Computer Software Review

ACD/HNMR Predictor and ACD/CNMR Predictor Advanced Chemistry Development, Inc. (ACD/Labs), 90 Adelaide Street West, Suite 600, Toronto, ON M5H 2V9, Canada. www.acdlabs.com. See Web site for pricing information.

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ACD/Labs' ^{13}C and ^{1}H NMR prediction software incorporates powerful features that generally result in remarkably accurate calculated NMR spectra. At the heart of the software is an extensive spectral assignment database: the ACD/HNMR Predictor includes more than 1,384,000 experimental chemical shifts and 449,000 experimental coupling constants; the ACD/CNMR Predictor is supported by 2,017,000 experimental chemical shifts. The databases include literature references and detailed information on how the original experiment was performed. Importantly, users can easily add their own spectral information to the database to improve the predictive capabilities, as well as weight the prediction to similar substituents on the structures. Browsing the database is also possible in conjunction with filtering by different criteria, such as structure, substructure, or similarity of structure.

The interface is intuitive, and the basic features are all obvious. Indeed, we have used a simpler version of the software in our sophomore-level organic courses for years. The students find that the ability to see a highlighted signal within the spectra from a particular hydrogen (or vice versa) by merely sweeping the mouse over the structure (or spectrum) is very helpful in learning to interpret NMR spectra and to assign structures.

Chemical structures to be predicted can be inputted from the chemical drawing software ACD/ChemSketch, or alternatively, ChemDraw and ISIS draw interfaces can be used by simply copying and pasting. The ChemSketch software contains a variety of templates that simplify entering complicated compounds, polymers, and organometallic structures. It also offers a convenient properties generator that can display chemical formula, molecular weight, percentage composition, and estimated macroscopic properties, such as molar refractivity, refractive index, molar volume, density, and others.

A slightly limited version of ChemSketch can be downloaded for free at http://www.acdlabs.com/chemsketch. The free version of ChemSketch can be used to name structures with up to 50 non-hydrogen atoms and three rings, and the full version handles an impressive 255 non-hydrogen atoms and 15 rings per polycyclic section. One weakness of ChemSketch is that its function buttons generally clutter the window without an easy way to organize them by toolbars or to hide and expand them as is common for many Windows applications. The result is that the ChemSketch work area appears cluttered. A second frustration voiced by nearly all users is that for no apparent purpose the commands are separated into two distinct alternate windows called "structure" and "draw." This arbitrary separation forces the novice user to switch frequently between windows in order to access (or search for) various commands.

We evaluated version 8 of the ACD/HNMR DB and CNMR DB software in our research laboratory for several months. There were some minor annoyances with the prediction software, such as default settings set to include second-order interactions and long-range coupling constants, which produced over-complicated predictions compared to authentic spectra. Fortunately, these can be turned off or adjusted to user specifications, and with a little familiarity the more advanced features are easy to navigate and master. We found no defects or flaws in the software; the program was quick and ran flawlessly under Windows XP Pro with multiple user accounts and simple file sharing disabled. Customer support was outstanding.

Many deployment options are available, including the standalone software as evaluated here, as well as access to predictions and databases over local networks and over the Internet at http://www.acdlabs.com/ilab/. Pricing varies according to deployment, and academic customers do receive discounts on the retail prices. Full pricing details can be obtained from sales@acdlabs.com.

The software is an extraordinarily practical and convenient compendium of NMR data that effectively replaces the time-consuming tasks of looking up individual NMR data from the Web, the primary literature, paper-based libraries of NMR spectra, or similar resources. Students less experienced in NMR-based elucidation of structures found the software a useful resource in the sometimes frustrating task of interpreting spectra and confirming structural assignments. However, one must consider the software's appropriateness in graduate chemistry education. The predictive accuracy of the software was insufficiently rigorous to assist in differentiation and assignment of challenging structures encountered in our research, such as the bis-THF domain of the annonaceous acetogenins and certain acyclic syn−anti aldol products.

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