



## Why upgrade from MestReC or MestReC Lite to Mnova?

### MestReNova: NMRPredict plugin

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**Mnova** is the natural evolution of our very popular application **MestReC**. However, it is more than a new version of MestReC. The fact is that **Mnova** is a redevelopment of MestReC which is intended to supersede the old software, so we would strongly recommend that you update for **Mnova**.

**Mnova** is a completely new development and a completely new concept which will open up a whole new range of possibilities when storing and sharing data within organizations, changing the way in which scientists process and report NMR data. **Mnova** has been designed to make NMR both more convenient and more powerful, and to give the user improved results with minimum effort.

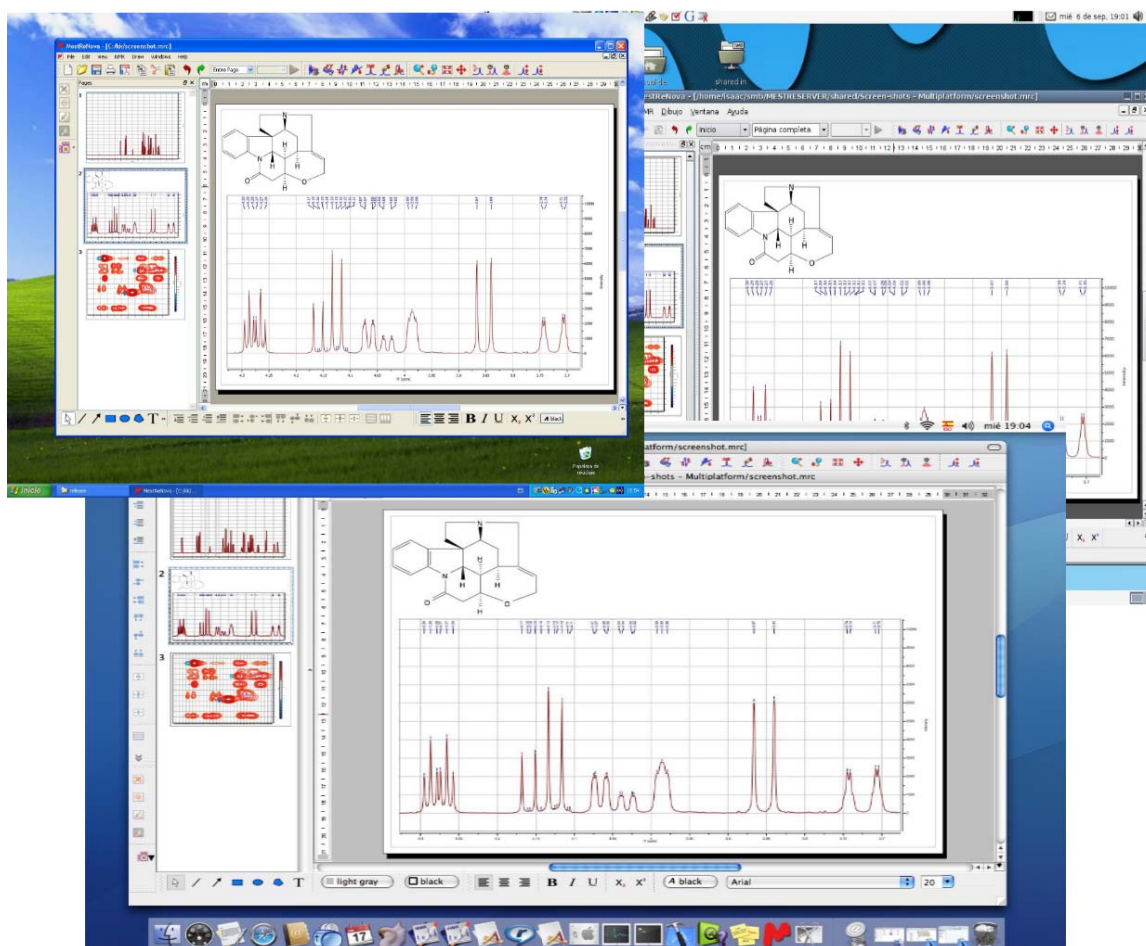
There are many reasons why we went to the effort to develop **Mnova**, focused around our aim to make Mnova even easier to use and learn that our previous software packages, whilst increasing processing power and capabilities and improving reporting, integration with other applications and many other areas MestReC and MestReC Lite users had highlighted in their feedback. Some of the most significant improvements above MestReC and MestReC Lite are itemized and detailed in the following pages, but here is a very concise summary of just some of the main ones, followed by the detail:

1. Mnova is multiplatform and runs on Windows, Mac, Linux and Unix-like systems
2. Mnova has a multipage interface and document, which allows users to handle and save many more spectra within one document.
3. Mnova has greatly improved annotations, making report preparation much easier
4. Mnova handles molecular structures and allows assignment, NMR prediction, etc.
5. Mnova is integrated with MS Office, ELNs and other Windows applications via OLE/COM.
6. Mnova includes very significant improvements to automation, with automated processing, automated reporting via templates and also a full scripting language which allows full automatic running of the application.
7. Mnova has many powerful additional processing and analysis features (Resolution Booster, Metabonomics Phase Algorithm, JCorrelator, etc.).

Now, let's look at these, and many others, in more detail in the following pages:



1. Mnova is **multiplatform**, running on **Windows, Mac, Linux** and Unix-like systems. From now on, multiplatform laboratories will be able to allow each researcher to work on their Operating System of choice, and to seamlessly share data and processing capabilities with other researchers working on different platforms. There is no longer a need to have three different software packages, and three different file formats, for different Operating Systems.

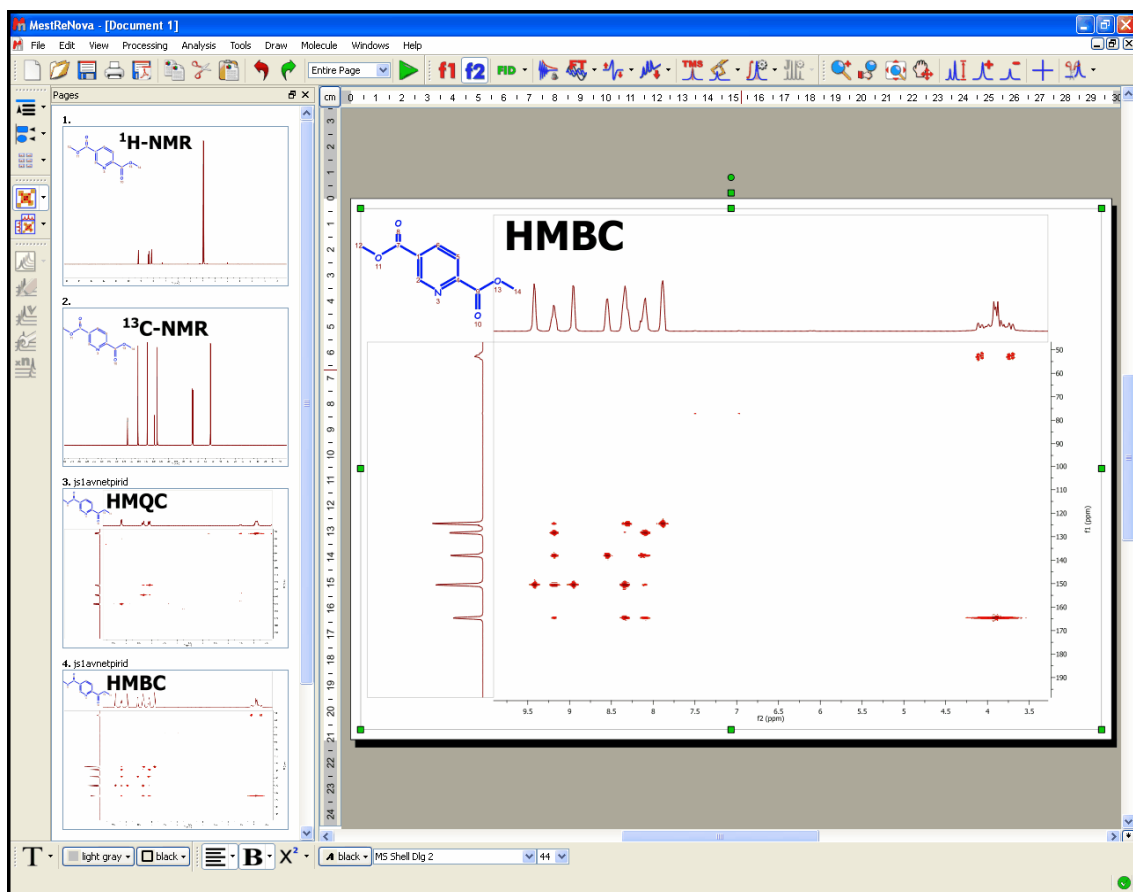




2. Mnova has a **multipage interface** similar to Powerpoint (this allows the user to work with and save several spectra in one document, maybe all experiments for a given sample, maybe a metabonomics or other multiple spectra study). The behavior of graphical objects in Mnova is also MS Powerpoint-like, as we think that the great majority of people in science are familiar with this presentation and reporting software, and that making our program behave in a very similar way to it will ensure that even new users find it very easy to work with from the very start.

The **page navigator** is placed, by default, as a column on the left hand side of the screen.

The **Mnova document** is also a **Multipage Document**. This means that *all pages within a single document will be saved as a single document*. This will allow you to keep, for example, different experiments for a certain sample ( $^1\text{H}$ ,  $^{13}\text{C}$ , homonuclear and heteronuclear 2D correlations) as a single, unified document.



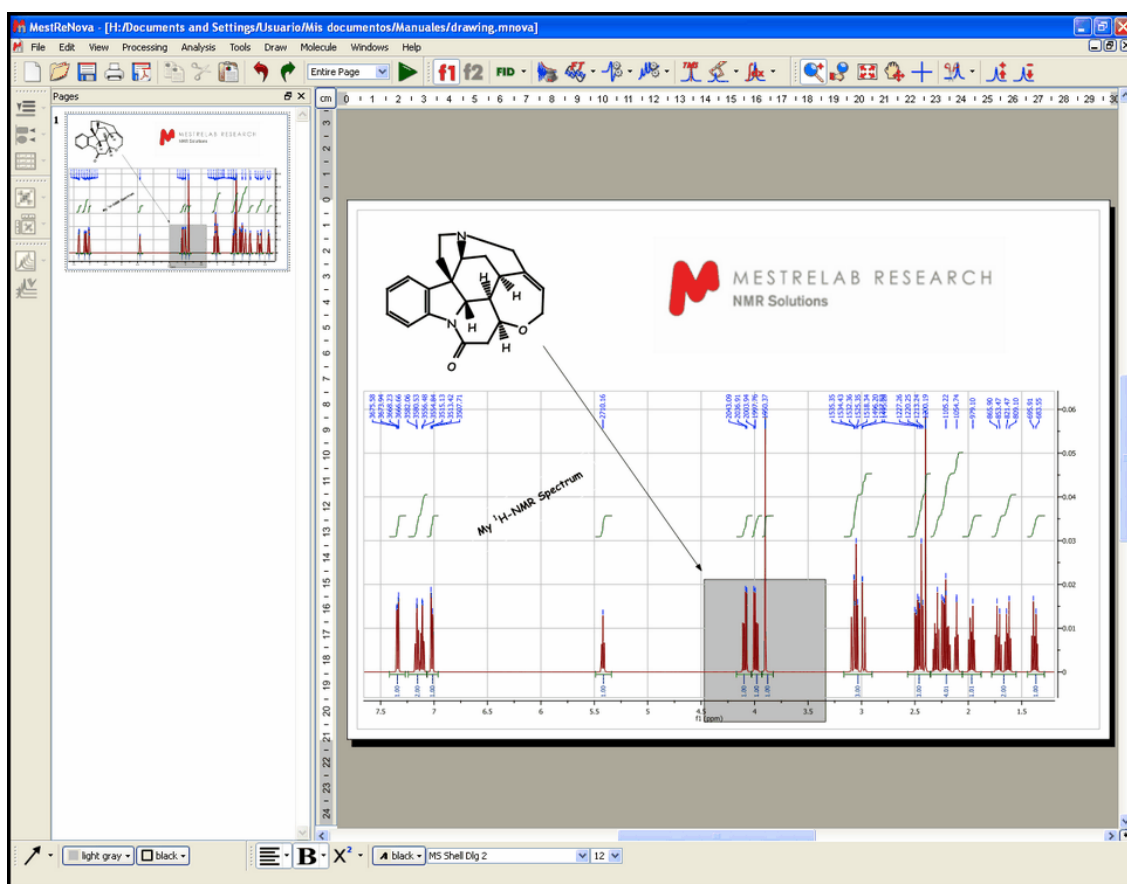


3. **Mnova** has the most powerful **graphics and annotations** capabilities available in any NMR software. This was very common feedback from MestReC and MestReC Lite users, who often found the annotations capabilities in these packages somewhat restrictive.

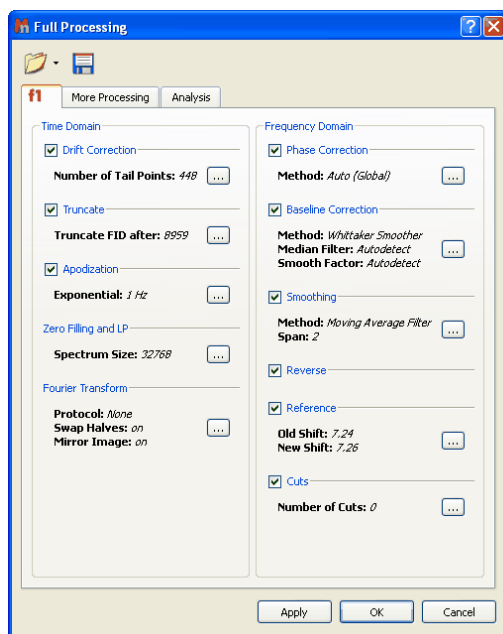
Most of the annotations and drawing available in MS Powerpoint are available in **Mnova** via the graphics toolbar placed by default at the bottom of the screen, below the page navigator and the document area.

The software supports Rich Text and so a wide range of fonts, font sizes and font embellishments (sub- and superscript, bold, italic etc) are available. In addition to text annotations, geometrical objects, arrows and other commonly used graphics are also available.

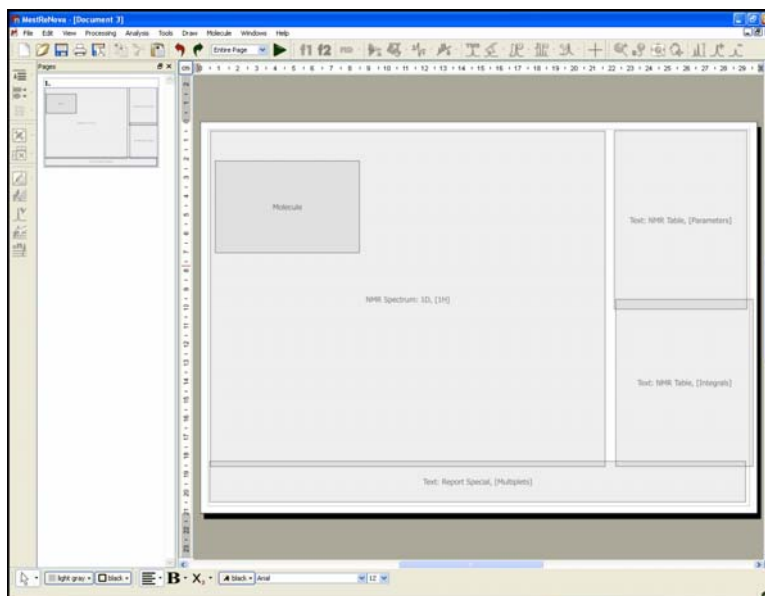
**Mnova** can import objects such as **molecular structures** or **images** by using the standard Windows Copy and Paste tools.



4. Automation is key to very important time savings and productivity enhancements, as it eliminates the need to spend valuable time on routine tasks. **Mnova** includes a powerful and flexible '**Processing Template**' feature which allows the user to easily automate the full processing of both 1D & 2D NMR data sets, and to save these processing templates for future use or for sharing with others. This is ideal for the batch processing of spectra of the same type, and can also incorporate analysis operations (peak picking, cuts, integration and multiplet analysis).



5. **Layout Templates:** It is now possible within Mnova to create '**Layout Templates**' for your NMR spectra. This feature includes the capability to create templates with the location, orientation and size of the spectrum, molecular structure, tables and multiplet reports. It is very easy to create a template with Mnova, just open a document and select the desired location and properties for the different objects present in it, once you are done, 'Save As...' a Mnova template.

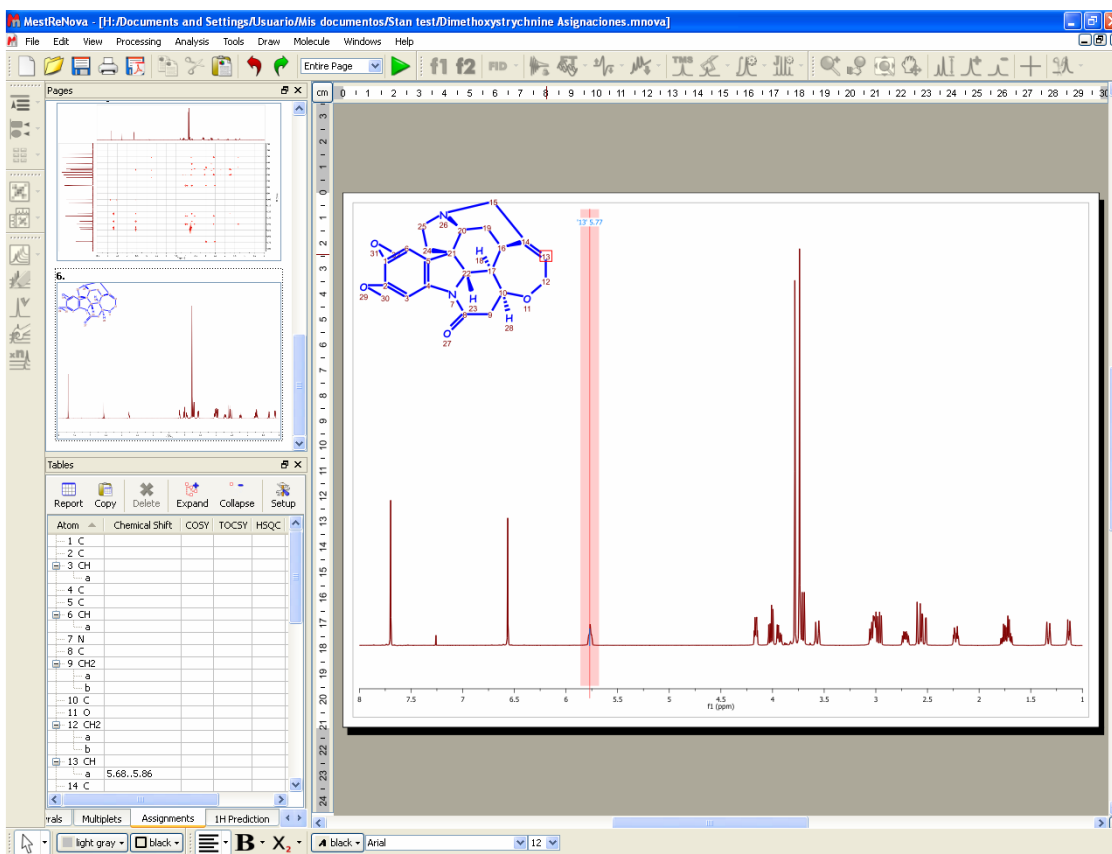




6. Mnova provides a molecular viewer and a very simple interface to **assign** your molecule.

Once the **assignment** has been made, hovering the mouse over the atom will highlight the corresponding peak or multiplet in the spectrum, and hovering the mouse over the peak will highlight the corresponding atom on the molecular structure.

Once you have finished with the **assignment** you can visualize the assignments list in a table where you will be easily able to edit/add/remove any entry by double clicking on it.



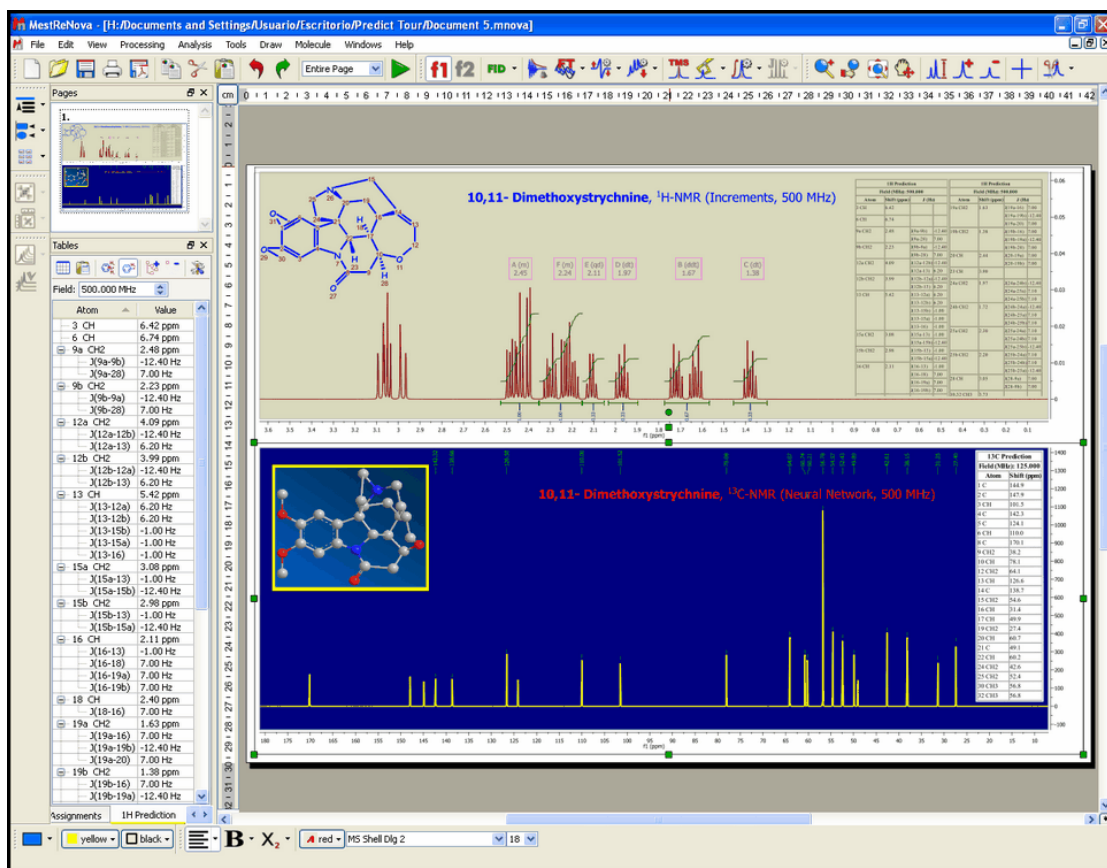
7. Mnova incorporates the ability to predict molecules as a separate plugin (**NMRPredict Desktop or Server**).

Our intention is for **Mnova** to support predictions with a range of prediction packages as wide as possible.

Currently, predictions can be carried out by using **NMRPredict**, the prediction software by Modgraph Consultants Ltd.

**NMRPredict** comes into two different flavours:

- NMRPredict Desktop**
- NMRPredict server-based**



**MestReNova Desktop** uses a Neural Network system for the prediction of  $^{13}\text{C}$ -NMR spectra, and the **increments** methodology of Professor Ernö Pretsch (ETH, Zürich) for a fast simulation mode of  $^1\text{H}$ -NMR spectra, as well as the **CHARGE** program which offers  $^1\text{H}$ -NMR prediction based upon partial atomic charges and steric interactions.

**CHARGE** offers the **first** quantitative prediction of the proton chemical shifts of a variety of organic compounds. It works by first generating 3D conformers from a 2D structure through a choice of *force fields* and then predicting proton spectra for all the conformers.

The inclusion of this prediction package within the Mnova interface generates the ideal environment for comparison of experimental and predicted data, as part of structure verification, elucidation or spectral analysis.

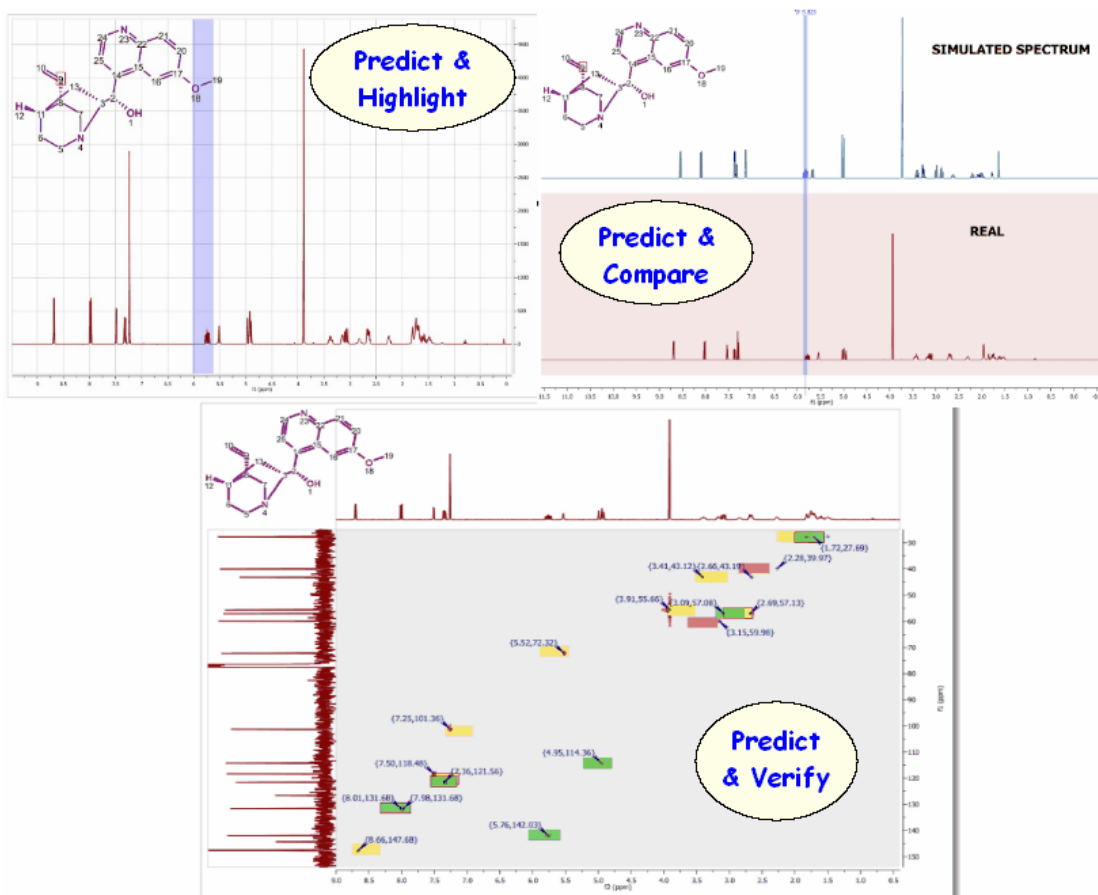
8. Mnova integrates the prediction feature to assist the user in the assignment of 1D and 2D NMR spectra by the incorporation of the **Predict & Highlight**, **Predict & Compare** and **Predict & Verify** features.

The **Predict & Highlight** feature will calculate, in the background, a simulation of the spectrum of the molecular structure present in the spectral window, replicating the experimental magnetic field, highlighting the expected chemical shifts when the user hovers the mouse over an atom of interest.

The **Predict & Compare** feature will display a simulation of the spectrum of the molecular structure present in the spectral window, stacked with the experimental spectrum present on the same window, highlighting the expected chemical shifts when the user hovers the mouse over each proton or carbon atom.



The **Predict & Verify** feature is based on the concurrent analysis of two simulated 1D ( $^1\text{H}$  and  $^{13}\text{C}$ ) NMR spectra and a real 2D NMR one-bond correlation spectrum, and will be very useful to validate molecular structures.

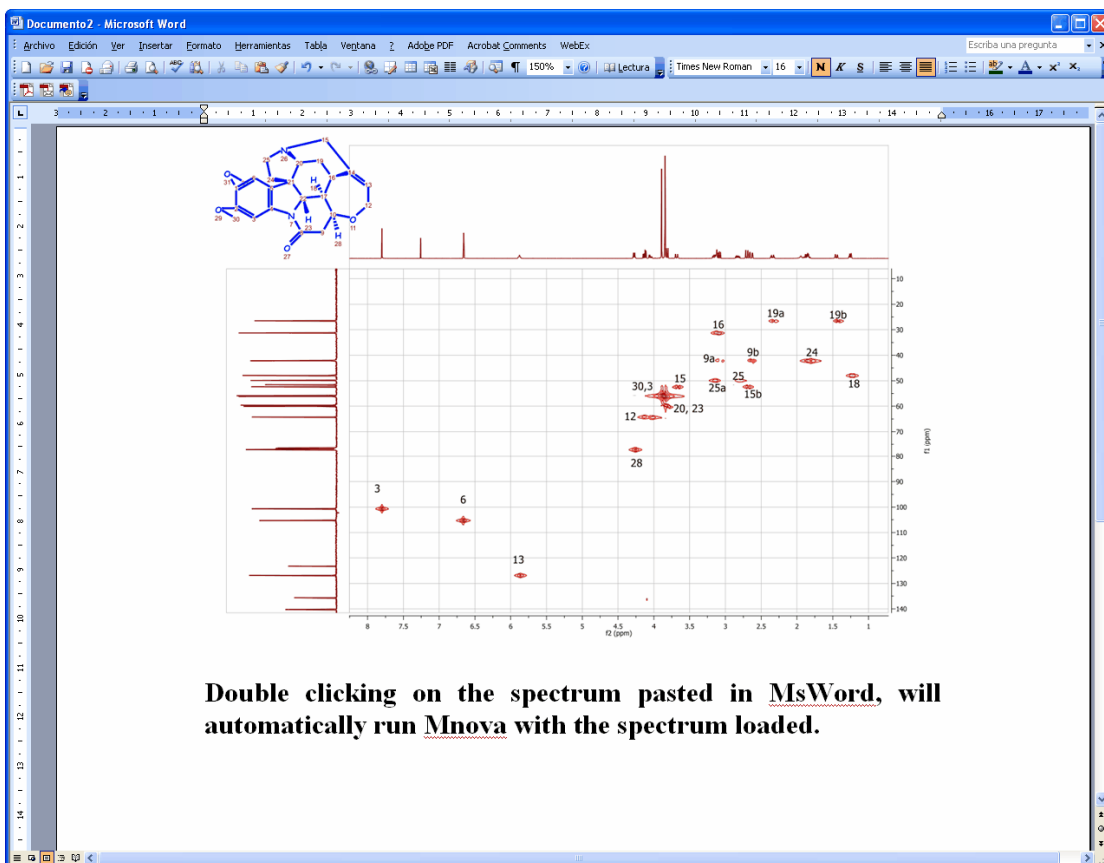





9. Mnova is fully integrated with MSOffice and several Electronic Lab Notebooks through **OLE/COM**.

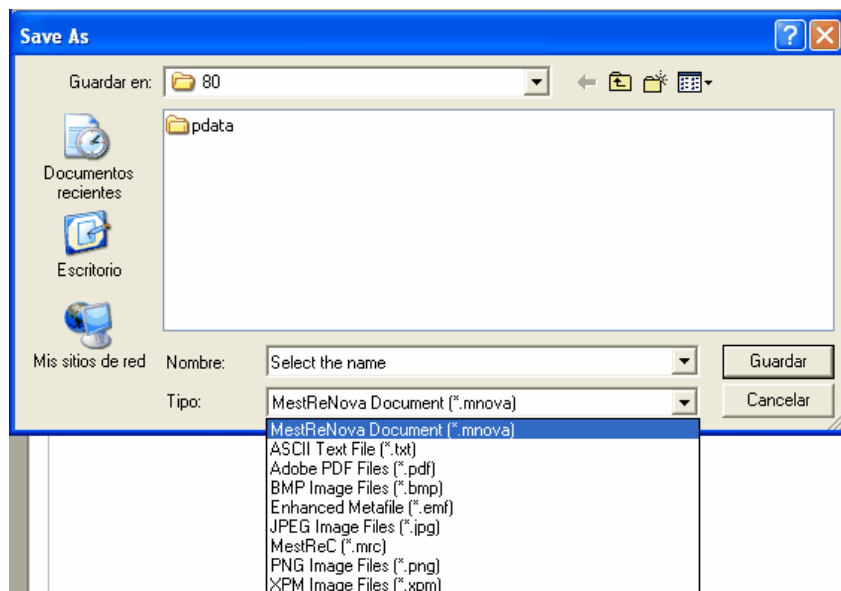
**Mnova** supports clipboard copying, drag & drop and the ability to link external software objects such as documents and images to the Mnova document or to embed them in the document known as **OLE** (Windows only).

This ensures data integrity by keeping the link between reports and the original data used to produce them, and allowing later changes to the original data to update the reports.

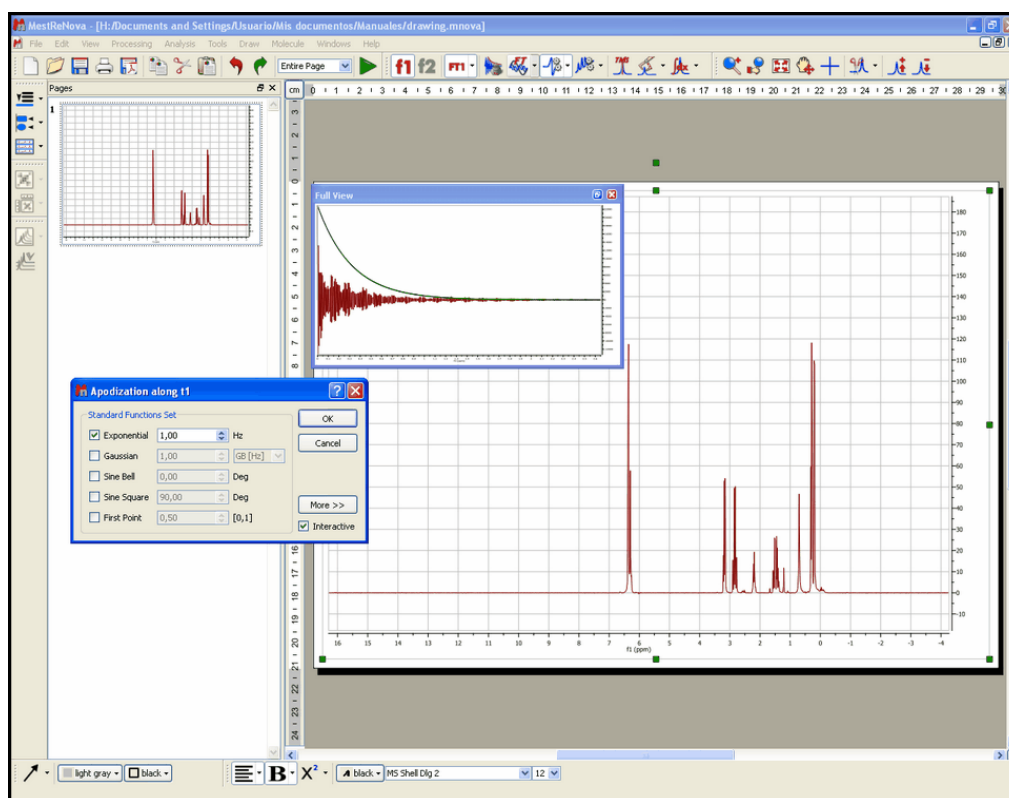




10. Mnova has integrated an 'export to PDF on-the-fly' feature  and many graphical formats such as \*.bmp, \*.png, \*.jpg, \*.emf, \*.xpm, etc.

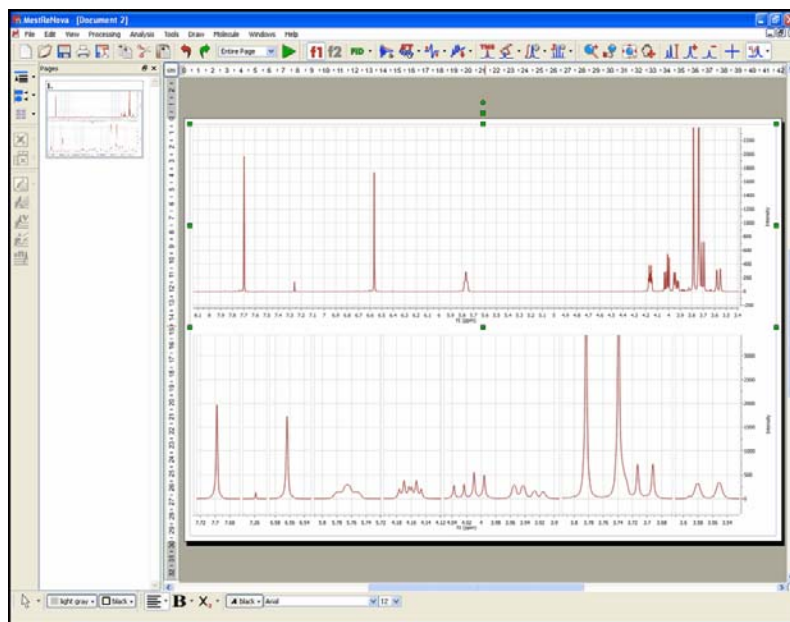


11. Mnova has fully **interactive processing**, given the user the ability to effect changes in the time domain and see the results in real time in the frequency domain, thus eliminating the need for tedious reloading and FTing of the spectrum when the optimal processing parameters are not immediately found.

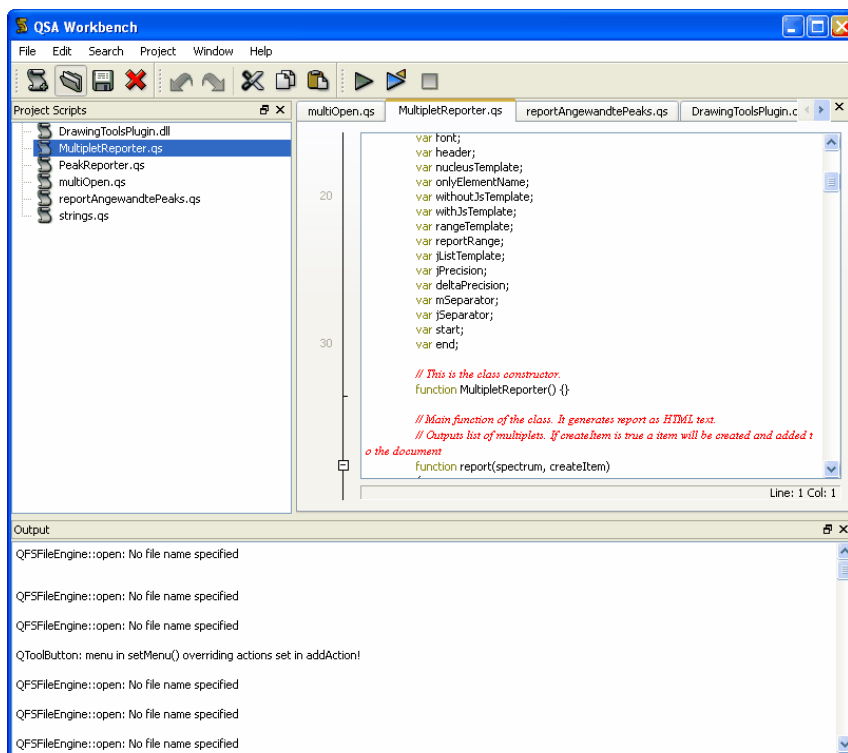




12. Mnova incorporates the '**Cutting**' tool, to allow the user to hide areas of the spectrum which are not of interest for a given study, thus maximizing the on-screen and on-report size of the important or significant ranges in the spectrum.



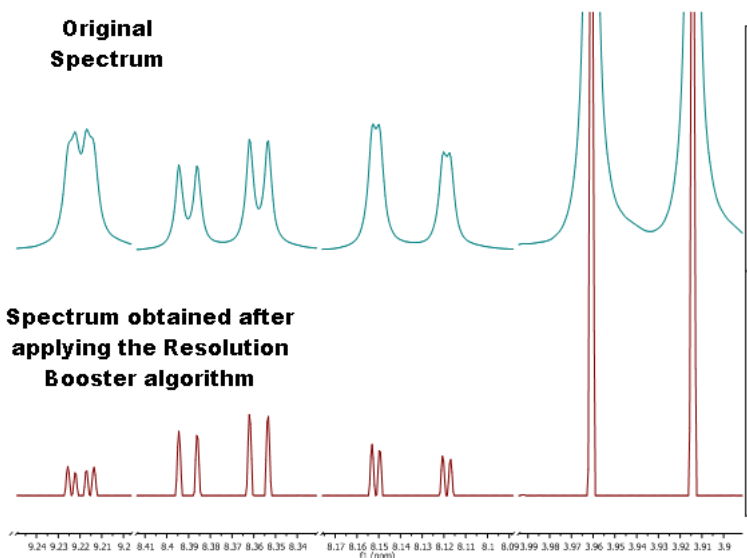
13. Mnova implements a very powerful **scripting** language for automation (based on Javascript), as well as a very simple interface for building macros. This scripting tool allows full customization of every aspect of Mnova and the running of the software in full automation, even from third party applications. Integration with other reporting or analysis applications can therefore be done a lot more effectively than with previous generation software packages.



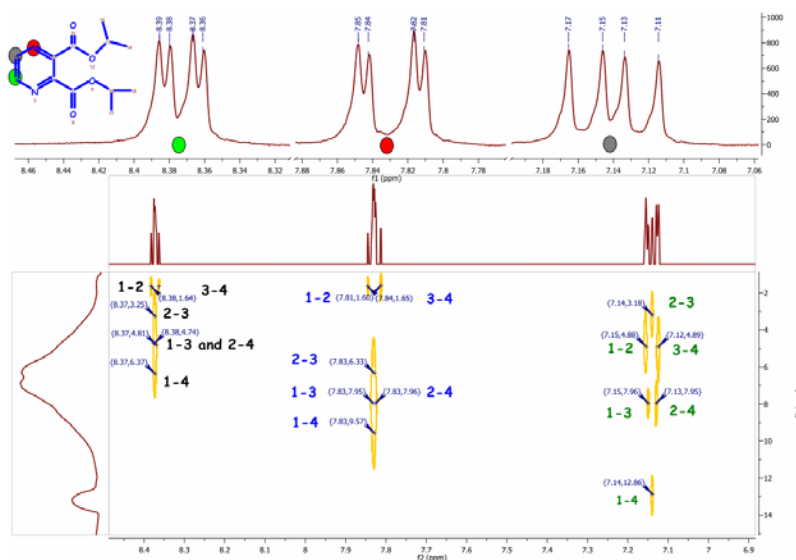




17. Mnova now includes the '**Resolution Booster**' feature, a new, revolutionary method for Resolution Enhancement of 1D and 2D NMR Spectra. This Resolution Booster algorithm is extremely fast and efficient, very simple to use and will very significantly improve the analysis capabilities of the software.



18. Mnova implements the '**J Correlation**' analysis feature: A New Method for Detecting Spin Connetivities in  $^1\text{H}$  NMR Spectra. The main goal of this tool is to convert a 1D spectrum into a 2D-like plot in which it is easy to correlate multiplets containing the same **splitting**. Its main purpose is to rule out couplings between multiplets.



19. Mnova incorporates a fast in-house developed wavelet-based **compression algorithm**, which is generally applicable to 2D NMR data sets (obtaining high compression rates; up to 800:1). We have tested this compression methodology with some examples of 2D spectra focusing on keeping the NMR signal information intact either on cases of qualitative purposes of signal assignment or on quantitative analysis as commonly required for solution structure calculations derived from nuclear Overhauser effects.



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20. And...many more: New **templates** for **Multiplet Reports**, **Contextual Menus**, **Predefined Integration**, **Binning**, **Smoothing**, **Arithmetics**...