COMPUTER SOFTWARE REVIEWS

MNova: NMR Data Processing, Analysis, and Prediction Software. Chemistry Research Laboratory, Department of Chemistry, University of Oxford Oxford OX1 3TA, U.K.

The MNova program by Mestrelab Research (www.mestrec.com) offers tools for the processing, analysis, and prediction of NMR data and is aimed primarily at chemists dealing with 1D and 2D spectra of small or midsized molecules. It is available for a variety of platforms, including Windows, Mac OS, and a range of Linux distributions. This multiplatform capability offers a significant advantage over some rival packages, especially for academic institutions where Mac systems find widespread use among research chemists but are often rarely catered for.

The structure of the graphical user interface is reminiscent of that of the well-known presentation software Powerpoint. In this, each "slide" or page contains a separate spectrum or sequence of spectra, and a collection of one or more pages comprise a single file that can contain all 1D and 2D data sets associated with a single compound. Thus, the layout feels familiar, and it becomes very easy to jump between different spectra for a given compound during a structure elucidation process. The software operates following the WYSIWYG (what-you-see-is-what-you-get) philosophy and the use of so-called antialiasing display technology produces soft line styles that are pleasing to the eye. Access to the main functionalities of the program is very convenient, either through icons, menus, or a fully customizable and context sensitive pop-out menu from the right mouse click.

The interaction with spectra is itself very sleek, and I found this highly intuitive and on the whole very well thought out. Raw data or spectra may be imported from a wide range of formats (including those of all major NMR vendors) with automatic recognition *via* a simple cut and paste from the original data file. Here, one immediately comes to one example of the attractive and well considered features that permeate this program; the software will automatically reproduce the processing previously applied to the raw data, such as used on the source spectrometer, including window functions (apodization) and phasing, presenting the chemist instantly with a workable spectrum without the need for manual application of these processing steps. Reprocessing of the data remains an option if required, as does further manipulation, and the automated modes for phasing and baseline correction worked very well. All the functionalities expected of a well developed NMR package are to be found including automated and/or manual peaking-picking and integration of both 1D and 2D spectra and 1D multiplet analysis, together with options for reporting in tabulated forms or, in the case of multiplets, in the formats dictated by primary journals (currently only JACS, RSC journals, and Angewandte). Beyond this core functionality, the program is enhanced by additional features that make it such a pleasure to use. Two I particularly liked were the ability to observe the influence of the interactive application of varying apodization functions on a spectrum in real time (impressively, for both 1D and 2D data!) and the (optionally automatic, but always reversible) "cut" feature that removes empty regions, or those containing solvents or impurities, from the spectrum display, allowing one to focus on those of interest, again for both 1D and 2D spectra. Other attractive features include the easy incorporation of expanded spectrum regions on a page, the ability to drag-and-drop structures onto any page, the ability to move and align images (spectra, structures, tables) around on the page as in standard graphical packages, and the ability to stack multiple 1D spectra very readily. Figures may also be annotated conveniently for inclusion in papers or theses. The WYSIWYG display then allows for the ready transfer of spectra *via* copy and paste into other documents or for export in a variety of formats including pdf, png, eps, and tiff. For the analysis of more complex data sets the ability to view multiple 1D and/or 2D spectra on a page simultaneously with correlated cursors provides yet another attractive feature.

The inclusion of chemical structures on a page also enables use of the NMR spectrum prediction functionality available as a plug-in through a separate license. This is provided by the Modgraph company and incorporates the ability to predict spectra for the ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{29}Si, and ^{31}P nuclides based on methods developed by the groups of Pretsch (ETH) or Abraham (Liverpool); further details may be found at www.modgraph.co.uk. Although it was not possible to test extensively the capabilities of the predictors, the evaluations made for ^{1}H and ^{13}C indicated the performance and accuracy to be at least competitive with other desktop predictor packages available.

The MNova program also contains a scripting language that could be used to automate a range of tasks, such as the processing of multiple spectra or the generation of layouts on a page. This programming capability is more likely to find use by the dedicated spectroscopist or NMR laboratory manager rather than the chemist looking to quickly interpret their spectra, and although no scripts were supplied with the software, some can be downloaded from the company Web site and one anticipates this repository will grow over time. The Web is also used extensively as part of the Help features in the form of short movies that illustrate various operations. The electronic Help documentation supplied with the software likewise contains a high graphical content with many screen-shots making it rather straightforward to find answers without the need to read pages of laborious text.

Overall I was very impressed with the package, finding it not only very comfortable and intuitive to use so well suited to non-NMR specialists but also well endowed with more advanced processing features for more experienced users. Examples include DOSY processing, covariance NMR, and the ability to perform spectrum simulation, again easily achieved through a simple tabulated input of shifts and couplings. Incidentally, a "lite" version is also available that contains only 1D processing functionality, which may be well suited to the bench chemist working primarily with such data. Inevitably there were a few points that could be improved; I found the "zoom out" option troublesome as using this

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repeatedly too quickly would instead open the page properties dialogue (the "double-click" function). I also found the program "encountered a problem" and "needed to close" on a number of occasions, and while not frequent these were nonetheless frustrating when they occurred; a background periodic autosave feature would have been useful here!

In conclusion, I would recommend highly this software to any chemist or spectroscopist seeking a desktop package for the analysis of 1D and 2D NMR data sets. Its attractive and intuitive graphical interface combined with some smart functionality will suit less experienced users, while dedicated spectroscopists will also be impressed with the more advanced functionality it contains.

Installation and Testing. The MNova version tested (5.3.0) was run under both Windows XP and Vista on moderately powered systems (XP desktop: 3 GHz CPU with 1 GB RAM or Vista laptop: 2 GHz CPU and 2 GB RAM) and with impressive speed in both cases. The software was available as a Web download, and installation was trivial taking only ~15 s. It may be configured to work in four languages: English, Japanese, Russian, and Spanish.

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