

Features Included in ChemOffice 2005

(W) - Feature available on Win only

No designation implies feature is available on the platform you purchase.

U,P	MOPAC Client	Chem3D interface to MOPAC. (Note: MOPAC application is required and must be purchased seperately.)
U	New Data Types / BioDraw	Conveniently store virtually any data type in its native format sequence data, restriction maps, literature, mass spec data, microarrays, presentations, Word & PDF documents, hyperlinks, etc.
U	New Integration / BioDraw	BioDraw works seamlessly with your other desktop programs so you can use your pathways in presentations and publications.
U	New Organize Data / BioDraw	BioDraw provides you with a single place to store and organize all of your important research data - regardless of the source.
U	New Pathway Diagrams / BioDraw	BioDraw includes drawing tools specifically designed for pathway diagrams; you can create beautiful pathway diagrams in a matter of minutes.
U,P,S	New Configurability / E-Notebook	(W) Design forms and add buttons that are tailored to your needs. (multiple -user configuration only)
U,P,S	New AutoText / E-Notebook	(W) Share prewritten protocols that dynamically add data from the experiment.
U	New BioViz/Office	The bio visualization add-on to ChemFinder allows you to create graphical representations of ChemFinder databases in order to identify trends and correlations within subsets of your data.
U	New ChemFinder/Oracle	Connects directly to Oracle, and carries out all searches and transactions on the server.
U,P,S	Molecular Modeling & Dynamics	Workstation quality molecular modeling.
U,P,S	MM2 & Tinker	Built in support for MM2 to generate realistic 3D structures.
U,P	New Stereo Hardware Support	Use Chem3D with a variety of stereo monitors, shutterglasses, & other hardware to provide a true 3-dimentional modeling experience.
U,P,S	Object Specific Settings	Create drawings with different styles in different parts of the document.
U	New Automatic Overlay	Select multiple molecules and let Chem3D automatically align them with a target molecule.
U	New Dihedral Driver	New conformational analysis tool allows the generation of MM2 energy plots.
U	New ChemDraw LiveLink	Simultaneous 2D & 3D editing! Draw structures using a ChemDraw window embedded in the Chem3D application. This powerful feature adds a 2D view that is always in-sync with the 3D view.
U	New Model Explorer/Chem3D	Hierarchical tree-control for exploring the structure of large models. Import a PDB file and examine chains, groups, and ligands. This new feature gives fine-grained control.
U,P	Structure Drawing	Draw chemical structures.
U,P,S	Graphical File Formats Enhanced	Import graphics stored in GIF, TIFF, PNG, JPEG, and BMP formats.
U,P,S	Chemical Warnings Enhanced	Mouse-over red box to read error description.
U,P	Query Properties	Efficiently search chemical databases by specifying properties for atoms and bonds.
U,P	Custom Templates & Nicknames	Ability to create & edit templates & nicknames.
U,P	New Expand Generic Structure	Generate multiple structures from an "abbreviated" generic structure.

U,P	New Chemical File Formats Enhanced	Reading & writing of chemical file formats including spectra & reactions.
U,P	New Mass & Other Fragmentation Tools	Now three fragmentation tools: Mass, Dissociation, & Retrosynthesis.
U,P	New TLC Plate Tool Enhanced	New customizable and crescent-shaped spots available from TLC tool for reproduction of TLC plates for inclusion in ChemDraw Documents.
U,P	New tPSA	Topological Polar Surface Area calculation is displayed on the Chemical Properties window.
U,P	New Properties LiveLink	Chemical names, formulas, molecular weights, and other physical properties added to the document are "live", and will now update automatically as modifications are made to structural diagrams.
U,P,S	Extensive Data Types / E-Notebook	(W) Notebook pages include ChemDraw reaction schemes, Microsoft Word and Excel documents, and spectral data using the Galactic Spectral Control.
U,P,S	ChemDraw & Stoichiometry Calculations / E-Notebook	(W) Stoichiometric calculations are long and tedious. E-Notebook tackles this troublesome problem by performing the calculations for you, dependant upon the drawn reaction and other entered parameters.
U,P,S	Microsoft Office & Galactic Spectra / E-Notebook	(W) E-Notebook manages all the other kinds of data chemists store in their notebooks. For free-form data, you can include Microsoft Word or Excel documents. For spectral data, you can take advantage of the Galactic Spectral Control embedded in the notebook that allows for analysis and storage of hundreds of kinds of spectra files.
U,P	New ChemNMR Enhanced	Enhanced display & calculation. Proton NMR prediction contains proton-proton splitting patterns. Enhanced accuracy of Carbon-13 shift values.
U,P	New Struct<=>Name Enhanced	Generate systematic names for chemical structures with support for the Cahn-Ingold-Prelog rules for stereochemistry. Many improvements & new classes of names.
U	3D Query/Finder	(W) Query ChemFinder database by 3D parameter.
U,P	3D Glasses	(W) Included glasses provide enhanced stereo-mode with depth shadings to give realistic 3-dimensional quality to all Chem3D renderings.
U,P,S	Enhanced Graphics	(W) Chem3D uses OpenGL to provide high quality graphics display.
U,P,S	Structure Perspective Tool	Adjust the perspective of ChemDraw molecules with simple horizontal/vertical mouse movements.
U,P,S	Floating Character Map	Add special characters from any font instantly to any ChemDraw document.
U,P,S	Floating Periodic Table	Element information available at all times with floating periodic table on the desktop.
U,P,S	Atom Numbering	Add sequential numbering indicators to atoms in a structure.
U,P	ChemSAR/Excel	(W) Through Excel, access and display calculations performed in Chem3D.
U,P	GAMESS Client	Chem3D interface to GAMESS. (Note: GAMESS application is required and must be purchased separately.)
U,P	ChemDraw/Excel	(W) Display and perform calculations on up to 1,400 chemical structures at a time in Excel.
U,P	BioArt	A ChemDraw palette of customizable common biochemistry symbols including membranes, cellular structures and more.
U,P,S	Polymer Draw	Represent and manipulate polymers in ChemDraw.
U,P,S	ChemProp/Chem3D	(W) Advanced property parameter including BP, MP and more.
U,P	Name=Struct/Excel	(W) Generate a ChemDraw structure in MS Excel by typing in systematic chemical names for most substances.
U,P,S	Multi-Page Docs	Create multiple page documents and posters within a single ChemDraw file.
U,P,S	Structure CleanUp	Improves poor drawings.

U,P,S	Online Menu	(W) Draw a structure or model and immediately get online vendor information ChemACX.Com with the click of a button.
U,P,S	Stereochemistry	Identifies stereocenters using Cahn-Ingold Prelog rules.
U,P	ChemFinder/Office	(W) Search on your computer or network for chemical structures in Word, Excel, Powerpoint, ChemDraw, ISIS files and more, and browse, search, refine, or export your hit list to any destination.
U,P	ChemSAR	(W) ChemSAR is a Chem3D Windows add-in for MS Excel with descriptive statistics and plots for structure-activity relationships.
U,P	CLogP	CLogP property server provides the latest methodology for calculating n-octanol/water partition coefficients.
U	CombiChem/Excel	(W) Use ChemFinder for MS Excel to build combinatorial libraries with embedded ChemDraw structures.
U,P	Gaussian Client	Chem3D interface to Gaussian. (Note: Gaussian application is required and must be purchased separately.)
U,P,S	LabArt	Publication-quality EPS glassware art for use within your ChemDraw documents.
U,P	ChemProp/Draw	Computes physical properties such as LogP, BP, MP and more.