Delivering a World of Discovery Information

ISIS

Integrated Scientific Information System

MDL®
Information Systems, Inc.

Flexible, Scalable Support for a World of Discovery Information

"We selected ISIS because of its speed, performance, and flexibility. ISIS enables us to enhance our current capabilities, to manage our chemistry data using modern information technology standards, and to integrate data seamlessly with existing applications. We have very aggressive productivity goals, and ISIS will help us manage the huge amount of information that results from our extensive discovery program."

Dr. Marcel Janssen
Vice President of Medicinal Chemistry
Janssen Research Foundation

Scientists who need robust, versatile, easy-to-use tools in today's fast-paced discovery environment overwhelmingly choose MDL's ISIS, the leading informatics system in the life science and chemical industries.

ISIS is extremely adaptable in supporting the data management needs of individuals, project teams, and corporate information groups, maintaining a consistent look and feel from the individual to the enterprise level. Built on a distributed-computing, client-server model, ISIS enables scientists to capture and manage data, collaborate with research groups, and synchronize information with corporate systems. ISIS also hosts a wide-range of applications for exploiting its foundation technology. Scientists can work in their environment of choice—Microsoft Excel, any Web browser, Visual Basic, or ISIS/Base. From all of these, ISIS provides a comprehensive, reliable informatics framework to deliver discovery information to the desktop. The system's scalability and breadth of application support integrates corporate workflow, increases productivity, lowers the cost of distribution—and distinguishes ISIS from the point solutions offered by other vendors.

Uniquely Suited for Data Capture and Validation

ISIS provides enormous flexibility to assist with creating scientific data and is uniquely suited for data capture and validation. Scientists working on either PCs or Macintoshes commonly use the system in a wide range of disciplines, including chemistry, therapeutic biology, agrochemical biology, analytical chemistry, metabolism, toxicology, and administration (e.g. in the sample room). MDL tools such as Cheshire for ISIS and the Flexmatch operators combine to provide ISIS with the most comprehensive and accurate chemical structure validation and novelty checking in the industry.

ISIS also supplies the most sophisticated tools for editing and registering chemical structures. The system sets no limits on the size of the molecules, and enables scientists to draw and register small molecules, polymers, proteins, models, reactions, mixtures, and formulations—the largest set of data types of any system on the market.

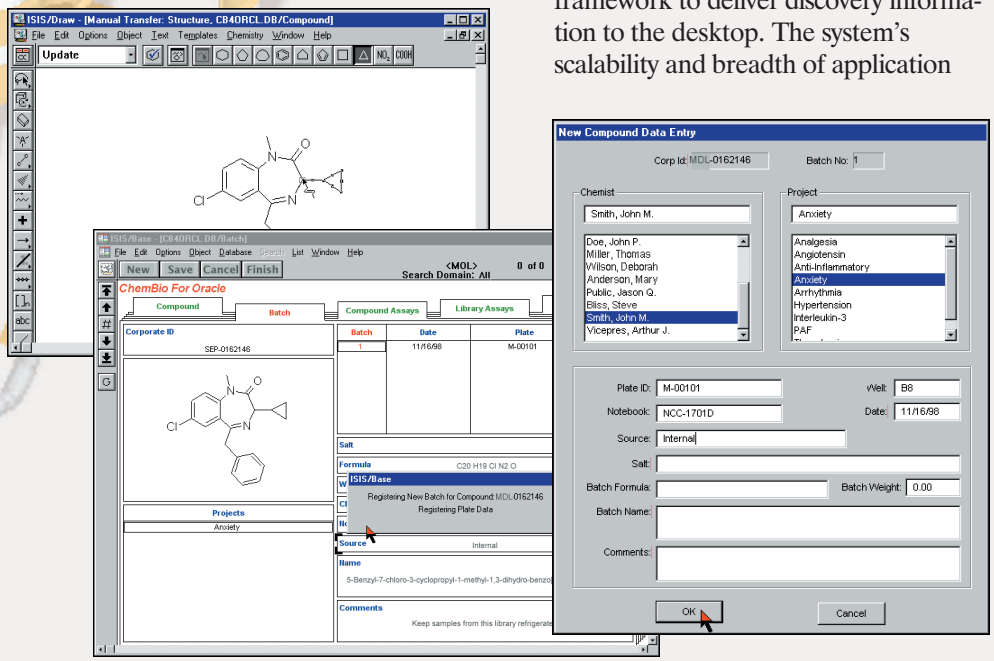
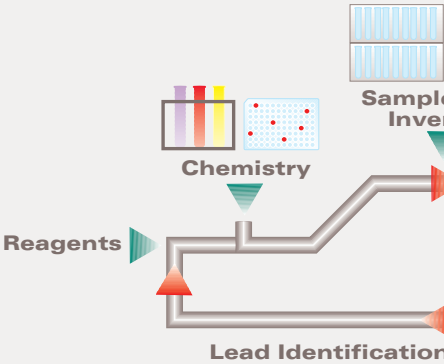
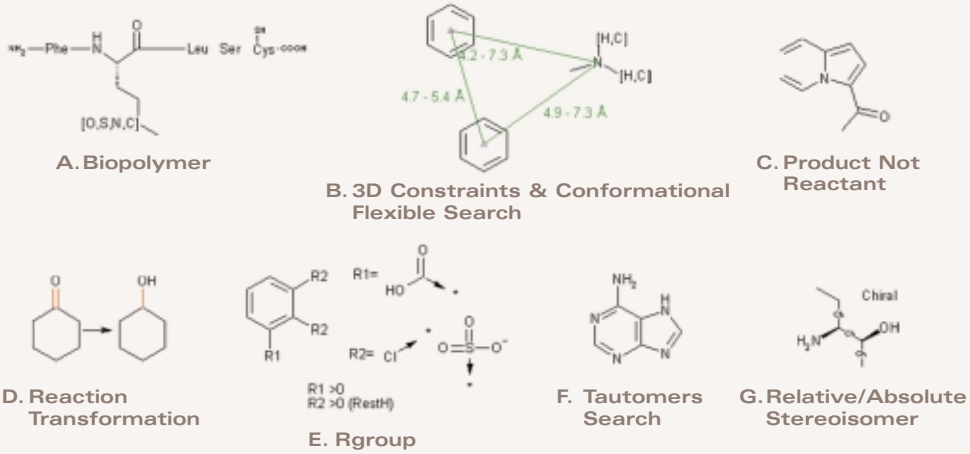


Figure 1: *Working either out of the box or, as seen here, with a custom data-entry dialog box, ISIS provides the high level of precision needed when registering chemical structures and streamlines the association of chemical, biological, or other experimental data with chemical structures or reactions.*



Cheminformatics Searching



A. Biopolymer

B. 3D Constraints & Conformational Flexible Search

C. Product Not Reactant

D. Reaction Transformation

E. Rgroup

F. Tautomers Search

G. Relative/Absolute Stereoisomer

H. Exact Structure

I. Substructure

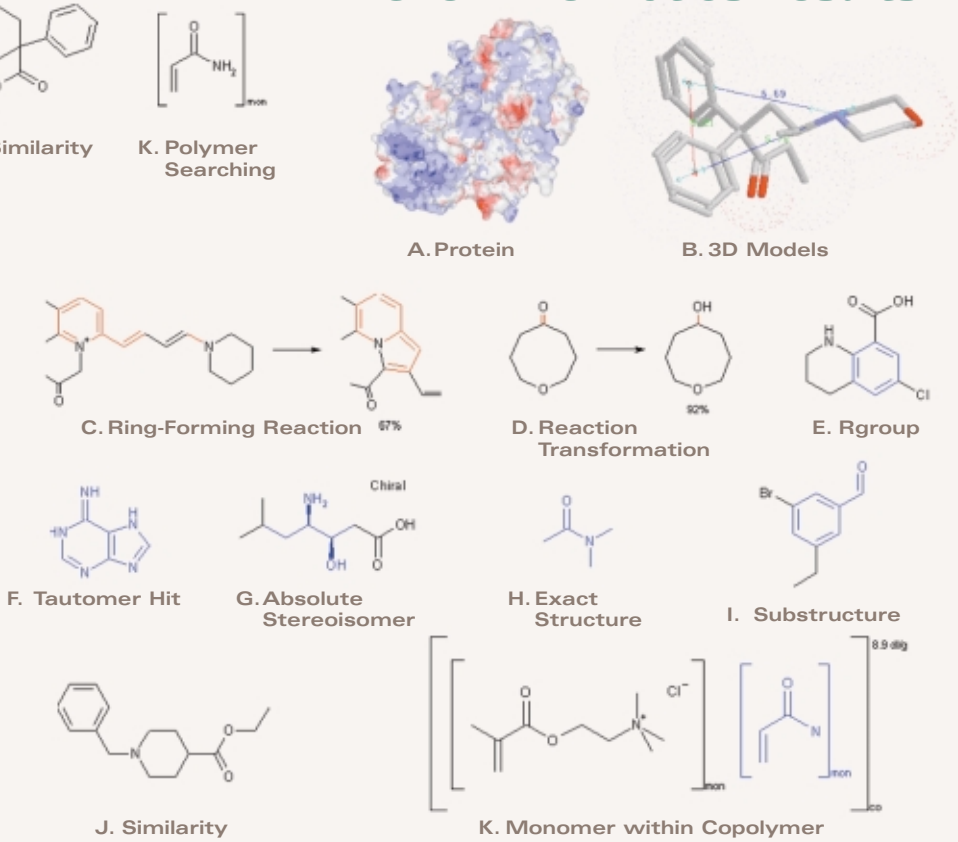
J. Similarity

K. Polymer Searching

Real-Life Data Types

With over 20 years of experience building decision-support systems and registration environments, MDL leads the industry in supporting the variety of chemical data types used in discovery research. The searching diagram (left) illustrates the breadth of chemistry available, with the results diagram (below) providing a glimpse into the types of chemical information returned to the user.

Cheminformatics Results



A. Protein

B. 3D Models

C. Ring-Forming Reaction

D. Reaction Transformation

E. Rgroup

F. Tautomer Hit

G. Absolute Stereoisomer

H. Exact Structure

I. Substructure

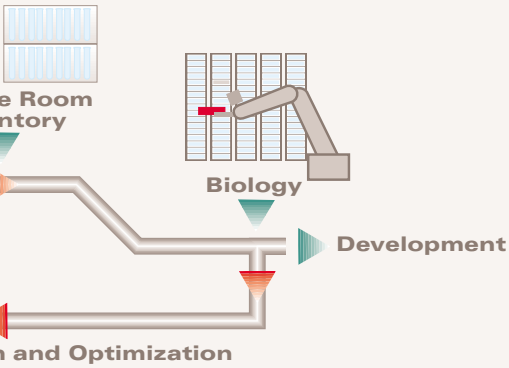
J. Similarity

K. Monomer within Copolymer

With ISIS, researchers know that what goes into a database has been properly validated, and that it is represented with the precision and accuracy necessary to meet diverse scientific requirements from the individual to the enterprise level.

Integration, Integration, Integration . . .

Integration is the mantra of today's discovery informatics. Yet only recently have RDBMS vendors rushed to support the hierarchical data structures that accommodate sophisticated data-mining and decision-support applications. MDL pioneered the integration of heterogeneous databases in the life science and chemical industries. In the early 1990s MDL patented a heterogeneous join technology to provide scientists with simple, yet powerful views of integrated data in a hierarchical context. ISIS allows researchers to bring together data from diverse sources—chemistry, biology, metabolism, toxicology, etc.—to produce actionable information that supports successful decisions. Scientists can use integrated data for reporting and for changing the presentation of information, or they can pass it along to sophisticated analysis software such as MDL's ISIS for Excel, SAR Table, SCULPT, or Spotfire from Spotfire, Inc.



Unlike other systems, ISIS does not simply look up small subsets of information via Open DataBase Connectivity (ODBC) from relational databases. The solution integrates very large repositories—relational, chemical, etc.—at the server level by establishing a heterogeneous join over many different database types. This approach allows scientists to query and explore the entire integrated database in real time, and to ask the questions they need to ask across the discovery enterprise. And the integration potential of ISIS is further enhanced with the release of ISIS/Direct, MDL's data cartridge for Oracle 8*i*. ISIS/Direct works with desktop chemistry tools from MDL such as ISIS/Draw, Chime Pro, and ISIS/Object Library, allowing an application to send chemically-extended SQL to the Oracle 8*i* engine.

Power Tools for Decision Support

The Web and distributed computing environments such as ISIS have made the deployment of business information easier than ever. New tools have evolved to provide effective access to the world of scientific information and to systems for presenting, analyzing, and visualizing the ever larger sets of discovery data. The data presentation, analysis, and visualization environments available through ISIS exploit the comprehensive integration capabilities of the system's server.

MDL supplies browsing applications with ISIS for easy, flexible access to MDL, customer, and third-party databases. Scientists, research management, and IT departments appreciate the common, consistent interface to both commercial and proprietary data.

Organizations can combine ISIS for Excel, Cheshire for ISIS, and SCULPT to provide decision support and analysis tools that work together for SAR spreadsheets, physicochemical property prediction, Rgroup decomposition, and 3D lead alignment. By automating the reporting and analysis, scientists can speed lead identification and lead optimization.

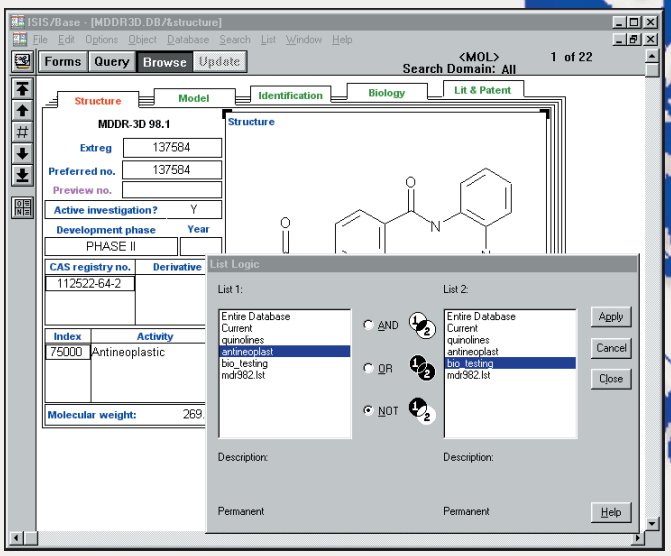


Figure 3: Scientists value the easy-to-use, yet powerful list handling in ISIS. Combinations of text, numeric, and chemical structure searching can be saved to individual lists and then correlated with Boolean operators to narrow or broaden search results.

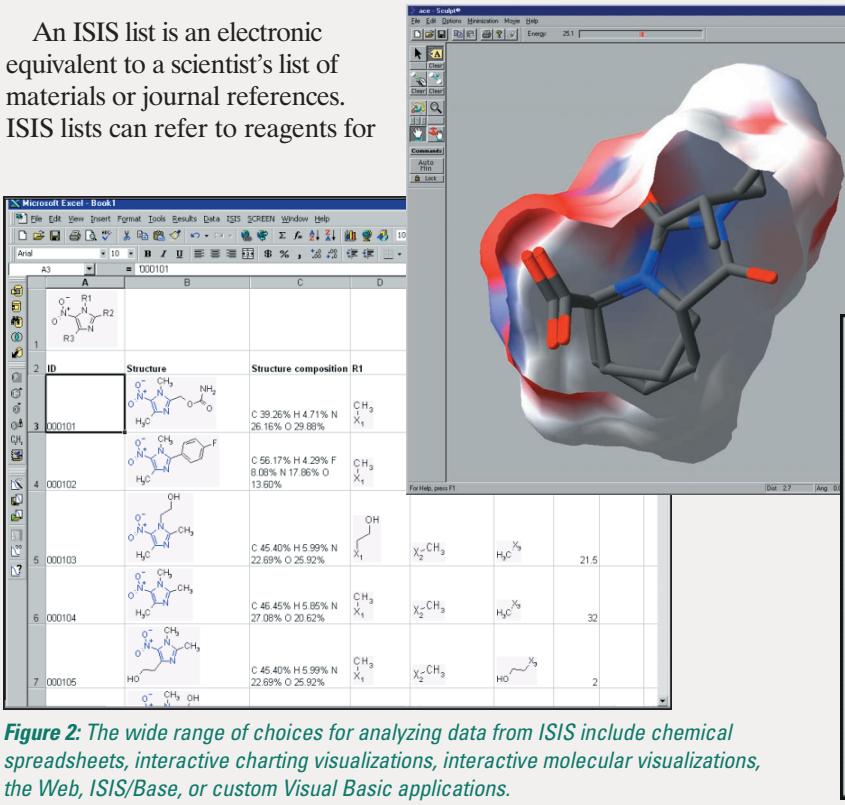
Control Over Search Results

An ISIS list is an electronic equivalent to a scientist's list of materials or journal references. ISIS lists can refer to reagents for synthesis, products for screening or SAR, citations of reactions, chemical suppliers, activity results—any logical combination that will help scientists focus their analyses and make the right decisions.

ISIS' sophisticated list management allows sorting, collecting, analyzing, and reporting. These capabilities provide a handle on corporate information as it is passed to desktop tools for easier analysis and visualization.

"We were looking for an easy-to-use interface for our discovery scientists that would integrate chemical structures from medicinal and combinatorial chemistry with biological data from therapeutic areas and high-throughput screening. Our scientists were able to build a browser that accesses these multiple data sources and pivots data from a single user interface. The new browser has proven its effectiveness very quickly."

Dr. Edward W. Petrillo
Director of Combinatorial Drug Discovery
Bristol-Myers Squibb



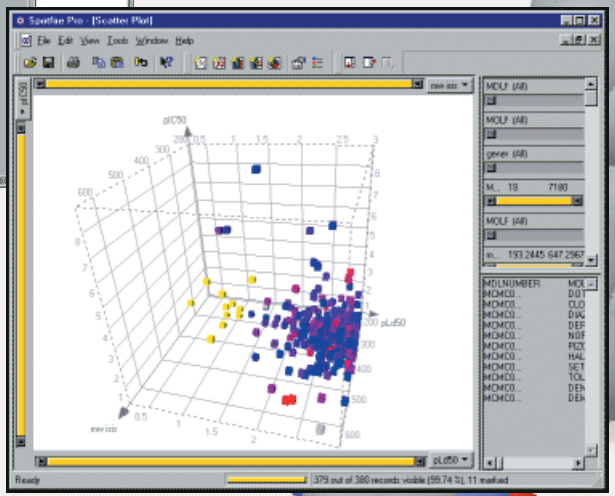


Figure 2: The wide range of choices for analyzing data from ISIS include chemical spreadsheets, interactive charting visualizations, interactive molecular visualizations, the Web, ISIS/Base, or custom Visual Basic applications.

"Cheshire for ISIS is based on a set of abstract concepts including 'collections' and 'mappings' within an object-oriented framework. The combination of these concepts with the rich dictionary of basic operations allows Cheshire to cover all the business rules we need in the process of structure registration. The Cheshire Studio will help us to do the programming and testing in a remarkably efficient way."

Dr. Upali Bandara
Business Analyst, ZDW Scientific Information
BASF Aktiengesellschaft

Developer Toolkits

The ISIS foundation includes a wide variety of application development toolkits that are available on the server and on the client in the environments supported by ISIS.

Whether your development goals are to centralize business logic on the server or to provide sophisticated chemistry components on the client (or both), ISIS provides the toolkits you need in your environment of choice.

Server

ISIS/Direct—an object relational implementation of MDL chemical search and indexing methods under Oracle 8*i*

Chemscape Server—a Web interface to ISIS/Host

ISIS/Host API—a C interface to integration of data sources and structure searching

ISIS/Host Command Line Interface—command line interface to ISIS

ISIS/Host Open Gateway—a programmable data source interface to data sources not supported by MDL

ISIS/PL—a chemistry procedural language called from ISIS/Host

Cheshire for ISIS—an object-oriented chemical structure automation environment

Client

ISIS/Object Library—a 32-bit OLE automation server for accessing ISIS from OLE supporting development tools

ISIS/ADK Pro—a collection of prepackaged OCX's for cheminformatics application development

ISIS/PL—a chemistry procedural language called from ISIS/Base and ISIS/Draw

ISIS Add-In Manager—a framework for packaged ISIS/PL routines

Cheshire for ISIS—an object-oriented chemical structure automation environment

Scalability Across User Environments

ISIS operates at the scale you need, allowing scientists to work locally on a client or on a network server at the client level. Designed with connection pooling, Oracle fetch constraints, and optional buffering of query results, ISIS can efficiently handle very large user communities. Server-side ISIS/Host can be installed on an individual machine and accessed by scientists across an organization, or it can be distributed among various departmental servers.

"After evaluating the options, we determined that MDL tools and technology will help us build the robust informatics infrastructure that we need to support the cutting-edge applications we plan for the future. We have aggressive goals for R&D productivity and our relationship with MDL will help us to provide our scientists with the tools to achieve them."

Martyn Wilkins
Director, Research Information Systems
AstraZeneca Pharmaceuticals

Popular Discovery Platforms

ISIS products run on the desktop client or on the server which hosts the system's integration capabilities. The foundation technology supports a wide range of platform configurations for both operating system support and development.

ISIS Technology on the Server

ISIS/Host, Cheshire for ISIS
- Sun Solaris
- SGI IRIX
- IBM RS/6000 AIX
- Microsoft Windows NT Server
- Compaq Open/VMS Alpha

Chemscape Server
- Netscape Enterprise Server (Sun, SGI, AIX, NT)
- Microsoft Internet Information Server (NT only)

ISIS Technology on the Client

ISIS/Base and ISIS/Draw
- Microsoft Windows 95, 98, and NT
- Macintosh

Chime and Chime Pro for Web Browsers
- Microsoft Windows 95, 98, and NT
- Macintosh

ISIS for Microsoft Excel
- Microsoft Windows 95, 98, and NT
- Macintosh

ISIS Gateways and Development Toolkits on the Server

Supported ISIS/Host Gateways
- MDL Molecule Database
- MDL Reaction Database
- ORACLE RDBMS
- MDL Relational Chemical Gateway
- Beilstein Crossfire Server Database Gateway

About MDL

MDL Information Systems ("MDL") is the recognized leader in discovery informatics for the life science and chemical industries. MDL software, content, and services provide the enterprise framework for identifying successful new products. MDL is an international business headquartered in San Leandro, CA with offices worldwide. MDL Information Systems, Inc. is a wholly owned subsidiary of Elsevier Science, Inc.

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