

Computer Software Review

ChemDraw Ultra 9.0. CambridgeSoft, 100 CambridgePark Drive, Cambridge, MA 02140. www.cambridgesoft.com. See Web site for pricing options.

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ChemDraw Ultra 9.0, the latest offering for chemical drawing from CambridgeSoft, is billed as the "Ultimate Drawing Suite". It performs as advertised for drawing in chemistry, providing a way to communicate structural information in documents such as reports and journal manuscripts, to manage chemical information, and to derive computed data from structures quickly. Thus, it is widely used in academia and industry. A number of the features would also be useful for teaching chemistry, but the price of the full package may be cost prohibitive. This review will focus primarily on recently added features. For more details, refer to the vendor's Web site and to recent reviews of previous versions and alternative packages of the program (see (a) Li, Z.; Wan, H.; Shi, Y.; Ouyang, P. *J. Chem. Inf. Comput. Sci.* **2004**, *44*, 1886–1890. (b) Mendelsohn, L. D. *J. Chem. Inf. Comput. Sci.* **2004**, *44*, 2225–2226. (c) Buntrock, R. E. *J. Chem. Inf. Comput. Sci.* **2002**, *42*, 1505–1506).

A significant number of improvements and new features are found in ChemDraw Ultra 9.0, and a number of enhancements and separate programs are offered in the "Ultra" package that are not included in the current "Pro" and "Standard" versions of ChemDraw. As with other recent packages from CambridgeSoft, some of the programs and features are not available for Mac OS. In particular, Chem3D, ChemFinder, E-Notebook, Excel integration, and the three databases included on ChemIndex do *not* run on Mac OS. The Windows version includes all of these features, in addition to the flagship application, ChemDraw, which runs on both platforms.

The package was tested on a Mac G4 running OS 10.3 and on a Pentium IV computer running Windows XP (SP2). Installation on both systems was straightforward. Note that MS Office must be installed in order to use the E-Notebook and Excel integration features. As with previous versions, the user is permitted to install the software on both a home and an office computer, so long as only one copy is in use at a time.

The interface and features of the ChemDraw application are very similar on the Mac and Windows platforms, and files were exchanged easily. The drawing tools will be familiar to prior users of even very old versions of the software, with enhancements to improve the drawing of structures and other objects, as well as to predict a number of physical properties. Users of earlier versions of ChemDraw should be able to create good quality structures and figures without assistance. However, completing the tutorials is recommended to facilitate learning how to use the new features. For example, one tutorial shows how to maintain structure alignment while moving copies, another demonstrates how to draw polymer structures using built-in shortcuts, and a third teaches the use of hot-key shortcuts. The tutorials were very easy to follow and should be considered mandatory for new users.

ChemDraw Ultra 9.0 includes a number of new or enhanced drawing tools and analysis features, including tools for drawing more realistic TLC plates, enhanced predicting of proton and C-13 spectra, automatic generation of up to 500 similar structures, and "Live" predicting of physical properties that provides updates to calculated values as a structure is edited. The tool for name-to-structure conversion has also been enhanced to recognize more names, and a tool for mass spectral/fragmentation has been added. Each new feature was easily located by inspection or with the help of included documentation, and each tool was easy to use. The fragmentation tool was particularly interesting, as it has two roles: (1) to enable rapid generation of retrosynthetic schemes by providing implied structural precursors when "breaking" designated bonds and (2) to discern candidate molecular fragments and their masses quickly in order to assist in interpreting experimental mass spectral data. The mass spectral feature is not automated: that is, the user must specify possible bonds to break. As such, it would likely make a good instructional tool for students. The tools for predicting proton and C-13 spectra, although not yet of research-grade quality, are adequate for generating approximate spectra to assist in interpreting experimental spectra, and are particularly effective for generating problem sets for students and for showing atom/peak correlations using projected images in a lecture hall.

Chem3D Pro looks much different from previous versions, and it now uses Open GL graphics for enhanced display of molecular models. Chem3D is seamlessly interfaced with ChemDraw: a three-dimensional model can be generated and displayed within ChemDraw, and a ChemDraw window appears in Chem3D for drawing two-dimensional structures. The Chem3D model can be displayed and manipulated in many ways for effective presentation. In addition, the program can be used to run MM2 calculations for determining conformational minima, MM2 dynamics analyses can be performed, and Hückel calculations can be performed for generating partial charges. Molecular surfaces can be generated and displayed, and movies of molecular manipulations can be generated and exported for presentation. A large number of file formats can be exported and imported, enabling Chem3D to display structures from most sources. As with ChemDraw, the tutorials were very helpful for learning to navigate the new interface and to use the new features. However, the documentation and tutorial notes for Chem3D Pro were inferior to those of ChemDraw Ultra. For example, one feature, automated structure overlay, presented in one of the tutorials was not available in the Pro version of Chem3D, but required the Ultra version (both versions share the same documentation). For chemists interested in using Chem3D as a graphical interface for computational chemistry, an upgrade to Chem3D Ultra would be appropriate to take advantage of enhanced features.

The E-Notebook portion of the package is intriguing, although not as well developed as other components. There are no

tutorials available, and not all features are transparent or adequately explained by searching the online help or paper manuals. E-Notebook is intended to replace paper laboratory notebooks, and includes security features that document changes, require passwords, and so forth, such that CambridgeSoft claims that E-Notebook entries are more secure than written records. E-Notebook uses ChemDraw tools for drawing reaction schemes, which can also be generated from lists of reagents and products obtained from internal or external databases. Tables of reagents and products are generated automatically, and stoichiometric calculations are performed as soon as any amount or ratio has been added or changed by the user. There is a word processing section for writing the procedure, with some common reaction templates prebuilt for modification. Any entry into the electronic notebook can be easily duplicated for use and modification in subsequent experiments. Also, data and spectra can be imported in a number of file formats to augment the notebook entry. Records (notebook entries) can be saved on a local database to allow access by co-workers or supervisors.

ChemFinder has also improved a great deal from earlier versions. The tutorials demonstrate clearly how to create a simple database from scratch, as well as how to build an interface to an existing database. ChemDraw tools can be used to draw structures within the database. The ChemFinder database could prove to be useful for maintaining a chemical inventory

or research catalog, or to build a user-friendly front end to many larger chemical databases. In fact, ChemFinder serves as the front end for the databases included in the ChemIndex Ultra DVD. This DVD, which is searchable by name, formula, structure, and more, comprises ChemIndex (a small molecule database), ChemRXN (an organic reaction database), and the NCI and AID databases, each containing bioactive compounds and activities. Using ChemFinderOffice, it is also possible to search for ChemDraw structures (and structures in several other chemical formats) within any MS Office document, other supported document, or ChemFinder database. Full structure, substructure, and similarity searches can be performed using user-generated structures as search terms. With this feature, even novice users can rapidly locate structures in, for example, old research reports or exams or in the databases provided on the ChemIndex Ultra DVD.

ChemDraw Ultra remains the premier drawing package for chemists. Before making a purchase, one can compare program capabilities among different versions of ChemDraw and ChemOffice; the page comparing features provided on the CambridgeSoft Web site can be helpful in making the appropriate choice.

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