THE LATEST SOFTWARE SOLUTIONS FOR CHEMICAL AND BIOLOGICAL PUBLISHING, MODELLING, AND DATA MANAGEMENT.





ChemOffice 2006

transforms your PC into a chemical and biological publishing, modelling, and database workstation.

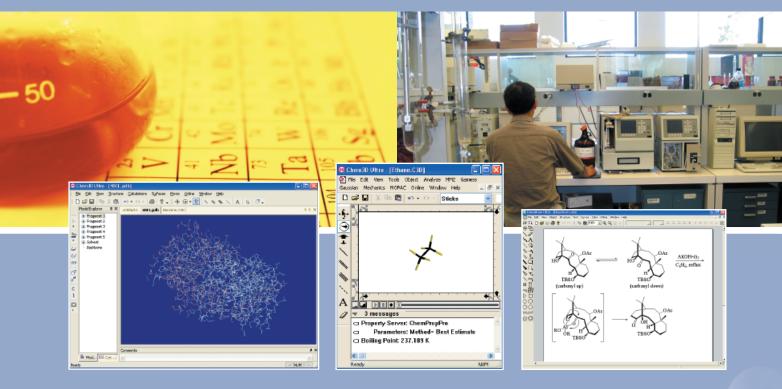
BioOffice 2006

the ultimate suite for managing biological data.

ChemDraw 10

the industry leader of chemical drawing programs.





ChemOffice Ultra 2006

ChemOffice Ultra 2006 is the ultimate drawing, modelling and information suite. It combines ChemDraw Ultra, Chem3D Ultra, ChemFinder Ultra, BioOffice Ultra, Inventory Ultra, E-Notebook Ultra, ChemACX Ultra, The Merck Index and the ChemInfo databases in the world's premier desktop chemistry suite.

PRODUCTS AND BENEFITS:

- ChemDraw Ultra The undisputed standard for chemical drawing, featuring proton NMR with peak splitting and highlighting, TLC plate drawing tool, Struct<=>Name, and structure perspective altering tool. ChemDraw offers integrated BioDraw for high-quality biological pathway drawing.
- Chem3D Ultra Open GL graphics and stereo glasses. Molecular mechanics, semi-empirical MOPAC calculations, and interfaces to GAMESS and Gaussian. ClogP and other property servers for ChemSAR/Excel.

- ChemSAR/Excel.

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

 Inventory Ultra Organise, 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. Pages now include history and have enhanced searching capabilities, plus improved reaction sections.

 The Merck Index Electronic version of the new Thirteenth Edition with complete contents searchable by structure, substructure, text and numeric fields. ChemDraw structures with ChemFinder searching.

 ChemInfo Ultra Scientific, reference and chemical databases structure searchable including ChemACX, ChemSCX, ChemMSDX, ChemINDEX, ChemRXN, NCI and AIDS databases.

 CombiChem/Excel Build combinatorial libraries in Microsoft Excel

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

 BioViz/Chem and BioOffice The bio visualisation add-on to Chem-Finder allows you to create graphical representations of ChemFinder databases in order to identify trends and correlations within subsets of your data.

 BioAssay Ultra This application fulfils the desktop data storage and modelling needs of both high and low throughput screening biologists.

 ChemFinder 10 Features much improved data plotting and visualisation integrated with your structure and data repositories, so you can analyse data, see trends at a glance and evaluate diversity among compounds in a library.

ChemDraw Ultra 10

ChemDraw Ultra 10 is the structure drawing suite for the serious professional, with advanced prediction tools and full Web integration using the ChemDraw ActiveX/Plugin. Also includes Chem3D Std, E-Notebook Std, ChemFinder Std, ChemInfo Std and the ChemDraw and Chem3D ActiveX/Plugins.

PRODUCTS AND BENEFITS:

- **BioDraw Tools** Create and edit biological entities from within your ChemDraw documents!
- Stoichiometry Grid Tool Automatically generate a table of reaction stoichiometry data using this powerful tool. You can customise the display, change units and even toggle visibility of specific information. Tabular data is automatically updated as you draw.

 Improved graphical display and image output Improved graphics engine adds greater detail to on-screen drawings and saved image files.
- ChemNMR display improvements, ChemNMR accuracy improvements Proton and carbon-13 NMR spectra have more accurate chemical shifts and splitting patterns, and the predicted spectra are displayed more clearly.

- spectra are displayed more clearly.

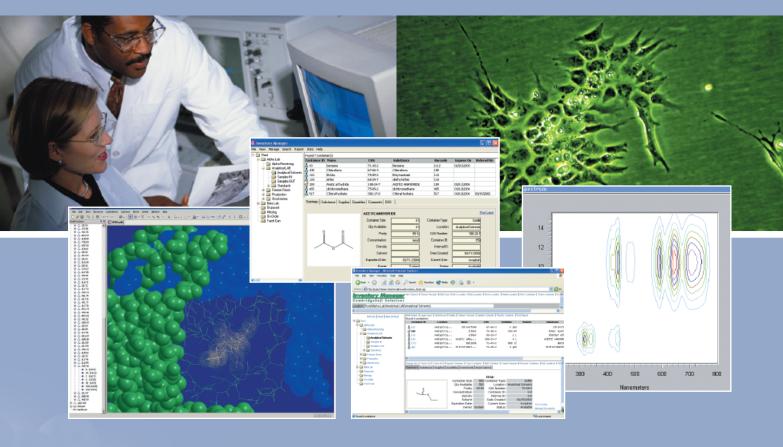
 Relative Stereochemistry support: Stereochemical representation has now been enhanced to allow specification of relationships between groups of stereocentres.

 Colour-faded shapes: The fill colour of shapes (circles, ovals, rectangles) and BioDraw objects can now be set to a faded version of the object's fill colour.

 Terminal Carbon labelling: When this setting is turned on, terminal carbon atoms will get labelled automatically, instead of remaining unlabelled. Having an appropriate atom label (usually CH3) is often more aesthetic that leaving a bare atom sticking off into space.

 Better ISIS/Draw compatibility: Compatibility with reading and writing of ISIS/Draw files has been greatly improved. Many new user-interface options have been added to ease the transition from using ISIS/Draw to using ChemDraw.

 ...and much, much more



Chem3D Ultra 10

The ultimate modelling, visualisation and analysis suite, **Chem3D Ultra 10** brings workstation-quality molecular surface graphics and rigorous computational methods to your desktop. Integration with molecular analysis and a built-in calculation set-up environment make Chem3D Ultra the ideal software for molecular modelling and analysis needs.

FEATURES AND BENEFITS:

- ChemDraw LiveLink Simultaneous 2D and 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.
- Measurements 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.
- PowerPoint Embed Chem3D models in PowerPoint files. Rotate and zoom Chem3D models while giving a presentation.
- models while giving a presentation.

 Netscape and Firefox New Chem3D plugin for Netscape and Firefox. Display Chem3D models using these browsers.

 GUI and Effects Improved Open/Save dialogues with options. New context menus on file tabs. New gradient and image backgrounds for the 3D view. New "rocking" demo mode.

 Plus MANY other new features and improvements, including improved Bio and Quantum functionality.

Inventory Ultra 10

Inventory Ultra 10 is the ultimate chemical materials management desktop application which includes the ChemACX Database and provides a complete tool for research chemical sourcing and purchasing.

FEATURES AND BENEFITS:

- **Cascading Locations** Easily supports locations as general as a lab or as specific as a rack in a refrigerator.
- Container Management Containers are assigned a unique barcode when created. Duplicate Checking Duplicates are detected according to key fields defined by the user (i.e. structure, CAS number).
- Custom Reporting Create reports of search results or location contents in numerous formats. Create your own templates.
- templates.

 Chemically Intelligent Search containers by any stored field including chemical structure, molecular formula and weight.

 ChemACX and ChemMSDX ChemACX Database contains over 350 catalogues from leading suppliers and the ChemMSDX Database contains over 20,000 material safety data sheets for commonly used laboratory chemicals.
- EHS Data Management Add Environmental Health and Safety data for Substances and Containers. EHS managers can use the built-in report engine to generate a variety of EHS reports.

E-Notebook Ultra 10

E-Notebook Ultra 10 is the ultimate electronic journal and knowledge suite, streamlining the daily record-keeping tasks of research scientists, while maintaining live chemical structures and information. Save time documenting work and retrieving chemical information.

FEATURES AND BENEFITS:

- Multiple Projects E-Notebook combines all your notebooks into one. Organise project notebooks into one. Organise project notebooks the way you work.

 Document Pages Pages contain Excel spreadsheets, Word documents, ChemDraw drawings and spectral data.

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

 AutoText Share prewritten protocols that dynamically add data from the experiment.

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

 Spectral Controls Spectral controls from Thermo Galactic are available.

 Additional sources of data in notebook

- Thermo Galactic are available.

 Additional sources of data in notebook pages You can now add PowerPoint slides and images to your experiment, allowing you to record a wider variety of data.

 Enhancements to reaction section With E-Notebook, you can:

 Select from a list of default numerical units when entering values in the stoichiometry grid.

 Select from a pre-defined list of solvents when adding solvents to your reaction.

 Have the preparation Auto-text update automatically based on changes you make to the reaction drawing or to the stoichiometry grid.

 Represent a compound in a salt or hydrated form with its formula in the stoichiometry grid.



The Merck Index 14

The Merck Index 14 is a structure-searchable encyclopedia of chemicals, drugs, and biologicals. It holds all the content of the hard copy 14th Edition (10,250 monographs), plus 230 new monographs, unavailable anywhere else, as well as 540 monographs retired from the 12th Edition.

EDITION AND BENEFITS:

- CD-ROM Stand-alone edition contains all the information in The Merck Index 14 Use ChemOffice Net to search, browse contents, view structures and stereochemistry.

 Online Access the complete contents of The Merck Index 14 through your Web browser. Search and retrieve information, view and analyse structures all with the ChemDraw Plugin. Annual subscription gives immediate access to all additions and updates as they become available.



ChemACX Ultra 10

Available Chemicals and Safety Data Suite

ChemACX Ultra on DVD is a collection of over 350 catalogues 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 326,000 unique chemical substances and their safety data (21,000 new), over 638,000 products (42,000 new).

DATABASES AND BENEFITS:

- ChemACX Over 350 catalogues from leading chemical suppliers, including Sigma-Aldrich, Fisher, Acros, Alfa Aesar and TCI America, provide rapid ordering information for over 638,000 products.

 ChemSCX A collection of fully searchable catalogues from leading screening compound suppliers.

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

ChemINDEX Ultra 10

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.

DATABASES AND BENEFITS:

- 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 Database Over 200,000 compounds
- NCI Database Over 200,000 compounds with anti-cancer drug dose-response data.

 AIDS Database NCI compiled database for AIDS anti-viral compounds.





BioOffice Ultra 2006

BioOffice Ultra 2006 is the ultimate assay, pathway and visualisation suite, to work with and manage your biological data. The suite includes BioAssay Ultra, BioDraw Ultra, Chem3D Ultra, Inventory Ultra, E-Notebook Ultra and BioViz/Chem.

FEATURES AND BENEFITS:

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

 BioDraw Ultra Manages biological data with common pathway elements, data sharing and annotations.

 Chem3D Ultra Open GL graphics and stereo glasses. Molecular mechanics, semiempirical MOPAC calculations, and interfaces to GAMESS and Gaussian. ClogP and other property servers for ChemSAR/Excel.

 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.

 Inventory Ultra Conveniently organise, store and search over inventory from your desktop.

- BioViz/Chem and BioOffice The bio visualisation 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.



BioAssay Ultra 10

The ultimate assay, screening and visualisation suite, **BioAssay Ultra 10** provides flexible storage, retrieval and analysis of biological data. Designed for complex lead optimisation experiments, the software supports the quick set-up of biological models.

FEATURES AND BENEFITS:

- The most flexible assay definition model in the industry Different facilities have the need to include multiple ways of calculating and displaying assay results. For this reason, CambridgeSoft has created software that allows you to easily translate any assay into a step by step automated procedure. Be it high or low throughput, you decide how and when to calculate results. After defining the necessary data tables, calculations and plots, simply load your data and the work is done.

 Built in graphing engine Visualise your data using the BioAssay graphing engine. Fit your data to any curve and adjust display options at will.

 Quickly upload large amounts of data to the database Data sets gathered from assays can become quite large. BioAssay Ultra allows you to load large amounts of assay data quickly and easily. Use specially designed wizards and templates to load your data efficiently.

 Perform calculations and curve fits on

- your data efficiently.

 Perform calculations and curve fits on your raw data Define calculations and curve fit algorithms for use in your assay to help analyse and interpret your raw data. Calculations are automated and do not include any data marked invalid by the user. Import data from a wide variety of instruments and Excel sheets Both columnar and plate block files are accepted for data import. This allows the application to accept close to all formats output by plate reading instruments. You tell the application where to find the data in the file and the import wizard does the rest.

- Built-in data validity management and QC functionality Users are able to validate and invalidate imported data. Invalid data is not included in calculations or curve fits, making it easier to interpret only data you deem relevant.

 Quickly find hits with well plate and data table colouring Colour wells or rows in a data table by any field associated with the data tale or plate. Define a gradient in order to quickly visualise which compounds are worth further testing.

 Numerous Visualisation Options Users have the ability to create custom plots and analyse them individually or compare them against each other. Attachment and picture handling make BioAssay ideal for everything from in vivo to high-throughput work.

 Compound/Curve Overlay Plot multiple compounds on a single graph, or multiple curves for a single compound and compare on the same graph.

 ...and much, much more

BioDraw Ultra 10

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

FEATURES AND BENEFITS:

- Drawing Elements Common pathway elements such as membranes, DNA, enzymes, receptors and reaction arrows.
 Sharing Data Export data to a Microsoft Office application, save as an image file or use the BioDraw viewer.
 Annotations Store annotations for each element in your drawing. Annotation data ranges from manually entered text to attached documents, literature references, or links.

Chem and Bio Office: Chemistry, Biology and Knowledge

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Software	*ChemDraw Ultra	Win/Mac													
	*ChemDraw Pro	Win/Mac													
	*ChemDraw Std	Win/Mac													
	*ChemDraw ActiveX/Plugin Pro	Win/Mac													
	*Chem3D Ultra	Win													
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	*Chem3D and E-Notebook Pro	Win													
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	*BioDraw Pro	Win													
	*BioAssay Pro	Win													
	BioViz Pro	Win													
	*Inventory Pro	Win													
	*E-Notebook Ultra	Win													
Applications & Features	CombiChem/Excel	Win													
	ChemFinder/Oracle	Win													
	ChemFinder/Office	Win													
	ChemDraw/Excel	Win													
	Struct<=>Name	Win/Mac													
	ChemNMR and ClogP	Win/Mac													
	Stoichiometry Grid	Win/Mac													
	TLC Plate Tool	Win/Mac													
	Mass Fragmentation Tool	Win/Mac													
	Structure CleanUp	Win/Mac													
	Polymer Draw	Win/Mac													
	LabArt and BioArt	Win/Mac													
	MOPAC Interface	Win													
	GAMESS	Win													
	Gaussian Interface	Win													
	Jaguar Interface	Win													
Databases	*The Merck Index	Win/Mac													
	*ChemACX Ultra (1 Year)	Win													
	*ChemINDEX Ultra	Win													
	ChemRXN, NCI and AIDS	Win													



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