

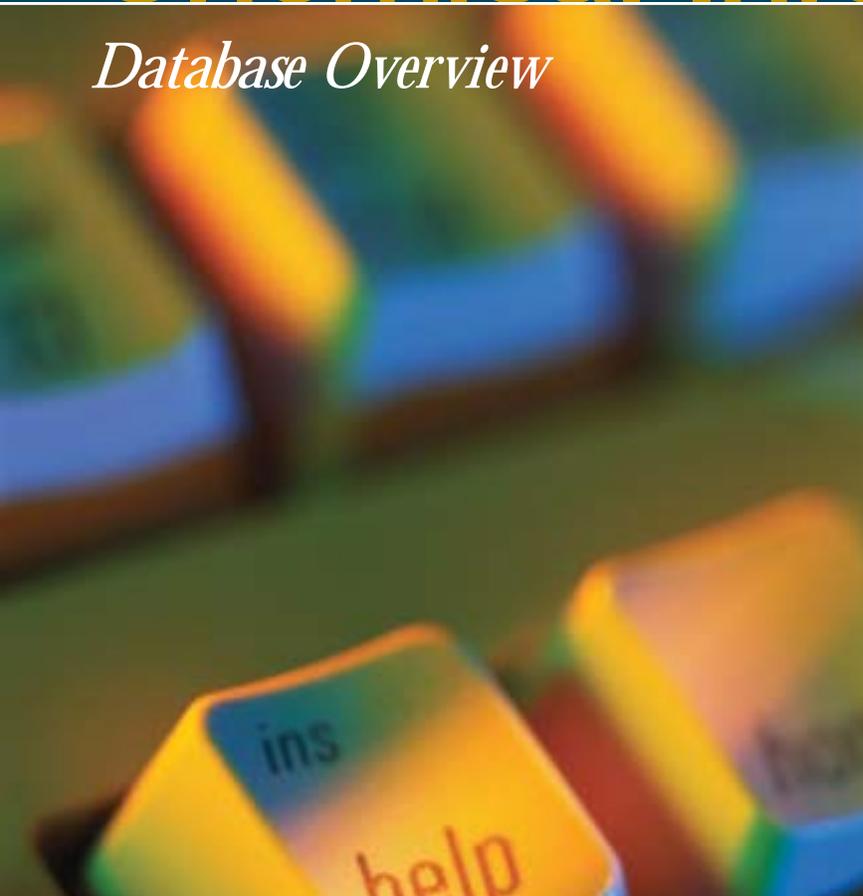
MDL® DISCOVERY KNOWLEDGE



discovery

Chemical Information

Database Overview



MDL Discovery Knowledge puts vast amounts of chemical and biological information at your fingertips. Search by any number of methods, including chemical structure. Or work with MDL Consulting to leverage the contents in custom discovery applications, such as chemical inventory systems. The table below highlights the depth, breadth, and utility of MDL Discovery Knowledge products.

Database Field Content	Chemistry Information		Synthetic Methodology Information										Pharmacology Information		Metabolism and Toxicology Information	Sourcing and Logistics Information	Chemical Safety Information				
REACTIONS																					
<i>Behavior</i>																					
Reagents	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
<i>Reaction Details</i>																					
Derivative Reactions	✓		✓					✓													
Mapping	✓		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
Markush-Like Reaction Scheme			✓					✓								✓					
Reaction Classification			✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
Reaction Conditions	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
Solvent	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
Yields	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
<i>Systematic</i>																					
Preparations	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
Synthetic Methods	✓		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
SUBSTANCES																					
<i>Biological Data</i>																					
Enzyme/Isoenzyme																✓					
Metabolism and Degradation Pathways	✓															✓					
Pharmacological Data	✓	✓											✓	✓	✓	✓					
Route of Administration and Excretion	✓	✓														✓	✓				
Species	✓															✓	✓				
Stability in Soil	✓												✓	✓							
Toxicity	✓															✓	✓				
<i>Chemical Data</i>																					
Characterization	✓	✓							✓	✓	✓	✓									
Isolation	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
MSDS																		✓			
Preparation	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
Reactivity	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓						
Stability	✓	✓							✓	✓	✓	✓									
Thermochemical and Electrochemical Data	✓	✓																			
Use	✓	✓							✓	✓	✓	✓		✓	✓						
<i>Physical Data</i>																					
logP	✓																				
Magnetic and Electrical Properties	✓	✓																			
Optical Data	✓	✓				✓															
Physical State	✓	✓																			
pKa	✓												✓								
Safety Data	✓	✓						✓													
Spectral Data	✓	✓																			
<i>Supplier Information</i>																					
Catalog Number																		✓			
Package Size																		✓			
Price																		✓			
Purity																		✓			
Supplier Addresses																		✓			
CITATIONS																					
Availability of Experimental Details in Article			✓					✓													
Conference Proceedings														✓		✓					
Corporate Communications														✓	✓						
Link to Original Electronic Article	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓				
Literature References	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓				
Patent Citations	✓	✓						✓						✓	✓						
	CrossFire Beilstein	CrossFire Gmelin	ChemInform Reaction Library	Current Synthetic Methodology	Derwent Journal of Synthetic Methods	MDL Reference Library of Synthetic Methodology	MDL Solid-Phase Organic Reactions	ORGSYN Database	Comprehensive Asymmetric Catalysis	Comprehensive Organic Functional Group Transformations	Comprehensive Organic Encyclopedia of Reagents for Organic Synthesis	Science of Synthesis	ADDS Database	MDL Comprehensive Medical Chemistry	MDL Drug Data Report	National Cancer Institute Database	MDL Metabolite Database	MDL Toxicity Database	MDL Available Chemicals Directory	MDL Screening Compounds Directory	OHS Safety Series

MDL provides knowledge to support every stage of discovery R&D—from developing hypotheses through synthesizing and testing compounds to selecting and optimizing promising leads. Read on for an overview of six of the MDL Discovery Knowledge families.

***Synthetic methodology information:
better, faster synthesis of novel compounds***

Search by structure to locate starting materials and intermediates, design solution-phase and solid-phase combinatorial libraries, and develop plans for entirely novel syntheses. Full chemical coverage, plus a reaction classification algorithm from InfoChem GmbH that speeds searching and organization of search results.

- **ChemInform Reaction Library:** Emphasizing 100 years of new and novel methodologies; developed by FIZ Chemie Berlin
- **CrossFire Beilstein:** Over two centuries' worth of chemical preparations in organic chemistry
- **CrossFire Gmelin:** Over two centuries' worth of chemical preparations in inorganic and organometallic chemistry
- **Current Synthetic Methodology:** The most innovative and significant new reactions since 1992; developed by FIZ Chemie Berlin
- **Derwent Journal of Synthetic Methods:** General methods as published in the print publication of the same name; developed by Derwent Information
- **MDL® Reference Library of Synthetic Methodology:** Functional group transformations, metal-mediated transformations, chiral chemistry, and heterocyclic chemistry over the last 100 years (through 1991)
- **MDL® Solid-Phase Organic Reactions:** New and novel methodologies on solid support, including data describing polymeric materials, linkers, solid supports, and protecting groups; developed by FIZ Chemie Berlin
- **ORGSYN Database:** General methods as verified and published in the print series, *Organic Syntheses*
- **Comprehensive Asymmetric Catalysis:** Major reference work focusing on the review of catalytic methods for asymmetric organic synthesis; developed by Springer Verlag
- **Comprehensive Organic Functional Group Transformations:** Major reference work focusing on the construction, introduction, and interconversion of functional groups; developed by Elsevier Science
- **Encyclopedia of Reagents for Organic Synthesis:** Major reference work focusing on the preparation, handling, and use of reagents in organic chemistry; developed by John Wiley & Sons Ltd.
- **Science of Synthesis:** The world's most comprehensive major reference work covering functional group transformations and synthesis of compound classes; developed by Georg Thieme Verlag

***Pharmacology information:
smarter lead generation***

Explore pharmacophores and lead compound structure-activity relationships (SAR), select scaffolds and R-groups for combinatorial libraries, compare ecotoxicology and biodegradation profiles, and monitor industry trends.

- **MDL® Drug Data Report:** Current bioactivity findings for newly launched or developmental drugs; developed by Prous Science
- **MDL® Comprehensive Medicinal Chemistry:** Searchable 3D models plus important biochemical properties, including drug class, logP, and pKa
- **CrossFire Beilstein:** Key data describing bioactivity, chemical and physical properties, and ecological fate
- **AIDS Database:** Compiled by the National Cancer Institute (NCI) and provided as a public service to MDL customers
- **National Cancer Institute Databases:** NCI's CAS Registry, Plated Compounds, AIDS, and Cancer databases, offered as a public service to MDL customers

For more detailed information, visit the MDL Web site at www.MDL.com or contact the MDL office nearest you.

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About MDL

Over 1,000 life science companies supercharge their discovery engines with MDL software solutions to generate fresh ideas and make breakthrough discoveries. By synchronizing and streamlining the sharing and management of vital information and knowledge, we enable scientists to work more efficiently and invent drugs faster. This saves time, money, and lives. In support of our customers and the momentous challenges they face, everything we do must be reliable, resourceful, innovative, and insightful.

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ChemData/11-02/5k

Chemistry information: more informed investigations

The largest, most comprehensive electronic sources of their kind, MDL's chemistry information provides a single point of entry to over two centuries of collected chemical structures, substances, reactions, and facts.

- **CrossFire Beilstein:** Organic chemistry coverage
- **CrossFire Gmelin:** Inorganic and organometallic chemistry coverage

Chemical sourcing and logistics information: streamlined, cost-effective sourcing

Make informed purchasing decisions and cut costs by using MDL's industry-standard, structure-searchable databases of supplier information to locate, evaluate, and purchase compounds.

- **MDL® Available Chemicals Directory:** Complete catalogs from every major chemical supplier, consolidated in one easily searchable database
- **MDL® Screening Compounds Directory:** Consolidated supplier data for product lines and sample collections suited for high-throughput screening

Chemical safety information: more efficient handling and hazard communication

OHS MSDS authoring, reference, and hazard communication products provide the most current, comprehensive, and accurate safety data available.

- **OHS Custom Services:** Custom data services and hosting and delivery systems support EH&S data projects and enterprise MSDS distribution

- **OHS Hazard Communication:** Full-service tools for employee safety and compliance comprising vendor MSDS; validation with OHS Inventory Match; the centralized OHS MSDS HazCom System; Emergency Response through Chemtec; and OHS Fast Fax for on-demand MSDS access
- **OHS MSDS Services:** Content from the leader in MSDS development, including individual MSDS creation, MSDS translation, and fully outsourced MSDS authoring
- **OHS Reference:** Premium data to underpin enterprise EH&S systems, including the OHS Complete Reference System, OHS Global Reference System, OHS MSDS on Disc, OHS MSDS Pure Substance Database, OHS MSDS Mixture Substance Database, and OHS EH&S Data Elements

Metabolism and toxicology information: more viable pipelines

Conduct more targeted structure-based design by applying data about metabolic fate and toxic effects earlier in the discovery process. Benefit from published research, or store results generated in-house for future reference.

- **MDL® Metabolite Database:** The world's largest and most comprehensive collection of xenobiotic transformations, compiled from the primary literature, conference proceedings, and NDAs; includes a browser for searching and displaying metabolic schemes and a registrar for archiving proprietary studies
- **MDL® Toxicity Database:** Complete contents of the Registry of Toxic Effects of Chemical Substances (RTECS)® database from the US CDC, the GENE-TOX database from the US EPA, and the CCRIS database from the National Cancer Institute
- **CrossFire Beilstein:** Toxicological, lethal dose, and metabolism information combined with bioactivity data