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ChemOffice Pro 13.0 Suite

ChemOffice Pro 13.0 Download Individual Perpetual English
by Perkin Elmer (formerly by CambridgeSoft)

System Requirements: XP Pro SP3 (32 bit only), Vista Business and Ultimate (32 bit only), **Windows 7 (Pro and Ultimate (32/64 bit);** MS Office 2010 (32 bit), MS Office 2003, MS Office 2007;

New Version of ChemOffice® Pro 13.0 with Scientifically Intelligent Productivity Suite for Chemists and Biologists

ChemOffice® Pro 13.0 is a full featured personal productivity solution for biologists and chemists who don't require the **electronic laboratory notebook** and inventory capabilities provided with ChemBioOffice® Ultra 13.0.

All of the other ChemBioOffice Ultra 13.0 applications and capabilities are included in this up to date scientifically intelligent suite that can transform a PC into a chemical & biological publishing, modeling, and database workstation.

Highlights in Version 13.0

The following are highlights of the features in ChemOffice Pro 13.0. For a full list of ChemOffice Pro features, please click on the Features tab below.

ChemBioDraw® - Scientifically Intelligent Drawing Tools

- Biopolymer toolbar with disulfide and lactam bridges, beta and D-amino acids, DNA, RNA, protecting groups and linkers

> *"The new Biopolymer Toolbar is a huge help to draw peptides or DNA sequences. It is easy to handle and saves a lot of time."*

- Paste peptide, DNA and RNA sequences and have them interpreted chemically with sequence wrapping and shaping
- New Gel Electrophoresis Plate Tool provides arbitrary rotation for lane labels, drag and position band labels, paste data from Excel or other sources, and copy and paste between lanes
- Calculators for pKa, LogD and LogS enable scientists explore important bioavailability properties such acid dissociation, distribution and aqueous solubility for putative compounds

ChemBio3D® - Molecular Graphics and Computational Methods

> *"I have just run Autodock using the default ligand and am amazed at the results... the ChemBio3D interface is markedly easy to use... the speed of execution, albeit for a rather small molecule is the fastest I've seen in a MS OS. Well done!"*

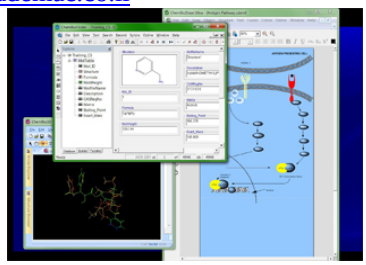

Figure 1: Transform your desktop into a chemical & biological publishing, modeling, and database workstation.

Use ChemBio3D to set up Autodock runs to dock flexible ligands into receptors of known 3D shape and compare the goodness of fit

- Set up CONFLEX® runs to quickly explore conformational space and identify minimum energy conformations for small and large molecules

ChemBioFinder™ - Database Management and Search

A chemically and biologically intelligent database manager and search engine

Cluster analysis helps scientists discover similarities within sets of compounds and properties.

Applications Included

ChemBioDraw Ultra 13.0

This ultimate chemistry and biology drawing application delivers all of the industry leading drawing, publishing and analytical features in ChemDraw combined with the biology features in BioDraw, providing a complete solution for chemical structure drawing and analysis combined with biological pathway drawing.

ChemBioDraw Ultra chemical structure analysis tools include 13C and 1H NMR prediction with peak splitting and highlighting and choice of solvent, Struct=Name, ChemDraw/Excel, stoichiometric analysis, property predictions including pKa, LogD and LogS live-linked to the structure, a live-linked Database Gateway, fragmentation tools, TLC and Gel Electrophoresis plate drawing tools, and 3D structures live-linked to the 2D structure. ChemBioDraw also offers customization options for Nicknames, Templates, and HotKeys, and adds a new Save to Dropbox feature. A new biopolymer toolbar enables creation of peptide, DNA and RNA sequences, including beta and D-amino acids, disulfide and lactam bridges and linkers and protecting groups. Biological pathway drawing elements include membranes, DNA, enzymes, receptors, and reaction arrows. tRNA, Ribosomes, Helix Proteins, Golgi Bodies, G-Proteins, Immunoglobins, Mitochondrion, new Freehand Pen Tool, Annotation, and a Plasmid mapping tool are also included.

ChemDraw ActiveX/Plugin Pro 13.0

This premier ActiveX Control/Plugin allows querying online chemical databases and viewing and publishing online structures. This installer automatically installs the necessary Plugin or ActiveX controls based on the web browser(s).

ChemBio3D Ultra 13.0

This ultimate application for desktop molecular modeling and state-of-the-art protein visualization is designed for chemists and biologists. Visualize detailed 3D protein-ligand complexes and DNA structures using open GL graphics and stereo hardware and display and analyze Hydrogen bonds and partial surfaces. Build small molecules using the ChemDraw interface and see the 3D structure appear simultaneously, perform basic Molecular modeling computations such as Alignment, Stochastic conformational sampling, Dihedral driver, MM2 experiments, Molecular Mechanics with support for MMFF94.and Dynamics. Perform ab initio and semi-empirical calculations, and predict and visualize

NMR, IR and Raman spectra with interfaces to MOPAC, Jaguar, GAMESS, Gaussian, and, **new in 13.0, Autodock and CONFLEX** for flexible ligand docking and conformational analysis

GAMESS Pro 13.0

ChemBio3D Ultra provides a graphical interface to the GAMESS program for ab initio quantum chemistry. A variety of wavefunctions (RHF, ROHF, UHF, GVB, and MCSCF, CI and MP2 energy corrections) and basis sets are available. Users can also calculate vibrational frequencies and a variety of molecular properties, such as dipole moments, hyperpolarizabilities. GAMESS is maintained by the members of the Gordon research group at Iowa State University

MOPAC 2009 for ChemBio3D 13.0

MOPAC is a general-purpose semi-empirical quantum mechanics package for the study of chemical properties and reactions in gas, solution, or solid-state. This premier molecular computation application features a number of widely-used, semi-empirical methods and allows you to compute properties and perform energy minimizations, optimize to transition states, and compute properties. It supports MOPAC sparkles, has an improved user interface, and provides faster calculations.

CONFLEX

ChemBio3D Ultra provides a graphical user interface to the CONFLEX program for high performance conformational analysis and energy minimization of small and large molecules. CONFLEX can completely search the conformational space of a flexible molecule to find every optimal structure of chemically significant conformers

Autodock

ChemBio3D Ultra provides a graphical interface to the Autodock suite of automated docking tools, which is designed to predict how small molecules, such as substrates or drug candidates, bind to a receptor of known 3D structure. This enables researchers to examine and compare the docking of flexible ligands to receptors via a user interface that steps through the process in in logical and simple steps

Gaussian

Gaussian is a series of electronic structure programs, used by chemists, chemical engineers, biochemists, physicists and other scientists worldwide. Starting from the fundamental laws of quantum mechanics, Gaussian predicts the energies, molecular structures, vibrational frequencies and molecular properties of molecules and reactions in a wide variety of chemical environments.

Jaguar

Jaguar is a high-performance ab initio package for both gas and solution phase simulations, with particular strength in treating metal containing systems, making it the most practical quantum mechanical tool for solving real-world problems.

ChemBioFinder Ultra 13.0

ChemBioFinder Ultra is the ultimate database management system for chemical structure and information databases. Browse, create, search, and update local databases with structural, numeric, and text data via user-customizable forms, including structural, sub-structural, and similarity queries, as well as linking to related data in sub-forms. Calculate values for physical properties, view and edit structures in a variety of modes, automatically create databases and forms for imported data, export and print. Easily manage saved queries, access favorite databases, and view database structure via the dockable Explorer Window. Features include the ability to perform RGroup Analysis, read graphic files from the database, Python programming and improved tautomeric searching.

ChemBioViz Pro 13.0

ChemBioViz Pro is a rich toolkit for visualizing numeric data in ChemBioFinder. Calculate and display structure activity relationships, clustering relationships, and statistical data, including histograms, scatter, logarithmic plots, and dendrograms. Descriptive statistics include minimum, maximum, mean, median, standard deviation and more. Create Compound Profiles and visually compare and rank structures based on values of selected properties and the cost profile associated with each property. Create plots within ChemBioFinder sub-forms.

ChemBioViz is a visualization application which works with ChemBioFinder Ultra and allows users to correlate biological activity with chemical structures. ChemBioViz transforms ChemBioFinder data into easy to understand graphics, allowing scientists to easily discern structure-activity relationships. ChemBioViz generates an interactive window containing a variety of plot types and allows researchers to analyze data using a variety of statistical analytical tools. Users can then filter their data on any field in the database in order to examine subsets of data in order to locate trends and correlations.

ChemDraw/Excel Pro 13.0

ChemDraw/Excel allows scientists to create chemically intelligent spreadsheets within the familiar Microsoft Excel environment. Build and manipulate chemical structures within Excel,

compute chemical properties and use structure and substructure searches to locate and group compounds.

ChemBioFinder for Office 13.0

ChemBioFinder for Office locates and searches structure files contained in documents on your computer or network drives. Multiple structure file types are recognized, including cdx, mol, sdf, rxn and skc, and search results can be displayed or exported as SDfiles.

BioDraw Ultra 13.0

BioDraw Ultra makes drawing and annotating biological pathways quick and straightforward, adding an unmatched level of uniformity and detail. Drawing elements include membranes, DNA, enzymes, receptors, and reaction arrows, tRNA, Ribosomes, Helix Proteins, Golgi Bodies, G-Proteins, Immunoglobins, Mitochondrion and a Plasmid Map Tool. BioDraw Ultra now includes a biopolymer toolbar for drawing and editing peptide and nucleotide sequences using single and three letter codes, including beta and D-amino acids. The sequences can be expanded and contracted and sulfide and lactam bridges can be easily added.

ChemNMR Pro 13.0

ChemNMR can be used to accurately estimate ^{13}C and ^{1}H (proton) NMR chemical shifts. The molecule and the spectrum appear in a new window. The chemical shifts are displayed on the molecule and the spectrum is linked to the structure so that clicking on a peak in the spectrum highlights the related fragment on the molecule. With ChemNMR 13.0, the solvent can be specified as DMSO or $CDCl_3$

Struct=Name Pro 13.0

Struct=Name contains the leading comprehensive methods for converting chemical structures into IUPAC chemical names and names to structures. It can be used for many types of compounds, including charged compounds and salts, bridged and fused ring systems, highly symmetric structures, isotopically labeled compounds and many other types of inorganic and organometallics.

MestRe Nova Std/Lite

MestRe Nova (MNova) Std is a 1D only application for data processing, visualization and analysis of NMR data. The program provides a variety of conversion facilities for most NMR spectrometer formats and includes the conventional processing, displaying and plotting capabilities of an NMR program, and more advanced processing techniques. MNova Std/Lite is a 1D only version of MNova which offers the user basic processing and analysis capabilities. The full version of MNova is available through the SciStore online store or directly through Mestrelab Research.