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COMPUTER SOFTWARE REVIEWS

NMRPredict. Modgraph Consultants, Ltd, 1348 Graham Place, Escondido, CA 92129. http://www.modgraph-usa.com. Contact company for pricing information.

NMRPredict (Version 2 Enhanced, released June 2006) is a useful and straightforward stand-alone product to facilitate the prediction and interpretation of NMR spectra. Given a chemical structure, it can accurately predict ^{1}H, ^{13}C, ^{19}F, ^{15}N, ^{31}P, ^{11}B, and ^{29}Si chemical shifts, based on calculations or comparison to library spectra. NMRPredict can also be used to search for compounds or mixtures that exhibit a particular set of resonances. It has a number of features that make it helpful for scientists in both industrial and academic settings. For example, once the appropriate one-dimensional spectra have been generated, the results expected for several important two-dimensional experiments can be viewed. The operating frequency of the instrument can be varied, and the solvent changed, allowing the predictions to be tailored to the user's own system.

NMRPredict's interface is simple, intuitive, and suitable for a wide range of user abilities. For example, students with little previous exposure to NMR were quickly able to utilize this program. Structures whose chemical shifts are to be predicted may be input from standard drawing programs, such as Isis Draw or ChemDraw, or they can be created with the embedded drawing program. Pull-down menus allow for selection of parameters such as solvent, operating frequency, and peak width. After the rapid spectral prediction routine is finished, an informative three-section report is displayed, showing the structure, a table of shifts, including the range of predicted values and coupling constants, if applicable, and graphical representations of the spectrum. The data for each nucleus are located under an individual tab, with a convenient Overview tab summarizing all results. Within each report, all three sections are linked, so that pointing to an atom in the structure, a line in the table, or a peak in the spectrum highlights the corresponding features in the other two sections.

Predictions of ^{1}H shifts are based on molecular-level effects such as partial charges, steric interactions, and the presence of functional groups. When compared to known shifts for a variety of compounds, the predicated values were found to agree quite well. Predictions of ^{13}C shifts are based on a library of over 130 000 compounds; an extended library with over 100 000 additional compounds is available at additional cost. The ^{n}X-nucleus (^{19}F, ^{31}P, etc.) library contains nearly 80 000 entries. An optional database-building application allows users to develop their own libraries (not included in the basic NMRPredict package).

Two methods for assessing similarity to library spectra are employed. The HOSE (Hierarchical Organization of Spherical Elements) approach centers spheres of increasing radii on a particular nucleus and searches the library for compounds with chemically similar spheres. The second approach, which utilizes neural networks, is more effective for structures with few analogues in the library. Results from both predictions are shown, with the one considered to be more reliable highlighted. Comparison of predicted ^{13}C shifts to known values for a wide variety of compounds confirmed that the calculations are acceptably accurate. Once the appropriate one-dimensional data have been generated, it is easy to predict two-dimensional spectra (COSY, HSQC, HMBC, and NOESY).

The ^{13}C peak-searching routine is also easy-to-use, fast, and reliable. Several search parameters can be specified, such as the minimum number of peaks to be matched, the acceptable shift tolerance, and the number of components, if the sample is a mixture. The best matches are shown, and structures can be displayed in a tiled pattern to provide an overview. The hit quality is indicated by the average deviation in chemical shifts, with a lower number implying a better fit.

Overall, the documentation for NMRPredict is excellent. As discussed above, most users will likely require little instruction, but the help files give clear and concise directions on how to run the program. They also provide helpful explanations of the various terms and abbreviations used. Additional information available on the Modgraph Web site describes the prediction approaches used.

One problem encountered sporadically was the tendency of the software to stop responding if the structure contained certain typographical features, even those supported by the embedded drawing program. For example, if an "R4" abbreviation is used to indicate a butyl group, or if a polymer structure is enclosed by "[ ]$_n$", the program halts, and must be restarted. While it is understandable that unrecognized characters might confound the calculations or the routines of library comparison, an error message or warning would be preferable to having the software stop functioning. This problem was never experienced for structures that did not contain abbreviations or brackets.

On balance, NMRPredict provides a simple, powerful, and versatile resource for analyzing NMR spectra. The basic industrial license includes a single-user license, although multiuser licenses are also available. While not inexpensive, its cost is competitive with similar packages. A server-based academic version is extremely cost-effective and would be a great value to anyone who teaches NMR spectroscopy.

Anita J. Brandolini,
Fairleigh Dickinson University

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