DiscoveryGate® and SciFinder®

SciFinder from CAS and DiscoveryGate from Elsevier MDL both provide bibliographic, molecule and reaction and textual descriptive information.

- **For access to the chemical literature, SciFinder is the place to start.**

- **For access to highly detailed bioactivity, sourcing, synthesis, drug safety and pharmacology data profiles, DiscoveryGate is the place to start.**

SciFinder enables users to comprehensively search journal abstracts to find all new reported molecule structures, but offers few experimentally determined data values. DiscoveryGate offers the best solution to examine reaction, sourcing and experimental data from representative articles, patents and other sources. With over 434 million experimental data values, DiscoveryGate excels at delivering more structure, bioactivity, synthesis and sourcing information to help scientists gain new insights into structure-activity relationships, discover new synthetic routes to novel compounds and save time in acquiring commercially accessible starting materials.

SciFinder

SciFinder is an application for searching five databases listed below.

- **Chemical Abstracts Plus**: a bibliographic database that covers journals, patent documents, technical disclosures and reports, books, conference proceedings, dissertations, electronic-only journals and Web preprints from 1907 to the present, with additional records for patents and journal articles dated before 1907.
- **CAS REGISTRY File**: a substance database containing records for substances identified by the Chemical Abstracts Service Registry. It contains organic and inorganic substances and protein and nucleic acid sequences.
- **CASREACT File**: a chemical reaction database with reaction information derived from journal and patent documents from 1840 to the present; contains single- and multi-step reactions.
- **CHEMLIST**: a database that identifies substances from inventories and regulatory lists from around the world; contains substance identity information, inventory status, source of information and summaries of regulatory activity, reports and other compliance information.
- **CHEMCATS**: a catalog file containing information about commercially available chemicals and their worldwide suppliers. Records contain catalog information for the substance provided by the supplier, e.g., the catalog name, chemical and trade names, grade information, CAS Registry Number, structure diagram, properties, regulatory information and prices.

SciFinder is best used to:

- Search cover-to-cover over the abstracts of nearly 1,500 key chemical journals for bibliographic information
- Determine if a given specific chemical structure is novel (not previously reported) and what its CAS Registry Number is
- Find records with common concepts using thesaurus text searches such as "resistance to antibiotics in pigs"
- Search over patents and articles with nucleic acid sequences

SciFinder content contains very few excerpted experimental values. CAS mitigates this deficiency by supplementing the CAS Registry File with over 1 billion *calculated* properties. Although calculated properties can be useful in some situations, they do not replace experimentally measured values.

DiscoveryGate

DiscoveryGate is an online content platform from Elsevier MDL with four linked applications (Database Browser, xPharm®, Integrated Major Reference Works and PharmaPendium™) for accessing 22 databases covering bioactivity, sourcing, synthesis, drug safety and pharmacology data.

DiscoveryGate is best used to:

- Find methods to synthesize new and existing compounds and determine the scope and limitations of synthetic methods, including representative reactions with general synthetic application, retrosynthetic schemes, highly specific reaction protocols and closely related information from *Science of Synthesis*[*], *Comprehensive Functional Group Transformations* and *Comprehensive Asymmetric Catalysis* reference works. All reactions can be linked and sorted by similarity using ChemInform Reaction ClassCodes.
- Associate structures with experimentally determined property data from selected articles and patent documents including ADMET profiles and over 11,000 metabolic schemes.
- Find drug safety information from the full text of hundreds of FDA Approval Packages and overviews of related pre-clinical, clinical and post-market safety data
- Delineate the pharmacology relationships among molecular targets, agents, related disorders and the principles that govern their interactions.
- Compare supplier data from multiple catalogs on the same page and order chemicals
- Use cross-referenced records to bring disparate data onto a single display page (e.g., link reactants to sourcing data, metabolism data to pharmacology relationships and link newly reported drugs to drug safety information).
- Link to data outside of DiscoveryGate, including Derwent WPI, ISI Current Chemical Reactions, Index Chemicus, PubChem and GeneGo (available October 2006) to find additional patent, reaction and biological activity information.
- Link molecules and reactions from applications external to DiscoveryGate to compile bioactivity, sourcing, synthesis, drug safety and pharmacology data profiles.

In contrast to SciFinder content, DiscoveryGate databases contain extensive *excerpted experimental data* from journals, patent documents, chemical catalogs, major reference works and FDA Approval Packages. This content is searchable by applications that are interlinked to retrieve closely related results from all databases from a given query. DiscoveryGate content provides a focused list of publications containing descriptive, explicative information.

DiscoveryGate and SciFinder Content July 2006

	Articles or Patent Documents Excerpted	Molecules	Single and Multi-step Reactions	Experimental Properties	Calculated Properties
SciFinder	24+ M	25+ M	<10 M	Few	1+ B
DiscoveryGate	3.4+ M	20+ M	>12 M	545+ M	110+ M

[*] *Science of Synthesis* is not available via DiscoveryGate for academic market

Data Sources and Applications Available on DiscoveryGate

- **Database Browser** accesses 17 bioactivity, chemical sourcing, synthesis and index databases from Elsevier MDL and other providers listed below.
- **Integrated Major Reference Works** offers synthetic methodology information and chemistry reference works from three major publishers listed below.
- **xPharm** is a unique electronic reference work of information on pharmacology principles, molecular targets, agents and related disorders.
- **PharmaPendium**, the essential drug safety resource, provides researchers with unprecedented access to best-in-class content, including searchable FDA Approval Packages.

Category	Application Data Sources
Index Database	Database Browser (**17 databases** below plus Derwent World Patents Index, ISI Current Chemical Reactions, ISI Index Chemicus and PubChem indexed in Compound Index) **MDL® Compound Index**
Bioactivity	**MDL® Drug Data Report** **MDL® Comprehensive Medicinal Chemistry** **MDL® Metabolite Database** **MDL® Toxicity** **National Cancer Institute Databases** **CrossFire Beilstein** **MDL® Patent Chemistry Database**
Chemical sourcing	**MDL® Available Chemicals Directory** **MDL® Screening Compounds Directory**
Chemistry	CrossFire Beilstein **CrossFire Gmelin** MDL® Patent Chemistry Database
Synthetic methodology	**ChemInform Reaction Library** **MDL® Solid-Phase Organic Reactions** **MDL® Reference Library of Synthetic Methodology** **Current Synthetic Methods (subset of ChemInform Reaction Library)** **Derwent Journal of Synthetic Methods** **ORGSYN** Integrated Major Reference Works (3 reference works) *Comprehensive Asymmetric Catalysis* (Springer-Verlag) *Comprehensive Organic Functional Group Transformations* (Elsevier) *Science of Synthesis* (GeorgThieme Verlag)* * not available for academic market
Drug safety	PharmaPendium FDA Approval Packages** *Mosby's Drug Consult*™** Adverse Event Reporting System** *Meyler's Side Effects of Drugs, 15th edition*** **Offered through PharmaPendium
Pharmacology	xPharm® xPharm Reference Work