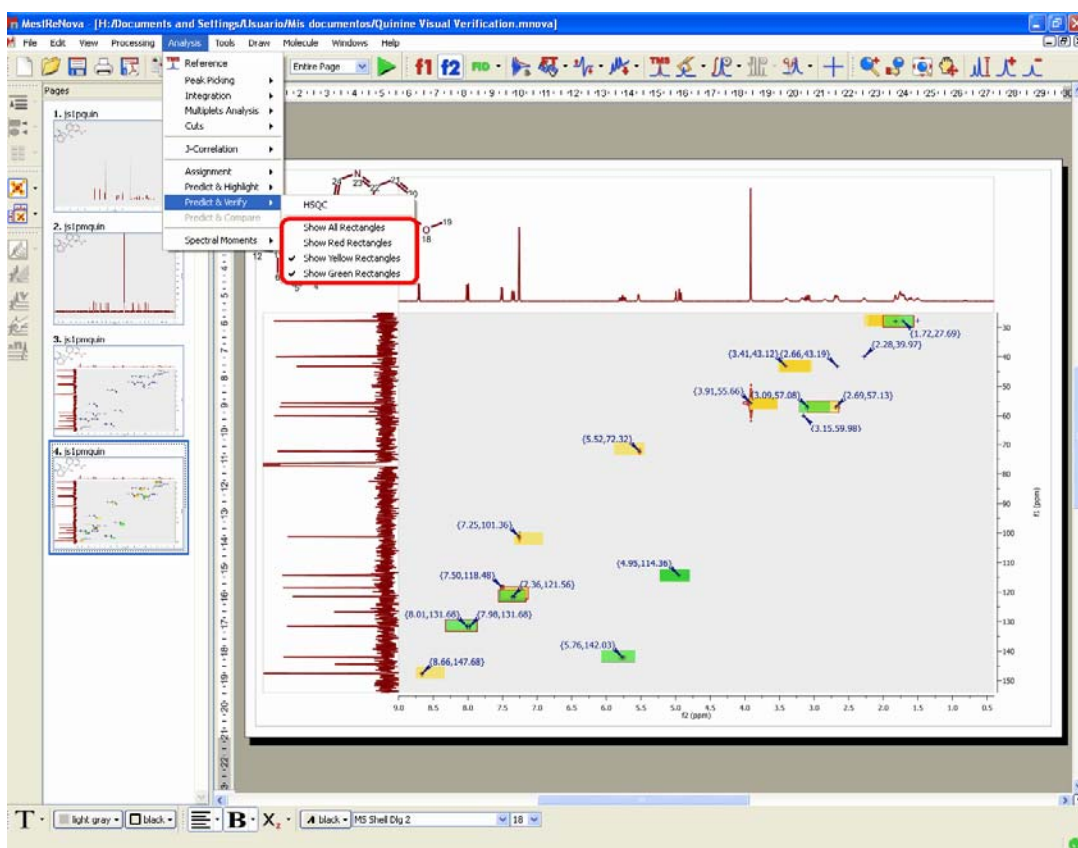


Finally, to know the "predicted assignment", just hover the mouse over the desired atom, (so that it becomes highlighted in a red box) and the corresponding signal in the spectrum will automatically highlight in blue and red; or vice versa (hovering the mouse over the peak will highlight the corresponding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

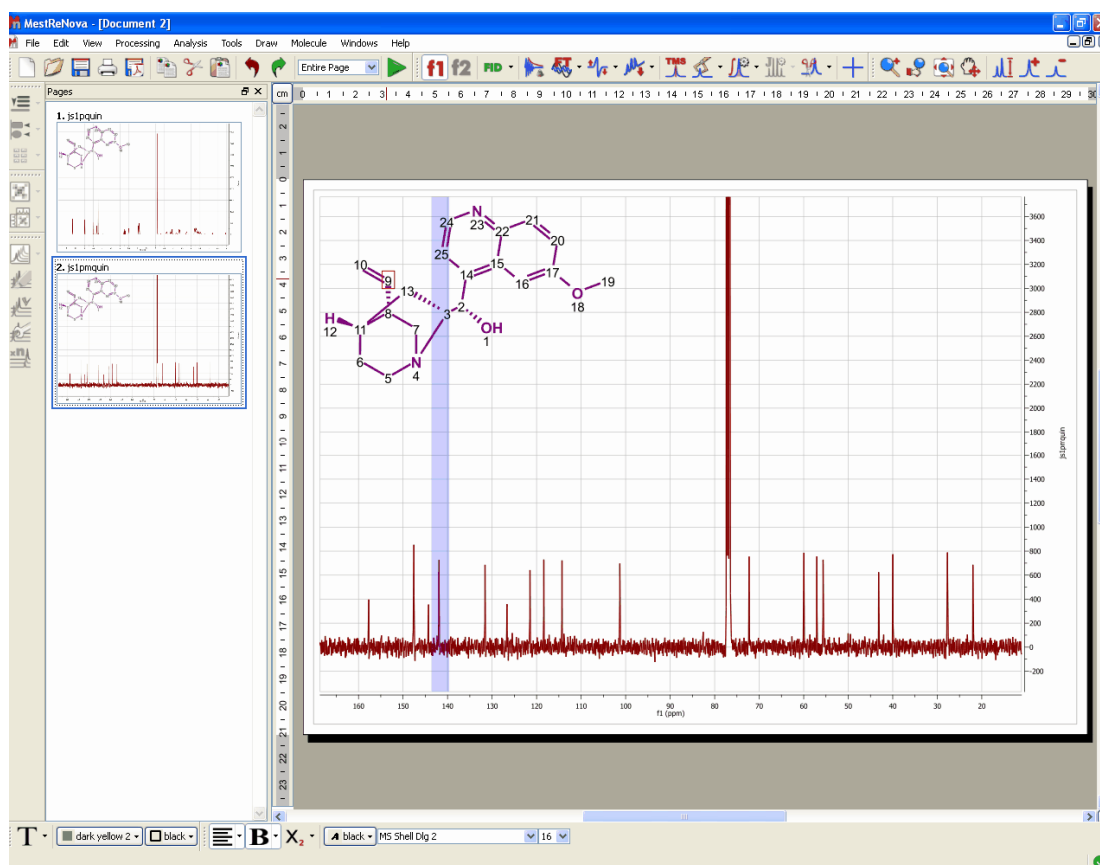


NMRPredict Desktop also incorporates three additional features to help the user in the process of assigning 1D NMR spectra:

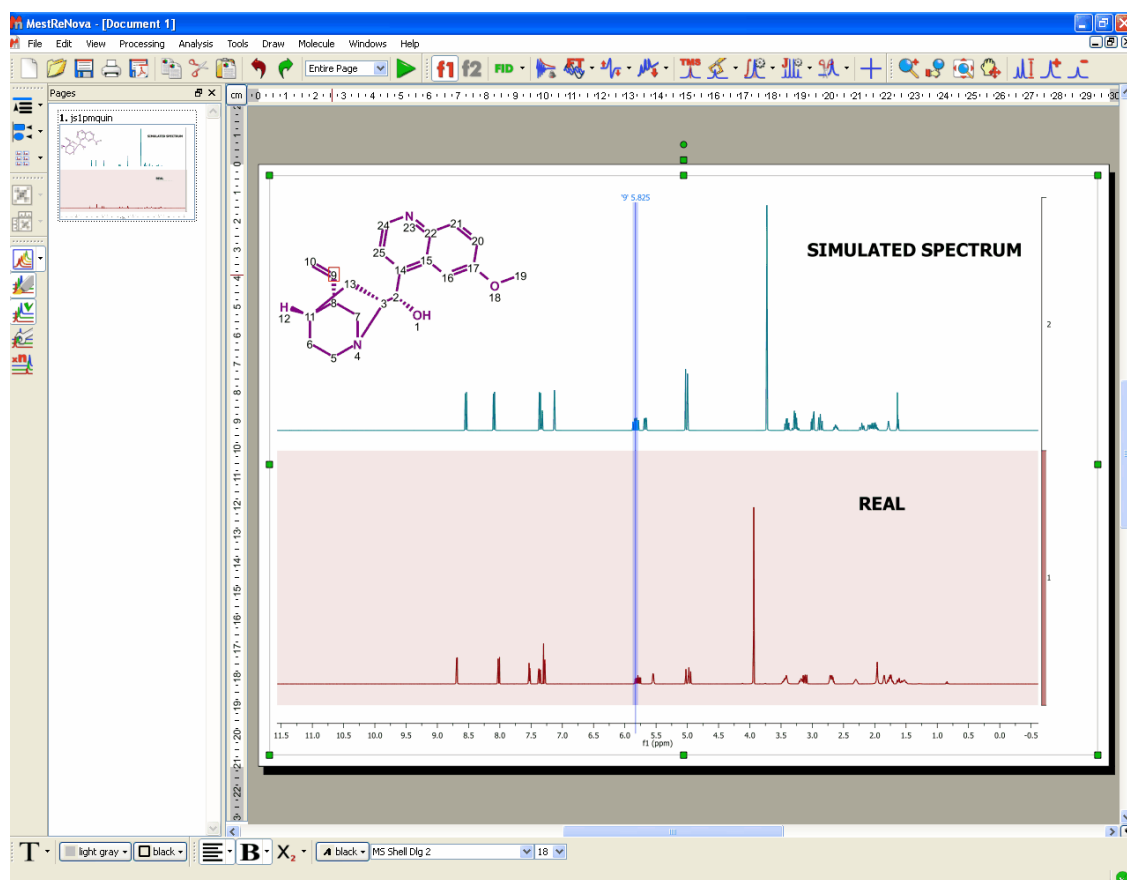
Predict and Verify: a new feature to validate molecular structures, which is based on the concurrent analysis of two simulated 1D (^1H and ^{13}C) NMR spectra and a real 2D NMR one-bond correlation spectrum, such as HMQC or HSQC (experiments which correlate the chemical shift of the proton with the chemical shift of the directly bonded carbon).



Predict & Highlight: This feature will calculate in the background a simulation of the spectrum of the molecular structure present in the spectral window, highlighting the expected chemical shifts when the user hovers the mouse over a proton or a carbon. This tool will be very useful to help the user in the process of assigning 1D NMR spectra.

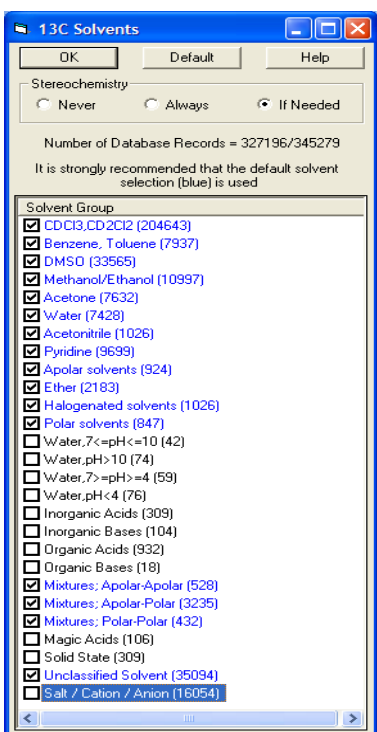


Predict & Compare: This feature will display, in stacked mode, an experimental spectrum and a simulation of the spectrum of the molecular structure present in the spectral window, highlighting the expected chemical shifts when the user hovers the mouse over a proton or a carbon. This tool can be used of assistance in the process of assigning ^1H and ^{13}C NMR spectra.



Setting ^{13}C prediction options in NMRPredict Online

All ^{13}C database records used for prediction have been measured in a certain solvent. In NMRPredict Online it is possible to change the default solvent setting and only use database records measured in that specific solvent. In NMRPredict Desktop the solvents are taken into account by the Neural Network but the solvents are hard coded to a default list of solvents and cannot be changed. The screen to change the solvents within NMRPredict is shown below:



By default stereochemistry is used automatically by both NMRPredict Online and NMRPredict Desktop. In NMRPredict Online it is possible to turn stereochemistry off. It is very unusual to need to do this and it is not possible to do this in NMRPredict Desktop.

So, which software do you need? That depends on how you intend to use it. It is common for companies and Universities to purchase a combination of a few copies of NMRPredict for the NMR specialists and many more copies of NMRPredict Desktop for the general chemists.