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COMPUTER SOFTWARE REVIEWS

**ChemBioOffice Ultra 2010 Suite**. CambridgeSoft. 100 CambridgePark Drive, Cambridge, MA 02140. www.cambridgesoft.com. See Web site for pricing information.

An impressive suite of software applications targeting both chemists and biologists, ChemBioOffice Ultra 2010 consists of 15 applications and a one-year subscription to three separate chemical databases. The core of ChemBioOffice Ultra consists of three tightly integrated software applications for the visualization, management, and analysis of chemical and biological data: ChemBioDraw Ultra 12.0, an enhanced version of the industry-leading software for rendering 2D chemical structures for publication; ChemBio3D Ultra 12.0, a molecular visualization and modeling application; and ChemBioFinder Ultra 12.0, a database management system for chemical structure and information databases. Within these three applications are additional software tools that enable rapid prediction of $^{1}$H and $^{13}$C NMR chemical shifts (ChemNMR Pro 12.0), conversion of chemical names to structures and vice versa (Struct=Name Pro 12.0), and the visualization of chemical data (ChemBioViz Pro 12.0). In addition, ChemBioOffice Ultra includes desktop applications for managing HTS data (BioAssay Pro 12.0), chemical inventories (Inventory Pro 12.0), and electronic notebooks (E-Notebook Pro 12.0). Elements of these applications are integrated with the Windows Office environment through ChemDraw/Excel Pro 12.0, which allows the drawing and manipulation of chemical structures and the calculation of chemical properties within Excel and ChemBioFinder for Office 12.0. This is a particularly helpful application that enables chemical structure and substructure searches within all Office file types. In addition to ActiveX support through plug-ins for ChemDraw and Chem3D, ChemBioOffice also includes the MNova Lite application for routine 1D processing and analysis of FT-NMR data as well as the statistics software package STATISTICA Base.

ChemBioOffice Ultra 2010 is fully supported only on PCs running Windows XP Professional SP2 or Vista operating systems (32-bit only for both. Vista Home/Home Premium is not supported). Limited support is provided for PCs running Windows 2000 SP4 (not supported for E-Notebook) as well as Windows 7 Professional (32-bit only) and Ultimate (not supported for BioAssay). Although ChemBioOffice Ultra 2010 is not supported for Windows emulation environments, such as Macintosh computers running Parallels software, all applications except E-notebook were found to run successfully on an Intel dual-core iMac under Mac OS 10.4.11 running Windows XP Professional SP3 32-bit emulation using Parallels Desktop 3.0, and this served as the primary evaluation environment for this review.

**General Remarks.** The manner in which CambridgeSoft bundles software in different packages can lead to some confusion. Previous versions of some of the applications discussed here were reviewed in this journal under ChemDraw Ultra 10.0 (*J. Am. Chem. Soc.* **2006**, *128*, 13646−13650) and ChemDraw Ultra 9.0 (*J. Am. Chem. Soc.* **2005**, *127*, 4115−4116), both of which were bundled with previous versions of Chem3D, E-notebook, and MNova Lite. As such, this review will focus on those applications and features in ChemBioOffice that are new or particularly noteworthy but not addressed in these previous reviews.

**ChemBioDraw Ultra 12.0.** Building upon the success of the widely used ChemDraw program, ChemBioDraw Ultra 12.0 seeks to appeal to both chemists and biologists by including templates for a wide variety of biological macromolecules and cellular structures along with an impressive array of tools for chemical drawing and analysis. The reviews of previous versions of ChemDraw, cited above, highlight many of the very useful features for chemical drawing and analysis that are shared with ChemBioDraw Ultra 12.0. New to this version are sequence tools that allow rapid input of DNA/RNA and protein sequences. These tools also allow the rapid input of modified sequences, such as disulfide bonds, covalent DNA, or peptide adducts, by expanding the structure of the residue of interest and drawing the specific modification. Unfortunately, these tools are not appropriate for large peptides or proteins since the entire sequence must be entered manually, and the formatting of long nonlinear (multiple line) sequences is not retained after expansion. Also included is a tool for plasmid annotation. An expanded array of biological templates, such as membranes, DNA, receptors, tRNA, ribosomes, helix proteins, and mitochondrion, is also new. Although support for enhanced graphics that include over 16 million colors is new, this is not reflected in the biological templates, which appear "flat" due to a lack of enhanced shading effects.

Nicknames, chemically interpreted text, e.g., Me, Ac, etc., have been an integral part of ChemDraw. New to ChemBioDraw Ultra 12.0 are user-defined nicknames that can include multiple attachment points. These and standard nicknames can be invoked through user-defined hotkeys. The Struct=Name tool is enhanced and now recognizes additional fused and bridge ring systems, along with salts and hydrates of organic compounds. Assigned names are live-linked to structures and are automatically updated as the structure is modified. In addition, limited support is provided for inorganic and organometallic compounds.

The ChemNMR routine within ChemBioDraw allows the rapid prediction of $^{13}$C and $^{1}$H NMR spectra, with peak splitting and highlighting. In this new version, this functionality is greatly enhanced by the ability to supplement the database used to predict $^{1}$H shifts with user-supplied data. Other new features include the ability to run ChemScript Pro 12.0, an enhanced Python scripting language, directly from within ChemBioDraw, export of SVG format files, and rotation of objects about user-defined centers.

**ChemBio3D Ultra 12.0.** The live-linked 3D structures generated by ChemBio3D Ultra of 2D drawings can be visualized within a ChemBioDraw window. The 2D to 3D conversion is often rather crude; however, once ChemBio3D Ultra is launched, the 3D structures can be refined by minimization of the molecular mechanics employing either the MM2 or MMFF94 force fields. Although this generates structures that are local minima, molecular dynamics or stochastic conformational search routines can be performed to aid in locating structures at global minima. ChemBio3D provides a graphical interface for Gaussian, GAMESS, Jaguar, and MOPAC, which are all sold separately. When tested with both Gaussian98 and


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Gaussian03, this interface worked nicely in both preparing and running simple jobs and in the analysis of the results, including the visualization of molecular orbitals.

ChemBio3D Ultra can interpret a wide range of file types, including protein pdf files. As a visualization tool for proteins, ChemBio3D is adequate but less functional than a number of freely available alternative programs. However, its ability to integrate visualization of biological macromolecules with molecular mechanics and dynamics is a significant feature, particularly with respect to protein−ligand complexes.

**ChemBioFinder Ultra 12.0.** ChemBioFinder is an SQL-based desktop relational database tool that provides support for chemical structure/reaction data through integration with both ChemBioDraw and ChemBio3D. The setup of the database is relatively straightforward and can include importation of data from a variety of file types. Databases are accessed through forms that can be easily created and edited. Structure windows within forms are edited via ChemBioDraw, and 3D structure windows are linked to ChemBio3D. Subforms can be used to access relational databases.

The utility of databases of ChemBioFinder lies in the ease with which they can be searched and analyzed. Searches for structures can be performed as exact, substructure, or similarity searches, the latter employing Tanimoto coefficients of molecular descriptors. Searches of databases of hundreds of thousands of structures/reactions can be performed in seconds. In addition to structural data, databases can include a wide range of predicted properties that are calculated within ChemBioDraw and ChemBio3D. Integration with ChemBioViz allows structures selected by ChemBioFinder to be clustered by structural similarity and the clusters color-coded by predicted or experimental properties, such as CLogP or biological activity.

**Other Applications and Documentation/Support.** ChemBioOffice Ultra includes an electronic notebook application, E-notebook—which could not be run on a Mac under Parallels but was successfully installed and tested on a Windows XP PC—an inventory program (Inventory Pro 12.0), and a BioAssay Pro program that enables analysis of raw data from plate readers. One additional application, ChemBioDraw for Excel, provides a very useful CombiChem utility. Within Excel, one can define generic reactions, import files of starting materials, and generate ChemBioFinder databases of combinatorial chemistry libraries.

Overall, the documentation and support for the ChemBioOffice suite is uneven and at times frustrating. Some programs, such as ChemBioDraw and ChemBio 3D, are extensively documented, with informative tutorials provided, whereas, for other programs, the documentation is less detailed or, as in the case of the CombiChem utility, missing altogether. As might be expected from such a large number of interacting applications, technical issues are common, but Web-based support requests were answered promptly.

In conclusion, the ChemBioOffice suite provides an extremely high level of functionality for chemists and biologists. The cost, in both time and money, for all this functionality can be an issue. Academic laboratories, which can purchase the suite at a discount, will benefit but must be prepared to devote significant time to troubleshooting and training to get the most out of this suite of software—a separate enterprise version, not reviewed here, targets industry. Overall, the real strength of the suite lies in the trio of ChemBioDraw Ultra, ChemBio3D Ultra, and ChemBioFinder Ultra. The additional functionality of the other applications may be very important to some, but few laboratories would actually require all of these additional programs.

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