

ELSEVIER MDL has 30 years of experience providing software, databases and services that improve the speed and quality of scientists' decision making and accelerate successful R&D. Tens of thousands of researchers around the world rely on MDL solutions to manage workflow and access scientific information.

About Elsevier MDL

Headquarters San Ramon, California, USA with offices worldwide

Founded In 1978, as Molecular Design Limited

Employees Approximately 400 in 12 offices worldwide

Solution Areas MDL discovery solutions encompass three broad categories:

Content—a comprehensive collection of databases, reference works and essential discovery content

Framework—the standard applications and integration technology that provide the basis of discovery informatics solutions

Workflow—an integrated set of applications for managing chemical and biological discovery workflows, including data acquisition, reagent logistics and electronic laboratory notebooks

Customers Tens of thousands of users worldwide in the pharmaceutical, biotechnology, chemical and agrochemical industries, government and educational institutions, hospitals and utility companies.

Consulting Expert consultants assess client issues and opportunities, supporting the design and implementation of processes and tools to improve productivity.

Customer Care Elsevier MDL professionals help customers gain maximum value from MDL solutions and provide reliable, high-quality product support—onsite, by telephone and via the Web.

Educational Services Experienced educators provide onsite training, documentation and electronic training products to improve customers' proficiency with MDL products.

Elsevier MDL is part of Reed Elsevier Group plc, a world-leading publisher and information provider.

Affiliations

ELSEVIER MDL is part of Elsevier and works closely with leading providers to offer optimum solutions for researchers.

Elsevier

Elsevier is a world-leading publisher of scientific, technical and medical information products and services. Working in partnership with the global science and health communities, Elsevier's 7,000 employees in 70 offices worldwide publish more than 2,000 journals and 1,900 new books per year, in addition to offering a suite of innovative electronic products, such as ScienceDirect (www.sciencedirect.com), MD Consult (www.mdconsult.com), Scopus (www.news.scopus.com), bibliographic databases and online reference works.

Elsevier (www.elsevier.com) is a global business headquartered in Amsterdam, The Netherlands and has offices worldwide. Elsevier is part of Reed Elsevier Group plc (www.reedelsevier.com), a world-leading publisher and information provider. Operating in the science, medical, legal, education and business-to-business sectors, Reed Elsevier provides high-quality and flexible information solutions to users, with increasing emphasis on the Internet as a means of delivery. Reed Elsevier's ticker symbols are REN (Euronext Amsterdam), REL (London Stock Exchange), RUK and ENL (New York Stock Exchange).

Solution Partners

Elsevier MDL works with leading providers to ensure that its software runs in multi-platform, multi-application environments. Elsevier MDL has partnerships with hardware, operating system and application vendors whose products are integral to MDL solutions, including Sun Microsystems, Microsoft Corporation, Oracle Corporation, Citrix Systems and others.

Content partners include Thomson-Derwent, FIZ CHEMIE Berlin, the U.S. Food and Drug Administration, the German Chemical Society (GDCh) and Prous Science, among others.

MDL® Isentris® Alliance

The Isentris Alliance is a community of companies joining forces to provide integrated, high-value solutions to researchers. The program maximizes opportunities for life sciences researchers using the MDL Isentris system by establishing relationships among industry leaders in software, content, hardware and other services. (see page 6).

Consulting and Services

During thirty years of providing leading discovery solutions to research organizations around the world, Elsevier MDL has amassed vast experience in improving the effectiveness and efficiency of research. To share this knowledge and expertise with customers every step of the way, Elsevier MDL offers a continuum of service and support via a global services organization.

Consulting

Elsevier MDL consultants combine experience in the discovery environment with an understanding of the latest technology advances to deliver performance-improving, custom, integrated solutions. Serving diverse organizations from small biotechs and start-ups to large pharmaceutical companies with global operations, Elsevier MDL tailors informatics solutions to suit customer requirements, using both MDL products and third-party technology.

Customer Care

Through comprehensive customer services, Elsevier MDL ensures that products are utilized properly and that customers stay productive. This global team supports customers both onsite and remotely, and provides the key contact point for any issue regarding MDL products. Product experts provide direct personal support (via phone and online) and extensive follow-up on customers' issues.

Educational Services

Elsevier MDL Educational Services helps customers master the product learning curve effectively and efficiently. Experience shows that instructor-led training programs with planned follow-ups increase user effectiveness. Educational Services provides electronic and paper-based product documentation and offers custom training materials for specific in-house or consulting-developed applications. Educational Services also offers Web-based, self-paced and electronic training options.

The **Elsevier MDL Learning Center** provides online access to training materials—anytime, worldwide. The up-to-date materials are suitable for self-paced training or classroom instruction, allowing hands-on, scenario-based practice in a simulated environment that includes explanations of key concepts. Four targeted Learning Center hubs address the specific needs of research communities, including academic CrossFire and DiscoveryGate researchers, smaller biopharma companies and global pharmaceuticals.

Content

ELSEVIER MDL offers the world's most comprehensive collection of factual databases and reference works covering bioactivity, chemical sourcing, synthetic methodology, pharmacology, metabolism and toxicology. In addition to local installations, Elsevier MDL offers most of these data sources via the hosted DiscoveryGate® platform with links to the primary literature and important third-party databases including Derwent World Patents Index®.

Access Platforms



DiscoveryGate®

DiscoveryGate provides unprecedented access to scientific information. With DiscoveryGate, scientists have the ability to ask questions and get immediate, comprehensive answers in a seamless, integrated environment. DiscoveryGate integrates, indexes and links scientific information to give immediate access to compounds and related data, reactions, original journal articles and patents, and authoritative reference works on synthetic methodologies and pharmacology. DiscoveryGate interlinks the content sources necessary for answering discovery questions—all from a single entry point:

Primary sources: Over 20,000 scientific, technical and medical journals

Databases: The most up-to-date versions of all MDL databases, featuring over 27 million structures and 17 million reactions with more than 500 million associated facts covering synthesis, bioactivity, physical property, pharmacology, metabolism, toxicology and sourcing. DiscoveryGate also offers access to information from partner databases, for example, indexed compounds referenced in PubChem and the Derwent World Patents Index.

MDL® CrossFire® Commander

MDL CrossFire Commander and MDL® CrossFire® Server are an integrated client/server application for searching CrossFire Beilstein, CrossFire Gmelin and the MDL® Patent Chemistry Database. The intuitive search interface in CrossFire Commander lets scientists quickly search the CrossFire databases and hyperlink to relevant, related data such as chemical structures, literature references, bioactivity data and the properties of molecules participating in a preparation.

A grouping and sorting feature organizes large hit sets to provide better overviews and greater benefits to scientists. CrossFire Commander uses the same reaction ClassCodes as DiscoveryGate, enabling scientists to search similar reactions in Beilstein, Gmelin or DiscoveryGate's other content sources.

CrossFire Commander accesses:

- **CrossFire Beilstein** (see description, page 4)
- **CrossFire Gmelin** (see description, page 4)
- **MDL Patent Chemistry Database** (see description, page 4)

Bioactivity Databases

MDL® Comprehensive Medicinal Chemistry

Derived from the Drug Compendium in Pergamon's *Comprehensive Medicinal Chemistry*, the MDL Comprehensive Medicinal Chemistry database provides 3D models and important biochemical properties, including drug class, logP, and pK_a values for pharmaceutical compounds (1900-present). Elsevier MDL updates the database annually with compounds identified for the first time in the United States Adopted Names (USAN) list.

MDL® Drug Data Report

The MDL Drug Data Report covers patent literature, journals, meetings and congresses. Produced by Elsevier MDL and Prous Science, the database contains biologically relevant compounds and well defined derivatives. It allows scientists to search by structure or across relevant data fields to explore 3D structure-activity relationships.

National Cancer Institute Databases

NCI's CAS Registry, Plated Compounds, AIDS and Cancer databases are offered as a public service to Elsevier MDL customers.

MDL® Metabolite Database

A complete metabolism information system, MDL Metabolite Database comprises a database, registration system and browsing interface. The Metabolite Database is the only source that uses published information from multiple studies to assemble structural metabolic database entries for particular parent compounds. The Metabolite Registrar enables scientists to create, edit and register metabolic schemes. The Metabolite Browser offers a graphical interface for searching and displaying metabolic schemes stored in either Metabolite or corporate databases.

MDL® Toxicity Database

MDL Toxicity Database contains data from *in vivo* and *in vitro* studies of acute toxicity, mutagenicity, skin and eye irritation, tumorigenicity and carcinogenicity, reproductive effects and multiple dose effects. It contains the contents of the Registry of Toxic Effects of Chemical Substances (RTECS®) database, from the U.S. Public Health Service and updated by Elsevier MDL, as well as the Chemical Carcinogenesis Risk Information System (CCRIS) produced by the National Cancer Institute, and Genetox database produced by the U.S. Environmental Protection Agency.

Chemical Sourcing Databases

MDL® Available Chemicals Directory

MDL Available Chemicals Directory provides access to 2D and 3D structures, supplier and pricing information for over 571,000 unique research-grade and bulk chemicals. The database contains over 1.7 million available products from over 720 suppliers. It can be searched by structure and data, and offers access to Safety Data Sheets available via Elsevier MDL OHS. The database is available in a variety of formats.

MDL® Screening Compounds Directory

MDL Screening Compounds Directory consolidates chemical data from suppliers specializing in compounds for high-throughput screening. With over 4.6 million unique, drug-like compounds in an electronic, structure-searchable format, MDL Screening Compounds Directory provides instantaneous access to comprehensive information from trusted global suppliers.

Chemistry Databases

Reaction Classification by InfoChem GmbH extends Elsevier MDL's reaction retrieval system to index all reaction databases (Chemistry and Synthetic Methodology databases and Integrated Major Reference Works), creating the world's most advanced system for selecting and evaluating synthetic methods. By grouping reactions in clusters of similar types, chemists can determine a cluster group's relevance to a synthetic problem without wading through reaction after reaction.

CrossFire Beilstein

The world's largest chemical facts database, CrossFire Beilstein, produced by MDL Information Systems GmbH, is an essential first step in the chemical discovery process. The database offers access to over 9.9 million compounds and over 10 million reactions in organic chemistry. With CrossFire Beilstein, scientists can locate starting materials, melting points, NMR spectra, MS spectra and other physical property data to validate syntheses. Bioactivity, chemical and physical property data in CrossFire Beilstein provide key information on how compounds interact with and affect organisms and the environment, including pharmacodynamics and environmental toxicology, transport, distribution and fate information. CrossFire Beilstein contains more than 320 million scientifically measured (not calculated) properties and facts for compounds and reactions. It also contains over 900,000 original author abstracts from 1980 to the present, as well as pharmacological and ecotoxicological data describing the bioactivity of organic compounds.

CrossFire Gmelin

Based on the Gmelin Handbook of Inorganic and Organometallic Chemistry, CrossFire Gmelin, from MDL Information Systems GmbH, is the world's largest compilation of inorganic and organometallic compounds and related physical properties. With over 100 million experimental facts covering over 2.4 million substances, over 1.8 million reactions and over 1.1 million citations, CrossFire Gmelin is an ideal tool for researchers engaged in designing new materials and catalysts. The database is maintained in partnership with the German Chemical Society, GDCh, the largest scientific organization of its kind in Europe.

Synthetic Methodology Databases

MDL® Patent Chemistry Database

Updated every 2 weeks, the Patent Chemistry Database indexes chemical reactions, substances and related substance information from World and European organic chemistry and life sciences patent publications since 1978, and U.S. patent publications since 1976. The database contains not only compounds with data, but also prophetic compounds. For reactions, the full reaction text from the patent document is given. For substances, the bioactivity*, application* and physical data are indexed. The database brings patent claim texts and Markush* structures/reactions to the desktop in an easy-to-view format, enabling an easy relevance check of patent documents (*for patent publications from December 2003 onwards).

ChemInform Reaction Library

This database focuses on novel methodology and reactions of current interest to synthetic chemists. The collection is selected, abstracted and organized by FIZ CHEMIE Berlin. The database provides convenient access to full reaction schemes.

MDL® Solid-Phase Organic Reactions

Produced by Elsevier MDL and FIZ CHEMIE Berlin, this database includes extensive data on solid-phase organic chemistry, such as information on polymeric materials, linkers, solid supports and protecting groups. The database provides convenient access to full reaction schemes.

MDL® Reference Library of Synthetic Methodology

This broad collection of novel organic synthetic methodologies covers functional group transformations, metal-mediated chemistry and asymmetric syntheses, as well as reactions abstracted from Dr. William Theilheimer's *Synthetic Methods of Organic Chemistry* and Pergamon's eight-volume *Comprehensive Heterocyclic Chemistry*.

Current Synthetic Methodology

This database, organized by FIZ CHEMIE Berlin, contains the most innovative and significant reactions since 1992, emphasizing new synthetic methodologies, reactions that use new reagents or important modifications of known reagents, and regio-, chemo- and stereoselective reactions carried out on multifunctional substrates.

Derwent Journal of Synthetic Methods

An electronic version of Derwent's *Journal of Synthetic Methods* (1980-present), this database compiles chemical reaction literature from international journals and patent sources. It contains detailed information about new synthetic methods, high-yield functional group transformations, improvements to existing methodologies and reactions representing the most significant new patents.

ORGSYN

An electronic version of the entire series of *Organic Syntheses* (first published in 1921), this database provides simple graphical access to general synthetic methods and proven compound preparations. *Organic Syntheses* also contains information on product purity, product yield and hazards, as well as references to the original procedures and journal sources.

Integrated Major Reference Works

Integrated Major Reference Works provides one-click, two-way linking between reaction databases and authoritative reference works, and single-click access to the primary literature. This electronic product affords the same high-quality content as the printed sources, but with the benefit of user-friendly navigation tools. From a single interface, multiple reference works can be easily searched using full-text, reaction-type and structure-based queries. The major reference works include:

- **Comprehensive Asymmetric Catalysis**—Published by Springer-Verlag
- **Comprehensive Organic Functional Group Transformations**—Published by Elsevier

Environmental, Health and Safety

Elsevier MDL OHS offers a variety of databases, software and services for material safety data sheet (MSDS) authoring, reference and hazard communication.

MSDS Services

OHS delivers professional services to support the centralized and cost-efficient creation and maintenance of MSDSs, including:

- OHS MSDS Authoring Outsourcing
- OHS MSDS Translations and International Formats
- OHS MSDS Distribution Services
- OHS Web Hosting Service
- OHS e-Link

Reference

OHS offers a variety of EH&S data for reference or use in populating existing systems. These premium data sources are regularly updated and distributed for professional use and decision making:

- OHS Global Reference System
- OHS Complete Reference System
- OHS Pure Substance Database
- OHS Mixture Substance Database
- OHS MSDS ON DISC
- OHS EH&S Data Elements

Hazard Communication

OHS provides valuable tools for employee safety and compliance, each featuring the highest OHS standards for quality and employee safety.

- OHS Inventory Match
- OHS HazCom System
- Emergency Response through CHEMTREC
- OHS Fast Fax

Custom Data Services

OHS offers customizable and unique solutions for virtually any environmental, health and safety project.

Framework

ELSEVIER MDL provides the foundation for discovery application development and integration. With MDL technology, MDL and third-party content and applications benefit from rapid development and optimum interoperability. The newest technology is the MDL® Isestris® system—an open, flexible, and scalable n-tier architecture that improves R&D efficiency by integrating business processes, data and applications.

MDL® Isestris®

MDL Isestris is a complete, out-of-the-box solution for searching, browsing, organizing and reporting on data and information needed in research organizations. Isestris streamlines the storage, integration, calculation, manipulation and retrieval of a broad range of chemistry and biology data, enabling scientists to access the right information at the right time, in the right context and format.

MDL Isestris enables global project teams to collaborate more effectively and to better exploit data and applications in the decision-making process, reducing costs, saving time and sharpening the focus on science in support of a more efficient and effective discovery process. The types of applications developed on Isestris include integrated chemical and biology data access, experiment management, data capture, procurement, inventory management and analysis applications.

MDL Isestris has a three-tier architecture containing the following main components:

- The MDL® Isestris client user interface and MDL® Draw chemical drawing and rendering software are desktop applications for accessing and managing scientific data; they offer application developers an environment for application building, extension and integration.
- MDL® Core Interface middleware provides the unifying logic and data integration for all applications built on or integrated with Isestris. MDL® Cheshire provides the environment for building and applying consistent enterprise-wide chemistry rules.
- MDL® Direct chemical data cartridge technology provides specific support for storing, searching, and retrieving molecules and reactions in Oracle® databases.



Isestris Alliance

MDL® Isestris® Alliance

Elsevier MDL and a community of partner companies are joining forces to provide integrated, high-value solutions to researchers. The Isestris Alliance program maximizes opportunities for life sciences researchers using the MDL Isestris system by establishing relationships among industry leaders in software, content, hardware and other services. By combining partners' core

competencies and a powerful integration framework, Isestris Alliance offers new opportunities and integrated discovery research solutions that rapidly provide a high return on investment. Partners include ACD/Labs, Aureus-Pharma, BioWisdom, DeltaSoft, Eidogen-Sertanty, InfoChem, InforSense, Klee, Osthus GmbH, Spotfire, Symyx, Tripos and Waters.

MDL® ISENTRIS® client

The MDL ISENTRIS user interfaces enable scientists to collaborate in an optimized workflow environment, sharing and exploring data across chemical and biological research domains. The ISENTRIS user interfaces provide easy-to-use tools for accessing data using defined business rules and powerful integration facilities in the middle-tier. With tools such as drag-and-drop form design, dynamic query building, automatic form design, tight Excel integration, history tracking and public and private data integration, researchers are able to access and share scientific information when they want, in a format and context that best meets their needs. With ISENTRIS, scientists can move seamlessly between applications and data with a single logon, integrate chemical structures, reactions, biological activity and property data, and access and share global data throughout a research community.

Highlights

- **Researcher:** Easy-to-use interface, self-service data access, collaborative environment; ISENTRIS for Excel enables scientists to access, browse, collate, manage and share data in the familiar Microsoft® Excel® spreadsheet environment
- **Developer:** Open .NET development, faster development, simplified management, scalable, high performance; easy-to-use, flexible MDL® ISENTRIS® controls enable developers to rapidly build custom applications, extend applications and integrate existing applications that have a consistent look and feel
- **Administrator:** Centralized storage of data and management of business rules, reduced support

MDL® Draw

For advanced structure drawing, rendering and structure queries, MDL Draw enables scientists to draw and edit complex molecules and chemical reactions with unprecedented ease. A single all-purpose drawing tool lets scientists continuously draw a structure, assign atom properties and apply query features. Dragging and dropping a drawn structure over a button creates a custom template. Right-clicking on atoms or bonds of interest enables scientists to explore query options for searching MDL databases. Because it can be easily built into custom applications, MDL Draw Enterprise Edition offers organizations programming flexibility. Developers can drop components into existing Microsoft Visual Studio® .NET and Java applications, and use XML configuration files to change the look-and-feel according to their organization's workflow needs.

Highlights

- **All-purpose drawing tool:** Draw bonds, pull out rings of any size, add atoms and query features using one tool

- **Sequence tool:** Draw, register, search and report on chemically modified peptide and nucleotide sequences
- **Custom template toolbars:** Drag and drop commonly used functional groups and queries for instant reuse
- **Easy development:** Drop into .NET or Java applications, use in Internet Explorer, configure look and feel with XML

MDL® Core Interface

MDL Core Interface is a middleware platform specifically designed to support Web and desktop application building and consistent, accurate management of researchers' data. Researchers gain improved access to chemical and biological research data with rich tools for processing data. For application developers, Core Interface streamlines integration and accelerates application development with a set of services and discovery-focused tools that can be shared by multiple applications. In combination with other MDL products, Core Interface provides a complete solution for connecting discovery scientists with their data and applications.

Highlights

- **Application developers:** Supports Java and .NET environments for rapidly building, extending and customizing applications
- **System administrators:** Web-based console for managing user sessions, license tracking, user interfaces, security and database connections
- **Database administrators:** Enables metadata-driven use of information to build hierarchical views from relational data; quickly create, select and modify data views without scripting

MDL® Direct

MDL Direct data cartridge technology makes chemical databases accessible to scientists and developers working with Oracle's standard SQL syntax. It enables research organizations to manage fully relational molecule structure and reaction databases while integrating other enterprise data in an open Oracle environment. A single chemistry data cartridge handles both molecule structure and reaction management. The MDL Direct technology features industry-leading chemical and stereochemical representation, and is compatible with existing application infrastructures and a wide range of commercial databases. MDL Direct improves search speed, reduces maintenance costs and facilitates performance for networked chemical information searching and management.

Highlights

- **Enhanced stereochemistry:** Meets the challenges of representing stereochemically relevant structures including tetrahedral and non-tetrahedral stereoisomers
- **Powerful searching:** 2D/3D exact and substructure searches; ISIS flexmatch searching; similarity, formula, Rgroup, Sgroup, polymer and mixture queries; tested against databases with over five million reactions and at least 20 million structures
- **Flexible:** The reaction cartridge is model independent, no restrictions on the size of molecules

MDL® Cheshire

An object-oriented chemical structure automation environment, MDL Cheshire adds sophisticated chemical representation tools for manipulating chemical structures. Using familiar programming constructs such as objects, methods and properties, organizations can define cheminformatics business rules that can be called by different applications to perform a variety of operations, such as chemical convention checks, chemical structure validation and physicochemical property calculations.

Highlights

- **Features:** Molecule, reaction, Rgroup and Sgroup handling
- **Cheminformatics Business Rules Manager:** Enables Oracle-based business rule organization and administration
- **Industry-standard interfacing:** Through Java, COM and C allow Cheshire to be used in a range of application environments

Other Tools and Technology

MDL® ISIS

MDL ISIS (Integrated Scientific Information System) serves as an information management framework for scientific data. It provides extensive chemical representation features and powerful capabilities for searching chemical structures, reactions and 3D molecular models. It is also an application development environment that enables organizations to deploy innovative scientific software applications, such as chemical inventory systems, electronic lab journals and systems for managing therapeutic-level lead candidates. Today, MDL ISIS remains the industry standard, with more than 50,000 users at approximately 500 customer sites worldwide.

MDL® Chemscape Server connects Web servers to MDL ISIS/Host, the server foundation for the ISIS family of products. It is a Web development tool that provides structure searching, registration, lists and other major functionality of MDL ISIS/Host. Chemscape Server is used with the MDL® Chime Pro browser plug-in, which provides the user interface for Web-based applications.

MDL® Report Manager

MDL Report Manager is a chemically intelligent tool that enables scientists to generate multi-sectioned reports in a matter of minutes. Report Manager simplifies enterprise-wide reporting by accessing and integrating chemical and other Oracle databases. Report Manager uses query filters and pre-formatted templates to extract and organize complex information from multiple databases into a broad range of reports. Report Manager is the ideal tool for checking inventory status, sharing experiment results, analyzing pharmacophore substructures—even creating HTML reports for the Web. Scientists can use the intuitive interface to build views of databases and customize report templates for repeated use. Report Manager makes all of an organization's scientific data readily accessible.

MDL® Central Library

This server-based system combines the data management capabilities of Oracle databases with Elsevier MDL expertise in handling chemical information. MDL Central Library supports the day-to-day activities of combinatorial chemists, allowing them to integrate commercial and corporate chemical structure databases, access reagent databases, automatically process reagents into libraries and register and manage libraries. Reagents or synthesized products can be accessed using MDL ISIS/Base, MDL® ISIS for Excel or MDL® Reagent Selector.

MDL® ISIS for Excel

This data-analysis tool combines the familiar spreadsheet environment of Microsoft® Excel with the chemical-structure handling expertise of MDL ISIS. The result is a flexible desktop application for retrieving, manipulating and analyzing data and chemical structures. MDL ISIS for Excel is excellent for SAR analysis and converts an Excel spreadsheet into a database search engine, eliminating the tedious job of importing and exporting data.

MDL® Chime Pro

MDL Chime Pro offers platform-independent chemical structure visualization and database searching. By using Chime Pro in conjunction with MDL® Chemscape Server or MDL Direct, scientists can search databases accessed through corporate intranets or the Internet. Chime Pro's JavaBean component enables developers to provide chemical structure rendering and visualization in pure Java applications and applets as well as in Web pages.

Workflow

ELSEVIER MDL delivers an integrated set of applications that enables scientists to manage the chemical and biological aspects of the discovery process. From designing chemical syntheses to managing plates and analyzing assay results, flexible MDL solutions leverage the value of MDL content and streamline workflows.

MDL® Logistics



MDL Logistics is a complete solution for managing the reagent procurement and reagent inventory process. It incorporates in-house inventory data with the MDL Available Chemicals Directory (the world's largest electronic collection of chemical supplier catalogs) and the MDL OHS database (an electronic encyclopedia of product safety information and MSDS sheets). This complete, flexible inventory management solution, built on the extensible MDL® ISENTRIS® system, provides an out-of-the-box solution for biopharmaceutical companies and can be customized to meet the needs of larger organizations. Integration with financial business systems and laboratory hardware devices increases the value of the investment by providing employee time savings and productivity gains. MDL Logistics is the only solution on the market offering regulatory capabilities; it also offers support for collections-based procurement for combinatorial chemists. MDL Logistics integrates out-of-the-box with hardware devices (balances, barcode scanners, printers and inventory robotics) and offers integration with purchasing systems.

MDL® Notebook



MDL Notebook supports the capture, authentication, integration, reporting and sharing of scientific data and the integration of critical workflow applications. MDL Notebook helps researchers work more efficiently together, save time, reduce costs, focus on science and make better decisions. MDL Notebook addresses the needs of scientists, including organic synthetic chemists, with a scope covering authentication, sign/witness, audit, record repository and reporting functions and with support for single-step, multi-step and parallel syntheses. The application integrates with MDL structure and reaction registration services, with the MDL Logistics materials management solution, and with both MDL and proprietary customer content. MDL Notebook also accesses hosted content via the DiscoveryGate and ScienceDirect® platforms.

MDL® Registration



MDL Registration is a flexible, new-generation registration system for building a corporate substance and batch database. Researchers can register single substances, load batches via SDF files and use comprehensive functionality tuned to meet multiple registration needs. MDL Registration enables organizations to effectively satisfy their own rules for drawing and storing substance data. With all the features of a fully developed system, MDL Registration is ideal for global pharmaceutical companies as well as startup and biotechnology companies.

MDL® Plate Manager



MDL® Plate Manager is a central repository for plate and sample information that integrates with MDL data management and chemical registration tools. It provides comprehensive sample and container management to accommodate different scientific workflows and the needs of IT managers. By enabling researchers to redirect resources from logistical tasks to decision making, Plate Manager facilitates an efficient discovery process and becomes a vital part of a laboratory workflow management solution. With MDL Plate Manager scientists can import plates and samples; request and create new samples and plates; cherry-pick samples; reformat plate layouts; browse and search for plate and sample information; track sample volumes, concentrations, genealogy and location; and view and search by chemical structure and custom properties.

MDL® Assay Explorer®

MDL Assay Explorer is a powerful, customizable and extensible biological data management system that provides biologists with the unparalleled ability to capture, analyze and store all of their experimental results within the well-known Oracle environment. Assay Explorer's unique open API and flexible data model make Assay Explorer the only commercial application that offers the flexibility that biologists need to capture both results and methodology. At the same time, IT departments can easily add extensions and customize Assay Explorer so that it fits into their company's unique workflow. Combined with a range of MDL cheminformatic tools, Assay Explorer provides the means for centrally storing and integrating biological and chemical data.

- **MDL® Assay Explorer Visualizer:** An integrated module exposes the analytical and statistical power of the Partek® Pattern Visualization System®, allowing researchers to easily visualize plate-based data, interact with the views and run statistics to validate experiments
- **Assay Explorer for Excel:** Integrated functionality enables biologists to create, view and analyze experiments in the familiar Excel® spreadsheet environment, providing easy access to Excel's flexible calculation and graphing capabilities

MDL® ChemBio AE

MDL consultants developed MDL ChemBio AE as a storage and retrieval system for chemical and biological data in response to frequently cited customer needs. Designed with small to mid-sized discovery research organizations in mind, ChemBio AE delivers an out-of-the-box system that combines an easy-to-use interface, integration capability with other applications, and administrative tools for simplified management of the database. Utilizing ChemBio AE, scientists can register chemical compounds and view biological data stored in Assay Explorer or other biological repositories. Searching and viewing features allow scientists to retrieve information and compare chemical and biological data side by side. To adapt to specific projects, ChemBio AE enables system administrators to quickly configure elements such as pick lists without the cost and complexity of additional programming.

MDL® Reagent Selector

MDL Reagent Selector offers scientists engaged in medium- and high-throughput synthesis a set of integrated tools for searching, selecting, locating and obtaining compounds from in-house inventories and “shopping” for reagents using MDL Available Chemicals Directory. Developed for synthetic, medicinal and combinatorial chemists, Reagent Selector’s architecture also helps IT professionals easily administer and customize the system in a variety of ways to consolidate and accelerate the scientist’s workflow. Reagent Selector readily links to other systems, including MDL ISIS and MDL Logistics.

Data Analysis and Visualization

MDL® QSAR

MDL QSAR is a comprehensive QSAR modeling system that enables scientists to establish reliable quantitative structure-activity and structure-property relationships, create new calculators for *in silico* screening and generate new compound libraries based on results—accelerating the discovery of lead compounds. MDL QSAR provides all the tools necessary to perform the most demanding QSAR analyses, including over 400 built-in 2D and 3D molecular descriptor calculators. Additionally, researchers can import their own or third-party descriptors or use measured endpoints as custom descriptors.

MDL® Carcinogenicity Module

Jointly developed by Elsevier MDL and the United States Food and Drug Administration (USFDA), the MDL Carcinogenicity Module predicts the toxicological activity of compounds based on structural properties. Scientists can use the carcinogenicity model built on the MDL® QSAR platform to screen, classify and prioritize compounds based on their predicted carcinogenicity risk. They can also search for and analyze related compounds in the USFDA/Center for Drug Evaluation and Research (CDER) rodent carcinogenicity database based on their chemical structure-related toxicological profiles.

Senior Management

Lars Barfod

President and CEO

Carmel Andrews

Senior Vice President,
Operations & Chief Financial Officer

Jean Colombel

Senior Vice President,
Sales & Services

Trevor Heritage

Senior Vice President and
Chief Scientific Officer

Howard Abels

Vice President and Chief Information Officer,
Information Systems and Technology

Bill Balke

Vice President,
Key Accounts

Greg Bartolo

Vice President,
Contract Management & Licensing

Carol Dockery

Vice President,
Business Operations

Doug Hounshell

Vice President,
Content Development and Production

David Hughes

Vice President,
Core Technology Product Management

John McCarthy

Vice President,
Consulting Services

Phil McHale

Vice President,
Solutions Product Management

Julie Page

Vice President,
Global Customer Care

Dana Ray

Director,
Human Resources

Media Contact

Jean Holt

Senior Director
Marketing & Communications
Tel: +1 (925) 543-5400
j.holt@mdl.com

Legal Contact

David Hall

Senior Legal Counsel
Tel: +1 (925) 543-7347
d.hall@mdl.com

About Elsevier MDL Worldwide Offices

USA Offices:

World Headquarters

Elsevier MDL
2440 Camino Ramon, Suite 300
San Ramon, CA 94583
TEL: +1 (925) 543-5400
FAX: +1 (925) 543-5401
Email: info@mdl.com

New Jersey

Elsevier MDL
60 Columbia Road-Bldg B, 2nd floor
Morristown, NJ 07960
TEL: +1 (973) 630-2000
FAX: +1 (973) 630-2001

Illinois

Elsevier MDL
2000 Clearwater Drive
Oak Brook, IL 60523
TEL: +1 (630) 288-8730
FAX: +1 (630) 288-8711

Tennessee

Elsevier MDL
OHS Products & Services
1281 Murfreesboro Pike, Suite 300
Nashville, TN 37217
TEL: +1 (615) 366-2000
FAX: +1 (615) 360-9538

European Offices:

Switzerland

Elsevier MDL
Gewerbstrasse 12
CH-4123 Allschwil 2
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Elsevier MDL
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FAX: +33-1-45 36 80 01

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Zweigniederlassung Koeln
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Germany
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FAX: +49-221-16025-68

Germany (MDL GmbH)

Elsevier MDL
Theodor-Heuss-Allee 108
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Germany
TEL: +49-69-5050-42-0
FAX: +49-69-5050 4245

UK

Elsevier MDL
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UK
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