

ChemBioOffice Ultra 2008

Ultimate Chemistry, Biology & Knowledge Suite

ChemBioOffice Ultra combines *ChemBioDraw Ultra*, *ChemBio3D Ultra*, *ChemFinder Ultra*, *BioViz Ultra*, *BioAssay Ultra*, *Inventory Ultra* and *E-Notebook Ultra* in the world's premier desktop suite designed for both chemists and biologists.

PRODUCT

ChemBioDraw Ultra

ChemBio3D Ultra

ChemFinder Ultra

BioViz Ultra

Inventory Ultra

E-Notebook Ultra

**CombiChem/Excel
Databases**

BENEFIT

The undisputed standard for chemical and biological drawing, featuring proton NMR with peak splitting and highlighting, amino acid and DNA sequence tools, TLC plate drawing tool, Struct=Name, and stoichiometric analysis.

State-of-the-art protein visualization, open GL graphics and stereo glasses. Molecular mechanics and semi-empirical calculations with interfaces to MOPAC, Jaguar GAMESS and Gaussian.

Store searching and analyze relational scientific data, either within a structure-searchable local database, or as interface to a shared scientific data (including data stored in Oracle tables).

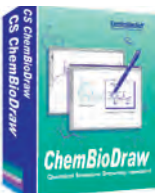
Correlate chemical and biological activity data, create graphical representations of *ChemFinder* databases in order to identify trends and correlations within subsets of your data, calculate descriptive statistics and display them on the plot.

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

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

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

Structure searchable scientific, reference and chemical databases including ChemINDEX, ChemRXN, NCI and AIDS and a 1-year subscription to the *ChemACX* and ChemMSDX databases.



ChemBioDraw Ultra 11.0

Ultimate Chemistry, Biology, Drawing & Query Suite

ChemBioDraw Ultra is the structure drawing suite for the serious professional, with advanced prediction tools and full Web integration using the *ChemBioDraw ActiveX/Plugin*. The *ChemBioDraw Ultra* suite also includes *ChemDraw/Excel*, *ChemBio3D Pro*, *ChemFinder Ultra with BioViz*, *E-Notebook Pro* and the *ChemInfo Databases*.

APPLICATION

BioDraw

Chem3D LiveLink

Database LiveLink

Struct=Name

ChemNMR

Stoichiometry Grid

Sequence Tool

Customizations

MS Office Integration

BENEFIT

Create publication quality Biological Pathways with common pathway elements, data sharing and annotations.

View your 2D structures live in 3D.

Perform dynamic database lookup using the Database Gateway HotLink. The database search results include links to information resources found in the databases, structural properties, names & synonyms and chemical identifiers such as ACX ID's and CAS numbers.

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. Produce structures from systematic and common chemical structure names.

Predict proton and carbon-13 NMR spectra from *ChemDraw* structures. Chemical shifts and splitting patterns are clearly displayed and live-linked to the structure for both proton and carbon-13 NMR predictions.

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

Draw peptide or nucleotide sequences using single letter codes. The atoms are labeled with amino acid or nucleotide nicknames. The sequences can be expanded and contracted.

Customize your ChemBioDraw experience with your own Nicknames, Templates, HotKeys and even newly added ChemBioDraw Themes.

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

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

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NEW ChemOffice Ultra 2008

Ultimate Chemical Modeling, Visualization & Analysis Suite

ChemOffice Ultra combines *ChemBioDraw Ultra*, *ChemBio3D Ultra*, *ChemFinder Ultra* with *BioViz*, *E-Notebook Ultra* and *CombiChem/Excel* in the world's premier desktop chemistry suite.

BENEFIT

Create publication quality graphics featuring chemical and biological elements. Create macromolecules with amino acid and DNA sequence tools. Simulate proton NMR spectra with splitting. Convert chemical names into structures and vice versa. Visualize proteins and other 3D structures with state-of-the-art open GL graphics. Perform molecular mechanics and semi-empirical calculations, and interface to MOPAC, Jaguar, GAMESS and Gaussian. Create, store and search chemical databases. Graphically identify trends and correlate biological activity with chemical structures. Maintain configurable lab notebooks with pages from *ChemDraw* and Microsoft Office products. Build combinatorial libraries in Microsoft Excel using reagents from databases.



NEW ChemDraw Ultra 11.0

Ultimate Chemical 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*. The *ChemDraw Ultra* suite also includes *ChemDraw/Excel*, *Chem3D Pro* and *ChemFinder Std*.

BENEFIT

Create publication quality graphics featuring chemical structures and lab ware elements. Automatically calculate and update stoichiometry data for chemical reactions. Draw peptide and nucleotide sequences using single letter codes. Preview chemical structures in 3D. Perform dynamic database lookups on structures. Convert systematic and common chemical names into publication quality structures. Generate systematic names for chemical structures. Predict proton and carbon-12 NMR spectra from structures, with splitting patterns and chemical shifts identified and linked to the structures. Customize *ChemDraw* with Nicknames, Templates, Hot Keys, and Themes.



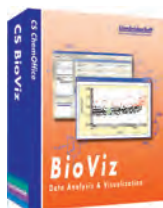
NEW ChemBio3D Ultra 11.0

Ultimate 3D Modeling, Visualization & Analysis Suite

ChemBio3D Ultra brings workstation-quality molecular graphics and rigorous computational methods to your desktop. Integration with molecular analysis makes *Chem3D Ultra* the ideal software. The *ChemBio3D Ultra* suite also includes *ChemDraw Std*, *ChemFinder Std* and *E-Notebook Pro*.

BENEFIT

Build and visualize 3D structures and macromolecules. Simultaneously edit structures using a ChemDraw window. Explore complex macromolecules using Model Explorer, a hierarchical tree-control. View and compare a set of small structures and their properties with the Structure Browser. Compute electronic properties and spectra with GAMESS, Gaussian, Jaguar and MOPAC. Select multiple molecules and align them with a target molecule. Analyze rotation about one or two dihedral angles and generate live-linked energy plots. View hydrogen bonds, kekule and delocalized aromatic bonds, ligands, and hydrating water molecules.



NEW ChemBioViz Ultra 11.0

Ultimate Data Mining & Visualization Suite

ChemBioViz Ultra brings basic data mining and visualization tools to the desktop by allowing users to create graphical representations of *ChemFinder* databases and identify trends and correlations within subsets of data. The *ChemBioViz Ultra* suite includes *BioDraw Ultra*, *ChemFinder Ultra* and *BioViz Ultra*.

BENEFIT

Graphically identify trends and correlate biological activity with chemical structures. Perform statistical analyses and utilize a wide variety of flexible options for plotting graphs of results. Visually compare and rank chemical structures based on values of selected properties and the cost profile associated with each property. Create publication quality graphics that include chemical structures and biological pathways. Create and search relational scientific data with chemical structures.

All specifications subject to change without notice. ChemOffice, ChemBio3D Ultra, and ChemBioViz Ultra are Windows only.

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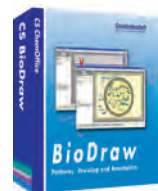
BioOffice Ultra 2008

Ultimate Biological Data Management & Analysis Suite

BioOffice Ultra is the ultimate suite for management and analysis of biological data including *BioDraw Ultra*, *ChemBio3D Ultra*, *ChemFinder Pro*, *BioViz Ultra*, *BioAssay Ultra*, *Inventory Ultra*, and *E-Notebook Ultra*.

BENEFIT

Create publication quality graphics featuring biological pathways. Add metadata with annotations. Create biological macromolecules with amino acid and DNA sequence tools. Create plasmid maps with multiple regions. Store, retrieve, and analyze assay data. Graphically identify trends and correlate biological activity with chemical structures. Visualize and explore complex macromolecules such as PDB file in 3D with state-of-the-art Open GL graphics. Organize, store, and search biological and chemical inventories. Maintain configurable lab notebooks with pages from *ChemDraw* and Microsoft Office products.



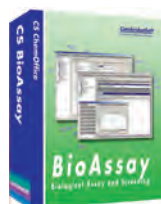
BioDraw Ultra 11.0

Ultimate Biological Pathway Drawing Suite

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

BENEFIT

Create publication quality graphics with common pathway elements such as membranes, DNA, enzymes, receptors, tRNA, ribosomes, helical proteins, and more! Annotate each element in a drawing with notes, literature reference, links, and attached documents. Create plasmid maps with specified regions, locations, and labels for markers. Draw peptide and nucleotide sequences using single letter codes. Copy drawings into Microsoft Office applications or save as a wide variety of image formats.



BioAssay Ultra 11.0

Ultimate Assay, Screening & Visualization Suite

BioAssay Ultra provides flexible storage, retrieval and analysis of biological data for both high and low throughput screening biologists and supports the quick set-up of biological models. The *BioAssay Ultra* suite also includes *BioDraw Ultra*, *ChemFinder Std*, and *BioViz Pro*.

BENEFIT

Store and visualize assay data using a flexible data structure. Define the observables and calculations for high-throughput, low-throughput or in-vivo studies. View associated data in one comprehensive screen. Automatically calculate data and plot graphs upon new data entry. Import data from instruments, excel, or enter manually. Fit data to curve equations. Validate or invalidate data and remove outliers and tainted results. Graphically identify trends and correlate biological activity with chemical structures. Export data to Excel or BioViz for additional analysis.



Inventory Ultra 11.0

Ultimate Chemical Materials Management Suite

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

BENEFIT

Supports location as general as a lab or as specific as a rack in a refrigerator. Containers are assigned a unique barcode when created. Usernames and passwords are linked to predefined roles in SQL Server. Changes to location, containers and compounds are logged to the database. Create reports of search results or location contents in numerous formats. *ChemACX Database* contains over 400 catalogs from leading suppliers, and *ChemMSDX Database* contains over 200,000 material safety data sheets for common laboratory chemicals.

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

NEW

ChemBioFinder.com

Chemistry Database Gateway

ChemBioFinder.com is an online chemistry and biology reference database. With more than 400,000 compounds cataloged and linked to other web sites, it provides a wealth of chemical information for professional chemists and students alike. *ChemBioFinder.com* serves as the gateway to all database offerings.

DATABASE

Online

BENEFIT

Records contain chemical structures, physical properties and hyperlinks to other websites containing information on your compound.

Searches yield results extending across all databases, including The Merck Index, ChemACX, Traditional Chinese Medicines, Ashgate Drugs, CambridgeSoft Patents and more.



NEW

The Merck Index 14th Edition

Chemistry's Constant Companion

The Merck Index is a structure-searchable encyclopedia of chemicals, drugs and biologicals. It is comprised of 10,200 monographs from the hard copy 14th Edition which cover over 18,000 compounds and over 50,000 synonyms including systematic and trade names. There are also 900 monographs, unavailable anywhere else, that were retired from the 12th and 13th Editions.

DATABASE

Online

BENEFIT

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.



NEW

R&D Insight/Chemists

Structure Searchable Drug Pipeline Database

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

DATABASE

Structure Searching

Adis Profile

BENEFIT

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

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).

NEW

ChemACX Database

Available Chemicals & Safety Data Suite

ChemACX Database is a collection of approximately 500 chemical supplier catalogs, searchable with a single query by structure, substructure, name, synonym, partial name and other text and numeric search criteria. It contains approximately 450,000 unique chemical substances and over one million products.

DATABASE

ChemACX

ChemMSDX

BENEFIT

Approximately 500 catalogs from leading suppliers such as Sigma-Aldrich, Fisher, Acros, Alfa Aesar and TCI America, provide rapid ordering information for over one million products.

Integrated into *ChemACX*, contains approximately 25,000 Material Safety Data Sheets (MSDS) for commonly used laboratory chemicals.

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

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		Available Suites											
		ChemBioOffice Ultra	ChemOffice Ultra	ChemBioDraw Ultra	ChemDraw Ultra	ChemDraw Pro	ChemBio3D Ultra	ChemBioViz Ultra	BioOffice Ultra	BioDraw Ultra	BioAssay Ultra	Inventory Ultra	E-Notebook Ultra
Software	Includes												
	*ChemDraw Ultra	Win/Mac	■	■	■	■	■	■	■	■	■	■	■
	*ChemDraw Pro	Win/Mac							■				
	*ChemDraw Std	Win/Mac								■		■	■
	*ChemDraw ActiveX/Plugin Pro	Win/Mac	■	■	■	■	■	■	■	■	■	■	■
	*ChemBio3D Ultra	Win	■	■					■	■	■		
	*ChemBio3D ActiveX Pro	Win	■	■					■	■	■		■
	*ChemBio3D Pro	Win			■	■							
	ChemBio3D Std	Win					■						■
	ChemFinder Pro	Win	■	■	■					■	■		
	ChemFinder Std	Win				■				■		■	■
	*BioDraw Pro	Win/Mac	■	■	■	■				■	■	■	■
	*BioAssay Pro	Win	■								■		■
	BioViz Pro	Win	■							■	■		■
*Inventory Pro	Win	■								■		■	
*E-Notebook Ultra	Win	■	■							■		■	
E-Notebook Pro	Win			■	■				■			■	
Applications & Features	CombiChem/Excel	Win	■	■						■			■
	ChemFinder/Office	Win	■	■	■	■				■	■		■
	ChemFinder/Oracle	Win	■							■			
	Ideal Compound Profiling	Win	■							■	■		■
	Struct=Name	Win/Mac	■	■	■	■	■			■			■
	ChemDraw/Excel	Win	■	■	■	■	■			■			
	ChemNMR & ClogP	Win/Mac	■	■	■	■	■			■			
	Database Livelihood	Win/Mac	■	■	■	■	■			■			
	Structure Clean Up	Win/Mac	■	■	■	■	■	■		■			
	Stoichiometry Grid	Win/Mac	■	■	■	■	■			■			
	TLC Plate Tool	Win/Mac	■	■	■	■	■	■		■			
	Polymer Draw	Win/Mac	■	■	■	■	■	■		■			
	Sequence Tool	Win/Mac	■	■	■	■	■			■	■	■	
	ChemScript	Win	■							■	■		
GAMESS	Win	■	■	■					■	■	■		
Gaussian Interface	Win	■	■						■	■	■		
Jaguar Interface	Win	■	■						■	■	■		
MOPAC Interface	Win	■	■						■	■	■		
Databases	*ChemACX Ultra (1 Year)	Win/Mac	■									■	
	*ChemINDEX Ultra	Win	■	■	■	■	■			■			■
	ChemRXN, NCI & AIDS	Win	■	■	■	■	■			■			■

*Available Separately

All specifications subject to change without notice.



E-Notebook Ultra 11.0

Ultimate Electronic Journal & Knowledge Suite

This ultimate electronic notebook suite includes *E-Notebook Ultra*, *ChemDraw Std*, *ChemBio3D Pro*, *ChemFinder Std with BioViz*, and *CombiChem/Excel*, as well as the *ChemINDEX* databases.

PRODUCT

Multiple Projects

Document Pages

Retrieval

Audit trail

AutoText

Configurability

BENEFIT

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

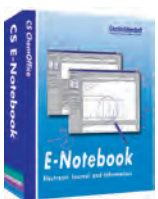
Notebook pages contain *ChemBioDraw* drawings, MS Excel spreadsheets, Word documents, PowerPoint documents, Images and spectral data.

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

Retain a complete copy of the experiment for each save, including username and timestamp.

Share prewritten protocols that dynamically add data from the experiment.

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



E-Notebook Enterprise 11.0

Chemistry, Biology, Process & Compliance Management

E-Notebook Enterprise provides a smooth web-based interface designed to replace paper laboratory notebooks. *E-Notebook* pages contain Excel spreadsheets, Word documents, *ChemDraw* drawings and reactions and spectral data. *E-Notebook* can be searched by text, structure or reaction.

FEATURE

Research & Development

Chemistry Research

Applied Biology

Analytical Services

Sample Management

BENEFIT

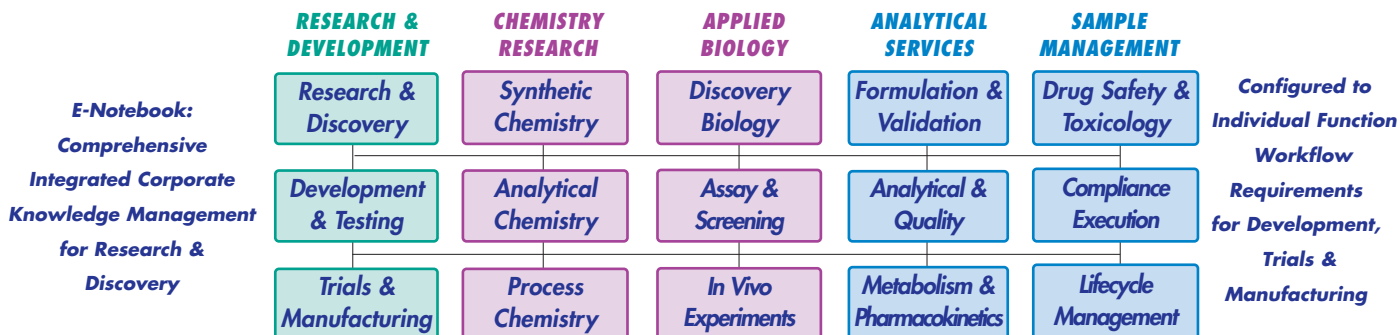
Improve collaboration, knowledge management, regulatory compliance, intellectual property (IP) protection, and project management. Flexible and configurable architecture allows for multiple workflows from early stage discovery through clinical development.

Record and share data using *ChemBioDraw*, MS Office, Adobe Acrobat and other industry standard applications. Protect IP with digital signatures. Create and enumerate libraries with *CombiChem* using flexible plate layouts, multiple reaction site checking, and multiple step parallel synthesis.

Capture information in from instruments into electronic experiments and protocols. Manage data with familiar tools such as Microsoft Word and Excel. Generate customizable reports. Centralize the collection and storage in vivo experiment SOP's and results. Track animal housing and breeding as part of the biology workflow.

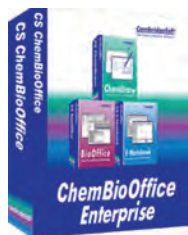
Support workflows for Formulations, Validation, Quality Control, Drug Metabolism and DMPK groups. Manage GxP and FDA 21CFR compliance. Implement an automated service request workflow with sample management. Create customized reports based on specific database fields or aggregates.

Customize sample logins with Inventory integration. Track and barcode samples, add information such as physical properties, non-chemical data and test results. Register proprietary compounds from *E-Notebook* with *Registration* integration and perform duplicate checks and assign registry numbers. Manage the chemical and biological sample lifecycles with full audit trails, and customizable reporting for GxP and 21CFR part 11 compliance.



All specifications subject to change without notice. E-Notebook Ultra and E-Notebook Enterprise are Windows only.

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NEW ChemBioOffice Enterprise Ultra 2008

Ultimate Chemistry, Biology & Knowledge Suite

ChemBioOffice 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 *ChemBioOffice Enterprise*.

PRODUCT

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 size.

ChemACX & ChemMSDX

The *ChemACX* Database contains approximately 500 catalogs from leading suppliers and *ChemMSDX* Database contains approximately 25,000 material safety data sheets for commonly used laboratory chemicals.

ChemINDEX Database

ChemINDEX, ChemRXN, NCI and AIDS databases include property and reaction data. ChemRXN has approximately 30,000 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 ChemBioOffice Workgroup Ultra 2008

Ultimate Chemistry, Biology & Knowledge Suite

ChemBioOffice Workgroup Ultra is the solution suite offering the workgroup versions of *E-Notebook*, *BioAssay*, *Inventory*, including *ChemACX* and *ChemIndex* Database using SQL Server. SQL Server is the application of choice for small to medium sized databases.

ChemBioOffice

Available Suites

	ChemBioOffice Enterprise Ultra	BioOffice Enterprise Pro	ChemOffice Enterprise Ultra	ChemBioViz Enterprise Std	ChemBioOffice Workgroup Ultra	ChemOffice Workgroup Pro
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Includes

*E-Notebook Enterprise or Workgroup	■	■			■	
*BioAssay Enterprise or Workgroup	■	■			■	
*BioSAR Enterprise	■	■		■		
*BioViz Desktop				■		■
*Registration Enterprise	■		■			
*Inventory Enterprise or Workgroup	■	■	■		■	■
*ChemACX Database	■		■		■	■
ChemBioViz Enterprise or Workgroup	■	■	■	■	■	
*ChemINDEX Database	■		■	■	■	■
*Oracle Cartridge	■		■	■	■	
SQL Server Compatible				■	■	■
*ChemFinder Ultra				■	■	■

*Available Separately

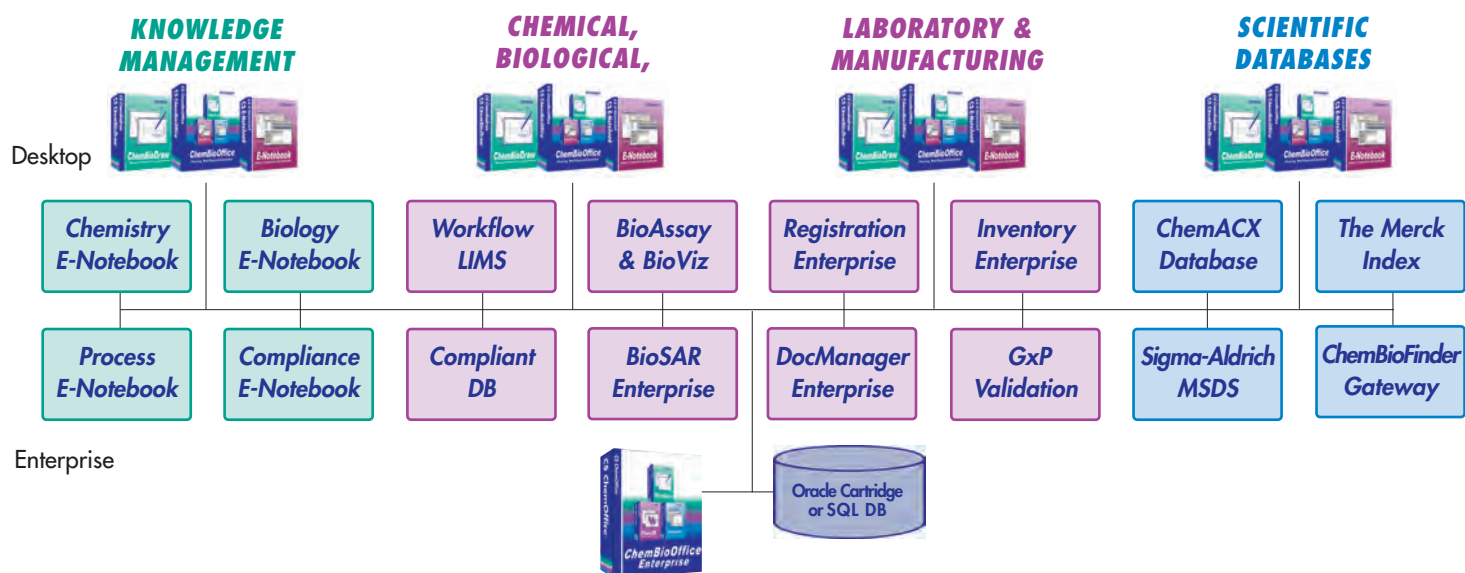
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Chem & Bio Office

Desktop Software to Enterprise Solutions



Research, Discovery, Development, Trials & Manufacturing

Enterprise Solutions include *Chem & Bio Office* with *Oracle Cartridge* and *Chem & Bio Office Workgroup*, based on SQL Server to help organizations from small workgroups to large enterprises collaborate and share information more effectively.

Knowledge Management with *E-Notebook*, including *Reaction Explorer*, *CombiChem*, *E-Signatures* for intellectual property protection and *21CFR11 Compliance*, streamlines daily record-keeping with rigorous security and efficient archiving.

Laboratory Informatics includes *Workflow LIMS* for instrumentation automation and *Compliant DB* for storage of your data.

Biological Informatics scientists use *BioDraw*, *BioAssay*, *BioSAR* and *BioViz* to set up biological models and visualize information, generate spreadsheets correlating structure and activity, search by structure, and draw and annotate pathways.

Chemical Informatics, including *Registration*, organizes new compound information. *Inventory* provides complete management of chemical and biological inventories including *GxP Validation*. *DocManager* indexes chemical structures in documents.

Manufacturing Informatics include *Inventory* to meet the chemical, reagent, sample and compound tracking needs of large multi-site chemical and pharmaceutical laboratories and *E-Notebook* for manufacturing compliance management.

Desktop Software includes *Chem & Bio Office*, a powerful suite of software, consisting of *ChemBioDraw*, *ChemBio3D*, *ChemFinder* and *ChemACX* for chemists, *BioDraw*, *BioAssay*, and *BioViz* and for biologists, and *Inventory* and *E-Notebook* for all.

Scientific Databases include the *ChemACX Database* of commercially available chemicals and *Sigma-Aldrich MSDS*. *The Merck Index* and other scientific databases provide information about chemicals, their properties, and reactions.

Professional Services include custom development, system deployment, educational training, and technical support for pharmaceutical, biotechnology, and chemical customers, including government and academia, by experienced staff.

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Naturwissenschaftliche Unternehmenslösungen
Solutions globales pour les sciences de la vie
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