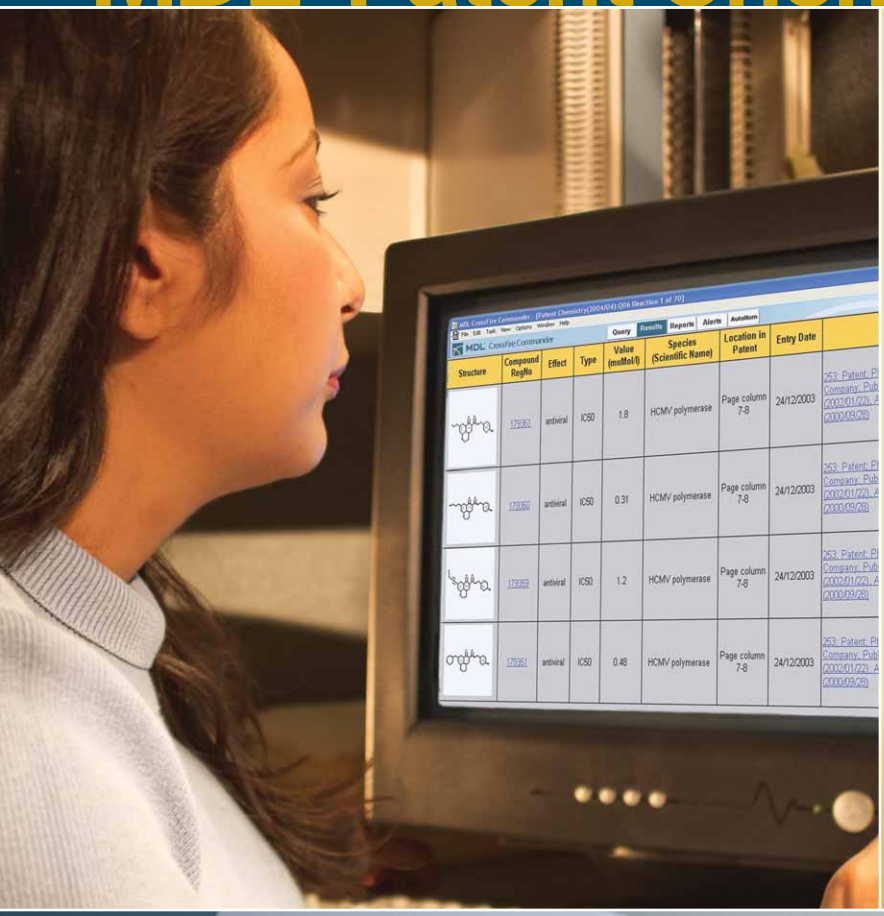
MDL® Patent Chemistry Database



Chemical reactions and substance data for scientists

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Finding reactions, substances and associated information in patent literature is an essential part of lead discovery. Expedite these essential searches with the structure-searchable MDL® Patent Chemistry Database, which provides access to over 28 years of organic chemistry and life science patents.

Powerful searching, experimental details on your desktop

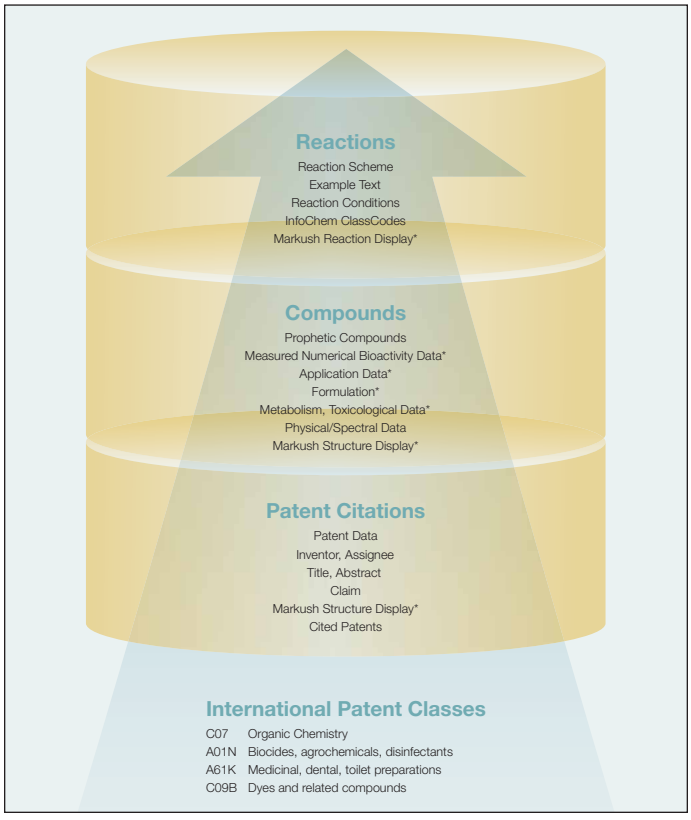
While much information on synthetic chemistry is published in journals, many novel substances, chemical reactions and processes appear only in patent documents. This makes patent databases a key information source in chemistry and life sciences research. Structure-based searching is a powerful and flexible way to mine highly relevant information from this vast source of information.

The MDL Patent Chemistry Database is structure-searchable and designed specifically for research scientists. It contains chemical reactions together with their complete experimental text from the patent document, as well as organic, inorganic, organometallic and polymeric* compounds and associated data. These are taken from World and European organic chemistry and life science patent publications since 1978, and U.S. patent publications since 1976. The MDL Patent Chemistry Database can be used to search for substances, develop drug profiles, select and optimize leads, design new synthetic methods and monitor competitor activities and industry trends.

Updated every two weeks, the MDL Patent Chemistry Database can be searched via MDL® CrossFire® Commander and DiscoveryGate® platforms.

Patent Chemistry Database highlights

- Displays Markush structures*, Markush reactions* and full claim text together
- Excerpts specific substances with data, as well as prophetic substances†
- Provides the full experimental text from the patent document in addition to the reaction scheme
- Contains substances with their bioactivity data and allows exporting to create structure-activity relationship tables



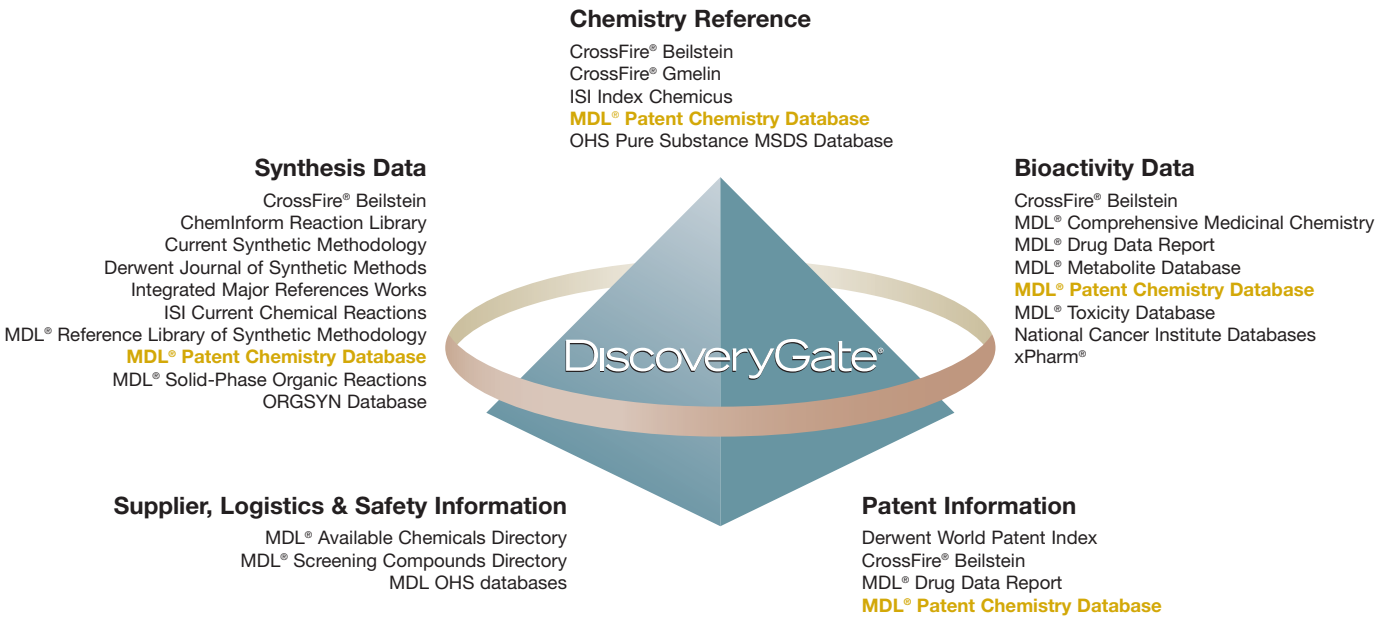
** Available from patent publications published beginning December 2003.*

† Prophetic compounds are patent-relevant compounds. The inventor states that they can be prepared analogously to described methods but gives no data (yield, physical properties, etc.). Typically, prophetic compounds can only be found as representatives of a generic structure from a Markush structure search.

Integration with other databases

MDL Patent Chemistry Database is integrated into DiscoveryGate, which allows researchers to use structure and text searches to explore patent information across a variety of integrated and complementary information sources such as Derwent Chemistry Resource/World Patents Index® or MDL Drug Data Report. All DiscoveryGate reaction databases are indexed with InfoChem ClassCodes.

MDL Patent Chemistry Database—Integration on DiscoveryGate



Find similar reactions in other MDL databases

Reactions in MDL Patent Chemistry Database and all other DiscoveryGate reaction databases are processed with InfoChem's CLASSIFY. This reaction classification algorithm categorizes reactions according to the type of chemical transformation they represent.

- Link to similar reactions in other DiscoveryGate reaction databases, Integrated Major Reference Works or ChemInform Reaction Library
- Group similar reactions
- Facilitate query formulations (Transformation Searches)

Find chemical reactions

By providing access to patent reaction data in an easy-to-search format interlinked to other important information sources, the MDL Patent Chemistry Database helps you develop effective synthesis plans based on a wider view of known chemistry.

More effective synthesis planning

- Provides the complete experimental section from the patent document
- Displays Markush* structures and reactions from the patent claim and patent description
- Interlinks, via Infochem ClassCodes, to ChemInform Reaction Library, Integrated Major Reference Works and other databases
- Summarizes all data for a given reaction derived from different patent documents

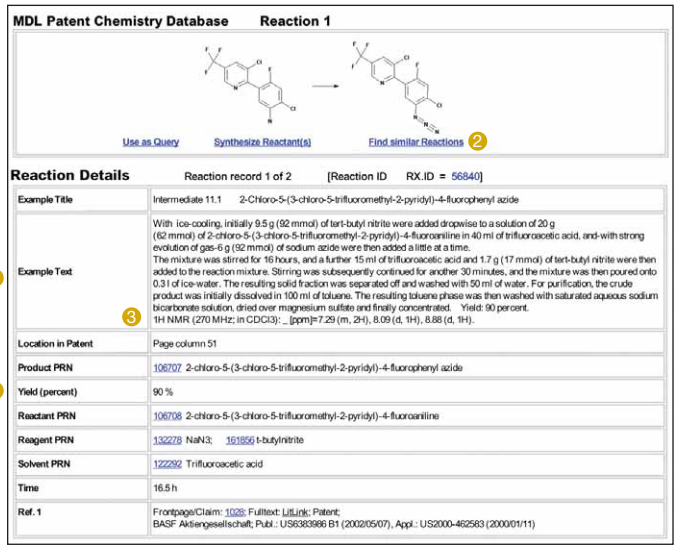
Find substances and their data

It is crucial to find the gaps in patent coverage for chemical processes, substances and their applications. Especially in the life sciences, researchers must compile comprehensive substance data sets for developing bioactivity profiles, selecting and optimizing leads or designing combinatorial libraries. By combining structural, text and numerical patent data with powerful visualization tools, the MDL Patent Chemistry Database helps you to quickly acquire an overview of compound and bioactivity information.

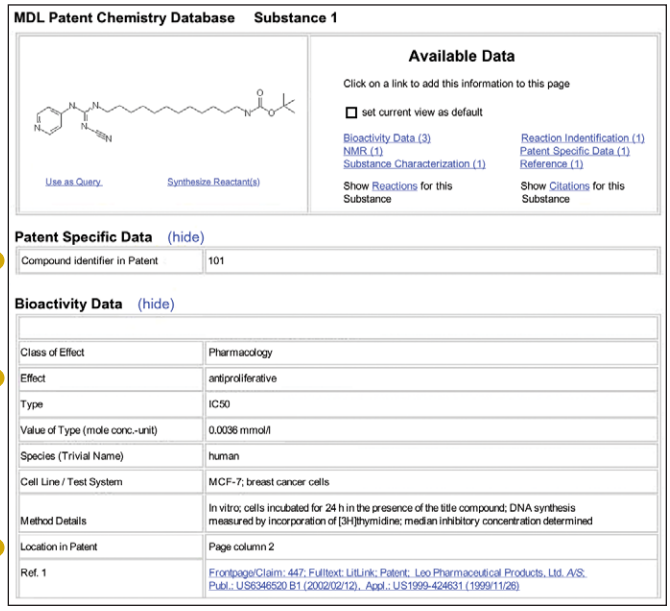
Better bioactivity profiling

- Provides searchable substance data including application and bioactivity data*, formulation*, spectral data (NMR, IR, UV, MS) including peak values and physical property data (e.g., logP)*
- Exports structures and their numerical bioactivity data into a tabular form, providing a clearly arranged structure-activity-relationship table
- Includes both defined and prophetic substances
- Displays Markush structures*
- Lists defined substances that are representatives of a given Markush formula and have been correlated to it*
- Collects all information for a given substance derived from different patent documents into one profile

Reaction hit set from a search using MDL Database Browser



Substance hit set from a search using MDL Database Browser



1. *Experimental Section: Almost all reactions have the full experimental section from the patent document.*
2. *InfoChem ClassCodes: This reaction classification enables integrated searches across all DiscoveryGate reaction databases and Integrated Major Reference Works.*
3. *Physical Data: Measured data including peak values and other physical data, e.g., logP, are often given for products.*
4. *Reaction Details: Specific conditions are in separate data fields.*

1. *Compound Identifier*: Compound number used in the patent document*
2. *Bioactivity Data*: Searchable numerical data (EC_{50}, IC_{50}, LD_{50}, etc.) plus details about bioassay and species used*
3. *Location in Patent*: Page where data appear in the patent document*

** Available from patent publications published beginning December 2003.*

Find patent citations

Quickly understanding the scope and relevance of patents enables you to save time, effort and money by avoiding patented compounds, reactions and processes. By bringing claim texts and Markush structures/reactions to the desktop in an easy-to-view format, the MDL Patent Chemistry Database helps you check the relevance of patent documents quickly and easily. The Patent Chemistry Database covers more than 360,000 patent publications (World and European since 1978, U.S. since 1976) and is updated every two weeks with the most current patents.

Easy relevance checking

- Displays Markush structures*, Markush reactions* and English-language claim text in addition to title and abstract for an easy-to-read display
- Appends indexed chemical structures and reaction schemes to the claim text
- Lists main patent family members (patent equivalents) under Publication/Application Data
- Links to patent full-text document providers including EspaceNet, US Patent Server and Delphion

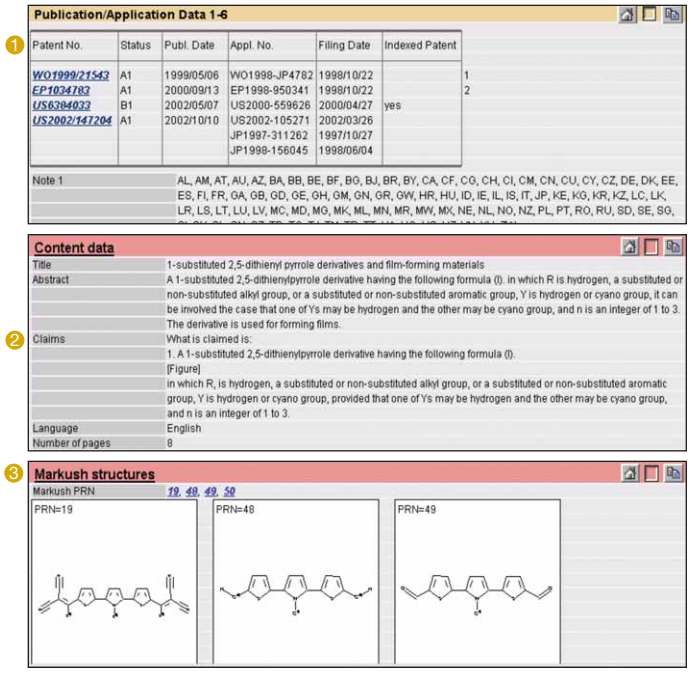
Display Markush structures and reactions

Displaying a specific Markush structure together with its related defined substances—the "**Markush Family**" gives a better understanding of the patent claim.

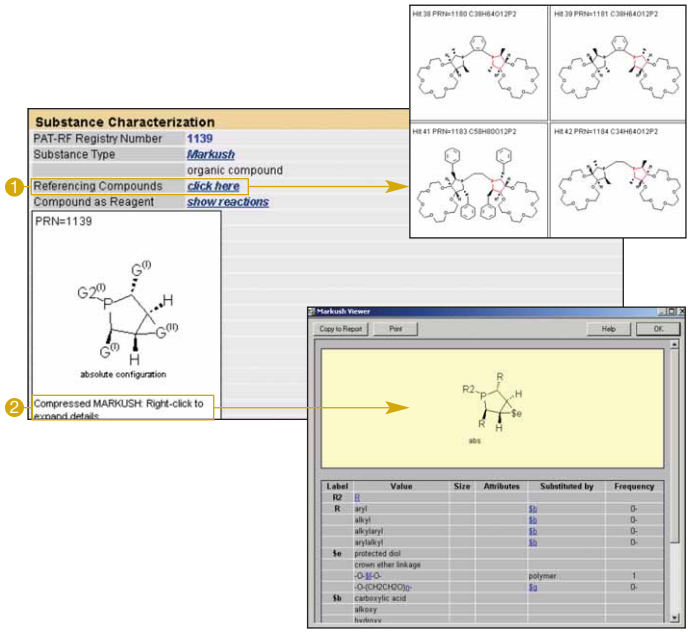
Better understanding of the claim

- Displays main Markush structures* from the claim text and patent description*. Substituents have the same symbols as in the patent full-text.
- Displays defined substances with their associated Markush formulae.

Citation hit set from a search using MDL CrossFire Commander 7.0



Markush structure display using MDL CrossFire Commander 7.0



❶ *Patent Family Members: Table lists main patent equivalents of a patent family (including the designated states for World and European patents*) with each patent number linked to the original patent document.*

❷ *Claim Text: Complete claim text is searchable.*

❸ *Markush Structure Display: The claim text is displayed together with the main cited Markush structures and reactions.**

❶ *Compounds related to Markush*: "Referencing Compounds" lists defined compounds that have been correlated to the given Markush structure.*

❷ *Compressed/Expanded Markush*: Markush structures are displayed schematically. Click on the Markush structure window to show the structure along with the meaning of all substituents. (Markush structures are not searchable.)*

** Available from patent publications published beginning December 2003.*

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Effective competitor watch

MDL Patent Chemistry Database is an effective tool both for investigating patent literature from the past and for continuous monitoring of competitors' R&D activities.

Create alerts

Once you have defined a specific query, an email query alert service automatically informs you of query hits relevant to your research at a frequency that you choose (every two weeks, monthly, etc.).

As the database is updated every two weeks, user-defined alerts will retrieve important new information on a regular basis.

Share alert results

Only the owner of the alert can view the alert results. However, you can share your results with colleagues by exporting your alert strategy and emailing it to them for implementation on their own system.

NOTE: At this time, the alert service is available only in CrossFire Commander 7.0.

Efficient access to chemistry patent literature

For fast, efficient access to chemistry patent literature, the structure-searchable MDL Patent Chemistry Database offers you the resources and tools to find the information you need quickly and easily. Updated every two weeks with in-depth information on chemical reactions, processes, substances and citations, the MDL Patent Chemistry Database is the essential first step in lead discovery.

For more information about the MDL Patent Chemistry Database, please contact an Elsevier MDL Account Manager or visit www.mdl.com.