J|A|C|S
COMPUTER SOFTWARE REVIEWS

MestRe Nova. Mestrelab Research S.L. Feliciano Barrera 9B, Bajo, 15706 Santiago de Compostela, Spain. http://www.mestrelab.com. See Web site for pricing information.

MestRe Nova (hereafter Mnova) provides a comprehensive set of computer programs for processing and displaying high-resolution NMR spectra. Some of the unique design features of Mnova are readily apparent. It accepts raw data (FID) input in many formats (Varian, Bruker, JCAMP, JEOL, Tecmag, and others), reads headers, and shows spectra with no intervention by the operator. These features are valuable to anyone who uses data from different spectrometers, especially raw data sent electronically from collaborators. However, attempts to confuse Mnova by inputting unusual data, such as raw MR images, results in the message "unknown format". The Mnova core code is cross-platform, and it is quickly installed in minutes on PCs, Linux systems, and Macintosh OSX platforms. Purchasers obtain a license for their operating system of choice. The Mnova manual is descriptive, well laid out, and written for the novice as well the expert spectroscopist. It is also available by download from the MestReLab Web site. The current release of Mnova, 5.3.1, handles 1D and 2D analyses. Overall, it is like a Swiss army knife, which has ordinary tools as well as little-used, specialized ones.

My experience with Mnova as a long-time user of NMR spectrometry took the following track. Mnova is GUI driven so I proceeded without reference to the manual. I collected raw data sets from my files, friends, and the Internet and read these into Mnova. Some data sets were from molecules I have known for a long time, whereas others would be considered a challenge and puzzle for any spectroscopist. In every 1D case, the first screen shown exhibited a high-quality spectrum. The 2D data sets behaved in the same way but were of varying quality. The user can enhance the appearance of any 2D spectrum by a series of ad-hoc corrections, especially after reading the manual. The incorporation of covariance methods for 2D is noteworthy. One method for testing GUI-driven computer programs is to click on icons and observe the effect. Some effects with Mnova were obvious but others were not.

An essential characteristic of Mnova is real-time processing. This is described in detail in the manual. Mnova reads and stores a raw data set as original FID, processed FID, spectrum after first FT, and spectrum after second FT for 2D inputs. The original FID is saved. When a command is changed, the spectrum is recalculated and displayed in real time—a feature that is both convenient and valuable. Zoom and integration commands behave well, although peak picking requires some operator intervention. Mnova offers enough computing options that most users will benefit from extensive use of the manual. After extensive testing of Mnova with different input data sets, I felt confident that I was exploiting its capabilities. However, reading the manual revealed that I had just scratched the surface of the program. As with many softwares, achieving a level of comfort with Mnova is the result of frequent use. Otherwise the user cannot remember what some commands do, or if these even exist.

Mnova outputs range from simple, e.g., a spectrum, to detailed, e.g., analyzed spectra and tables. Control of the format is through a user-defined template, the construction of which is provided in the manual. An output for inserting the processed spectrum and its associated tables in a paper is incorporated in Mnova, including a detailed text file for inclusion in a paper in JACS or RSC format as a menu choice and a labor-saving step. Many different tables are generated with ordinary use of the program. Aggregation of the tables on and around the spectral display can provide a comprehensive report with graphics, molecular structure, and tables, which can be saved in PDF format for distribution.

At least 30 individual processing commands can be used singly, and many thousands can be used in combination. If the user questions how a command changes the spectrum, Mnova has an answer. All commands are easily reversed by restoring the initial value. The processing template is hidden from the user, but it accepts the change, finds the original FID, and recomputes the spectrum. Mnova users can write scripts for special needs, which are in an accessible directory. Scripts are JAVA based and make full use of Object Oriented Programming (OOPS).

Mental acuity is important when using Mnova or any other NMR presentation software. For instance, I input a raw ^{13}C data file for codeine and obtained an attractive spectrum, but reference markers were missing. Comparing it with a published ^{13}C spectrum was hopeless. After a puzzling hour, I found the TMS marker at the downfield extreme; the Mnova spectrum was reversed. One keystroke remedied this shortcoming and provided a correct one. Wheeler's moral dictum "Never do a calculation before you know the answer" is in play here and should regularly be applied to processing NMR spectra.

The core code is C++-based. The core programs are inaccessible to the purchaser of Mnova; however, the Mnova GUI interface is driven by Java Script to which the user has complete access. The manual lists all functions and a built-in script editor facilitates script writing, where processing templates gives thousands of combinations, each with a different outcome. The balanced group of chemists and programmers of the MestReLab development team admits this program is a work in progress but that it is ready to be used for most data processing.

Mnova is a reliable and finished program, but it is not perfect. Bugs are not uncommon, although they can often be corrected by altering a script or by communicating with the MestreLab service desk. Features must be added by MestreLab, and the firm publishes a roadmap for the development of new ones. I found the extra complexity in cleaning up 2D spectra sometimes freezes the computer. Off-line processing and the feature for generating reports are excellent. Moreover, any laboratory group with extensive NMR processing needs will find Mnova a valuable means to free up spectrometer time by moving data processing off-line. I am impressed by the concept, packaging, and utility of Mnova. Both university and industrial laboratories will find it to be an asset.

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