



Predict & Highlight and Predict & Compare

MestReNova: NMR plugin

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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.

The user will be able to use this tool with ^1H and ^{13}C NMR spectra just by pasting the corresponding molecular structure (quinine, in this example) over the spectrum and following the menu 'Analysis/Predict/Predict & Highlight', as shown in the picture below:

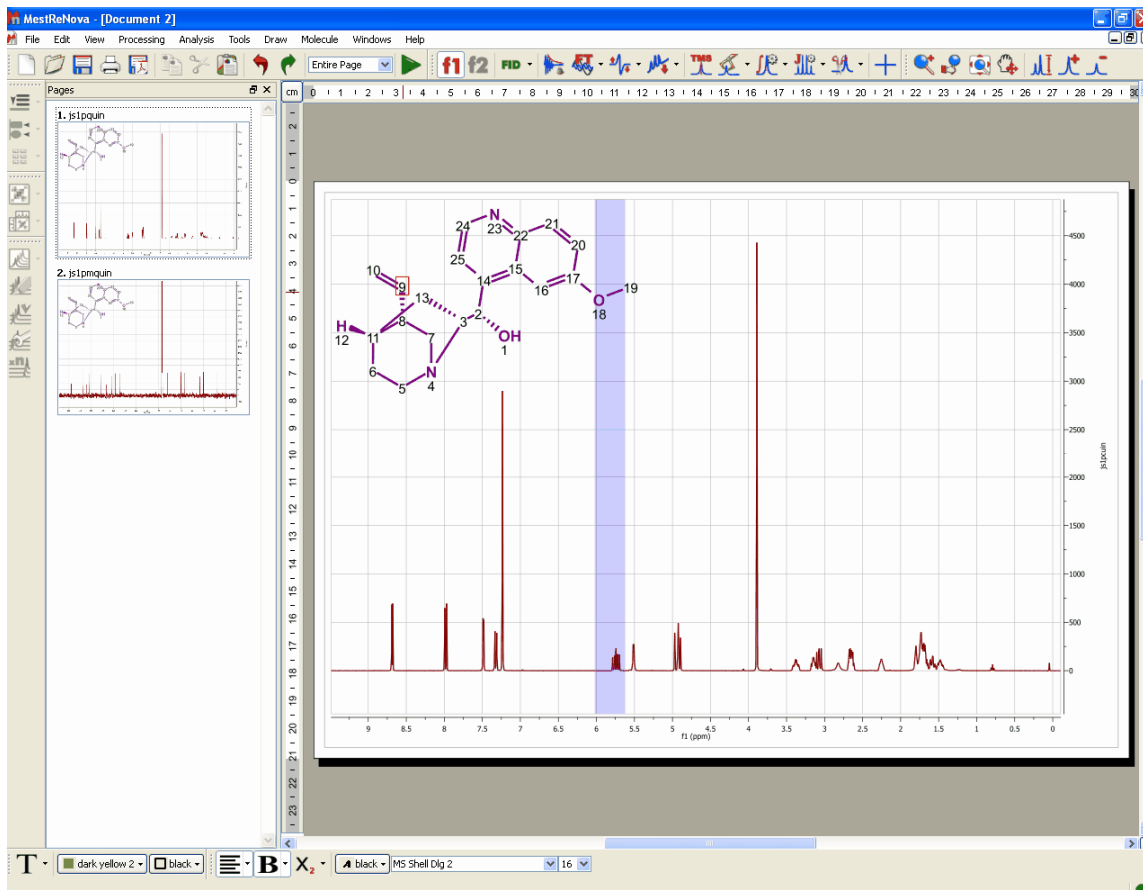
The screenshot shows the MestReNova software interface. The 'Analysis' menu is open, and the 'Predict & Highlight' option is highlighted with a red box. A blue arrow points from a callout box to this menu item. Another callout box points to the quinine molecule structure overlaid on the NMR spectrum, with the text '1st: Paste the molecular structure over the spectrum'. The NMR spectrum shows chemical shifts from 0 to 9 ppm. The quinine molecule is shown with atoms numbered 1 through 25. The '2nd: Select 'Predict & Highlight'' callout points to the 'Predict & Highlight' menu item.

The algorithm run for the simulation carried out in the background will be the one selected in the 'Molecule/Prediction Options' menu. The user will be able to select the 'Increments' or the 'Charge' algorithm in the ^1H simulation and the 'Neural Network' system (by using NMRPredict

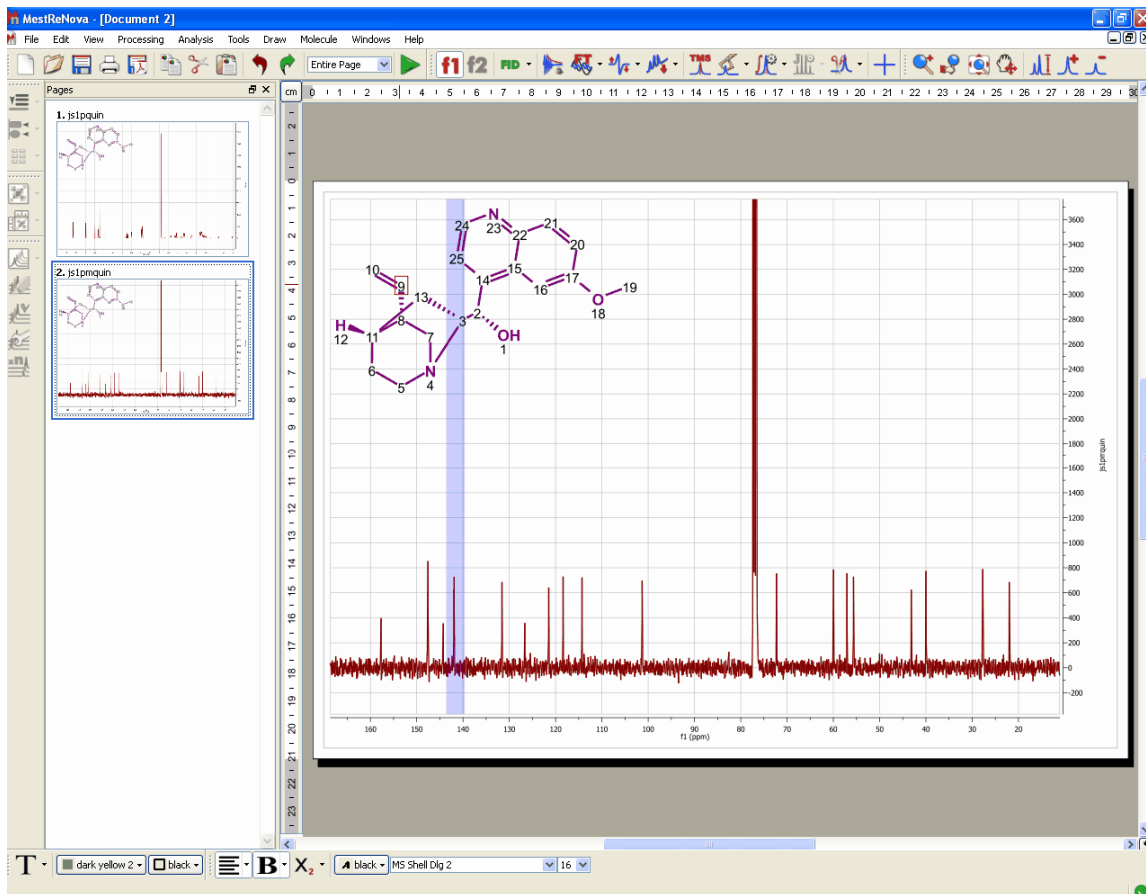


Desktop) or the **HOSE** database methodology (implemented in the server-based NMR Predict application only).

After having applied this feature, the user will notice that hovering the mouse over an atom will highlight the area on the spectrum corresponding to the simulated value for that atom. The user will therefore get an indication as to the fact that experimental signals falling within the highlighted area may correspond with the proton directly bonded to the carbon number 9 on the molecule.



The user will be able to apply the same feature with the ^{13}C NMR spectra, as shown in the picture below:



Predict & Compare

This feature will display, in stacked mode, a simulated spectrum for the molecular structure present in the spectral window, highlighting the expected chemical shifts when the user hovers the mouse over an atom on the molecule. This tool can be very useful as assistance in the process of assigning ^1H and ^{13}C NMR spectra.

The user will be able to use this tool with ^1H and ^{13}C NMR spectra just by pasting the corresponding molecular structure (quinine, in this example) over the spectrum and following the menu 'Analysis/Predict/Predict & Compare', as shown in the picture below:

