Mnova software for NMR and MS data processing

The Chemistry department has a site licence for the Mnova Suite of packages from MestreLabs, which includes tools for the processing and analysis of 1D and 2D NMR spectra and MS, GC-MS and LC-MS data. We also have additional licences for two further plugins for NMR Quantification and for Reaction Monitoring which can be installed optionally in addition to the main Mnova suite.

Key features

Some specific features of the Mnova software that make it attractive for use in the academic environment include:

- Platform independence: The software will run in native forms on Windows, Mac and Linux platforms.
- Flexible licence: The software uses a floating licence model that runs from a single Chemistry server. Once activated, the licence will remain valid for a continuous period of 90 days without the need to connect to the server or the university network. This is clearly ideal for working away from the laboratory.
- Familiar look and intuitive interface: The software has a similar appearance to Powerpoint, with separate spectra for a sample appearing as individual pages (slides) within one document.
- Data reporting and output: the software uses a WYSIWYG user interface and it is a simple process to extract information and copy spectra for reporting purposes.

Installation and licensing

The software may be downloaded as single executable files directly from the Mestrelab web site, allowing you to choose the appropriate version for your operating system:

http://mestrelab.com/software/mnova/download/

You will also need to copy to your system the zipped licence file (Mnova_University_of_Oxford_Campus_Licence2.zip) from the Chemistry NMR software server:

\\chem.ox.ac.uk\SRF\NMR\NMR Software

Now run the downloaded Mnova executable to install the software and then start the program, at which point a registration window similar to that below should appear.
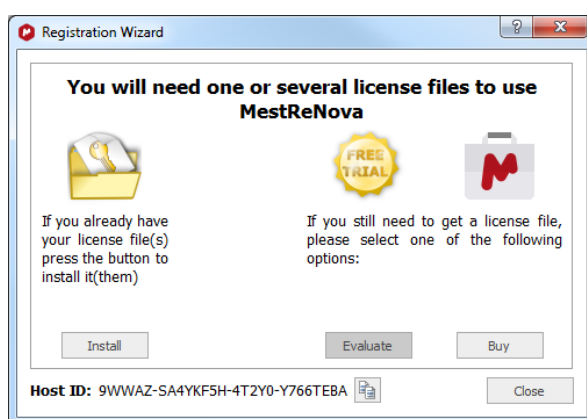

Select the **Install** option, browse to the licence zip file on your system and select this (there is ***no need*** to unzip the folder at any stage). You should then get confirmation that the licences were successfully installed. Restart the software to fully activate the program- ***you will need to be on the university network to have access to the chemistry licence server, such as via VPN***.

Optionally, you may also wish to install two additional modules for NMR Reaction Monitoring (RM) and for quantitative NMR (qNMR). If so, these may be downloaded from the Mnova website and then installed from within Mnova by selecting the ***Edit-> Advanced Plug-ins*** option.

NMR Processing interface

The basic interface for processing NMR data is shown below. The left had panel displays the main **Data Browser** in which your master NMR data folder(s) can be defined, and the **Pages** browser in which the different spectra for each sample are displayed in a manner similar to slides in Powerpoint (you can activate the pages display with the **View -> Pages** option). The main window displays the current data set. To open a data set, simply drag from the Data browser and drop into the main window; the data will be processed automatically if necessary.
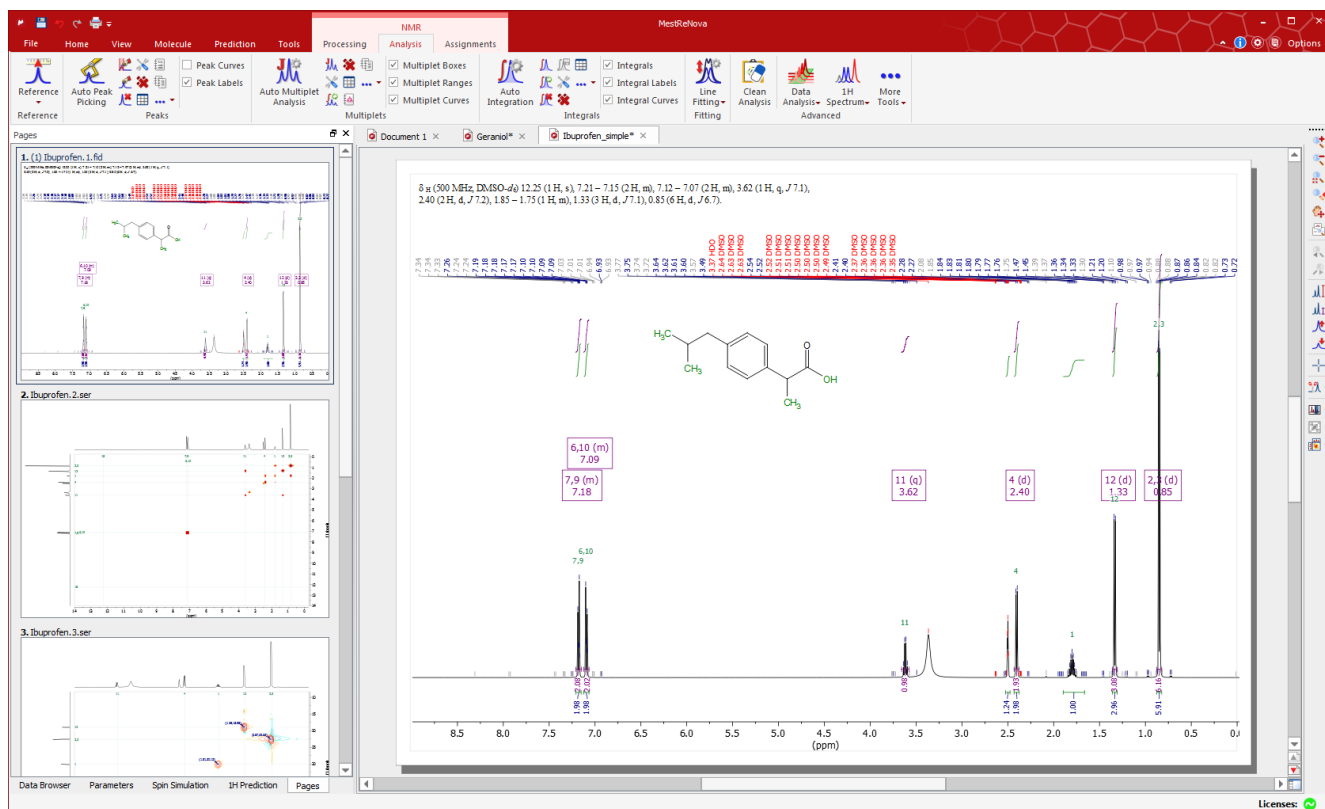
The main icon bar above the display provides tools for spectrum processing and analysis; placing the cursor over any one provides a pop-up banner describing its function. The icons down the right-hand side provide for interaction with 2D spectra, stacked spectra or with the optional modules. There are also tools for drawing of chemical structures, although it is usually preferable to directly paste Chemdraw structures onto the spectra.

Once spectrum assignment is complete, it is possible to report shift and coupling information in formats required for primary journals, and to copy & paste these directly into documents, as in the two examples below:

δ_H (500 MHz, DMSO-d_6) 12.25 (1 H, s, 15), 7.21 – 7.15 (2 H, m, 7, 9), 7.12 – 7.07 (2 H, m, 6, 10), 3.62 (1 H, q, J 7.1, 11), 2.40 (2 H, d, J 7.2, 4), 1.87 – 1.73 (1 H, m, J 6.8, 3), 1.33 (3 H, d, J 7.1, 12), 0.85 (6 H, d, J 6.7, 2, 1).

^{13}C NMR (126 MHz, DMSO) δ 175.95 (13), 140.01 (5), 138.94 (8), 129.43 (6, 10), 127.56 (7, 9), 44.75 (11), 44.69 (4), 30.09 (3), 22.65 (2, 1), 19.00 (12).

NMR Spectrum Prediction

The software includes the capability to predict NMR spectra for a range of common nuclides (^{1}H, ^{13}C, ^{19}F, ^{31}P, ^{15}N, ^{11}B, ^{29}Si) based on extensive databases built-up by a number of academic groups. These predictions **do not provide answers** to assignment problems, but can act as **helpful guides** in this process. Note that proton predictions in particular can be far less reliable than those of heavier nuclides, and that carbon predictions tend to be the most robust.

Mnova Manual

In addition to the Help files within the program, there is a very comprehensive PDF manual for Mnova available from the Mestrelabs website that will serve as a useful reference and covers all NMR and MS functionality.

Mass Spectrometry Processing interface

The software will open all the data file formats represented by the MS systems in the Chemistry Department including LC/MS and GC/MS and open access (chromatograms and spectra). Note there are some data file format restrictions for Mac users (http://mestrelab.com/resources/ms-supported-formats/). The basic interface for processing MS data is very similar to NMR (see below). It includes *a mass browser* (MS browser, right hand side) enabling easy access to all data file functions associated with the file you have open. These could include positive or negative ion TIC, MS/MS data (MS2) and/or UV/Diode array data. Each function can be selected from the MS browser and the appropriate chromatogram will be loaded. MS browser can be opened from the 'Mass Analysis' dropdown at the top of the page. The *Data Browser* can be used in the same way as for NMR. The MS tools automatically become active when you load MS data and the NMR tools grey out. The software tools can be used to predict and search your data files for peaks corresponding to chemical formulae or molecular structures which can be cut and pasted from Chemdraw. It can be used for accurate mass analysis and generating mass extracted chromatograms (it does not have the capability for de-convoluting protein charge state envelopes). It is primarily developed for manipulation of 'small molecule' data.
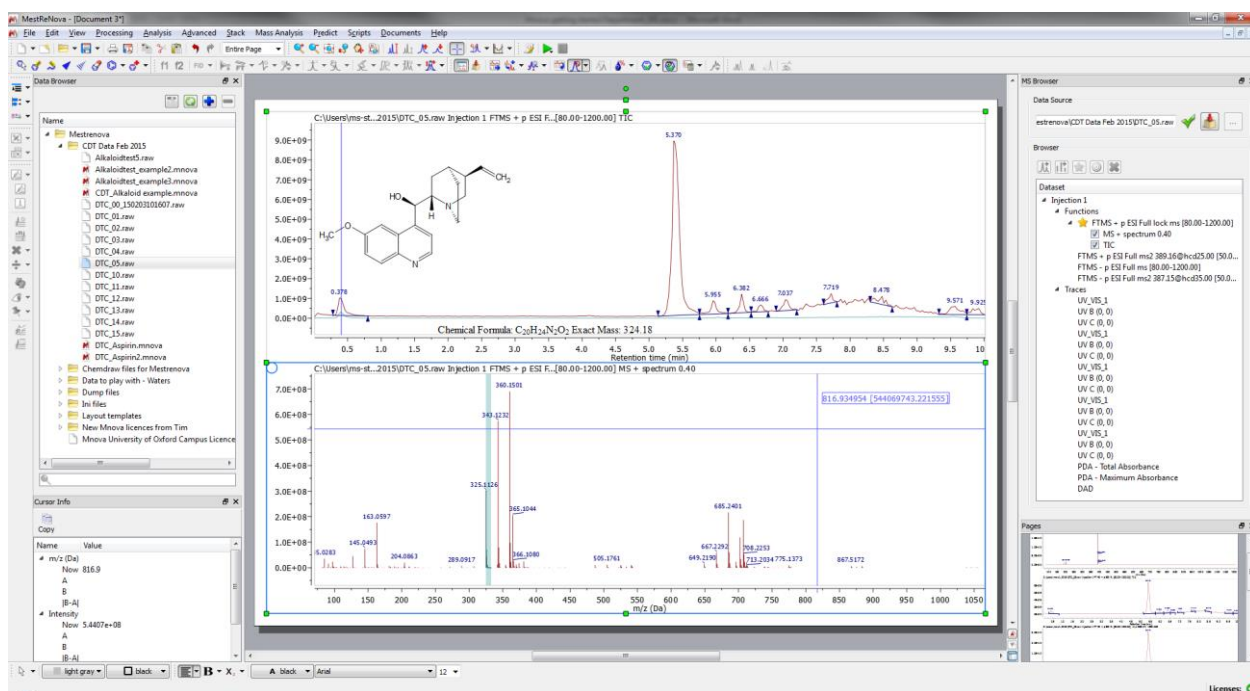
The software is very useful for displaying, manipulating and annotating chromatograms and spectra for display purposes, for example in publication or presentations. For example raw data files, from the small molecule open access system, can be uploaded (copy to your pc from the chem server first), viewed and manipulated.