Chemistry Software Package ChemOffice Ultra 2005

A. Zielesny*

University of Applied Sciences Gelsenkirchen, Section Recklinghausen, August-Schmidt Ring 10, D-45665 Recklinghausen, Germany

Received July 3, 2005

ChemOffice is an established comprehensive chemistry software desktop package for Microsoft Windows PCs and was partly or completely reviewed several times over the years.[1−4] ChemOffice Ultra 2005 is the latest release.[5] It consists of three core applications: the chemical structure editor ChemDraw, the chemical structure database ChemFinder, and the molecular modeling application Chem3D. In addition ChemOffice offers an E-Notebook (a personal electronic LabJournal solution), an Inventory, and a BioAssay tool as well as a number of chemical structure databases for ChemFinder with available chemicals, material safety data sheets, or selected chemical reactions. Several add-ins for Microsoft Office applications are provided, e.g. a CombiChem add-in for Microsoft Excel. The following review comprises the main current features of the core applications.

ChemDraw provides all basic drawing support functions for chemical structures and reactions as well as several well organized templates for organic and biochemical compounds (rings, aromatics, bicyclics, sugars, DNA/RNA templates, etc.). Style sheets support the preparation of drawings for corresponding scientific journals, and specific tools/clipware support lab drawings or the drawing of realistic TLC plates. Common chemical structure exchange formats for import and export are supported, e.g. MDL molfiles or Daylight SMILES. For the interplay with ChemFinder various structure and reaction query options are available like atom-to-atom mapping or the definition of reactive bond behavior. Especially helpful in practice is the integrated name-to-structure conversion for systematic chemical names and many trivial or trade names. The conversion is able to work in both directions: name to structure or structure to name.[6] As an example the trivial name "valium" can be converted into its corresponding chemical structure which in turn can be named "(*Z*)-7-chloro-1-methyl-5-phenyl-1H-benzo[*e*][1,4]-diazepin-2(3H)-one" (Figure 1). Stereochemistry is correctly evaluated, ambiguous drawings are detected, and the user is notified. ChemDraw provides basic fragment/increment based estimation methods for the prediction of ^{1}H NMR and ^{13}C NMR spectra which also show spectrum-structure assignments (Figure 1).[7] Fragment based methods are also used for the estimation of some physicochemical properties such as the octanol−water partition coefficient (logP), melting/boiling point, or the heat of formation.[8] These fragment based estimation methods must in principle be used with caution; their uncritical use may be misleading at best. In interplay with Chem3D a force-field optimized 3D structure of a 2D drawing in ChemDraw can quickly be obtained (Figure 1, the obtained local minimum 3D structure may again be misleading and is a "3D sketch" at best). In summary ChemDraw is still one of the most comfortable and developed chemical structure editors available today.

ChemFinder is a relational desktop database management system and end user front end that supports chemical structure/reaction retrieval in addition to common SQL functionality. The data can be browsed with record or table views (see Figure 2). Numeric data of a whole database or a queried hitlist can be visualized by various data plots with sorting and filtering functions. Structure and reaction queries are defined via interplay with ChemDraw. The available search modes include exact, substructure, and similarity searches. The latter are performed on the basis of molecular descriptors (e.g. existence of a six-membered ring or specific functional groups) that define a fingerprint vector ("bitscreen") for each compound. Similarity is then evaluated using the Tanimoto coefficient (the ratio of the number of intersected "bits" to the number of united "bits" of query and database structure) with a user-defined similarity threshold. The bitscreens also support the obvious sequential chemical substructure search. On a common desktop PC ChemFinder is able to manage databases in the order of hundred thousands of structures/reactions with search times in the order of seconds. MDL SDfiles can be directly imported without further a priori definitions into a flat generic ChemFinder database, and the export of SDfiles is available as well. With standard Microsoft Windows database access technology (ODBC) relational data of other local or networked relational databases are accessible. In summary local desktop ChemFinder databases are easy to build and to manage and do not require computational expert knowledge. They can be regarded as a useful chemical data store for individual research needs or those of small local project teams. An enterprise oriented chemical database and retrieval solution is not part of the reviewed ChemOffice package but another product line of CambridgeSoft (ChemOffice Enterprise, CambridgeSoft Oracle cartridge) and other vendors.

Chem3D is a molecular modeling front end with functions for building and analysis of 3D chemical structure models in combination with computational chemistry calculations. The application consists of a professional Open GL 3D structure and molecular surface rendering engine with common display options for structures (ball and stick, cylindrical bonds, space filling etc.) and surfaces (solid, wire mesh, translucent etc., see Figure 3). For computational chemistry calculations Chem3D comes with three force fields[9] and a limited implementation of the semiempirical package MOPAC (computations are limited to 250 heavy

* Corresponding author e-mail: achim.zielesny@fh-gelsenkirchen.de.

10.1021/ci050273j CCC: $30.25
Published on Web 08/27/2005

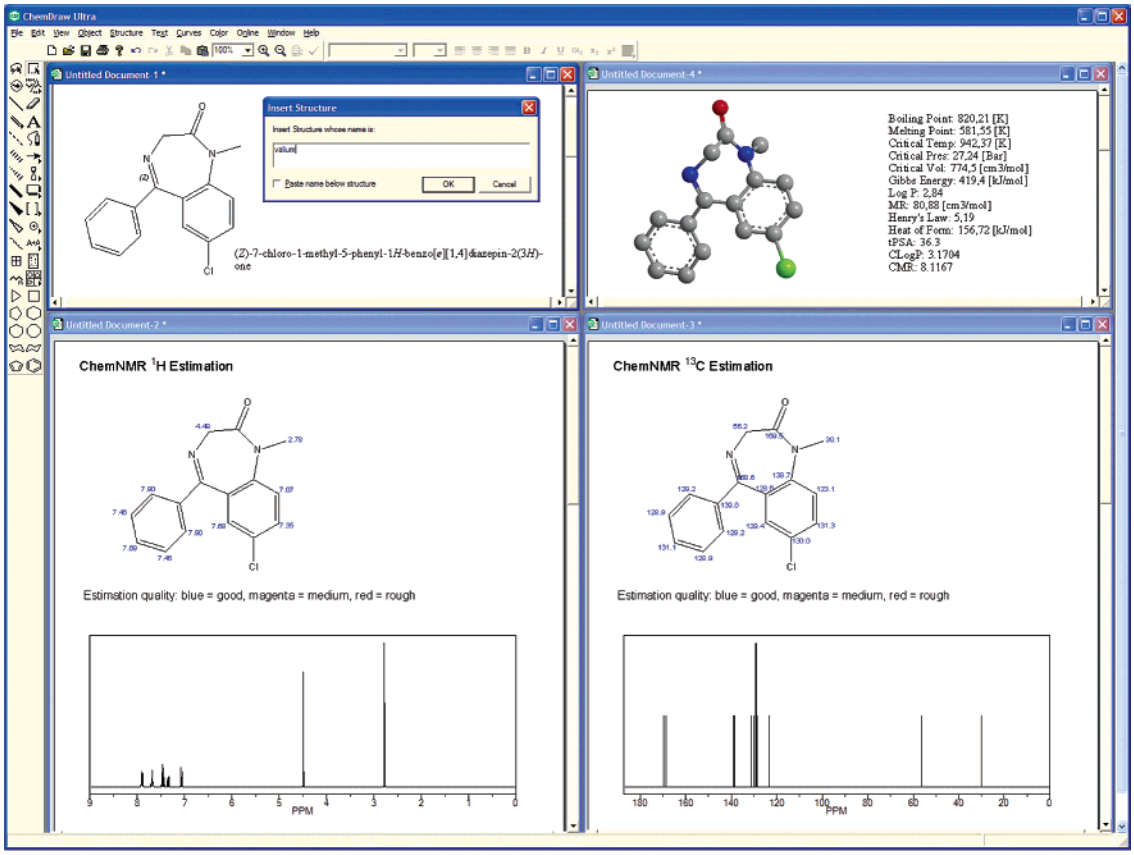

Figure 1. ChemDraw: Name-to-structure conversion and vice versa (upper left), 3D structure generation via force-field optimization and physicochemical property estimation (upper right), proton and carbon NMR spectra estimation with spectrum-structure assignment (lower left and right).

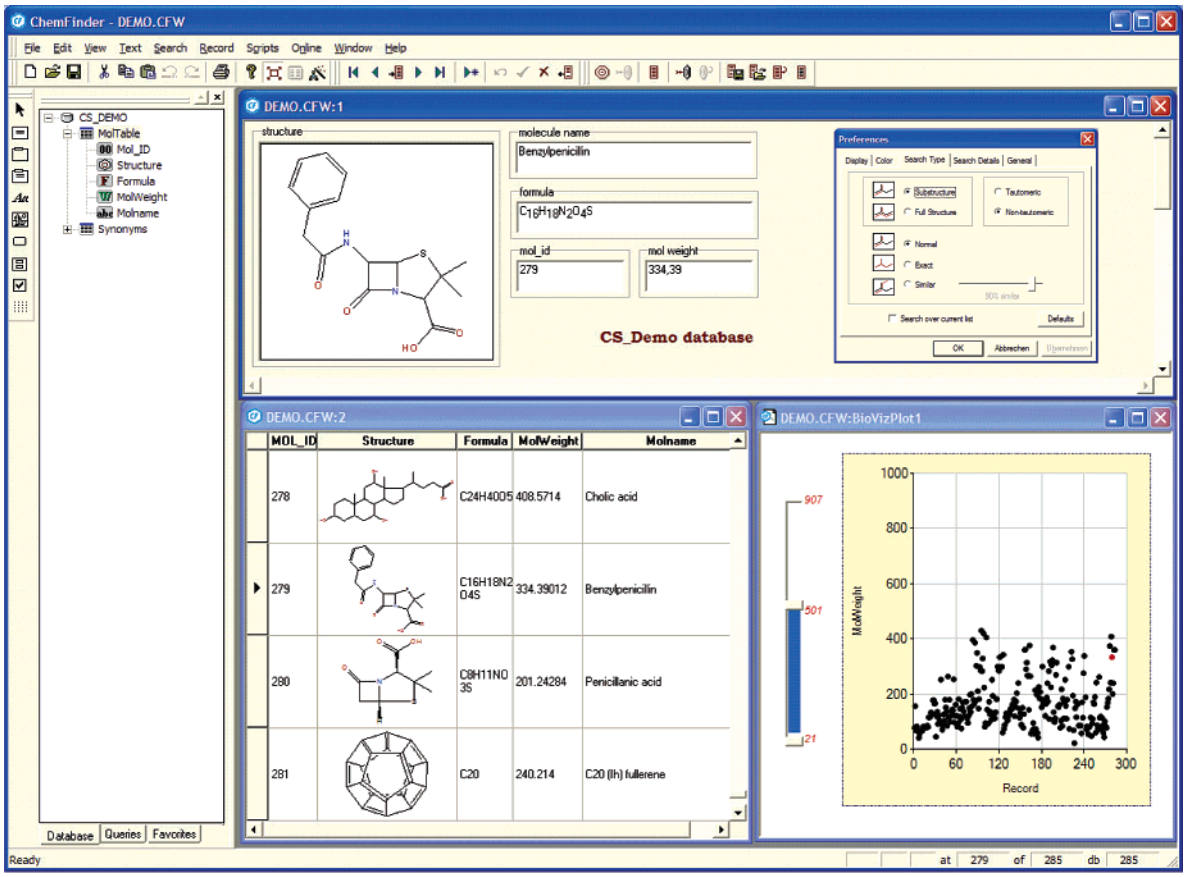

Figure 2. ChemFinder: Relational database schema (left), record view and structure search options (upper right), table view and filtered data plot (bottom right).

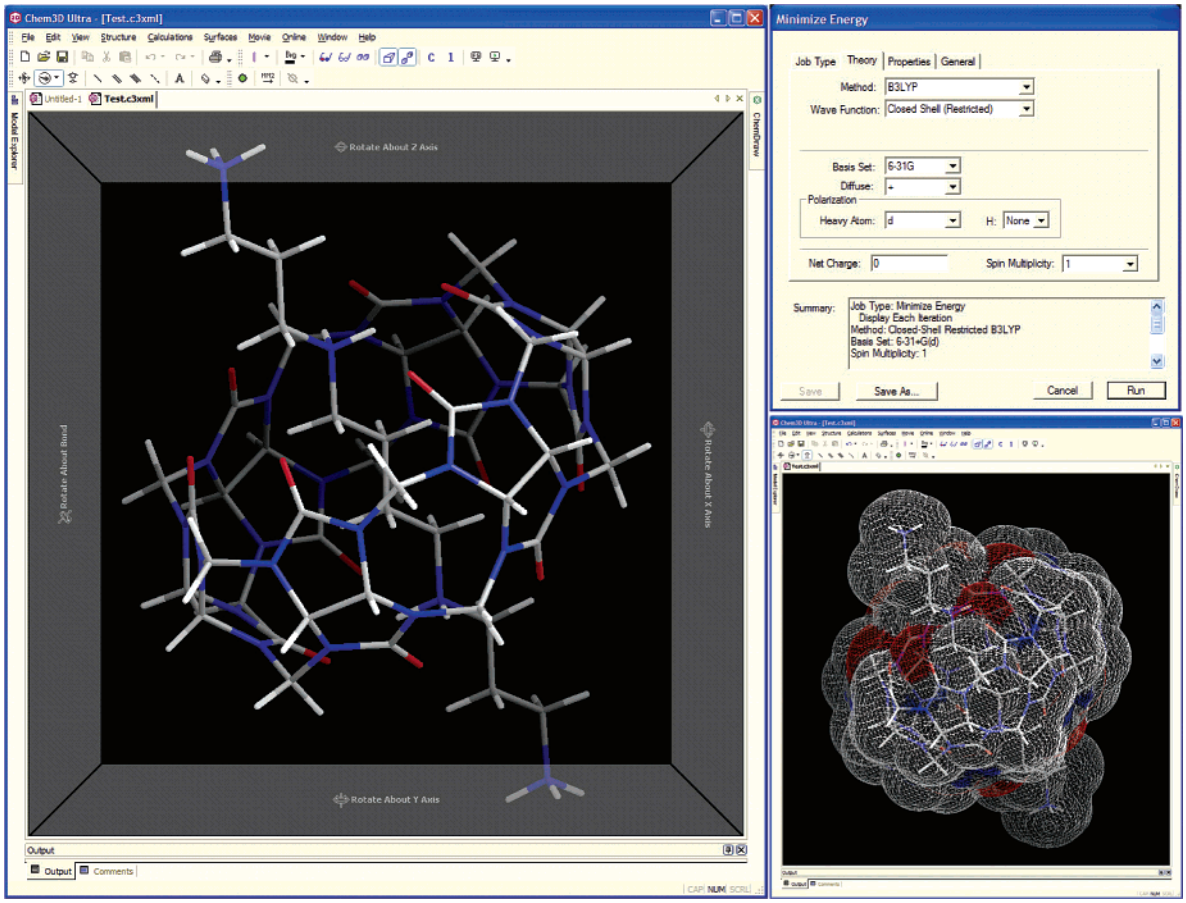

Figure 3. Chem3D: 3D structure display (left), Gaussian setup wizard (upper right), wire mesh surface plot (bottom right).

atoms).[10] Comfortable setup dialogue tabs are provided for calculations with the implemented force-fields, MOPAC, and the quantum chemical ab initio packages GAMESS[11] and Gaussian[12] which are not included in ChemOffice. The dialogue tabs allow a "point and click" definition of common computational chemistry tasks such as a single point calculation or an energy minimization. They do, of course, not map the complete range of possible settings of MOPAC, GAMESS, or Gaussian which require a thorough expert knowledge. Therefore they must be dealt with caution: An inspection of the resulting job file for the addressed computational engine is indispensable. For data exchange Chem3D supports several 3D structure file formats (e.g. MDL molfiles, MOPAC/Gaussian job files, PDB files, SYBYL files). 2D structures prepared with ChemDraw can easily be copied. Another dialogue box supports the calculation of topological, geometrical, or quantum chemical molecular descriptors for structure−activity relationships. A corresponding Microsoft Excel add-in allows automation of the calculation procedure for a (small) molecule set (large virtual substance libraries are outside the scope of this desktop product). Again, this feature must be used with caution due to the underlying subtleties of molecular descriptor calculations. Altogether Chem3D is a useful tool in setting up computational chemistry calculations for the expert. Nonexperts can easily get a "3D sketch" but must be cautious with the interpretation of the calculation results.

In summary ChemOffice Ultra 2005 is a matured and helpful software package for a chemically oriented scientist's desktop. It is intuitive and easy to use (concerning the computational chemistry part sometimes "too easy") and supports many of the common chemical R&D tasks from documentation to research design. Concerning chemical education in undergraduate and graduate chemistry courses the package is a nearly ideal set of tools due to its integration and comprehensiveness in chemoinformatics and computational chemistry. Last but not least ChemOffice Ultra 2005 comes with extensive electronic and printed documentation. Specific use-cases are illustrated at the CambridgeSoft Web site. A "Q&A" section tackles many of the problems a common user will encounter, and a download section provides necessary software patches. For current pricing information the CambridgeSoft Web site should be consulted.

REFERENCES AND NOTES

(1) Buntrock, R. E. *J. Chem. Inf. Comput. Sci.* **2002**, *42* (6), 1505−1506.

(2) Mendelsohn, L. D. *J. Chem. Inf. Comput. Sci.* **2004**, *44* (6), 2225−2226.

(3) Li, Z.; Wan, H.; Shi, y.; Ouyang, P. *J. Chem. Inf. Comput. Sci.* **2004**, *44* (5), 1886−1890.

(4) Cousins, K. R. *J. Am. Chem. Soc.* **2005**, *127*, 4115−4116.

(5) ChemOffice Ultra 2005 for Microsoft Windows 2000 or Windows XP, CambridgeSoft Corporation, 100 CambridgePark Drive, Cambridge, MA 02140-9802, U.S.A. Web site: www.cambridgesoft.com.

(6) ChemDraw uses a proprietary naming algorithm developed by CambridgeSoft.

(7) The prediction of NMR spectra is based on the work of E. Pretsch. For details see ChemDraw documentation.

(8) The calculation methods for property prediction are not documented: some seem to be proprietary to CambridgeSoft, and some use third

party algorithms (e.g. for ClogP the BioByte algorithm, BioByte Corp., is used). For explanations and details see ChemDraw documentation.

(9) The implemented force fields are based on the force fields MM2 and MM3 of N. L. Allinger and are extended by CambdridgeSoft. For details see Chem3D documentation.

(10) MOPAC 2000: Fujitsu Ltd., Web site: www.fujitsu.com (Note: At the "Q&A" section of the CambridgeSoft Web site it is remarked that the current Chem3D Ultra update version 9.0.2 is "no longer able to install the MOPAC application as part of our ChemOffice suite. You can however preserve the version of MOPAC that came with our 9.0 release."). The described preservation process is outside the scope of a normal end user.

(11) GAMESS is maintained by the Gordon research group at Iowa State University. Home page: www.msg.ameslab.gov/GAMESS/GAMESS.html. A GAMESS version for Chem3D can be downloaded from this Web site.

(12) Gaussian 03: Gaussian Inc., 340 Quinnipiac St Bldg 40, Wallingford, CT 06492, U.S.A. Web site: www.Gaussian.com.

CI050273J