COMPUTER SOFTWARE REVIEWS

ChemBioDraw 12.0. CambridgeSoft, 100 CambridgePark Drive, Cambridge, MA 02140, United States. http://www.cambridgesoft.com/software/ChemBioDraw/

The central component of ChemBioOffice, a tightly interwoven combination of ChemBioDraw, ChemBio3D, and ChemBioFinder is ChemBioDraw, the structure drawing program that was first developed in 1986 (a quarter century ago!) and has since been enhanced considerably. The two-dimensional (2D) structures produced by ChemBioDraw are live-linked to the corresponding 3D structures in ChemBio3D so that any change in either the 2D or the 3D structure, such as stereochemistry, is faithfully reflected in the counterpart structure. In addition to chemical structure drawing, ChemBioDraw includes many templates for biological structures, including membranes, nucleic acids, proteins, microorganisms, bioinstruments, and anatomical figures.

The name↔structure functionality accepts chemical structures or names as input. Systematic nomenclature is generally required, but the software can recognize trivial names, such as cholesterol and non-U.S.A. spellings, such as sulfur or aluminum. A variety of line notations are supported by these programs, but the interface presented to the user is confusing. SMILES and InChI strings of structures developed in either ChemBioDraw or ChemBio3D can be saved on the clipboard with the "copy as" command. Such strings, generated in ChemBioDraw or elsewhere, can be "specially pasted" into ChemBioDraw or ChemBio3D. The SLN and the InChIKey codes created in ChemBioDraw however cannot, inexplicably, be used as input to ChemBioDraw or ChemBio3D but are useful for external transfer, for example to NLM's PubChem or ChemSpider. The ChemBioFinder command in ChemBioDraw presents summary information about the structure at hand and includes commercial sources, synonyms and some properties, such as molecular formula and weight (MF and MW) and so on. A hotlink to ChemSpider is provided in this summary.

The ^{1}H and ^{13}C NMR shifts of input structures can be predicted and listed or presented graphically. These are the more accurate of predicted properties. Other properties, such as melting and boiling points (mp and bp) and log P, can be predicted but with less reliability. ChemBioDraw gives the estimated mp and bp of phenol, for example, with errors of 34° and 19°, respectively.

Energies of structures in ChemBio3D can be calculated, and energy minimization by MM2 or MMFF94, with or without rotation of specific bonds, is possible to obtain local minima. Molecular dynamics or stochastic conformational searching can be used to search for global minima. Interfaces to Gaussian, Jaguar, and MOPAC are available, but these programs must be purchased separately.

ChemBioOffice offers database analysis programs which are useful for the management of bioassay or chemical inventory data from bioassays. Structure-searchable Excel spreadsheets can be created with a ChemDraw/Excel program.

The documentation provided for all of these programs is voluminous but quite uneven. The more established programs, such as ChemBioDraw, are well documented, and the tutorials that are offered are helpful, but when seeking information on a specific topic, consulting the manuals or the online help can be frustrating. Color in ChemBioDraw structures can be key, and the absence of color in the printed documentation is a problem. ChemBio3D and ChemBioFinder online help appears to be simply copied from the user manuals.

Development of the ChemBioDraw programs has been continuous, and many interesting new capabilities have been added. But this user gets the impression that these additions are only icing on the cake that is ChemDraw. A stripped down structure drawing program, which is sought by many chemists, is apparently no longer offered. One is now faced with the purchase, at considerable expense, of the complete ChemBioDraw suite. The accompanying documentation is a reflection of the software in that the ChemDraw functionality is well described, with tutorials, while the subsequent enhancements are bundled into a series of later chapters.

The advertised commercial price of the ChemBioDraw Ultra 12.0 Suite is $2330; the government price is $890. Upgrades from earlier versions of the software are not available.

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