ChemDraw 8 Ultra, Windows and Macintosh Versions

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ChemDraw Ultra is one of the standard chemical drawing software packages. Over the years, its progressively more sophisticated versions have been reviewed in this and other chemistry journals.[1−3] ChemDraw Pro, a version with fewer features, is available at a lower price. As with previous versions, the standard single-user license permits loading the software on one workstation at the user's place of work or laptop at the user's home.

The structure drawing capabilities of ChemDraw remain fundamentally unchanged. The interface provides a standard palette of chemical drawing tools that can either be anchored to any of the four edges of the ChemDraw window or torn loose from the anchor for use in free-floating mode. Any of the pop-up menus within the palette can also be torn loose, as also can the other toolbars. A new and extremely useful feature of ChemDraw Ultra 8.0 is the periodic table palette, which functions as both a reference and a drawing tool. Clicking on an element will yield a short list of physical and chemical properties. If the user then clicks on a node of a molecule currently being drawn, the selected element will be inserted at that node. Also new is the character map palette, which enables the user to quickly and easily insert any symbol that is part of the installed font set. The character map tracks which characters are being used most frequently and displays the user's "top eight" characters in a row of boxes at the top of the palette, making them readily available for immediate selection. All other aspects of the user interface are typical of chemical drawing software. ChemDraw "knows" chemistry and identifies apparent errors (pentavalent carbon atoms, for example) by highlighting them in red. This feature can be turned on or off as needed.

Structures produced with ChemDraw can be supplemented using the drawing elements tool, which can insert a number of nonstructural shapes. The orbital tool can be used to insert molecular orbitals where appropriate, and the pen tool can be used for freehand drawing where necessary. The arrow tool palette enables the user to draw simple or complex reaction schemes. A new drawing feature is the TLC plate tool, enabling the generation of thin layer chromatography plates with any number of tracks and spots. Also available are several chemistry and molecular biology clip art palettes, which provide images of laboratory glassware and elements of cellular and molecular biology structures.

Among the numerous features of ChemDraw Ultra, several deserve special mention. The software includes a name-structure translator and will produce a structure given either common or the IUPAC name of most substances. The software will recognize and automatically correct many common typographical errors in chemical names. Similarly, ChemDraw will produce the IUPAC name of a substance when given the structure. This feature has been rewritten for the current version and now supports Cahn-Ingold-Prelog rules for absolute stereochemistry. Related to this feature, ChemDraw includes a chemical properties database and will generate a standard list of physical properties of any substance in its database. It is not possible to add or edit new names, structures, or associated properties. In addition to providing known property information, the software predicts several physical properties, such as chemical shifts for both ^{1}H and ^{13}C NMR and thermodynamic properties such as melting points, boiling points, and similar data. The chemical shift prediction function has been improved in this version. CambridgeSoft claims that ^{13}C predictions are on average twice as accurate as they have been in past versions, and ^{1}H predictions now include splitting patterns that more closely resemble actual spectra. Another new feature, the mass fragmentation tool, mimics the fragmentation that occurs in mass spectrometry. This feature is not predictive (the user determines which bonds will be broken); nevertheless, it facilitates interpretation of mass spectra by allowing the user to view in advance the structures and masses of possible molecular fragments. While ChemDraw can generate a 3D model of a drawn structure, it seems to work better to copy the structure to the Chem 3D module that is bundled with the software. The internal conversion process can place a strain on memory resources: several times when such a conversion was attempted, an "Out of memory" message popped up. This never occurred while using the copy and paste option.

Structures can be saved in numerous formats including several standard graphics formats and can easily be transferred to word processed documents. Images pasted to word processed documents can also be transferred back to ChemDraw for further editing with no loss of chemical information. A comprehensive list of file types available for import and export can be found at http://www.cambridgesoft.com/services/ftypes.cfmn?FID=2. Additionally, ChemDraw and Chem 3D structures can be inserted in MS Office documents using the Object function under the Insert pull-down menu. Such structures can be edited through OLE.

ChemDraw can also be used to draw query structures; that is, structures that can be used to search chemical databases. The user can designate any of several characteristics or properties for multiple atoms or bonds, such as indicating that a particular atom can be any halogen or that a particular bond may be single or double. Additional properties such as bond angles and exclusion spheres can be included in

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query structures. The atom mapping feature permits generation of reaction queries, indicating correspondence of specific atoms in different structures. Once generated, such structures and reactions schemes can easily be transferred into the appropriate database searching software. Related to this feature is the ChemFinder software bundled with ChemDraw. ChemFinder enables the user to locate chemical structures embedded within numerous standard file types, including all MS Office files as well as files produced by several other word processing, database, and graphics software packages. Thus, it is possible for chemists to create and manage a local database based on the chemical structures within their documents. ChemFinder will perform searches with both exact and query structures but will only locate structures that were saved or pasted in one of the chemical structure formats. Structures saved as gif, pict, tiff, or other graphics formats are not searchable.

The ChemDraw manual as received by the reviewer was fairly easy to use and generally accurate, but it contained several editorial errors. These errors were limited to the "What is New in ChemDraw 8" section on page 1, sending the user to the wrong pages for additional information, and have been corrected in subsequent editions and in the online pdf version. An html version of the manual is also available under the ChemDraw Help menu. The index of the print, pdf, and html versions seems incomplete, not including direct references to several of the new or enhanced functions. Hopefully, this is an oversight that will be corrected in subsequent editions of the manual. Until then, such information can be located by using the search function under the help menu. A limited form of context-sensitive help is included: on selecting "Help Mode" (Shift+Fl) from the Help menu, the user is presented with a "?" cursor. When in Help Mode, clicking on any menu or palette function or using a keyboard shortcut will bring up the appropriate section of the html manual.

The new features of ChemDraw, most of which have been documented above, offer an improvement over previous versions, but it will be up to individual users to determine whether the new features are worth the cost of upgrading. In any case, any research or instructional facility working with chemical structures and databases will find this software useful, especially if they are generating in-house structure databases.

Contact and pricing information is as follows: ChemDraw 8.0 Ultra. CambridgeSoft Corporation, 100 CambridgePark Drive, Cambridge, MA 02140. http://www.cambridgesoft-.com/. Price for CD-ROM: $1790 (commercial); $790 (academic). Price for annual subscription (2004): $640 (commercial); $290 (academic). ChemDraw Ultra comes bundled with the Chem 3D Pro and ChemFinder modules of ChemOffice, which is a comprehensive software package for chemistry laboratories. The software is shipped in both Windows and Macintosh versions; therefore, it was reviewed on both Windows (350 MHz Pentium PC with 192 Mb RAM running Windows NT 4.0) and Macintosh (600 MHz G3 Macintosh iBook with 256 Mb RAM running OS X) platforms. Other than variations associated with the respective operating systems, no significant differences were noted between the Windows and the Macintosh versions.

REFERENCES AND NOTES

(1) Klein, F. M. CS ChemDraw Pro, Version 3.1 for Windows. *J. Chem. Inf. Comput. Sci.* **1995**, *35*(1), 166−7.

(2) Cousins, K. R. ChemDraw 6.0 Ultra. *J. Am. Chem. Soc.* **2000**, *122*(41), 10257−10258.

(3) Engel, T.; Valenzen, B.; und Orbitale, S. *Nachr. Chem.* **2003**, *51*(4), 450−453. This review is possibly the most interesting, since it is the only recent comparative review, discussing ChemDraw and several other chemical structure software packages.

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