



MDL DISCOVERY KNOWLEDGE

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# MDL Patent Chemistry Database



## Access over 28 years of chemistry patents

*Finding reactions, compounds 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.*

### Your first step in lead discovery

While much information on synthetic chemistry is published in journals, many novel compounds, chemical reactions and processes appear only in patent documents. This makes patent databases a key information source in chemistry and life sciences research. They are used to search for compounds, develop drug profiles, select and optimize leads, design new synthetic methods and monitor competitor activities and industry trends.

The MDL Patent Chemistry Database is a structure-searchable database designed specifically for research scientists and information professionals. Structure-based searching is a powerful and flexible way to mine highly relevant information from this vast source of information.

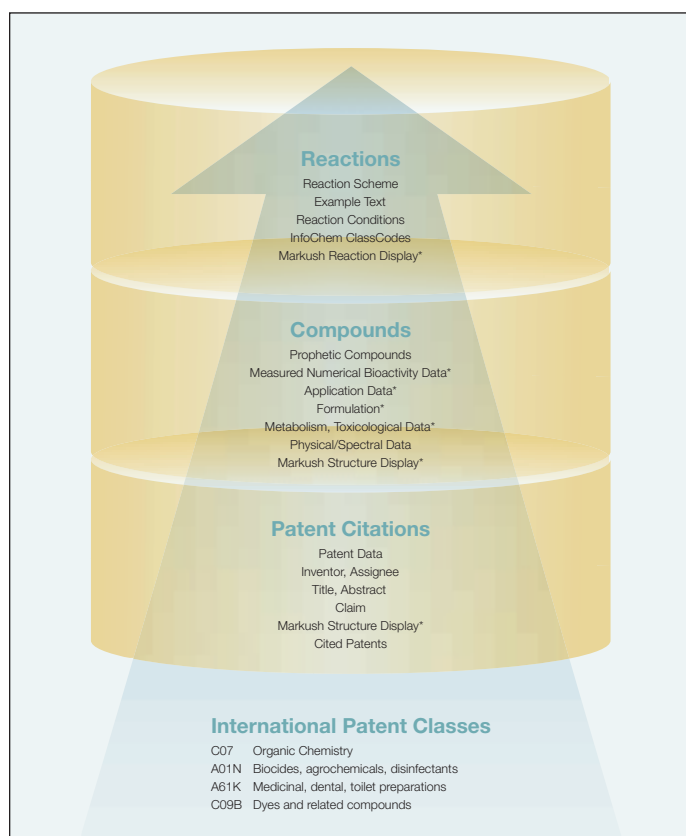
The first release of the MDL Patent Chemistry Database contains approximately 1.5 million reactions, along with over 1.6 million organic, inorganic, organometallic and polymeric\* compounds and associated data. These are taken from approximately 340,000 organic chemistry and life science patents (World, U.S. and European) since 1976.

### Powerful, flexible searching

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

### Patent Chemistry Database highlights

- Excerpts compounds and reactions with data, as well as prophetic compounds and analogous reactions<sup>†</sup>
- Incorporates complete and searchable claim text
- Displays Markush structures\*, Markush reactions\* and full claim text together
- Classifies all reactions with InfoChem ClassCodes, enabling seamless linking to similar reactions in all MDL databases and Integrated Major Reference Works



\* Available from patent publications published beginning December 2003.

<sup>†</sup> 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 MDL reaction databases are indexed with InfoChem ClassCodes.*

### Find similar reactions in other MDL databases

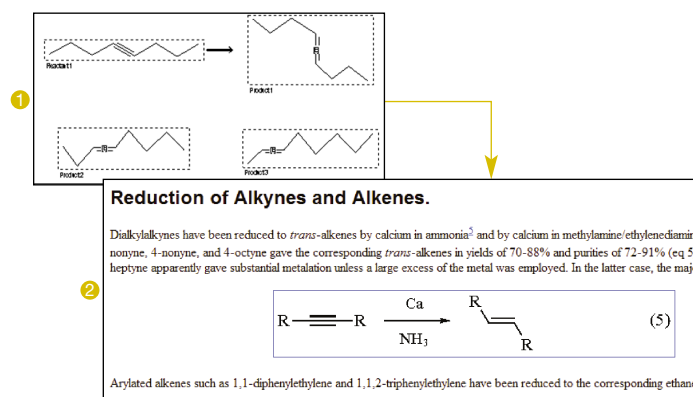
Reactions in MDL Patent Chemistry Database and all other MDL reaction databases are processed with InfoChem's CLASSIFY. This reaction classification algorithm categorizes reactions according to the type of chemical transformation they represent.

Indexing is based on changes occurring at atoms and bonds involved in the reaction (reaction center) and the immediate vicinity (alpha and beta atoms) and is expressed as a hash code (ClassCode).

InfoChem ClassCodes may be used to:

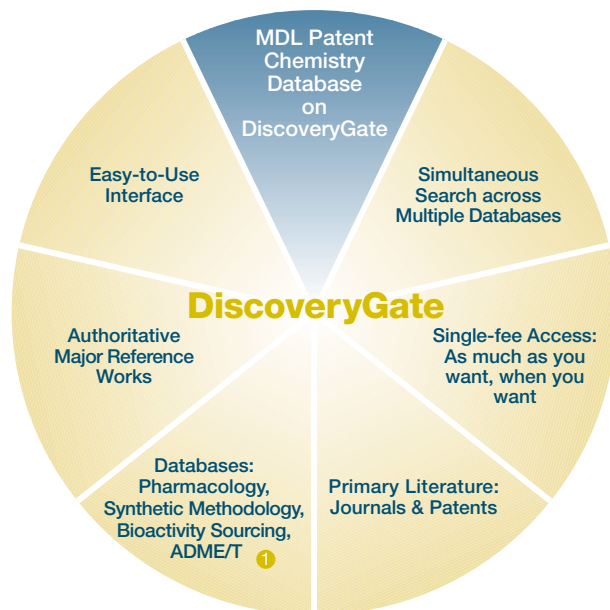
- Link to similar reactions in other MDL reaction databases, Integrated Major Reference Works or ChemInform Reaction Library
- Group similar reactions
- Facilitate query formulations (Transformation Searches)

Find similar reactions using InfoChem ClassCodes



- ① Reaction from MDL Patent Chemistry Database  
 ② Similar reaction in Integrated Major Reference Works

MDL Patent Chemistry Database—Integration on DiscoveryGate



### ① Synthesis

CrossFire Beilstein  
 CrossFire Gmelin  
 ChemInform Reaction Library  
 Current Synthetic Methodology  
 Derwent Journal of Synthetic Methods  
 ORGYSN Database  
 MDL Solid-Phase Organic Reactions  
 MDL Reference Library of Synthetic Methodology  
 ISI Current Chemical Reactions  
 ISI Index Chemicus

### Bioactivity

MDL Drug Data Report  
 MDL Metabolite Database  
 MDL Toxicity Database  
 National Cancer Institute Databases  
 MDL Comprehensive Medicinal Chemistry  
 xPharm  
 Derwent World Patents Index

### Sourcing

MDL Available Chemicals Directory  
 MDL Screening Compounds Directory



## 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 compounds and their data

It is crucial to find the gaps in patent coverage for chemical processes, compounds and their applications. Especially in the life sciences, researchers must compile comprehensive

compound 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 compound 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 compounds
- Displays Markush structures\*
- Lists defined compounds that are representatives of a given Markush formula and have been correlated to it\*
- Collects all information for a given compound derived from different patent documents into one compound profile

### Reaction hit set from a search using MDL Database Browser

**MDL Patent Chemistry Database Reaction 1**

Use as Query   Synthesize Reactant(s)   Find similar Reactions ②

**Reaction Details**   Reaction record 1 of 2   [Reaction ID   RX.ID = 56840]

Example Title	Intermediate 11.1   2-Chloro-5-(3-chloro-5-trifluoromethyl-2-pyridyl)-4-fluorophenyl azide
Example Text	With ice-cooling, initially 9.5 g (92 mmol) of tert-butyl nitrite were added dropwise to a solution of 20 g (62 mmol) of 2-chloro-5-(3-chloro-5-trifluoromethyl-2-pyridyl)-4-fluoroaniline in 40 ml of trifluoroacetic acid, and with strong evolution of gas 6 g (92 mmol) of sodium azide were then added a little at a time. The mixture was stirred for 16 hours, and a further 15 ml of trifluoroacetic acid and 1.7 g (17 mmol) of tert-butyl nitrite were then added to the reaction mixture. Stirring was subsequently continued for another 30 minutes, and the mixture was then poured onto 0.3 l of ice-water. The resulting solid fraction was separated off and washed with 50 ml of water. For purification, the crude product was initially dissolved in 100 ml of toluene. The resulting toluene phase was then washed with saturated aqueous sodium bicarbonate solution, dried over magnesium sulfate and finally concentrated. Yield: 90 percent. 1H NMR (270 MHz; in CDCl3): ... [ppm]=7.29 (m, 2H), 8.09 (d, 1H), 8.88 (d, 1H).
Location in Patent	Page column 51
Product PRN	106707   2-chloro-5-(3-chloro-5-trifluoromethyl-2-pyridyl)-4-fluorophenyl azide
Yield (percent)	90 %
Reactant PRN	106708   2-chloro-5-(3-chloro-5-trifluoromethyl-2-pyridyl)-4-fluoroaniline
Reagent PRN	132278   NaN3; 161856   t-butyl nitrite
Solvent PRN	122292   Trifluoroacetic acid
Time	16.5 h
Ref. 1	Frontpage/Claim: 1026; Fulltext: LitLink; Patent: BASF Aktiengesellschaft; Publ.: US638396 B1 (2002/05/07); Appl.: US2000-462583 (2000/01/11)

**MDL Patent Chemistry Database Substance 1**

**Available Data**

Click on a link to add this information to this page

☐ set current view as default

[Bioactivity Data \(3\)](#)   [Reaction Identification \(1\)](#)  
[NMR \(1\)](#)   [Patent Specific Data \(1\)](#)  
[Substance Characterization \(1\)](#)   [Reference \(1\)](#)

[Show Reactions for this Substance](#)   [Show Citations for this Substance](#)

**Patent Specific Data (hide)**

Compound Identifier in Patent	101
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**Bioactivity Data (hide)**

Class of Effect	Pharmacology
Effect	antiproliferative
Type	IC50
Value of Type (mole conc. -unit)	0.0036 mmol/l
Species (Trivial Name)	human
Cell Line / Test System	MCF-7; breast cancer cells
Method Details	In vitro; cells incubated for 24 h in the presence of the title compound; DNA synthesis measured by incorporation of [3H]thymidine; median inhibitory concentration determined
Location in Patent	Page column 2
Ref. 1	Frontpage/Claim: 447; Fulltext: LitLink; Patent: Leo Pharmaceutical Products, Ltd. A/S; Publ.: US6346520 B1 (2002/02/12); Appl.: US1999-424631 (1999/11/26)

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 MDL 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<sub>50</sub>, IC<sub>50</sub>, LD<sub>50</sub>, 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 initially covers approximately 340,000 World, U.S. and European patent publications from 1976 and is updated every two weeks with the most current patents.

### Easy relevance checking

- Lists main patent family members (patent equivalents) under Publication/Application Data.
- Provides English-language claim text in addition to title and abstract.

### Citation hit set from a search using MDL CrossFire Commander 7.0

**1** Publication/Application Data 1-6

Patent No.	Status	Publ. Date	Appl. No.	Filing Date	Indexed Patent
WO1999/21543	A1	1999/05/06	WO1998-JP4782	1998/10/22	1
EP1024783	A1	2000/09/13	EP1998-950341	1998/10/22	2
US6384032	B1	2002/05/07	US2000-559628	2000/04/27	yes
US2002/147204	A1	2002/11/01	US2002-105271	2002/03/26	
			JP1997-311262	1997/10/27	
			JP1998-156045	1998/06/04	

Note 1: AL, AM, AT, AU, AZ, BA, BB, BE, BF, BG, BJ, BR, BY, CA, CF, CG, CH, CI, CM, CN, CU, CY, CZ, DE, DK, EE, ES, FI, FR, GA, GB, OD, OE, OH, OM, ON, OR, OW, HR, HU, ID, IE, IL, IS, IT, JP, KE, KO, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MC, MD, MG, MK, ML, MN, MR, MW, MX, NE, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, SM, ST, SV, TD, TG, TH, TJ, TT, TZ, UA, US, UZ, VN, YU, ZA, ZM, ZW

**2** Content data

Title: 1-substituted 2,5-dithienyl pyrrole derivatives and film-forming materials

Abstract: A 1-substituted 2,5-dithienyl pyrrole derivative having the following formula (I), in which R is hydrogen, a substituted or non-substituted alkyl group, or a substituted or non-substituted aromatic group, Y is hydrogen or cyano group, it can be involved the case that one of Ys may be hydrogen and the other may be cyano group, and n is an integer of 1 to 3. The derivative is used for forming films.

What is claimed is:

1. A 1-substituted 2,5-dithienyl pyrrole derivative having the following formula (I).

[Figure]

In which R, is hydrogen, a substituted or non-substituted alkyl group, or a substituted or non-substituted aromatic group, Y is hydrogen or cyano group, provided that one of Ys may be hydrogen and the other may be cyano group, and n is an integer of 1 to 3.

Language: English

Number of pages: 8

**3** Markush structures

Markush PRN: 19, 48, 49, 50

PRN=19

PRN=48

PRN=49

- 1** 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.
- 2** Claim Text: Complete claim text is searchable.
- 3** Markush Structure Display: The claim text is displayed together with the main cited Markush structures and reactions.\*

- Appends chemical structures and reaction schemes to the claim text for easy-to-read display.
- Links to patent full-text document providers including EspaceNet, US Patent Server and Delphion.

## Display Markush structures and reactions

Displaying a specific Markush structure with its related defined compounds (compounds with data or prophetic compounds) gives you 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 compounds with their associated Markush formulae.

### Markush structure display using MDL CrossFire Commander 7.0

**1** Substance Characterization

PAT-RF Registry Number: 1139

Substance Type: Markush

organic compound

Referencing Compounds: [click here](#)

Compound as Reagent: [show reactions](#)

PRN=1139

**2** Compressed MARKUSH: Right-click to expand details

Markush structure display showing chemical structures and a table of substituents.

Label	Value	Size	Attributes	Substituted by	Frequency
R2	aryl	0			0
R	alkyl	0			0
	alkenyl	0			0
	alkynyl	0			0
S6	protected diol	0			0
	crown ether linkage	0			0
	di-OR	0			0
	di-OR(OH)2	0			0
Sb	carboxylic acid	0			0
	alkoxy	0			0
	hydroxy	0			0

- 1** Compounds related to Markush\*: "Referencing Compounds" lists defined compounds that have been correlated to the given Markush structure.
- 2** 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 release, 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, compounds 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](http://www.mdl.com).**

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PAT DB/11-04/5b