CambridgeSoft Solutions
featuring
E-Notebook

Desktop Software Enterprise Solutions

Chemical & Biological Research Informatics

Laboratory, Development & Manufacturing Informatics

Knowledge Management Scientific Databases

CambridgeSoft
Life Science Enterprise Solutions
Naturwissenschaftliche Unternehmenslösungen
Solutions globales pour les sciences de la vie
ライフサイエンス・エンタープライズ・ソリューション
Innovation is an organizational must in pharmaceutical, biotechnology, and chemical industries.

Effective new ideas, developed through collaboration and communication, free from organizational boundaries, will determine your long-term success. In today’s connected world, information flow within organization can be overwhelming. Large amounts of data—some structured and some unstructured—can cloud an R&D organization’s ability to focus on what is important. Since 1986, CambridgeSoft has been solving the problem of electronic storage and communication of chemical structures, models, and information. Starting with ChemDraw, then broadening to ChemOffice in 1992 and BioOffice in 2004, CambridgeSoft extended its software to include enterprise-wide solutions with ChemOffice Enterprise in 1998, E-Notebook in 2000 and biology with BioAssay in 2001. Today, CambridgeSoft products are used by hundreds of thousands of chemists, biologists, scientists, and engineers who work in pharmaceutical, biotechnology, and chemical industries, including government and academic research. These systems work within your research, discovery, development, trials and manufacturing, and information technology to help you capitalize on your organization’s intellectual assets. By turning information into explicit knowledge, you accelerate innovation and drive organizations forward.

Chemists, biologists, scientists, and engineers need timely, convenient access to critical information, whether structured or unrefined. CambridgeSoft, which began by helping scientists manage desktop chemical and biological information with Chem & Bio Draw, now addresses enterprise-wide scientific information problems with Chem & Bio Office Enterprise and Workgroup. These solutions are flexible and powerful to deal with today’s complex projects which span functional organizations and geographical boundaries. Eliminating data barriers and bringing information to all—in the form they need to interpret it—aligns all of the members of your teams, focusing their collective knowledge and diverse skills toward the common goals of problem solving and innovation. The results can be dramatic:

- Information transparency and group collaboration improve productivity and reduce costs.
- Faster and smarter research decisions cut time to market and increase productive efforts.
- Empowered employees contribute increased value to the research, discovery, development, trials and manufacturing organization.

Outpace your competitors. As the speed of business continues to accelerate, leading organizations constantly seek faster and better informed decision-making as well as new business efficiencies. For the individual chemist, biologist, scientist, and engineer who needs to capture, organize, and communicate chemical and biological data, through the complex and widespread workgroup and enterprise scientific information systems needs, CambridgeSoft Solutions can help.
Research, Discovery, Development,

**KNOWLEDGE MANAGEMENT**

Research organizations thrive when information is easily captured, well organized and readily available. *E-Notebook Enterprise* streamlines record keeping with rigorous security and efficient archiving, and facilitates text and structure searching. *E-Notebook* provides organizations with a powerful mechanism to transfer mission critical work product from shared drives to a well-organized, compliant and searchable Oracle application. MS Office, chemical structures and workflow support modules are provided for the full range of research and development activities.

**LABORATORY INFORMATICS**

Laboratory Informatics includes *Workflow LIMS* for instrumentation automation, *Compliant DB* for storage of your data and the *Oracle Cartridge* which is the industry’s only enterprise content management system developed by a large pharmaceutical company.

**BIOLOGICAL INFORMATICS**

Finding structural determinants of biological activity requires processing masses of biological assay data. Scientists use *BioAssay Enterprise* and *BioSAR Enterprise* to set up biological models and visualize information. The *BioViz* application allows you to create graphical representations of data.

**CHEMICAL INFORMATICS**

Managing huge data streams is a key challenge. *Registration Enterprise* organizes information about new compounds according to an organization’s business rules.
Good research depends on reference information, starting with the structure-searchable ChemACX Database of commercially available chemicals and Sigma-Aldrich MSDS. The Merck Index and other scientific databases provide necessary background about chemicals, their properties, and reactions.

MANUFACTURING INFORMATICS
CambridgeSoft’s Inventory Enterprise application is designed to manage the chemical, reagent, sample and compound tracking needs of large multi-site chemical and pharmaceutical laboratories. Inventory Enterprise is an Oracle-based, ChemOffice Enterprise product that is designed for multiple users with diverse container types, racks, and multi-well plate formats.

DESKTOP SOFTWARE
Success begins at the desktop, where scientists use ChemOffice, ChemDraw, BioOffice and BioDraw to pursue ideas and communicate with the natural language of chemical structures, biological pathways, and models. Scientists organize information and manage data with E-Notebook and Inventory. ChemBio3D provides modeling, ChemBioFinder aids searching, while BioOffice adds BioDraw, BioAssay and BioViz. All are integrated with Microsoft Office to speed research tasks.

SCIENTIFIC DATABASES

PROFESSIONAL SERVICES
CambridgeSoft’s scientific staff has the industry experience and the chemical and biological knowledge to maximize the effectiveness of your information systems.
**Desktop to Enterprise**

Since the company’s founding, CambridgeSoft’s desktop software, starting with its industry-leading Chem & Bio Draw, has been the cornerstone application for scientists who draw and annotate molecules, reactions, and pathways. This suite of enterprise applications has developed and now provides solutions in virtually all areas of discovery.

**Research and Discovery**

Researchers can record and share their experimental information using E-Notebook, while protecting intellectual property with digital signatures and 21 CFR Part 11 compliance. They can design both single experiments or design combinatorial libraries of compounds. They can find and purchase reagents in ChemACX database, store and use them from Inventory, record newly made compounds within a proprietary Registration system, record the results in BioAssay, analyze the results with BioViz, and generate reports linking activity and structure with BioSAR.

Virtually every aspect of discovery, from synthesis planning, library enumeration, reagent selection, primary and secondary screening, in vivo testing, through to analysis of results and reporting is covered by this integrated application suite.

**Development and Testing**

Building on productivity software, CambridgeSoft created enterprise applications to meet the needs of an ever expanding research and development community that relies on data sharing across scientific disciplines, research campuses, and even oceans as globalization has increased demands. Since the software takes advantage of the latest web based technologies, it is deployed readily throughout a research and development organization. Using the integrated suite, scientific teams are well armed to solve the daily challenges of development. These teams include scientists who scale up and design manufacturing procedures, toxicologists who determine the metabolic fate of drug candidates, formulation scientists who determine drug dosing and delivery systems, as well as many others.

**Trials**

A suitable drug candidate is one that has the desired activity to provide disease therapy while meeting drug safety requirements, can be manufactured in a cost effective and reproducible fashion under 21 CFR Part 11 and Good Manufacturing Processes (GMP) guidelines, and is stable under normal formulation and storage conditions. With a drug candidate in hand, the final challenge is to determine safety and efficacy, beyond the laboratory in a patient population.
Manufacturing

Manufacturing requires the transfer of data and batch process records from the pilot plant studies using Inventory, E-Notebook, and Registration systems under Good Laboratory and Manufacturing Processes (GxP).

The handling of materials, including chain of custody requirements, material documentation, material workflow, such as availability states and recertification dates, are tracked and handled by the system.

These systems meet the requirements and provide the basis to manage materials and records during clinical trials. Clinicians can design and record results from protocols, and all of these web based software systems provide the access required by clinicians who are removed from the sponsoring company.

Chem & Bio Office Enterprise

Chem & Bio Office Enterprise is a comprehensive knowledge management and informatics solution, covering electronic notebooks, biological screening and chemical registration over your intranet. ChemBioOffice Enterprise Ultra includes E-Notebook for record keeping, BioAssay for low and high throughput screening with integrated plate inventory, BioSAR for SAR reports, Registration System, Inventory for reagents and biologicals, and ChemACX database of available chemicals. Technologies include ChemDraw ActiveX and Oracle Cartridge.

Chem & Bio Office Workgroup Ultra

Chem & Bio Office Workgroup Ultra is a comprehensive knowledge management and informatics solution, covering electronic notebooks, biological screening and more over your intranet.

Chem & Bio Office Workgroup Ultra includes E-Notebook for record keeping, BioAssay for low and high-throughput screening, BioViz for visualization, Inventory for reagents and ChemACX database of available chemicals. Technologies also include SQL Server for affordability and ease of administration.

Research, Discovery, Development, Trials & Manufacturing Workflow
**Overview & E-Notebook’s Flexible Architecture**

**E-Notebook**

Used for collaboration and knowledge sharing, regulatory compliance, intellectual property protection, LIMS, document management, project management, and workflow support, *E-Notebook* is the leader in a new class of applications. Configurable, multi-purpose, and enterprise-scalable, it provides a solution to a large set of requirements across R&D and manufacturing. *E-Notebook*'s foundation layer of features includes support for 21 CFR Part 11, 37 CFR and GxP compliance, on top of which a widely configurable design interface provides support for specific scientific and regulatory workflows. Because this diverse portfolio of requirements is met in a single application platform, *E-Notebook* both lowers the total investment required to meet these needs, and provides a substantial increase in productivity due to a far more integrated environment for scientists and technical staff.

**E-Notebook Architecture**

CambridgeSoft’s *E-Notebook* provides a comprehensive, easy-to-use interface designed to replace paper laboratory notebooks in a variety of settings. Underneath is a fully configurable, secure system for organizing the flow of information generated by your organization. Scientists can enter chemical reactions, Microsoft documents (Word, Excel, PowerPoint), spectra, biological data and images, and other types of information and documents. It also allows you to search by text, chemical substructure, metadata tags, organizational hierarchy, or other keys.

**E-Notebook Architecture**

*E-Notebook* Enterprise edition is a globally-deployable, Oracle-based application designed for everyone from small research groups to global organizations. Oracle Cartridge manages chemical structures and reactions in a common data repository, layered with detailed security and is 21CFR Part 11 Compliant (audit trails, digital signatures). The enterprise edition works with procurement databases and services including ChemACX database and Inventory management systems to save time locating chemicals and entering structures.

**Flexible and Configurable Architecture**

The *E-Notebook* architecture is designed to provide organizations with an unparalleled level of flexibility. A powerful configuration layer is provided to make it possible to modify substantially the look and feel of the application in order to meet very diverse workflows. Detailed workflow support in the same application is provided for researchers in early stage discovery through early clinical development even though the requirements for these groups are totally different. Beyond configuration, a rich API is provided for custom development and system integration.

*E-Notebook* is also in production with integrated inventory systems including CambridgeSoft’s Inventory manager, as well as in-house systems, analytical data capturing systems, and compound registration systems. *E-Notebook* supports limiting access to certain information at the project or group level if desired, as security is granular. Information can be shared or secured as desired throughout the framework.

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All specifications subject to change without notice.

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General R&D

CambridgeSoft’s E-Notebook is a solution that enables pharmaceutical and biotechnology companies to improve the efficiency of the process from diseased target identification to product launch. Its core Oracle database manages the workflow to be compliant with Good Laboratory Practices (GLP), Good Manufacturing Processes (GMP), and the FDA’s 21 CFR Part 11; while the client interface is highly configurable and flexible. Anywhere a shared drive is used, E-Notebook can offer a better solution.

Through the R&D process, using CambridgeSoft’s E-Notebook in each subsequent stage adds increasing scientific and economic value by providing workflow automation and knowledge sharing.

Research and Discovery

E-Notebook Enterprise is capable of providing knowledge management, chemical- and biological-focused solutions in virtually all areas of discovery. Researchers can record and share their experimental information, while protecting intellectual property with digital signatures and 21 CFR Part 11 and 37 CFR compliance.

- Chem & Bio Draw—draw and annotate molecules, reactions, and biological pathways
- ChemACX—find and purchase reagents
- Inventory—store and track reagents and samples
- Registration—record newly made compounds
- BioAssay—model complex protocols and record results from biological testing
- BioSAR—generate reports linking activity with structure
- BioViz—analyze biological results

Virtually every aspect of discovery—from synthesis planning, library enumeration, reagent selection, primary and secondary screening, *in vivo* testing, through to analysis of results and the reporting of data—is covered by the integrated E-Notebook solution.

Developed and Testing

CambridgeSoft’s Enterprise E-Notebook meets the needs of ever expanding research and development communities that rely on data sharing across scientific disciplines and campuses as globalization has increased demands.

E-Notebook allows custom integration of a large array of modules, in-house applications, lab instruments, and end-end data storage to provide a true end-to-end solution for development and testing. Designing workflows and calculations is much faster and requires far less programming using the E-Notebook than existing lab information systems. End users include scientists and process chemists who scale up and design manufacturing procedures, toxicologists who determine the metabolic fate of drug candidates, formulation scientists who determine drug dosing and delivery systems, as well as many others.

Trials and Manufacturing

A suitable drug candidate has the desired activity to provide disease therapy while still meeting safety requirements, can be manufactured in a cost effective fashion under 21 CFR Part 11 and GMP guidelines, and is stable under normal formulation and storage conditions. The handling of materials, including chain of custody requirements, material documentation, material workflow, such as availability states and recertification dates, are tracked and handled by the E-Notebook application. CambridgeSoft’s E-Notebook meets these requirements under Good Laboratory and Manufacturing Processes (GxP) and provides the basis to manage materials and records during clinical trials.
Chemistry

Under the R&D value chain, chemistry can be further divided into three separate stages: synthetic chemistry (research/discovery), analytical chemistry (pre-clinical) and process chemistry (development). The flexibility and configurability of E-Notebook enables a successful data repository, analysis, sharing, reporting, and searching efficiently and paper-free.

Synthetic Chemistry

Synthetic Chemists take advantage of many features tied into a smooth interface within CambridgeSoft’s Enterprise E-Notebook. Reactions are drawn with in-place editing; a stoichiometry grid dynamically fills with the formulas, molecular weights, and chemical names. Reagents can also be imported from other systems, such as available chemicals from the ChemACX database or Registration system.

CombiChem is one important aspect of library generation for Synthetic Chemists. For some, E-Notebook serves as the complete CombiChem solution, taking advantage of features such as the enumeration of products from a virtual library on a flexible plate layout, a multiple reaction site checker, and multiple step parallel synthesis. Others simply import a list of compounds from an external source or SDFile so that they can record and calculate data on a library-wide stoichiometric table.

Analytical Chemistry

E-Notebook serves as a repository for analytical data, and it also acts as a communication portal with which scientists and analysts communicate with each other. Scientists can create and send service requests directly to an analyst with the click of a button. Paper is eliminated: when results are obtained, the analyst can send the images and chromatograms directly back to the scientist’s E-Notebook.

Process Chemistry

The objective of process research is to identify efficient processes for the synthesis of active pharmaceutical agents at the scale required for clinical trials and commercial use. It is necessary to provide precise descriptions of these processes so that they can be executed by different groups in different locations. It is also required that such processes be compliant with Good Laboratory Practices (GLP), Good Manufacturing Processes (GMP) and the FDA’s 21 CFR Part 11 regulation. E-Notebook’s process chemistry modules are designed to support these dual workflow and regulatory compliance needs of process chemists.
**Discovery Biology**

These scientists are involved at the very start of the drug discovery process, as genomics and genetics are essential disciplines used when identifying a disease target. This work is methodical but unscripted, and so requires an electronic notebook pallet that is as free form as its paper predecessor. This is where the benefit of E-Notebook’s flexibility is unmistakable. While the system can be set up with rigid form based data entry appropriate for later stage research and development, discovery biology configurations are typically open and boundless. Genomic map and DNA, RNA and protein sequence files can be dragged-and-dropped into E-Notebook, sequencing results can be sent directly from instruments to electronic experiments, and protocols and data can be managed with familiar tools such as Microsoft Word and Excel.

The beauty of capturing data in E-Notebook is that information can be compiled and viewed in a meaningful way. For example, the creation of a new biological strain entails many steps, potentially involving nonconsecutive workdays of various individuals. E-Notebook can generate customized reports that meaningfully summarize the process in real time. These reports are navigable—clicking on each step will bring you to the corresponding experiment.

**Assay & Screening Biology**

One of E-Notebook’s strengths is its ability to integrate with existing electronic methods of data capture, including using it with CambridgeSoft’s BioAssay module to provide full screening experimental support. In addition to this, Microsoft Word and Excel are also embedded directly in E-Notebook, as is image and movie capture. Scientists benefit from the functionality of these tools implanted in a rich, searchable environment. Biological experiments can be managed and organized in a way that is not possible with a traditional file system.

**In vivo Experiments/Animal Management**

In vivo experiments are important aspects of target discovery and validation, and are critical paths to determine the efficacy of selective therapeutic candidates. CambridgeSoft’s E-Notebook becomes the centralized location to collect, store and interpret in vivo experiment results. Again, when used with BioAssay, the full end-to-end experimental workflow is supported, from creation, to data analysis and quality control, to summary and reporting. In conjunction with in vivo experiments, animal housing and breeding can also be tracked. Traditionally, the workflow consists of paper-based record keeping across the animal facility, lab bench, and researchers desktop. With E-Notebook, paper tracking and recording is eliminated. Instead, form tools can be designed to:

- Track animal status
- Track animal pedigree
- Record Genotype
- Create mating records
- Create litter records
- Track experimental data

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**Database Structure**

All specifications subject to change without notice.

**Chemical Synthesis, Scale-up and Analytical**

**DMPK, Screening Biology, Genetics, and Microscopy**

**LIMS, Method Execution, 21 CFR Part 11, and GxP**
Formulation and Validation

*E-Notebook’s* formulation module is designed to support the dual workflows and regulatory compliance needs of formulation engineers. The flexibility allows any number of formulations to be created, and security allows only designated administrators to create a new formulation.

**Analytical & Quality Control**

Analytical and Quality Control Laboratories must execute defined procedures to test material that may be administered during preclinical and clinical trials. This work must also be compliant with both GxP and 21 CFR Part 11. Templates for standard analytical tests are provided and analytical procedures are implemented as *E-Notebook* forms, which are easily designed and controlled. Equally important, *E-Notebook* provides workflow enforcement that monitors data entry and ensures that the forms are completed in sequence for proper method execution.

For example, rules can be configured such that the ‘Day 3’ form of a multi-day process will not accept any entries unless all required fields on the ‘Day 2’ form are first completed. The forms can contain automatic calculations to compute totals, averages, differences, and much more. *E-Notebook* can further streamline the procedure by allowing for electronic management of solutions, equipment, and other resources that are needed for experiments.

**Drug Metabolism**

*E-Notebook* supports the DMPK laboratories in testing the metabolism and longevity of compounds in various *in vitro* and *in vivo* models. DMPK data capture needs can vary significantly, and the flexibility of the *E-Notebook* solution addresses this. For example, an *in vivo* enzyme induction test may create relatively small amounts of data for which scientists utilize *E-Notebook* integration with Microsoft Excel. Conversely, large quantities of data, such as those generated by *in vitro* enzyme inhibition studies, are often collected and analyzed by applications such as BioAssay. Therefore, integration with BioAssay and Excel are fundamental to DMPK *E-Notebook* usage.

**Pharmacokinetics (DMPK)**

There is a holistic approach to Drug Metabolism and Pharmacokinetics. No single study describes the behavior of a compound; it is the combination of data from disparate experiments that represents the pharmacological profile for a compound. It is here where *E-Notebook* reveals one of its most significant capabilities: the reporting feature. *E-Notebook* reports are flexible: any field (e.g. compound ID, study type, etc.) can be used to query the system and any field (e.g. conclusion, dose, etc.) or field aggregate (e.g. average radioactivity) can be displayed in the report. Reports are dynamic and navigable: results are displayed with links that provide quick access to experiments.

Reports are viewed directly in the *E-Notebook* interface, but they can also be exported to Microsoft Word or PDF to share with those who do not have *E-Notebook* access.
Drug Safety / Toxicology

Paper notebooks have traditionally been considered to be the record source for the entirety of an experiment, but they often miss non-experimental information generated shortly after conception. For example, toxicity studies are often initiated not by the scientist who ultimately runs the experiment, but instead by a manager or coordinator who assigns the study to the scientist. Important material related to this first step in the process, such as ideas, emails, and other communications are often left out of traditional paper notebooks. The E-Notebook toxicology workflow addresses this concern: studies are first created by a manager, and subsequently assigned to the scientist for execution.

Compliance Execution

E-Notebook is also useful for capturing the Standard Operating Procedure (SOP) corresponding to the experiment. These documents are often stored separately from the actual data, leading to error and confusion, thus causing risk to the validity of the data. Storing and displaying procedures and other related documents in concert with the data eliminates this risk and helps build perspective on the study.

Sample Lifecycle Management

E-Notebook can manage the entire sample lifecycle through tight integration with Inventory. Sample lifecycle management is essential for the registration, testing, evaluation, and reporting in various analytical and manufacturing stages. Manual tracking of samples and test results is labor-intensive and time-consuming; and compliance with GxP guidelines requires expensive manual audits.

The controlled flexibility of CambridgeSoft’s E-Notebook is well suited for these detail and compliance-oriented environments. E-Notebook’s Sample Lifecycle Management module is compliant with Good Laboratory Practices (GLP), Good Manufacturing Processes (GMP) and 21 CFR Part 11.

Sample Login

E-Notebook is able to easily configure sample logins (registration of sample, assignment of barcode label, and initiation of sample tracking) by incorporating CambridgeSoft’s Inventory application. Through E-Notebook, forms can be created to keep track of newly synthesized or acquired compounds, tracking their physical properties and tests, and assigning unique identifiers. New compounds are entered directly via the E-Notebook form, and chemical, along with non-chemical, data is kept alongside the sample. When a proprietary compound is registered, if desired, it is compared for uniqueness via a configurable, stereoselective duplicate check and assigned a registry number.

Sample Tracking

Tracking samples, requesting analysis and establishing chain of custody can all be simply managed within the E-Notebook interface. E-Notebook serves as a repository for analytical data and experiments, linking such data directly to the sample ID, and it acts as a communication portal with which scientists and analysts communicate with each other during the service request lifecycle. Scientists create and send service requests directly to an analyst with the click of a button. Paper is eliminated: when results are obtained, the analyst can send the images and chromatograms directly back to the scientist’s E-Notebook (which appear in the person’s E-Notebook inbox, and are then accepted into the experiment if desired). To establish chain of custody, each step of sample ownership is tracked, recorded and made compliant with FDA’s 21 CFR Part 11.
Workflow LIMS Automation

CambridgeSoft’s Workflow LIMS is a scientific data and workflow management tool for lab automation and in silico experimentation. Workflow LIMS eliminates the need for custom programming by providing a visual experiment design and workflow layout with built-in laboratory automation and analytics.

By using Workflow LIMS, researchers can connect their laboratory processes, instruments, and decision points in a conceptual manner that directly couples to instrumentation—for both automation and data gathering—and provide real-time results. The Workflow LIMS solution enables a scientific team to design procedures, execute those procedures, capture the results and integrate lab equipment to automate part or all of the process. Procedures typically revolve around lab activities, but may also draw in decision support tools on a scientist’s desktop, and queries/updates to databases.

Interactivity and Integrity

1. The modeling environment, Workshop Configuration Editor, in which the scientific team models the capabilities of the lab—for example, the kind of basic processes which are available in the lab, and their inputs and outputs.
2. The design environment, Workbench, in which researchers create workflows from these basic processes.
3. The runtime Operations Manager, which manages the assignment of tasks to agents, tracks the progress of tasks and workflows, and manages the storage of captured data.
4. The agent tier, made up of a number of applications that handle specific types of task, either manually (through a user interface), or automatically (by driving equipment through a control interface or performing automated data processing).
5. The monitoring tier consists of a reporting tool that provides historical utilization information, and a live activity viewer that allows scientists to drill into individual workflows and samples.

Applied Technologies and Benefits

Workflow management enables discovery teams to rapidly trial new procedures, capture best practices and scale successful designs from a manual prototype right up to a fully automated high-throughput lab. But discovery and research, by its very nature, demands that processes be flexible and that workflow execution rapidly adapt to new techniques and equipment.

Conventional laboratory information workflow applications cannot meet this requirement because of their heavyweight configuration needs, their lack of adaptability and the cost and complexity of integrating them with rapidly changing lab technology. Workflow LIMS addresses these problems by providing a visual, easy-to-use environment for describing processes and building workflows out of those processes, enabling scientists to rapidly trial new procedures, and by offering a rapid development tool kit for equipment integration which supports gradual automation to minimize up-front costs and ongoing risk.

CambridgeSoft’s Workflow LIMS simplifies even manual lab procedures by managing the breakdown of a procedure into tasks, and by automating the majority of data capture and transfer tasks; but by capturing process as well as data, Pathways reduces the costs and risks of implementing discovery techniques, and enables companies to accelerate the entire discovery process.
Compliant DB

CambridgeSoft’s Compliant DB is the industry’s enterprise content management system developed by a large pharmaceutical company. It serves as an electronic library that collects, organizes, warehouses, indexes and safely archives all your structured and unstructured electronic records. From raw data and laboratory reports to compliance records, Compliant DB also will support any of CambridgeSoft’s workflow solutions, including E-Notebook, BioAssay, and Inventory. As its name implies, Compliant DB is fully compliant with the requirements of 21 CFR Part 11 for electronic records and electronic signatures.

Compliant DB can be used directly over your company’s intranet, extranet, or over the Internet with a simple web browser. Compliant DB gives your organization a secure, 21 CFR Part 11 compliant centralized electronic library for all electronic data files. Not only can machine-readable instrument data files be stored, but also images, multimedia files, presentations, human-readable word processing and Adobe PDF documents, spreadsheets and hundreds of other formats. This data can serve as source data (instrument data to BioAssay), and also repository (for signed E-Notebook experimental records). Although Compliant DB can operate as a stand-alone application, only CambridgeSoft provides fully-integrated Knowledge Management and Enterprise Informatics applications integrated with compliant storage. Compliant DB makes this possible.

Oracle Cartridge

The CambridgeSoft Oracle Cartridge is used by all ChemOffice Enterprise applications for storing, searching, and analyzing chemical data. It can also be used in the development of your custom Oracle applications. Chemical structure and reaction data is difficult to manipulate without utilizing special software, and Oracle data cartridges define new, recognized data types. CambridgeSoft’s Oracle Cartridge utilizes this technology, making it possible to manipulate chemical structure and reaction data from within Oracle, improving portability and consistency in applications. Since the Oracle Cartridge is accessed through native Oracle SQL, programmers can interact with chemical structure data directly in the database.

The CambridgeSoft Oracle Cartridge supports CDX, CDXML, MolFile, MolFile v.3000, RXN and SMILES formats, making it flexible enough to be included with both new and legacy data applications, without the need for file conversion. Chemical information can originate from either ChemDraw or ISIS Draw, E-Notebook, Inventory, or Registration. Oracle Cartridge has extensive support for stereochemistry, relative stereochemistry, tautomers and structure normalization. There is also a built-in structure enumerator (for nonspecific structures), basic property predictors, nomenclature algorithms (name=struct), and dynamic utilities for molecular file format conversions.
**BioAssay**

For modeling complicated *in vivo* experiments, or supporting an ultra-HTS platform, *BioAssay* has become the leading choice for managing biological experimental data. It is the only application of its kind to provide a best-of-breed solution for both ultra-high volume laboratories and lower-throughput settings. *BioAssay* includes support for laboratory automation, calculation, and statistics, and also complicated low and medium throughput assays such as animal models and *in vivo* experiments.

*BioAssay* is designed to tackle the needs of high and low throughput screening biologists alike by providing an application flexible enough to model any assay, regardless of complexity, through an easy-to-use interface for importing, storing and analyzing the data. The software supports the quick set-up of biological models, automated calculations and curve fitting, data validation, and the creation of customized structure activity reports.

**BioAssay Extends E-Notebook**

*BioAssay* Enterprise is a scalable, flexible biological screening solution utilizing Oracle’s role based security and the Oracle Cartridge. When used as part of *ChemOffice* Enterprise, *BioAssay* is integrated with *E-Notebook* for experimental data, *Inventory* Enterprise for plate tracking and management, *Registration* Enterprise for the registration of new compounds and *BioSAR* Enterprise for customized reporting.

*BioAssay Ultra* is designed to deliver much of the functionality of our enterprise level applications, without a widespread roll-out. *BioAssay Ultra*, coupled with *BioViz*, offers a user friendly interface for importing, viewing, validating, and plotting your biological assay data from your desktop.

- *BioAssay* effectively manages data from complex biological assays involved with lead optimization.
- *BioViz* integrates with *BioSAR* for one step in-depth data analysis from a *BioSAR* report.

**BioDraw**

Diagramming and presenting cellular pathways is made easier and more effective with *BioDraw*. Formerly called Pathworks, *BioDraw* does for biologists what *ChemDraw* has done for chemists—saving time and producing a more professional representation of the science.

*BioDraw* makes drawing and annotating biological pathways quick and easy, adding a level of uniformity and detail which is unmatched. Common pathway elements such as membranes, enzymes, receptors, DNA and reaction arrows are built into the *BioDraw* toolbar. *BioDraw* also allows the import of images in GIF, PNG or JPEG formats. *BioDraw* offers many ways to share your drawings and accompanying data. Users can export data to Microsoft Office applications for inclusion in presentations and grant proposals or save data as an image file for use in journal article submission.
BioSAR & BioDraw
Data Mining and Pathway Drawing

BioSAR

BioSAR Enterprise, a strategic must for any discovery organization interested in serious data mining, is a data dictionary driven structure-activity analysis program. Users may choose among assays registered in the dictionary or search for assays of interest.

The power of BioSAR lies in the researcher’s freedom from dependence on IT support for dynamically working with all available scientific data. For example, once an assay is registered into the data-dictionary, it is automatically included in the powerful analysis framework. By reducing the time between question and answer, BioSAR gives researchers the ability to explore new ideas and avoids this issue by placing SAR report creation in the researcher’s control.

BioSAR Enterprise allows the researcher to create custom reports and views of their data. You decide what is displayed, and BioSAR takes care of the rest.

While most SAR tools provide only a table-based interface, BioSAR provides both a form view and table view, and connects to BioViz for high-dimensional analysis. BioSAR merges the sophistication of a powerful data catalog technique with knowledge gained through years of working closely with scientist users. The result is a SAR application that is as intuitive as it is powerful. Security within BioSAR Enterprise is highly granular; different roles exist for administrators, publishers, and browsers.

Administrators may add assays to the data catalog engine, publishers may create reports and publish them, and browsers may use data query and analysis. Most data mining tools provide a mechanism to store queries, but the interface for creating queries is too complex. With BioSAR, each set of assays is a complete report with a query form, a view form, and a table view, combining the convenience of a ChemFinder or ISIS application with the power and flexibility of a data catalog-driven mining program.

• BioSAR is a catalog driven mining and structure-activity analysis program
• BioSAR provides both form and table views within a simple and powerful web interface
• BioViz provides one-step in-depth analysis of several variables

• BioSAR is a catalog driven data-mining and structure activity analysis program.
• BioSAR provides both form and table views within a simple and powerful web interface.
• BioDraw makes it easy to draw and annotate biological pathways including common elements such as membranes, enzymes, receptors and DNA.

BioViz

BioViz with ChemFinder transforms the numbers in your database into graphics on your screen. Retrieve or search for a set of compounds, choose the data you want to see, whether it is biological test results in Oracle tables, physical property values calculated automatically or prices in a catalog, and BioViz will generate an interactive window showing a scatterplot, histogram, or other useful data graphic.

The Plot Window, the key to data visualization in BioViz, is able to show two variables plotted against each other in a scatterplot with each point representing a structure from the current hit list. If you, for example, modify the list by performing a search, the plot updates to show the new set of points. You can drag a rectangle around a set of points to select them or zoom in to see them more closely.
Chemicals and Biologicals

Inventory is an application designed to manage the chemical and biological reagent tracking needs of laboratories and research centers in multiple contexts: lab reagents, freezers/racks, plate management, proprietary compounds and stockroom are just some of the areas where Inventory has been deployed.

The system manages data associated with both commercially procured and internally produced chemical substances from procurement or initial production through depletion and disposal. Inventory Enterprise is an Oracle-based ChemOffice Enterprise product and can be used with other modules, such as E-Notebook, to track batch records in manufacturing, or to look up reagents from stockroom when planning a synthesis, BioAssay when supporting a high throughput screening environment, Registration for tracking proprietary compounds, DocManager for linking certificates of analyzes, analytical reports, or other documents associated with samples, and ChemACX available chemicals database for sourcing new compounds.

Inventory Enterprise includes plate handling and interfaces to liquid handlers for HTS environments, freezer/rack layout and targeting for managing biologicals, full chain of custody, audit trails for GxP compliance, request/disbursement workflow for use in both manufacturing and pre-clinical settings, and features tailored to specific material domains.

- Reagent handling and stockroom reporting
- Request/disbursement workflow for stockroom and GxP environments
- EH&S module, and links for MSDS data sheets
- Freezer/rack layout for biological materials
- Extensive plate handling for HTS and uHTS settings
- Full Oracle SDK for system integration and extensions

Inventory is also available in two other editions: Workgroup and Desktop. Inventory Workgroup is a rich-client SQL Server-based product geared at managing stockrooms and reagents. Inventory Ultra is a desktop edition based on the Workgroup product, and includes the ChemACX database.

Registration Enterprise

Registration Enterprise is built around robust data model for pure compounds, batches, salt management, automatic duplicate checking and unique ID assignments. Built on the Oracle Cartridge, it handles stereochemistry (including advances in relative stereochemistry), tautomerization and structure normalization for duplicate checking. Using ChemScript, it also can enforce drawing business rules, such as orientation around a scaffold and functional group normalization. Compounds may be entered individually through a user-friendly web form, or directly from a batch loader, from Inventory, or directly from E-Notebook.

As compounds are registered, regardless of whether through the web user interface, E-Notebook, or from a batch file, they are compared for uniqueness via a configurable, stereoselective duplicate check, and assigned a registry number. All information about the compound, including its test data and other syntheses, is tracked by the registry number, and this is used to link data throughout ChemOffice Enterprise. Registration Enterprise is the only true n-tiered application of its kind that is designed around thin clients and thin servers, with interfaces directly to Inventory, batch file registration and E-Notebook. Oracle is supported on a variety of platforms and operating systems. Using Oracle secures your proprietary data through the use of Oracle's role-based security and allows all chemical and non-chemical data to be stored directly in the Oracle tables.
DocManager & ChemFinder
GxP, Registration and Enterprise Infrastructure

Formulations & Mixtures
Formulation scientists face different challenges from those working with individual molecules, yet many of the tools they are forced to use emerge from the drug discovery world, where single-molecule research is the norm. Take an essential task such as compound registration and you will find that most systems are designed for registration of single molecules, with little thought for the world of formulations and mixtures. CambridgeSoft has developed a system specifically designed for this registration need called Formulations & Mixtures.

ChemFinder Enterprise
ChemFinder Enterprise is a multiple-user system designed for sites with comprehensive chemical and biological data needs. ChemFinder Enterprise contains its own engine for working with local and shared databases, and it is also delivered with the CambridgeSoft Oracle Cartridge, the powerful Oracle-hosted structure engine based on ChemFinder search technology. The face of ChemFinder Enterprise is the same friendly form-oriented interface as the desktop version, but underneath is a fast direct connection to Oracle and the robust, scalable Oracle Cartridge running on the server.

DocManager Enterprise
- DocManager parses Word, Excel and PowerPoint documents, including free text and structures
- ChemFinder is tightly integrated with BioSAR, BioViz and Oracle
- Support for advanced form layout and design

Web browser based, DocManager Enterprise extends the capability of standard search engines to include full free text searching and chemically intelligent structure searching of electronic documents including Text, Microsoft Word, Excel, PowerPoint, and Adobe PDF. The DocManager Enterprise interface allows users to easily submit documents through a series of simple-to-navigate web forms. When a new document is submitted, DocManager builds a free text index of the document, and extracts chemical information into a chemically-aware, substructure searchable database. Chemical information can originate from either ChemDraw or ISIS Draw.

DocManager Enterprise includes a batch loading utility for administration level users to load multiple documents at one time. The system can be configured to submit a batch of documents as one event, or as a reoccurring submission to be executed daily. The administrator specifies a time for the submission to take place and the location of the files. DocManager Enterprise utilizes the searching intelligence of the ChemOffice Enterprise suite.
Inventory Enterprise

CambridgeSoft’s Inventory Enterprise application is designed to manage the chemical, reagent, sample and compound tracking needs of large multi-site chemical and pharmaceutical laboratories. Inventory Enterprise is an Oracle-based, ChemOffice Enterprise product that is designed for multiple users with diverse container types, racks and multi-well plate formats.

Entities in the Inventory system include locations, containers and substances. A location is defined as any physical location where a container, plate or another location can be stored. An inventory container represents a container capable of storing chemical substances. An inventory substance represents a chemical compound, mixture, sample, etc. Inventory Enterprise manages an unlimited number of diverse locations, containers and substances.

Containers are created to represent the actual storage vessels used by the organization. Each container is assigned a unique barcode identifier which can be printed, using customizable report templates, from the Inventory interface. Updating the inventory becomes as easy as scanning barcodes into the system and adjusting parameters for one or multiple containers. Users are able to order, check-in/out, move, split and merge containers at will. Typical containers include: bottles, vials, tubes, cylinders, boxes, racks, multi-well plates, etc.

Multi-well Plates

Inventory Enterprise manages multi-well plate information. In addition to creating, storing, moving and deleting plates, the application allows users to create daughter plates, reformat plates and utilize plate maps. Inventory also supports user-interfaces or machine-interfaces for these operations (including reading files from liquid handler robots). Inventory Enterprise has the capability to import datafiles from other computer systems such as liquid dispensershandlers, Microsoft Excel spreadsheets, etc. to accommodate automated updating of information in the Inventory database.

Reference Standards, Regulated Materials Management,

- Request/Dispense/Reference Standard Materials from Central Group to Sites
- Certification/Expiration/Certificate of Analysis of Containers and Aliquots
- Create/Manage Container History and Genealogy

Searching

Every field in a record is searchable. The application includes a number of specially designed inventory search forms. Search results are returned in list form and can be exported into a document (PDF, RTF, HTML) via the report engine.

Workflow Support

Supported user transactions include the ability to request, dispense, modify, duplicate, dispose, etc. entities throughout the system. These and other transactions are an integral part of Inventory workflows.

For example: a user logs-on, finds the substance(s) they’d like to request and makes a request entry in the system; the request is fulfilled directly by changing the location the substance or by taking an aliquot and creating a new container of the substance. The new substance/container is also tracked in the system and inherits all of the critical properties of its parent container. If a quality control test is run on the parent, then the results are viewable in the daughter’s properties.

The multi-select capability allows the user to select several containers and perform a transaction on all of the selected containers simultaneously, including check-in/out, move, retire, delete and update. For instance, if a request is made of the system that is fulfilled by another user (such as dispensing), the requester can automatically receive e-mail notification of the progress. Likewise, users can be alerted to pending requests in the system.
Conflict Resolution

The Conflict Resolution processes flags and corrects duplicates in the system automatically. You may also search for duplicates at any time. If a conflict is found, the screen identifies the conflicting field(s) by highlighting it in red. The user has the option to select the existing substance and edit the conflicting substance or create a duplicate substance and resolve the conflict later.

Printed Reports & Labels

The Inventory interface allows for printing labels and can generate elaborate reports. Inventory Desktop and Workgroup use a report engine that incorporates wizards that allow for the quick creation of simple report/label templates that can be shared across an organization. A user has the ability to design a label based on templates for a number of commercially available label sheets (e.g. Avery Dennison). The Inventory manager makes extensive use of barcodes and web-based user interfaces to speed use, but substantial gains come in the automated reporting and alerting. Examples include notifying all users of samples derived from a single standard of some change in status, such as different analytical results or failure to recertify.

Electronic Data Files

In addition to storing, moving and disposing containers, the application allows users to reformat plates and create daughter plates as well as integrate with liquid dispensers/handlers for plate reformatting from pipette log files.

Compliance

Handling FDA regulations in an organization is an area that lends itself to automation. Thus, systems must be carefully implemented in order to meet the letter and spirit of FDA guidelines. Underlying the system are the controls expected by systems in regulated environments: audit tables, security and validated development methods. All transactions on all containers in the system are tracked and audit reports are customizable for simple presentation.

Document Management

To manage the myriad of documents that get generated in research and regulated environments, CambridgeSoft stores documents securely in Oracle where they are indexed (by chemistry and text) and managed by database security. Storing the associated documents in Oracle preserves system integrity such that you can backup to a known point, and be assured that the documents and data are entirely in sync with each other. It also provides tight document security, reduces IT overhead associated with file shares and attaches directly to Inventory containers.
# Desktop

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## Databases

| *ChemACX Ultra (1 Year)* | Win/Mac | | | | | | | | | | | | | | |
| *ChemINDEX Ultra | Win | | | | | | | | | | | | | |
| ChemRXN, NCI & AIDS | Win | | | | | | | | | | | | |

*Available Separately

All specifications subject to change without notice.

Chem & Bio Draw includes Struct-Name, ChemDraw/Excel and ChemNMR, BioDraw, a biological sequence tool, hotlinks to 3D structures, Stoichiometry grid, live linked chemical property calculations, a TLC plate tool and more. The ChemDraw ActiveX/Plugin adds chemical intelligence to your browser for querying databases and displaying information.

ChemBio3D provides state-of-the-art visualization and display of protein structures, molecular surfaces, molecular orbitals, electrostatic potentials, charge densities and spin densities. Chem3D provides basic computational tools such as 3D Molecular Overlay and Dihedral Driver and utilizes MOPAC, Jaguar, Gaussian, GAMESS and extended Hückel to compute molecular properties. ChemProp computes Connolly surface areas, molecular volumes and properties, including ClogP, molar refractivity, critical temperature and pressure.


BioDraw provides support for biological pathway drawing and annotation. A wide variety of customizable drawing tools are available, including membranes, DNA, enzymes, receptors, tRNA, ribosomes, and a plasmid map tool.

BioAssay manages both high and low throughput biological screening data. Designed for complex lead optimization experiments, the software supports the quick set-up of biological models.

BioViz offers automated statistical analysis, curve fitting, and customized structure activity reports, including a user-friendly interface for importing, viewing, validating and plotting chemical and biological data.

Inventory manages your reagent and biological tracking needs. Using MSDE as the desktop database, you organize, store and search over your inventory. Inventory integrates with the ChemACX database of available chemicals and ChemMSDX database of safety data for commonly used laboratory chemicals.

E-Notebook is an efficient, accurate way to write notebooks. It stores Microsoft Office documents, ChemDraw structures and reaction drawings, and related data in a notebook searchable by text or chemical structure. Organize pages by project, experiment or in your own style. Use CombiChem/Excel to build libraries.

Databases include ChemINDEX, including the NCI and AIDS databases. The ChemACX database contains nearly 400 catalogs from leading suppliers and ChemMSDX Database contains over 20,000 material safety data sheets for commonly used laboratory chemicals.
ChemDraw, Chem3D, Structure Drawing and Molecular Modeling


ChemDraw Ultra adds Struct=Name, ChemDraw/Excel, ChemNMR, Stoichiometry Grid, CLogP, tPSA as well as the added capabilities of Chem3D Pro and ChemFinder Std to the ChemDraw Pro application. With rich polymer notation, generic structure expansion, fragmentation tools, and a modern user interface, ChemDraw is more powerful than ever before. Create tables of structures, identify and label stereochemistry, estimate NMR spectra from ChemDraw structures, obtain structures from chemical names, assign names from structures, and create multi-page documents and posters.

ChemDraw Pro will boost your productivity more than ever. Draw quality publications with structures, reactions, chemical queries, polymers, relative stereochemistry, generic structures, TLC plate depictions and a biological sequence tool. Publish on the web using the ChemDraw Plug-in. Create precise database queries by specifying atom and bond properties and stereochemistry. Display spectra, structures and annotations on the same page.

Struct=Name contains the leading comprehensive methods for converting chemical structures into chemical names and names to structures. It can be used for many types of compounds, including charged compounds and salts, highly symmetric structures and many other types of inorganic and organometallics. Struct=Name is available in two forms: a batch application, and an interactive version that is also available in ChemDraw Ultra.

ChemDraw’s improved Struct=Name feature produces names for more types of compounds.

Live ChemDraw window embedded in Chem3D application allows simultaneous 2D and 3D editing.

Chem3D brings workstation-quality molecular graphics and rigorous computational methods to your desktop.

ChemDraw/Excel allows the user to create chemically knowledgeable spreadsheets within the familiar Microsoft Excel environment. You can build and manipulate chemical structures, compute chemical properties and perform database searches.

ChemNMR can be used to accurately estimate 13C and 1H chemical shifts. The structure and the spectrum appear with the chemical shifts displayed on the molecule and the spectrum is linked to the structure so that clicking on a peak in the spectrum highlights the corresponding fragment on the molecule.

ChemBio3D Ultra includes visualization and molecular modeling capabilities for both small molecules and protein structures designed for the bench chemist. Small molecule computational methods include Molecular Overlay and Dihedral Driver. It also includes interfaces to the MOPAC, Jaguar, Gaussian and GAMESS semi-empirical and ab initio computational packages. High quality Chem3D graphics can be viewed on the web using the Chem3D ActiveX.

Chem3D Pro brings workstation quality molecular visualization and display to your desktop. Convert ChemDraw and ISIS/Draw sketches into 3D models. View molecular surfaces, orbitals, electrostatic potentials, charge densities and spin densities. Use built-in extended Hückel to compute partial atomic charges. Use MM2 to perform rapid energy minimization and molecular dynamics simulations. Chem3D can also be used to estimate physical properties such as logP, boiling point, melting point and more. Visualize Connolly surface areas and molecular volumes.

**ChemFinder & ChemInfo**

**Structure Searching and Scientific Databases**

**ChemFinder Ultra** is a chemically intelligent database management and search system designed for chemical and biological data. *ChemFinder Ultra* can be used with local (MSDE) or shared (Oracle) databases. Either way, the face of *ChemFinder* is the same friendly form-oriented interface. *BioViz*, included in *ChemFinder Ultra*, provides data visualization features to help the user understand relationships between biological data and chemical structures. These features allow you to plot structural and biological data in a variety of styles, perform statistical analysis, filter plots based on your criteria, highlight lists and intersecting sets on plots, generate histograms of data distributions, and more.

*BioViz*, included in *ChemFinder Ultra*, provides statistical analysis and visualization tools for structural and biological data. *BioViz* transforms *ChemFinder* database information into easy to understand graphics, allowing users to discern structure-activity relationships more easily. With *BioViz* it is easy to retrieve a set of compounds using filters or searching capabilities; and generate an interactive window showing a wide variety of useful graphical information.

**ChemFinder Pro** is a fast, chemically intelligent, relational database search engine for the Desktop. The integration with Microsoft Excel and Word adds chemical searching and database capability to spreadsheets and documents. Compatibility with MDL ISIS databases is provided by SDfile and RDfile import/export.

**ChemACX Database** includes over 1 million chemical products available for purchase from 472 supplier catalogs, searchable with a single query by structure, substructure, name, synonym, partial name, and other text and numeric criteria.

**ChemMSDX Database** provides material safety datasheets and is integrated into *ChemACX*, and contains over 23,000 Material Safety Data Sheets (MSDS) in PDF format.

**ChemINDEX Database** includes 100,000 chemicals, public NCI compounds, AIDS data and more.

**NCI Database** contains over 200,000 compounds with anti-cancer drug dose-response data.

**AIDS Database** is an NCI compiled database for AIDS anti-viral compounds.

**ChemRXN Database** is a collection of 30,000 fully atom-mapped reactions selected and refined from chemical literature. It also includes reactions from InfoChem’s ChemSelect database and ISI’s ChemPrep database.

**ChemBioFinder.Com** is the award-winning web site within formation and WWW links for over 100,000 chemicals. Users can search by name or partial name, view structure drawings, or use the *ChemDraw ActiveX/Plugin* for structure and substructure searches.

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<table>
<thead>
<tr>
<th>US</th>
<th>1 800 315–7300</th>
<th>INT’L</th>
<th>1 617 588–9300</th>
<th>FAX</th>
<th>1 617 588–9390</th>
<th>EMAIL</th>
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<td>EU</td>
<td>00 800 875 2000</td>
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<td>0120 146 700</td>
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<td><a href="http://www.cambridgesoft.com">www.cambridgesoft.com</a></td>
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CambridgeSoft Corporation 100 CambridgePark Drive Cambridge, Massachusetts 02140 USA

BioAssay, BioViz, BioDraw, Biological Assay, Visualization and Pathways

BioAssay Ultra

BioAssay Ultra, the cornerstone of BioOffice, provides flexible storage, retrieval and analysis of biological data. BioAssay easily manages both high and low throughput biological screening data.

Designed for complex lead optimization experiments, the software supports quick set-up of biological protocols, automated calculations and curve fitting, and the creation of customized structure activity reports. BioAssay brings all of this functionality to your desktop. BioAssay Ultra, compatible with the MSDE database, offers a user-friendly interface for importing, viewing, validating and plotting your biological assay data.

BioViz

Combining biological data with chemical structures is of the utmost importance in any drug discovery environment. BioViz allows you to visually analyze and perform statistical analysis on structure-related data combined with biological data in ChemFinder.

Users can search over structural and biological data and construct various plots such as scatterplots or histograms. The plots are interactive; allowing you to select subsets of your data, perform statistical analysis, filter plots based on your criteria, highlight lists and intersecting sets on plots, generate histograms of data distributions and more.

BioDraw

Reporting on and presenting findings is a task familiar to every biologist. Making this process easier and more effective benefits everyone involved. BioDraw is doing for biologists what ChemDraw has done for chemists for years—saving time, and resulting in a more professional representation of the science. BioDraw makes drawing and annotating biological pathways quick and easy, adding a level of uniformity and detail which is unmatched. Typical drawings of biological pathways include many elements that are difficult to draw with the standard presentation and word processing software. Common pathway elements such as enzymes, receptors, DNA, tRNA and plasmid maps are built into the BioDraw toolbar. BioDraw is built into the same backbone as ChemDraw, allowing users to take advantage of the wide variety of the publishing capabilities available in ChemDraw such as the ability to import and export images in GIF, PNG or JPEG formats. In addition, the integration of ChemDraw and BioDraw in Chem & Bio Draw application provides a great communication mechanism between chemists and biologists.
Inventory Ultra

Inventory Ultra allows users to manage the tracking needs of chemical and non-chemical inventory data for laboratories and research centers. The system manages data associated with both commercially procured and internally produced chemical substances from their procurement or initial production through their depletion and disposal. Inventory Ultra is an MSDE based product and includes the ChemACX database with over 450 catalogs of chemical reagents.

The three primary entities in an Inventory system are locations, containers and substances. Users or administrators configure a network of locations, which represent locations within an organization. Containers are created to represent actual containers in your facility. Each container is assigned a unique barcode, which can be printed using a customized template from the Inventory interface.

Each container stores a substance. Additional text fields are available to track other chemical contents such as the solvent. Custom fields may also be defined. To keep track of substances the system maintains its own internal chemical structure database containing unique substances that can be associated with inventory containers. Advanced duplicate checking is incorporated in the system. Every field in a record, including the chemical structure, molecular formula and molecular weight are searchable.

The application includes a number of specially designed inventory search forms. Search results are returned in list form and can be exported into a document (PDF, RTF, HTML) using the report engine. The Inventory interface allows for printing labels as well as generating reports. Inventory uses a report application that incorporates wizards that allow for the quick creation of simple reports and label templates that can be shared across an organization.

E-Notebook Ultra

E-Notebook Ultra is an efficient, accurate way to store lab notebook information. It stores Microsoft Office documents, ChemDraw structures, reaction drawings and related data in an electronic notebook that is searchable by text or chemical structure. You can organize pages by project, experiment or in your own style with the MSDE database. CombiChem/Excel builds combinatorial libraries. E-Notebook is configured exactly like a chemist would like his or her own notebook to be. Reactions can be easily drawn into the reaction template by either selecting from the generous list of preloaded reagents or by entering or drawing one's own chemicals. Commonly used reagents can be stored in a separate folder for easy access. Another fantastic feature is the procedural section. This section contains pre-written procedural sentences with the ability to easily drop in the specific names of reagent chemicals present in the reaction. One can also easily add other data to the notebook page such as spectra and Microsoft Word or Excel documents.

CombiChem/Excel

CambridgeSoft provides you with the tools to effectively plan combinatorial chemistry experiments in Excel. The CombiChem/Excel add-in introduces additional functionality for handling combinatorial chemistry. Users can generate products from a reaction and lists of reagents, you can view all the products arising from a given reagent or all the reagents of a given product, and you can lay out reagent and reaction plates.
The Merck Index, NCI, AIDS, Scientific Reference, Chemical Reactions and Patents

ChemBioFinder Gateway

ChemBioFinder Gateway allows searching of the complete CambridgeSoft reference collection of databases with a single query. Search such databases as The Merck Index, R&D Insight for Chemists and Traditional Chinese Medicines with only one click of a search button. All results federate back to the specific databases for complete information.

The Merck Index

Known for its integrity, detail, and longevity, The Merck Index contains over 10,000 monographs on drugs, chemicals and other biologically active molecules. Each monograph contains information on the compound and its derivatives; common, trade, and systematic names; trademarks and associated companies; CAS Registry Numbers, physical and toxicity data, therapeutic and commercial uses, literature citations, as well as chemical structures, formulas and molecular weights. The electronic versions include archived monographs from previous editions and is updated twice a year.

R&D Insight/Chemists

Information on current drug products under development is essential for those working in research and development, licensing and marketing at pharmaceutical and healthcare institutions. R&D Insight for Chemists, a collaborative product from Wolters Kluwer Health and CambridgeSoft, combines the power of chemical structure searching with a wealth of drug development data to give subscribers a competitive edge when making decisions relevant to the direction of their research. Updated weekly, users can search the collection of over 20,000 compounds by structure, substructure, names, partial names and synonyms.

Patent Database

Researchers, chemists and patent analysts are now able to easily search full text patents for chemical structures using CambridgeSoft’s powerful search and analysis tools. The new CambridgeSoft Patent Database portal, co-developed by CambridgeSoft and Reel Two, will give users access to all the chemical compounds named in a patent, and enable them to search by structure, keyword or chemical name.

Traditional Chinese Medicines

Access to this wealth of knowledge is now available with the Traditional Chinese Medicines database. The database consists of monographs for 10,458 chemicals isolated from 4,625 natural sources used in traditional Chinese remedies. The monographs feature bio-activity data for many of the compounds, effects and indications of the medicines, English, Latin, and Chinese names for the natural sources, and over 2,000 references.

ChemINDEX, NCI AIDS & Cancer

Scientists have used the award-winning ChemFinder.Com database since 1995. Now, the data on ChemFinder.Com is integrated into ChemOffice as ChemINDEX. ChemINDEX contains data from over 75,000 compounds including structures, names and synonyms, physical properties and Internet links. Additionally, three informative databases have been integrated into one powerful application with the NCI and AIDS database, a collection of over 200,000 molecules studied by the National Cancer Institute.

ChemReact and ChemSynth

These reaction database collections from InfoChem GmbH comprising essential information on chemical reactions published in the literature between 1974 and 2001. The largest is ChemReact500, with almost 500,000 reactions selected with an eye toward synthetic utility. ChemSynth is a subset of the reactions found in ChemReact500 chosen because they have greater than 50% yield and have been sited in leading journals more than once. ChemReact68 has 68,000 reactions that have greater than 50% yield and have appeared in more than five example reactions.
ChemACX Database

Sifting through chemical catalogs is a poor use of time for any researcher. ChemACX database solves this problem by offering a complete tool for research chemical sourcing and purchasing. With an emphasis on up-to-date information of high quality, ChemACX allows you to purchase chemicals fast, efficiently and without worry or cumbersome paper catalogs. The database can be accessed from both desktop and enterprise environments and boasts nearly 500 catalogs from major suppliers, from Alfa Aesar and Aldrich, to TCI and Zeneca, with hundreds in between.

Sigma-Aldrich MSDS

Environmental, Heath and Safety (EH&S) is an important component of today’s research institutions. A key document that aids in the management of EH&S tasks is the Material Safety Data Sheet, also commonly referred to as MSDS. In every organization, there are several groups of personnel who require access to MSDSs. Everyone who comes into contact with chemicals needs to be aware of their proper handling, storage, disposal and emergency procedures. Helping to fulfill these diverse needs is the Sigma-Aldrich MSDS collection. The database contains over 130,000 MSDSs for the products of the Sigma-Aldrich family of catalogs (Sigma, Aldrich, Fluka, Supelco, Riedel-de Haën) in HTML format. With a click of a hyperlink, users will be able to view the Sigma-Aldrich MSDS in their preferred browser. This information is smoothly integrated with the ChemACX database and other enterprise applications.

Drugs: Synonyms and Properties

Drugs: Synonyms and Properties from Ashgate, provides comprehensive coverage of the 8,000 drugs currently in common use worldwide. A key component of this reference is the extensive coverage given to synonyms. The electronic version adds almost 70,000 synonyms and trade names that did not fit into the print version. This information is also available as an SD file to facilitate in-silico research.

Nanogen Index

The Nanogen Index contains data on over 1,000 pesticides and other environmental contaminants. The database is the up-to-date and authoritative source for information on all pesticides and agricultural chemicals in worldwide use, those which are currently under development in R&D pipelines, and compounds which were once marketed or reached a development status. Data fields include chemical structures and SMILES strings, names (CAS, IUPAC, trade), the various registration codes assigned to the compounds (RTECS, EINECS/ELINCS, CAS, US EPA, CA DPR, Tariffs, etc.), Hazard and Safety codes, the developing company and use.

### Scientific Databases

**REFERENCE DATA**

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**SOURCING & SAFETY DATA**

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<td>ChemMSDX Database</td>
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**REACTION & SYNTHESIS DATA**

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<td>ChemReact68</td>
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<tr>
<td>ChemSynth</td>
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</table>
When processes and technologies are disjointed, organizations lose efficiency and decision making capability. CambridgeSoft Professional Services uses technology to bring business processes together, integrate systems and assist with strategic informatics planning.

**Informatics Planning**

**Strategic and Operational Planning**

A formal review of the discovery and development process and human/system interfaces is mapped to form the basis of a roadmap for successful technology utilization.
- Analysis of the current laboratory and technology workflows
- An analysis of the current state of the science technology environment, including architecture/operational processes
- A view of strategic goals and the barriers to achievement
- The delivery of a phased technology transition plan

**Requirements Analysis & Proof of Concept**

With years of experience meeting the needs of the scientific community, CambridgeSoft understands the user. The prototyping process allows definition and testing of the functional and technical feasibility of potential technology solutions. The process provides a baseline for the future development and deployment of a tailored solution. Users gain valuable first-hand knowledge in experiencing how the system can help achieve individual and workgroup goals.

**Legacy System Migration**

Legacy systems, with private data structures and architecture, can be barriers for migrating systems to new technologies. CambridgeSoft’s consultants have significant experience with these systems and can successfully migrate chemical and biological data, business workflow, and other aspects of legacy informatics technologies.

**21 CFR Part 11 Compliance and GxP Validation**

As an integral part in creating 21 CFR Part 11 and GxP validated applications, CambridgeSoft offers services to:
- Audit the software and process
- Create conforming systems design specifications
- Create IQ/OQ/PQ documentation
- Generate test plans and validation matrices
- Insure systems compliance with functional guidelines

With custom development, CambridgeSoft works collaboratively with your team to create a system that meets your needs while executing our quality driven software development process. We deliver what you need, on time and within budget, without surprises.

**Product Development**

**Development Consulting**

With custom development, CambridgeSoft works collaboratively with your team to create a system that meets your needs, while executing our quality driven software development process. We meet your needs, on time and within budget, without surprises.

**Systems Integration**

Process improvement often requires integrating systems designed for focused areas of work. CambridgeSoft has integrated various E-Notebook, registration, inventory, and biological assay systems in a variety of settings. Whether these are CambridgeSoft, a third-party product or an in-house developed solution. CambridgeSoft has the expertise to unite these systems in order to they improve business processes, laboratory efficiency and decision making.

**Application Configuration**

Your organization will see the benefit from implementing a CambridgeSoft application, but would like to customize it for a unique environment. Our professional services teams provide those specific features by developing market add-ins, or other modifications that are supported in the future.

**Systems Deployment**

**Installation and Configuration**

CambridgeSoft has a tested methodology for system deployment that consists of an IT architectural review, a business workflow and process review as relates to specific scientific areas, a process integration review, and maintenance guidelines. By carefully following this proven methodology, CambridgeSoft installs and configures systems that are easy to maintain and have the flexibility to accommodate variations in the science or business workflow that come from extensive experience in these areas.

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Training & Support
Educational Training and Technical Support

Systems Optimization
CambridgeSoft’s systems deployment team will work with you to make sure that your computing environment has been optimized for high performance. Your systems, networks, applications and databases are assessed and designed to deliver maximum achievement.

Beta and Pre-Release Programs
Committed to maximizing your productivity through the use of our products, as well as exposing you to the newest technologies, our beta and pre-release programs provide you with first-hand product knowledge and allows CambridgeSoft to improve applications with your feedback.

Pilot Software Evaluations
It makes sense to pilot an application before a major commitment to an enterprise-wide implementation is made. CambridgeSoft will work closely with you to plan the evaluation, deploy the application, and gather feedback regarding systems design, API’s and technology specifications.

Training
Effective user, administrator and help desk training is often an afterthought in many systems deployments. However, the productivity returns generated by an investment in systems training can be dramatic. CambridgeSoft offers a complete array of powerful, user-focused training services.

Managed Informatics allows your organization to focus on science, while CambridgeSoft plans, implements and manages your technology environment.

Systems Management
Managed Informatics
Informatics outsourcing provides the people, processes and technology to develop a unique level of service for your organization. For a monthly fee, CambridgeSoft will deliver the informatics applications and the technology staff required to maximize productivity. This service allows your organization to focus on science, while CambridgeSoft plans, implements and manages your technology environment.

Systems Hosting
A hosting service that allows customers to use our state-of-the-art enterprise applications over the extranet from any location 24 hours a day, seven days a week is available. With this hosting service, our customers can shift the responsibilities of application development and IT infrastructure management to CambridgeSoft, allowing more time to focus on core science, research, discovery and development functions.

Ultra Services
The Ultra Services program is CambridgeSoft’s personalized, premium service for supporting our customers. Organizations can take advantage of both telephone and electronic access to CambridgeSoft’s support scientists who can address:

• Usage and installation questions
• Product compatibility and interoperability questions
• Diagnostic review to help isolate the cause of a problem
• Configuration assistance
• Planning information for software updates and upgrades
• Assistance with problem resolution

Technical Support & Remote DBA Services
Technical Support and Remote DBA Services for Oracle and SQL Server are also available.
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.


**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.