Computer Software Reviews

ChemDraw 6.0 Ultra. CambridgeSoft Corporation, 100 Cambridge Park Drive, Cambridge, MA 02140. http://www.camsoft.com. Commercial Price: $1395. Academic Price: $699.

ChemDraw has long been the standard for preparing chemical structures for publication and presentation using both PC and Mac platforms. ChemDraw 6.0 Ultra offers more capabilities than any other current or previous release of ChemDraw. Although other ChemDraw products (Pro, Standard, and Limited) include the chemical structure drawing features of the Ultra package at a more modest cost, they do not include the additional programs and add-ins (see http://products.camsoft.com/familycompare.cfm?FID=2 for comparison of features).

The product was tested on both a Macintosh G3 266 (PPC required), running Mac OS 8.1, with 96 MB RAM (32 MB required), and on a 300 MHz/AMD K-3, running Windows 95, with 32 MB RAM. The CambridgeSoft License permits a single user to install the software on a workplace as well as on a home or portable computer, so long as two copies are not used simultaneously. Installation on each machine required two to three minutes, and most features of the software were available on both platforms and had similar interfaces. Only a single ChemDraw user manual is provided, with the small differences between Macintosh and Windows versions being noted in the text. The tutorials in the manual were particularly helpful in introducing some of the new drawing features and shortcuts. No problems were encountered when exchanging files between platforms, making this product a good choice for users sharing files. The new version also successfully read files of several types created by previous versions of ChemDraw and Chem3D. Some of the desired files were not installed during standard installation, including documentation in Adobe pdf (portable document format) and the glassware templates in Clip Art Pro; these required manual retrieval from the CD-ROM. During the course of the review, ChemDraw and Chem3D crashed only rarely on either Windows or Macintosh and only when a "save" function was not performed prior to drawing and editing, as was recommended in the documentation.

The ChemDraw drawing program is the cornerstone of the product, and this upgrade has several new features, including the ability to make multipage posters. An enhanced "chemical intelligence" is built into the program, not unlike spelling and grammar checking in a word processor. A mistake such as an incorrect valence is highlighted with a red box on the computer screen (but not on the printed copy). Many mistakes can be automatically corrected using menu commands or during drawing. For example, when the number of bonds to a carbonyl oxygen atom was reduced to one, the oxygen atom was automatically changed to an OH group. "Hot keys" aid in typing common functional groups, and defined "nicknames" can be replaced with their structures in one step. Subscripts are automatically generated on atom labels and formulas, although defaults can be manually overridden. Additional tools automatically align structures and reaction schemes. The basic drawing package is the same for all versions of ChemDraw (Standard, Limited, Pro, and Ultra); only the additional features, including those detailed below, differ.

The structures generated in ChemDraw 6.0 Ultra can be exported into numerous other molecular and graphics formats [including SMILES, SMD, Molfile, ISIS, as well as GIF, TIFF, and PICT (Mac only)], and likewise a number of other file types can be imported into ChemDraw.[1] Other ChemDraw versions do not support all of these file types.

Additional features of the ChemDraw 6.0 Ultra package are included as "add-ins" to the drawing program, or as separate programs in the package. The add-ins include AutoNom, Name=Struct, ChemNMR, ChemProp, ChemSpec, ClipArt, and Excel Add-on. The additional programs included are Chem3D Std 5.0, ChemFinder Pro 5.1, and the ChemDraw Net Pro (6.0) and Chem3D Net Std (4.0) plug-ins.[2] Most of these additional features are simple to use and will enhance presentations, lecture notes, exams, posters, proposals, manuscripts, and other documents for both academic and industrial chemists. Some features can assist in the organization or interpretation of research data, and many would be valuable for use in instruction, particularly in organic chemistry, to help students learn structural concepts, check answers for spectroscopy or nomenclature problems, and prepare laboratory reports.

With AutoNom,[3] a user can type in an IUPAC (or in some cases, common) name, and the program will draw the corresponding structure. Alternatively, a structure created with the drawing tools can be selected, and "Name=Struct" will print the IUPAC name on the page. These features worked well on both platforms.

Experimental data can also be generated from a highlighted ChemDraw structure, such as calculated ^{1}H and ^{13}C NMR chemical shifts;[4] approximate physical data such as melting point, boiling point, and log(*p*); and molecular formulas, exact masses, and elemental composition. The spectral and physical data are calculated using additivity rules and fragmentation methods, respectively, and hence are approximations only.

The data for ^{1}H and ^{13}C NMR spectra appear in a separate report as (1) a list of chemical shifts (with the factors used to calculate them); (2) a spectral window; and (3) a structure labeled with predicted chemical shifts on the appropriate atoms. The spectrum is hyperlinked to the structure so that as a peak on the spectrum is "moused over", the corresponding atom(s) and shift labels on the structure are highlighted. Likewise, the peak(s) on the spectrum is highlighted when the corresponding atom is chosen. Experimental spectra in JCAMP format can be imported and linked to ChemDraw structures in the same fashion, a feature with potential application for presentations in the classroom and at conferences. No information about peak intensities (integration) or multiplicity is included for the NMR spectra generated.

Chem3D Std 5.0 is a simple molecular modeling and display program closely integrated with ChemDraw. In the Macintosh version, a Chem3D model can be created automatically from a highlighted structure in a ChemDraw document, and the resulting molecular model will be embedded in the ChemDraw document. The Chem3D application can then be activated to provide rudimentary molecular computation (MM2 geometry optimization and extended Huckel calculations), generate numerous views, create surfaces (i.e., solvent accessible surface, electrostatic potential maps, frontier molecular orbitals), and save the structure in several formats for import into other programs. Changes saved in the Chem3D application are updated in the original ChemDraw document. The model can also be moved or resized on the ChemDraw document. The process requires additional steps for the Windows version of the software; i.e., the chemical structure from ChemDraw must be copied and pasted into Chem3D, manipulated, and then copied and pasted back into ChemDraw. On either platform, the ChemDraw/Chem3D combination is a powerful tool for communicating structural information.

To manage chemical information, ChemDraw Ultra includes ChemFinder Pro, a front end for viewing and searching databases of chemical and alphanumeric information (no databases are included in this product). Chemical information can then be displayed in ChemDraw and Chem3D format structures, as well as other structure types that can be translated into these formats. ChemFinder Pro could be used for numerous purposes, in either academic or industrial laboratories, to maintain chemical inventories, for example, or to record laboratory notebook entries containing structure, reactions, and experimental data, or even to organize results from computational chemistry studies, including optimized structures. The Windows and Macintosh versions of ChemFinder Pro are entirely different, but both versions are somewhat difficult to use, and reference to the pdf documentation was required; printed documentation would have been nice! ChemFinder Pro for both Mac and PC can exchange data with Microsoft Excel.

The glassware templates ("clip art") included on the CD-ROM required manual installation and were not documented in the manuals. The selection of glassware was somewhat limited but adequate for drawing a variety of basic organic chemical apparatuses. While the

(1) See http://products.camsoft.com/ftypes.cfm?FID=2 for a complete list of input and output file types.

(2) The plug-ins are available for download without additional purchase, http://products.camsoft.com/Downloads.cfm.

(3) Version 2.1 under license from Beilstein Informationssysteme GmbH, Beilstein Institut fuer Literatur der Organischen Chemie.

(4) CS ChemNMR 6.0 Pro, Upstream Solutions GmbH, Scientific Software Engineering, CH-6052 Hergiswil, Switzerland.

images looked professional on laser printer output (600 dpi), they are of relatively poor quality on a computer monitor (17 in. set to 832 × 624). Thus, the glassware clip art would likely prove valuable to authors of printed versions of laboratory procedures or publications but would not work well for creating electronic or Web-based presentations. Some of the drawings were not completely "grouped", a deficiency that resulted in incomplete selection when moving or rescaling.

ChemDraw 6.0 Ultra can also be used to embed structures into MS Word (Windows only) documents through OLE. An embedded structure can be edited by clicking on it in the Word document, and the structure will be updated in the Word document. Unfortunately, Macintosh users can only take advantage of embedded objects if they are using an older version of MS Word (5.0 or 5.1) that supports Publish and Subscribe. On either platform, structures created in ChemDraw and Chem3D can be pasted as static images into any clipboard-compatible program.

ChemDraw Ultra components contain several useful Internet-related features. ChemDraw and Chem3D formatted files can be viewed with the plug-ins included.[2] The program links directly to technical support at the CambridgeSoft Web site (currently identical to the documentation on the installation CD-ROM). ChemDraw and Chem3D documents can also be saved in GIF format for easy incorporation into Web pages, and ChemDraw files can be saved in MDL molfile format, for viewing with Chime-enabled browsers. Chem3D can also view and edit files in protein data bank format (although there is, unfortunately, no option to save files in this format). In the Windows version only, a highlighted ChemDraw structure can be used to search in ChemStore.com (ChemACX.com) for a supplier. For example, a search for the structure of adenine identified 17 suppliers of 33 different products, along with catalog numbers, descriptions, and prices for each.

In conclusion, ChemDraw Ultra 6.0 goes far toward meeting the needs of chemists for structure drawing, modeling, and display and provides an assortment of information features. The structure drawing program continues its tradition of excellence. ChemDraw and Chem3D are well developed and easy to use. However, some features of the package (especially Clip Art templates and ChemFinder) are less user-friendly, and in some cases, their documentation is weak. Although ChemDraw is the product of choice for Macintosh and Windows users, it would be nice to see a consistent set features in versions for the two platforms. For those who need to draw chemical structures, no product on the market surpasses ChemDraw. Those chemists requiring some of the additional features of the package may want to upgrade to ChemDraw Ultra 6.0.

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Book Reviews

Stereoselective Biocatalysis Edited by Ramesh N. Patel (Bristol-Myers Squibb Pharmaceutical Research Institute). Marcel Dekker Inc.: New York and Basel. 2000. xiii + 932 pp. $250.00. ISBN 0-8247-8282-8.

Biocatalysis, the use of enzyme catalysts in chemical synthesis, is an increasingly important alternative to purely chemical methods for the production of fine chemicals, pharmaceuticals, and agrochemicals. The aim of this book is to provide state-of-the-art knowledge to organic chemists, chemical engineers, biochemists, microbiologists, and medicinal chemists on the use of enzymes for the synthesis of chiral molecules. This is an ambitious goal covering numerous publications, which is further complicated by rapid advancement in all of these areas. The goal, however, is well met in 30 chapters containing over 4000 references and written by leading academic and industrial researchers.

Virtually all applications of isolated enzymes and whole cells for asymmetric synthesis or chiral resolution are covered. There are many examples of detailed case histories that cover all of the steps from screening for the desired enzyme activity, cloning and mutagenesis, to optimizing desired catalytic properties, implementation, and process scale-up. These include chapters on hydantoinase, carbamoylase, and aminoamidase processes for the preparation of amino acids and their further conversions written by Ogawa and Shimizu and by Sonke et al.; (−)-lactam by Taylor et al.; and β-hydroxy acid and arylpropionic acid production processes by Hasegawa and Nagashima and Alcántara et al. Specific chemical transformations including hydroxylations (Holland; Azerad), epoxidations (Abraham), decarboxylations (Ward and Baev; Ohta and Sugai), C−C bond formation (Fessner), Baeyer−Villager oxidations (Banerjee), esterifications, and acylations (Santaniello et al.; Berglund and Hult) are extensively covered. I particularly liked the brief historical perspectives most authors included in their descriptions of the evolution of different enzyme technologies and the pure chemical alternatives. Lipases, monooxygenases, dioxygenases, epoxide hydrolases, hydroxynitrile lyases, and dehydrogenases are well covered in chapters on applications and on individual enzymes. There are excellent comparisons of whole cell microbial and yeast processes with isolated enzyme alternatives. My personal favorites were the chapters on enzyme protecting group techniques and on aldolases, and the summary of biocatalysis for the production of chiral pharmaceutical intermediates. General coverage of enzyme immobilization, poly(ethylene glycol) modification, and reactions in supercritical CO_2 complement the chapters on synthetic applications. The text is easy to follow with extensive use of synthetic schemes and tables.

In summary, this is an excellent text covering all aspects of biocatalysis for the synthesis of chiral compounds. It is an invaluable source book for both academic and industrial researchers with interests in biotransformations.

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