**Chem3D Ultra 10.0**

**Ultimate Modeling, Visualization & Analysis Suite**

Chem3D Ultra brings workstation-quality molecular surface graphics and rigorous computational methods to your desktop. Integration with molecular analysis makes Chem3D Ultra the ideal software.

**FEATURE**

ChemDraw LiveLink

Hydrogen Bonds & Partial Surfaces Measurements

PowerPoint Computation

**BENEFIT**

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.

Automatically display hydrogen bonds in the 3D view! Generate and display partial surfaces for protein active sites. One of the best tools in the industry for doing this.

Display distance and angle measurements graphically in the 3D view linked to the Chem3D measurements table. Report average range and standard deviation of measurements after a molecule dynamics run.

Embed Chem3D models in PowerPoint files. Rotate and zoom Chem3D models while giving a presentation.

Compute electronic properties with MOPAC, GAMESS, Gaussian, and Jaguar.

**Inventory Ultra 10.0**

**Ultimate Chemical Materials Management Suite**

Inventory Ultra is the ultimate desktop application, which includes the ChemACX Database, and provides a complete tool for research chemical sourcing and purchasing.

**FEATURE**

Cascading Locations

Container Management

SQL Server Role Based Security

Audit Trails

Custom Reporting

ChemACX & ChemMSDX

**BENEFIT**

Supports locations as general as a lab or as specific as a rack in a refrigerator, with ease.

Containers are assigned a unique barcode when created.

Usernames and passwords are linked to predefined roles in SQL Server. Users may define custom attributes. These roles control which buttons and links are available after login.

Changes to location, containers and compounds are logged to the database.

Create reports of search results or location contents in numerous formats. Create your own templates.

ChemACX Database contains over 400 catalogs from leading suppliers and ChemMSDX Database contains over 20,000 material safety data sheets for commonly used laboratory chemicals.

**E-Notebook Ultra 10.0**

**Ultimate Electronic Journal & Knowledge Suite**

E-Notebook Ultra streamlines the daily record-keeping tasks of research scientists and maintains live chemical structures and information. Save time documenting work and retrieving chemical information.

**FEATURE**

Multiple Projects

Document Pages

Retrieval

AutoText

Configurable

Spectral Controls

**BENEFIT**

E-Notebook combines all your notebooks into one. Organize project notebooks the way you work.

Pages contain Excel spreadsheets, Word documents, ChemDraw drawings, spectral data, images and PowerPoint slides.

Search by structure, keyword, dates and other types of data.

Share prewritten protocols that dynamically add data from the experiment.

Design forms and add buttons that are tailored to your needs.

Spectral controls from Thermo Galactic are available.

All specifications subject to change without notice. Chem3D, Inventory and E-Notebook are Windows only.

CambridgeSoft Corporation 100 CambridgePark Drive Cambridge, Massachusetts 02140 USA
BioOffice Ultra 2006
Ultimate Assay, Pathway & Visualization Suite


PRODUCT
BioDraw Ultra
BioAssay Ultra
BioViz Ultra
Bio3D Ultra
Inventory Ultra
E-Notebook Ultra

BENEFIT
Biological pathways drawing tool with common elements such as membranes, DNA, enzymes, receptors, and reaction arrows.
Provides flexible storage, retrieval and analysis of biological data. Designed for complex lead optimization experiments, the software supports the quick set-up of biological models.
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.
Open GL graphics and stereo glasses. Molecular mechanics and semi-empirical calculations with interfaces to MOPAC, GAMESS, Gaussian, and Jaguar. Also includes ClogP and other property servers for ChemSAR/Excel.
Conveniently organize, store, and search over inventory from your desktop.
Maintain configurable lab journals with pages from ChemDraw, Microsoft Word, Excel and spectral software. Search by structure and text, and navigate through a complete visual audit trail.

BioDraw Ultra 10.0
Ultimate Pathway & Drawing Suite

BioDraw Ultra makes drawing your biological pathways straightforward and quick, adding a level of uniformity and detail which is unmatched. Includes ChemDraw Std.

FEATURE
Drawing Elements
Sharing Data
Rotation & Integration

BENEFIT
Common pathway elements such as membranes, DNA, enzymes, receptors, and reaction arrows.
Export data to a Microsoft Office application, save as an image file or use the BioDraw viewer.
Rotate BioDraw objects and combine them with chemical structures.

BioAssay Ultra 10.0
Ultimate Assay, Screening & Visualization Suite

BioAssay Ultra provides flexible storage, retrieval and analysis of biological data. Designed for complex lead optimization experiments, the software supports the quick set-up of biological models.

FEATURE
Flexible Assay
Data Management
Data Analysis & Visualization
Calculations & Graphing
Curve Fitting & Validation
BioViz Ultra

BENEFIT
A flexible data table structure allows users to define the observables and calculations that make up almost any assay from high-throughput screening to low-throughput and in vivo studies.
Data tables are linked allowing you to view associated data in one comprehensive screen. Use BioViz to create custom forms for viewing data. Export data to Microsoft Excel.
Calculations are performed automatically whenever new data is entered or imported. Many options including bar, stacked bar, point, and line charts facilitate data analysis.
Fit data to any curve equation defined by the user. Remove outliers and tainted results.
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.

All specifications subject to change without notice. BioOffice, BioDraw and BioAssay are Windows only.

CambridgeSoft Corporation 100 CambridgePark Drive Cambridge, Massachusetts 02140 USA
www.cambridgesoft.com

US 1 800 315–7300 INT’L 1 617 588–9300 FAX 1 617 588–9390 EMAIL info@cambridgesoft.com
EU 00 800 875 20000 UK +44 1223 464900 JP 0210 731 800 WWW www.cambridgesoft.com
**The Merck Index 13.4**

*Chemistry’s Constant Companion*

*The Merck Index* is a structure-searchable encyclopedia of chemicals, drugs, and biologicals. It contains all the content of the hard copy 13th Edition (10,250 monographs), plus 230 new monographs, unavailable anywhere else, as well as 540 monographs retired from the 12th Edition.

**EDITION**

**CD-ROM**

Stand-alone edition contains all the information in *The Merck Index*. Use ChemOffice Net to search, browse contents, and view structures and stereochemistry.

**Online**

Access the complete contents of *The Merck Index* through your web browser. Search and retrieve information, view and analyze structures all with the ChemDraw Plugin. Annual subscription gives immediate access to all additions and updates as they become available.

**R&D Insight/Chemists**

*R&D Insight/Chemists* is a structure searchable drug pipeline database with over 20,000 drug candidates in various stages of development. Profiles include: a synopsis of chemical information, commercial information, phases of development, properties, Adis evaluation, review of clinical information, drug development history and references.

**DATABASE**

**Structure Searching**

Search the database using chemically intelligent structure and molecular formula searching.

**Adis Profile**

The profiles in *R&D Insight/Chemists* contain extracts of the clinical and commercial information about the drug candidate from the parent database, R&D Insight from Wolters Kluwer Health. Links to the full R&D Insight record are available (additional subscription required).

**ChemACX Ultra 10.0**

*Available Chemicals & Safety Data Suite*

*ChemACX Ultra* on DVD is a collection of over 400 catalogs from leading chemical suppliers, searchable with a single query by structure, substructure, name, synonym, partial name, and other text and numeric selection criteria. It contains over 381,000 unique chemical substances (29,000 new), over 843,000 products (110,000 new).

**DATABASE**

**ChemACX**

Over 400 catalogs from leading chemical suppliers, including Sigma-Aldrich, Fisher, Acros, Alfa Aesar and TCI America, provide rapid ordering information for over 843,000 products.

**ChemMSDX**

Over 20,000 material safety data sheets for commonly used laboratory chemicals.

**ChemINDEX Ultra 10.0**

*Scientific Reference & Reaction Database Suite*

*ChemINDEX Ultra* on DVD is an extensive chemical reference library for Windows. Databases of organic reactions and small molecule properties transform your desktop computer into a chemical information resource.

**DATABASE**

**ChemINDEX**

Small molecule physical property data on over 70,000 compounds.

**ChemRXN**

Organic reaction databases include ChemSelect from Infochem GmbH and a selection from ISI’s ChemPrep, for a total of over 29,000 reactions.

**NCI & AIDS Databases**

Over 200,000 compounds with anti-cancer drug dose-response data. NCI compiled database for AIDS anti-viral compounds.

All specifications subject to change without notice. All CD-ROM and DVD databases are Windows only.

**CambridgeSoft**

www.cambridgesoft.com
# Chem & Bio Office

**Chemistry, Biology and Knowledge**

**New**  The Merck Index · E-Notebook · CombiChem · BioAssay · BioViz · Inventory · ChemDraw/Excel

## Includes

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## Software

- CombiChem/Excel Win
- ChemFinder/Oracle Win
- ChemFinder/Office Win
- ChemDraw/Excel Win
- Struct<>Name Win/Mac
- ChemNMR & ClogP Win/Mac
- Stoichiometry Grid Win/Mac
- TLC Plate Tool Win/Mac
- Mass Fragmentation Tool Win/Mac
- Structure Clean Up Win/Mac
- Polymer Draw Win/Mac
- LabArt & BioArt Win/Mac
- MOPAC Interface Win
- GAMESS Win
- Gaussian Interface Win
- Jaguar Interface Win

## Applications & Features

- The Merck Index Win/Mac
- *ChemACX Ultra (1 Year) Win
- *ChemINDEX Ultra Win
- *ChemRXN, NCI & AIDS Win

*Available Separately

All specifications subject to change without notice.
E-Notebook Workgroup

Optimized for mid-sized rollouts, E-Notebook Workgroup provides a thick client interface for creating, editing, and searching your electronic notebook.

BioAssay Workgroup

A flexible solution for the storage and analysis of biological data. Although optimized for high throughput screening, BioAssay Workgroup is also well suited for low throughput and in vivo studies.

BioViz Ultra

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.

Inventory Workgroup

Inventory Workgroup, intended for use with up to 50 users, offers much of the functionality delivered in Inventory Enterprise, while using SQL Server as the database.

ChemACX & ChemMSDX

ChemACX Database contains over 400 catalogs from leading suppliers and ChemMSDX Database contains over 20,000 material safety data sheets for commonly used laboratory chemicals.

ChemINDEX Database

ChemINDEX, ChemRXN, NCI and AIDS databases include property and reaction data. ChemRXN has 29,000 reactions, ChemINDEX has 70,000 compounds, and NCI has 200,000 compounds.

SQL Server Support

ChemOffice Workgroup is compatible with SQL Server and is accessed through a client side application.

All specifications subject to change without notice. ChemOffice is Windows only.

NEW

ChemOffice Enterprise Ultra 2006

Ultimate Enterprise Solution & Scientific Database Suite

ChemOffice Enterprise Ultra is the ultimate solution suite offering the enterprise solution versions of E-Notebook, BioAssay, BioSAR, Registration, Inventory, including ChemACX and ChemINDEX Database, and Oracle Cartridge with ChemOffice Enterprise.

 Application

E-Notebook Enterprise

E-Notebook pages contain Excel spreadsheets, Word documents, ChemDraw drawings and reactions and spectral data. Pages can be searched by text, structure or reaction.

BioAssay Enterprise

Flexible storage, retrieval and analysis of biological data. Designed for complex lead optimization experiments, the software supports the quick set-up of biological models.

BioSAR Enterprise

Offers chemical and biological data mining and structure activity relationship analysis.

Registration Enterprise

Assigns corporate registration numbers for compounds based on an organization’s business rules. Includes duplicate checks with stereochemistry, salt/batch/lot management, data validation and security.

Inventory Enterprise

Manages and tracks data associated with both commercially and internally produced chemical substances for chemical and pharmaceutical research centers of varying sizes.

ChemACX & ChemMSDX

The ChemACX Database contains over 350 catalogs from leading suppliers and ChemMSDX Database contains over 20,000 material safety data sheets for commonly used laboratory chemicals.

ChemINDEX Database

ChemINDEX, ChemRXN, NCI and AIDS databases include property and reaction data. ChemRXN has 29,000 reactions, ChemINDEX has 70,000 compounds, and NCI has 200,000 compounds.

Oracle Cartridge

Adds chemically intelligent searching to Oracle; integrates with ChemOffice Enterprise solutions.

NEW

ChemOffice Workgroup Ultra 2006

Ultimate Workgroup Application & Scientific Database Suite

ChemOffice Workgroup Ultra is the ultimate application suite offering the workgroup application versions of E-Notebook, BioAssay, BioViz, Inventory, including ChemACX and ChemINDEX Database with a SQL Server database backend.

 Application

E-Notebook Workgroup

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SQL Server Support

ChemOffice Workgroup is compatible with SQL Server and is accessed through a client side application.

All specifications subject to change without notice. ChemOffice is Windows only.
ChemOffice Ultra 2006

Ultimate Drawing, Modeling & Information Suite


PRODUCT

ChemDraw Ultra

BENEFIT

The undisputed standard for chemical drawing, featuring proton NMR with peak splitting and highlighting, TLC plate drawing tool, Struct<>Name, and stoichiometry grid tool.

Chem3D Ultra

Open GL graphics and stereo glasses. Molecular mechanics and semi-empirical calculations with interfaces to MOPAC, GAMESS and Gaussian. ClogP and other property servers for ChemSAR/Excel.

CombiChem/Excel

Build combinatorial libraries in Microsoft Excel using reagents selected by ChemFinder.

BioOffice Ultra

The ultimate suite which includes all of the applications needed to manage your biological data.

BioViz Ultra

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.

Inventory Ultra

Organize, store, and search over inventory from your desktop. Assign unique barcodes.

E-Notebook Ultra

Maintain configurable lab journals with pages from ChemDraw, Microsoft Word, Excel and spectral software. Search by structure and text, and navigate through a complete visual audit trail.

ChemInfo Ultra


ChemDraw Ultra

is the structure drawing suite for the serious professional, with advanced prediction tools and full Web integration using the ChemDraw ActiveX/Plugin.

FEATURE

Improved Struct<>Name

Produce names for many more types of compounds, including charged compounds and salts, highly symmetric structures, many types of inorganic and organometallic compounds, and others.

Improved ChemNMR

Proton NMR spectra have more accurate chemical shifts and splitting patterns, and the predicted spectra are displayed more clearly for both proton and carbon-13 NMR predictions.

Stoichiometry Grid

Automatically track and update stoichiometry data for any user-defined chemical reaction.

Graphic Display & Image

Adds greater detail to on-screen drawings and saved image files.

New Arrows Tool

Control every aspect of arrows drawn, including arc, length, headstyle, dipole, no-go and more.

ActiveX Edit in ChemDraw

Separate ChemDraw window in which to edit your structures with more space when using the ActiveX control.

MS Office Integration

ChemDraw/Excel and ChemFinder/Office offer chemical spreadsheets with structures and searching of chemical structures in documents, folders and volumes.

And More...

Also includes Chem3D Std, ChemFinder Std, BioDraw Std, E-Notebook Std, ChemInfo Std and the ChemDraw and Chem3D ActiveX/Plugins.

All specifications subject to change without notice. ChemOffice and parts of ChemDraw are Windows only.

NEW

ChemDraw Ultra 10.0

Ultimate Drawing & Information Query Suite

ChemDraw Ultra is the structure drawing suite for the serious professional, with advanced prediction tools and full Web integration using the ChemDraw ActiveX/Plugin.