Computer Review of ChemDraw Ultra 12.0

ChemDraw Ultra 12.0. CambridgeSoft, 100 Cambridge Park Drive, Cambridge, MA 02140. www.cambridgesoft.com. See Web site for full pricing information.

The name ChemDraw has long been synonymous with the drawing of chemical structures, and CambridgeSoft has branched into additional tools for enhancing presentation and productivity. The current version of ChemDraw Ultra is a full-featured package for chemical communication with additional tools for bench and computational chemists in both industry and academia. This package is one of twelve "Suites" and three stand-alone products that include chemical structure drawing, according to the comparison chart on the CambridgeSoft Web site.

The software reviewed is packaged as a Windows/Mac DVD. Although all of the ChemDraw-based drawing features are available on both platforms, the add-on applications bundled in this Suite, i.e., ChemBio3D Pro, ChemBioFinder Std., MNova Ste/Lte, and Excel integration, are only available for Windows. Installation of ChemDraw Ultra was straightforward on both Mac OS X and Windows XP. Installation on two partitions of a single computer, along with an additional copy on a laptop or home computer, is permissible with the license.

In contrast to the editing issues encountered previously when using ChemDraw with a Mac OS, ChemDraw 12 structures pasted into MS Office 2011 documents can be returned to ChemDraw for further editing. Structures saved in MS Office 2004 files (but not in MS Office 2008) can also be edited in ChemDraw 12. However, Mac/MS Office integration has not yet reached the ease of the Windows versions; in Windows, a ChemDraw structure pasted into an MS Word, PowerPoint, or Excel document can be chosen and modified in ChemDraw, and the edits will be transferred automatically in the embedding MS Office document.

The user interface and drawing features in ChemDraw 12 are the same in the Mac and Windows versions and continue to set the standard for function and usability. Incremental improvements in features include tools for drawing and maintaining disulfide bonds as well as other biomolecules, saving as scalable vector graphics (to avoid the "pixelation" in structures that are expanded, for example), and better support for polycyclic structures when using the "structures to names" feature. It is also easier to rotate structures and manipulate arrows than in previous versions of the product. Drawing curves has been significantly improved with the new "draw curve" tool.

ChemDraw Ultra 12 is integrated with CambridgeSoft's subscription online databases; one year of access to the databases is provided with this product. When the ChemBioFinder hotlink window is activated for a highlighted structure, data from databases, including the Merck Index and the Encyclopedia of Reagents for Organic Synthesis, are retrieved and commercial sources for the substance are identified.

A number of tools in ChemDraw are intended to help experimental chemists be more productive. For example, a variety of physical properties for a structure are calculated using empirical methods. To assist in interpreting mass spectra, exact mass, m/z, is calculated, and with the mass fragment tool, a user can specify fragments of a structure while associated fragment masses are displayed. The tools for predicting ^{1}H and ^{13}C NMR spectra can be used to simplify the interpretation of experimental spectra. The clear correlation between nuclei and calculated spectral resonances makes this a natural instructional tool as well. For synthetic chemists, "chemically intelligent" reaction arrows define a balanced chemical reaction, which can be highlighted to create an interactive table of reagents and products. This editable table includes the theoretical yield, and all entries are updated appropriately when one entry is altered.

Although many of the features of the software are obvious, the multitude of features demands good documentation. ChemDraw's help menu brings up the complete electronic manuals, which are easily accessible using the table of contents, index, and search function. The included tutorials introduce novice users to program tools, while additional documents and video tutorials on the CambridgeSoft Web site are particularly effective in describing the newer, more advanced features. However, the local and online documentation could be better integrated.

The add-on applications in the package incorporate ChemDraw structures and are almost as easy to use as ChemDraw itself. ChemBio3D Pro provides tools to create publication-quality three-dimensional molecular models and includes entry-level molecular modeling, including molecular dynamics simulations, and the calculation and display of electronic surfaces. The program can read and save in a variety of chemical formats and could be used to generate molecular structures for other modeling programs. MestReNova Lite is an NMR processing and display program that can import one-dimensional NMR spectra or FIDs as well as process and manipulate these data for presentation or publication. The Excel Plugin, in conjunction with MS Excel, and ChemBioFinder Std provide different ways of storing chemical information. With the Excel Plugin, chemical structures and a variety of chemical calculations can be stored and searched in an MS Excel spreadsheet. Modest stand-alone, searchable databases of chemical information, including structures, can be created using ChemBioFinder.

Overall, this powerful package will find wide use among a variety of chemists in industry and academia. Potential users are urged to carefully consider the features they need before choosing the appropriate version of the product.

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