Solutions—At Every Stage in the R&D Process

MDL Databases

MDL®
Information Systems, Inc.

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MDL Databases

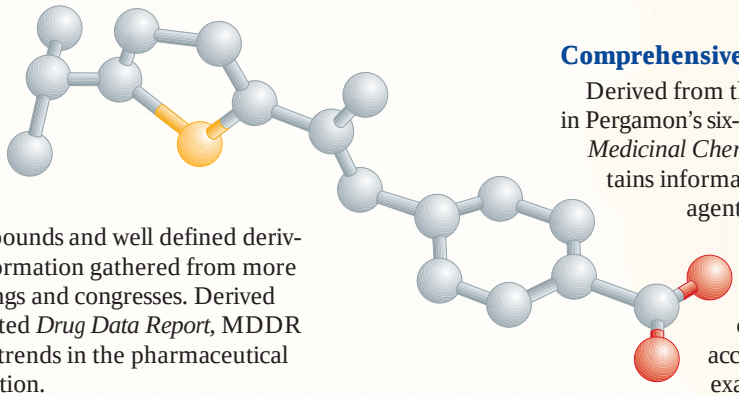
Many of the problems scientists encounter during research and development can only be solved with timely access to comprehensive information organized in an efficient, usable way. This is the rational that underlies the design, contents, and remarkable range of MDL electronic databases. Our databases contain a vast amount of chemical information; they can be searched easily by a number of methods, including by chemical structure; and they support every phase of the R&D process–from the development of hypotheses to the synthesis and testing of compounds, the refinement of results, the choosing of candidates, and the optimization of development processes. You can generate pharmacophores, for example, with our bioactivity databases; plan your syntheses or evaluate alternate development processes with our databases of synthetic methods; explore the metabolic fate of compounds, storing in-house experimental results with our metabolism information system; and stay up-to-date on the latest discoveries in genetics with our genomics database. If you need information on the price, purity, and safety of chemicals, MDL provides the world's largest collection of chemical supplier information and an extensive database of independently-researched Material Safety Data Sheets (MSDSs). MDL databases are always relevant, regardless of your area of biological or chemical research or where you are in the R&D process.

MDL databases are also specifically designed to complement and facilitate our information management solutions for chemistry, biology, genomics, automated synthesis and screening, materials science, and environmental health and safety. MDL software systems integrate multiple databases in a variety of ways to accommodate overlapping customer needs in all of these areas.

What follows is a brief overview of MDL databases and how they enable you to solve problems and make critical decisions. For more detailed information, please contact an MDL representative.

Generate Leads with MDL's **Bioactivity Databases**

Explore pharmacophores, evaluate hypotheses and the potential of lead candidates, select scaffolds and Rgroups for combinatorial libraries, perform SAR analyses, monitor industry trends—all with the aid of MDL's bioactivity databases. Our databases give scientists a head start on lead discovery by providing maximum leverage on what has already been done.



MDL Drug Data Report

Stay up-to-date and competitive with MDDR, which selectively covers patent literature from 11 international patent offices. This database contains biologically relevant compounds and well defined derivatives, and is supplemented by information gathered from more than 1,500 journals and 300 meetings and congresses. Derived from Prous Sciences' highly-respected *Drug Data Report*, MDDR keeps you informed about current trends in the pharmaceutical industry—and about your competition.

MDDR—especially MDDR-3D, with its capacity for conformationally-flexible substructure searching—is ideal for identifying pharmacophores and refining pharmacophore models. MDDR can help you develop the right scaffold and Rgroups for a combinatorial library. Researchers can use the structure activity data to select a scaffold for an area of therapeutic interest by analyzing scaffolds of new drugs in the same area.

Comprehensive Medicinal Chemistry

Derived from the Drug Compendium in Pergamon's six-volume *Comprehensive Medicinal Chemistry*, CMC-3D also contains information on pharmacological agents and logP and pKa values. The capacity for 3D searching provides researchers with very convenient and flexible access to the data. For example, a scientist can easily perform a conformationally-flexible substructure search to determine whether a pharmacophore has the same 3D arrangement of functional group atoms as a well tested compound that exhibits the desired biological activity.

Explore Metabolic Fate with MDL's **Metabolism Database**

With help from MDL's database of metabolic transformations, medicinal chemists can guide the structure-based design of novel, in vivo efficacious pharmaceuticals by blocking undesirable degradation pathways or by allowing metabolic clearance through a planned pathway. Perhaps a company's most valuable metabolism data is generated from in-house studies. By storing it in an electronic database, researchers can share this data throughout a corporation and utilize it in future studies.

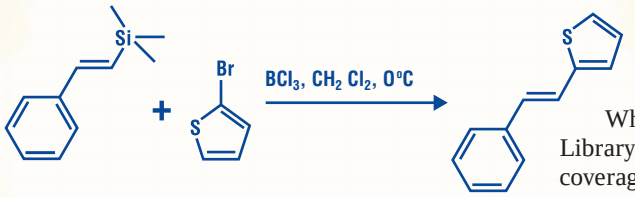
Metabolite

A complete metabolism information system, Metabolite includes an extensive database of metabolic transformations of xenobiotic compounds, the Metabolite Browser for searching and displaying metabolic schemes, and the Metabolite Registrar for adding proprietary research. Covering research since 1901, the database contains abstractions of both *in vivo* and *in vitro* studies, and provides all of the necessary information on metabolic transformations and associated data. Metabolism studies are selected by reviewing over 40 relevant metabolism journals. In addition, studies reported in *New Drug Applications* (NDAs) are entered into the database as the information becomes nonproprietary.

Plan the Synthesis of Novel Compounds with MDL's
Synthetic Methodology Databases

MDL designs its synthetic methodology databases to facilitate the synthesis of novel compounds. We select reactions based on synthetic methodology, enabling researchers to develop plans for novel syntheses when preparatory methods do not exist. Chemists can also use MDL's synthetic methodology databases to plan solution-phase and solid-phase combinatorial libraries. We have developed each database in the synthetic methodology group to complement the scope and chemistry of the others. The coverage ranges from functional group transformations to heterocyclic chemistry to metal-mediated and enzymatic transformations to solid-phase chemistry.

ChemInform Reaction Library



The premier synthetic methodology database, this compilation of 100 years of chemistry literature is selected, abstracted, and organized by FIZ CHEMIE Berlin, and then classified according to reaction type using InfoChem's reaction classification technology. Unlike databases oriented towards the preparation of specific compounds, ChemInform RXL's focus is on unique and novel methodologies so that when you decide to synthesize a new molecule, you have a *range* of synthetic methods from which to choose and a far better selection of relevant examples.

One of the most important issues when performing a synthesis is the scope and limitations of a given methodology. ChemInform RXL addresses the aspects of selectivity in synthesis by providing several examples for reactions or methodologies that illustrate the effect of substituents, the topology of the substrate, stereochemistry, and reaction conditions.

Solid-Phase Organic REactions

A perfect complement to MDL's solution phase reaction databases, SPORE contains extensive data from solid-phase organic chemistry, including polymeric materials, linkers, solid supports, and protecting groups. Developed jointly by MDL and FIZ CHEMIE Berlin, SPORE comes with an application that allows point-and-click access to the data, enabling chemists to make informed decisions when planning their solid-phase syntheses. Updated quarterly, SPORE provides comprehensive information in this rapidly expanding area of chemistry.

Reference Library of Synthetic Methodology

Reference Library combines reactions from a wide variety of sources into a single database, covering the synthetic chemistry literature from 1946 to 1991—from functional group transformations and metal-mediated transformations to the synthesis of chiral compounds. Providing convenient access to established methodologies, the database includes reactions from Dr. William Theilheimer's *Synthetic Methods of Organic Chemistry*.

Current Synthetic Methodology

Produced jointly with FIZ CHEMIE Berlin, CSM provides quick and easy access to the most innovative and significant reactions since 1992. This database emphasizes new synthetic methodologies, novel organic reactions, reactions which use a new reagent or an important modification of a known reagent, and regio-, chemo-, and stereo-selective reactions carried out on multifunctional substrates. Whereas the ChemInform Reaction Library abstracts several representative reactions for a reported methodology, CSM selects only the most novel methodologies for representation in the database. When combined with Reference Library, the two databases provide excellent coverage of the novel synthetic methodologies published since 1946.

REACCS-JSM

An electronic version of the *Journal of Synthetic Methods*, published by Derwent Information Limited, REACCS-JSM compiles chemical reaction literature from international journals and patent sources, and contains detailed information about new synthetic methods, high-yield functional group transformations, improvements to existing methodologies, and reactions representative of the most significant new patents. REACCS-JSM is the only database to extend the selection criteria established by Dr. William Theilheimer. In addition, the database includes worldwide patent literature information.

ORGSYN

An electronic version of the entire series of *Organic Syntheses* (first published in 1921), ORGSYN provides simple, graphical access to information that manual searches would take hours or days to find. For example, in just seconds you can locate preparations of a specific compound by sketching the target structure and initiating a search (each preparation has already been independently tested before being included in the database). ORGSYN also contains information on product purity, product yield, and hazards, as well as references to the original procedures and journal sources.

Comprehensive Heterocyclic Chemistry

CHC provides quick and easy access to data on heterocycles, which account for up to 75 percent of the new chemical entities introduced for human therapeutic use. Based on the popular, eight-volume compendium *Comprehensive Heterocyclic Chemistry* published by Pergamon Press, this database covers 100 years of chemistry (through 1983) and focuses on the synthesis of heterocyclic compounds, reactions of heterocyclic systems, and the use of heterocycles as synthetic precursors. Literature on heterocyclic synthesis published after 1983 is now covered in MDL's ChemInform Reaction Library.

THEILHEIMER

This database of high-yield functional group transformations and synthetic methods contains all reactions from Volumes 1-35 (1946-1980) of Dr. William Theilheimer's *Synthetic Methods of Organic Chemistry*, published by Karger.

Make Informed Purchasing Decisions with MDL's **Chemical Supplier Databases**

Streamline the complex process of locating, evaluating, and purchasing compounds with MDL's industry-standard databases of supplier information.

Available Chemicals Directory

An electronic collection of the complete catalogs from every significant chemical supplier, ACD provides all of the information you will need to locate the commercial sources of chemicals, compare price, purity, and grade, and select the particular products that meet your requirements. The ACD/Finder application offers easy access to the ACD database, entirely eliminating slow, error-prone manual searching and allowing users to search by chemical structure, substructure, or similar structure, chemical name or synonym, and CAS Registry Number. ACD can help you select Rgroups for combinatorial libraries, find scale-up alternatives, and avoid unnecessary syntheses by finding suitable starting materials and intermediates. Scientists can even access chemical safety information through an application that links ACD to MDL's database of Material Safety Data Sheets. The information available in ACD can also be loaded into inventory systems. MDL's Professional Services organization can assist customers in developing complete chemical inventory systems for compounds acquired through ACD, as well as ordering systems and interfaces to purchasing systems.

Available Chemicals Directory-Screening Compounds

Designed to complement ACD, the Available Chemicals Directory-Screening Compounds consolidates supplier data from several new vendors with product lines and sample collections specifically designed to meet the demands of high-throughput screening programs.

ACD-SC's initial release contains over 500,000 structures, merging over 700,000 individual compounds from ten companies. MDL ensures that the structures are chemically consistent and identifies and flags any duplicates. ACD-SC includes 3D models so scientists can use 3D search and analysis tools to assess diversity and locate compounds of interest. ACD-SC comes with easy-to-use search and display software based on MDL's field-tested ACD-Finder. As with all of our databases, ACD-SC is refined and updated on a regular basis.

Meet Health and Safety Challenges Using MDL's **Chemical Safety Databases**

Environmental health and safety information is as important as any other data required for chemical research and for handling chemicals in general. MDL specializes in providing the most current and comprehensive safety data available.

The OHS Safety Series

Covering thousands of pure substances and chemical mixtures, OHS MSDS databases are ideal for finding health, safety, and regulatory information about chemicals for research or scale-ups and for complying with OSHA, EU, and WHMIS regulations. MDL's OHS Material Safety Data Sheets (MSDSs) are complete, consistent, and reliable. All of our data sheets are independently researched and include detailed information on toxicology, exposure limits, storage, environmental impact, government regulations—and much more. Every MDL MSDS is formatted according to ANSI Z400.1, a 16 section format which meets requirements worldwide. MDL also ensures that the same type of data is located in the same place on each MSDS. The OHS Cornerstone and Reference databases are updated quarterly, and can be provided with optional one- to two-page summary sheets written in simplified language for easy reference and training of workers at all levels. These databases come with the popular MSDS Intranet Search Software, and can be linked to the Available Chemicals Directory. MDL also provides the Pure Substance Database in a growing list of European and other languages.

For a self-contained, desktop approach to health and safety reference data, try OHS MSDS ON DISC. The database software allows you to search and print MSDSs or summary sheets quickly and access the Related Code of Federal Regulations either directly or from within an MSDS.

MDL also offers OHS MSDS Outsourcing and Inventory Match services. OHS MSDS Outsourcing is a service MDL provides to chemical manufacturers, writing, updating, and translating high-quality MSDSs for their products. With Inventory Match, MDL will customize a database to cover all of the substances in a company's inventory, writing new MSDSs where necessary and updating them on a regular basis.

Access Secure, Up-to-Date Genomics Data with MDL's **Genomics Database**

The volume of data resulting from large scale gene sequencing projects is growing rapidly, and scientists have a critical need for the most up-to-date information. Sequence data is key to the development of gene therapies and diagnostic products, and to accelerating small molecule discovery projects by identifying the best targets for biological testing. A centralized, in-house source of genomic data makes access easier and more secure.

Genomes Today

Genomes Today is a daily feed of the latest published discoveries from genetics research and includes full sequence data with associated annotations. The data is collected in cooperation with the major DNA sequence database sources and is subjected to a series of quality checks. The database provides all of the data in valuable public genomics databases in a relational format that can be searched and annotated with proprietary information within the security of your own network. The data feed is easily automated to run unattended and at off-peak hours. Genomes Today is accessible using MDL's BioMerge or Bioinformatics Workbench software.

About MDL

MDL Information Systems, Inc. is a leading provider of integrated solutions to industrial, government, and academic producers and users of chemical and biological products. Our pioneering software systems, databases, and services help customers manage, communicate, and analyze the volumes of data associated with modern research, manufacturing, and business workflows. MDL has specialized applications in the areas of chemical and biological information management, bioinformatics, automated synthesis and screening, materials science, and environmental health and safety. MDL has offices worldwide with headquarters in San Leandro, California.

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