



Introduction to DiscoveryGate

Presented to Chulalongkorn University



What is DiscoveryGate?

- ❑ An internet service that increases the productivity of the drug discovery process.
- ❑ Allows one-query access to over 27 million compounds found in synthesis, bioactivity, physical property, and sourcing databases.
- ❑ Provides links to authoritative major reference works in synthetic chemistry.
- ❑ Provides links to over 15,000 journals and patent archives.

DiscoveryGate home page

The screenshot shows the DiscoveryGate home page with a dark blue header and a white main content area. The header includes the DiscoveryGate logo, a 'Quick Start Guide' link, and user settings for 'Chris'. A navigation bar contains 'Home', 'Support', and 'Logout chrismarth'. The main content is divided into several sections: 'How Do I?' with links to an 'Online Guide' and 'Flash Videos'; 'QuickSearch' with a search box and a 'start search' button; 'Applications' with links to 'Search Databases', 'Integrated Major Reference Works', and 'xPharm'; and a right-hand sidebar with 'FDC Reports - The Pink Sheet', 'My Company Links', and 'My Company Alerts'. A red box highlights the 'Applications' section, and a callout box points to it with the text 'Links to main DiscoveryGate search engines'. The footer contains copyright information and system requirements.

DiscoveryGate® Quick Start Guide Useful information to get you started

DiscoveryGate Chris' Settings Company Settings

Find the information you need Home | Support | Logout chrismarth

Quick Start Guide

How Do I?

- Online Guide**
Quickly view steps to complete common tasks. Query, browse and filter data with ease...
- Flash Videos**
Macromedia Flash video clips showing you how to complete various tasks...
 - [Molecule Search](#)
 - [Reaction Search](#)
 - [Data Search](#)

Administrator Quick Links

What Is New?

QuickSearch

Search all databases for which you have a license.

If you see a gray box below, [click here](#).

1. Double-click to draw structure

2. Select a **Search Type:** Automatic

? start search

Applications

- Search Databases**
Synthesis, bioactivity, physical properties, metabolism, toxicity or sourcing.
- Integrated Major Reference Works**
Review synthetic methods and learn about their scope and limitations.
- xPharm**
Browse pharmacology articles.

[Remove descriptive text](#)

FDC Reports - The Pink Sheet

My Company Links

My Company Alerts

© Elsevier MDL | Terms: rev.04-Apr-2005 System Requirements Layout: Standard view MDL-EdServices

Links to main
DiscoveryGate
search engines

Help for DiscoveryGate

The image displays a multi-windowed help system for DiscoveryGate. On the left, a 'How Do I?' sidebar lists 'Online Guide' and 'Flash Videos' with sub-links for 'Molecule Search', 'Reaction Search', and 'Data Search'. The top window, 'DiscoveryGate Quick Start Guide', lists categories like Searching, Personalize, and Support. The middle window, 'DiscoveryGate "How Do I Guide"', features buttons for 'Locate', 'Find', 'Identify', 'Compare', and 'Discover'. The bottom window, 'DiscoveryGate "What's New in DiscoveryGate"', contains a 'QuickSearch' section with 'Search Databases' and 'Integrated Major Reference Works', and a 'START' button for a lesson on 'Synthetic Methodology Information'. Red arrows connect the sidebar items to their corresponding content in the other windows. A large orange text box at the bottom left reads 'Interactive simulation'.

Interactive simulation

Today's objectives

- ❑ Conduct structure and data searches using the MDL Compound Index and individual databases
- ❑ View the search results using the Grid, Database, and Properties views
- ❑ Save search results and combine lists
- ❑ Link to literature
- ❑ Create reports
- ❑ Modify query forms and save as default forms
- ❑ Introduce synthetic methods

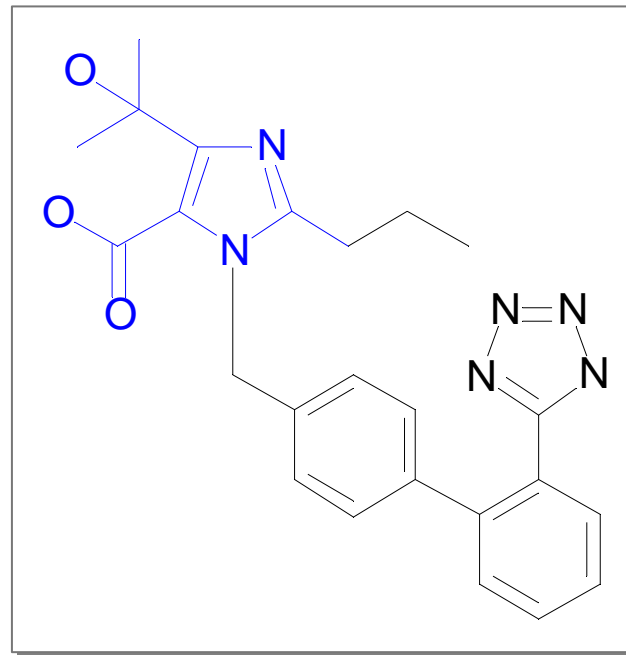
Structure searching

In this section, you will learn how to:

- ❑ Conduct an exact match and substructure search using the MDL Compound Index
- ❑ View search results using the Grid, Database, and Properties views
- ❑ Conduct a combination structure/data search

Search scenario




Olesmesartan is an antihypertensive agent, acting as an angiotensin II receptor agonist. You want to retrieve available information for the compound, as well as determine other known 2-alkyl-, 4-carboxy-, 5-alkylhydroxy-imidazole derivatives.



Draw the structure query

The screenshot shows the MDL Draw for the Web software interface. The main window displays a chemical structure of a complex organic molecule. The interface includes a menu bar (File, Edit, Chemistry, Help) and a toolbar with various drawing tools. Two tools are highlighted with red boxes: the Lasso tool (top left) and the All-Purpose Drawing tool (middle left). The right-hand side of the window contains a help panel with the following text:

Adding and sprouting atoms, atom lists, or templates using the keyboard

When either the Lasso tool , the Select tool , or the All-Purpose Drawing tool  is active, you can use **keyboard sprouting** to add or sprout an atom or template structure. Sprouting an atom or a template adds an extra single bond, whereas adding an atom or a template does not.

1. Click the atom where you want to add or sprout the atom or template structure, or click the drawing area to add a new one.
2. Do one of the following:
 - * To **add** an atom or template, click one or more atoms and type the name of the atom or

Conduct an exact match search

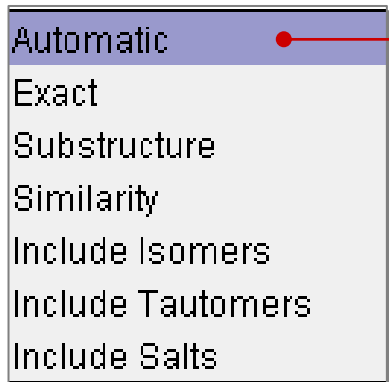
Compound Index looks at an index of molecules for all databases

The screenshot displays the DiscoveryGate MDL Database Browser interface. The main header includes the logo and navigation tabs for 'queries', 'results', and 'reports'. Below the header, there are links for 'start search', 'import', 'save', 'clear form', 'help', and 'logout', along with the text 'MDL® Compound Index'.

The interface is divided into several sections:

- Database:** A dropdown menu is set to 'MDL® Compound Index'.
- Find in Field Index:** A text input field is empty, with a 'Next' button to its right.
- Field Index:** A tree view on the left lists various categories: Molecular Formula, Molecular Weight, cdbregno, molstructure, Adverse Effects, Pharmacological, Physical Chemical, Preparation, Safety, Analytical, Structure based, Toxicity, and ADME. The 'Molecular Weight' category is currently selected.
- MolStructure:** A central area showing a chemical structure of a complex organic molecule.
- Select Search Type:** A dropdown menu is open, showing options: Substructure, Exact (highlighted), Include Tautomers, Include Isomers, Include Salts, Similarity, and Automatic.
- Search Criteria:** A row shows 'AND' in a dropdown, followed by 'Molecular Weight' in a text field, an equals sign (=) in a dropdown, and an empty text input field.
- Buttons:** 'start search', 'show brackets', and 'save form' are located at the bottom.
- Utility Links:** On the right side, there are links for 'Reset', 'Delete', 'Duplicate', and 'Info'.

Search types



DiscoveryGate conducts a series of searches until it retrieves at least one compound that matches your query. Each subsequent search is more general than the preceding search. The order is listed below.

- ❑ **Exact Match:** Search for substances that match your structural query exactly.
- ❑ **Include Isomers:** Search for all stereoisomers (all R and S configurations, all E and Z configurations, and so on).
- ❑ **Include Tautomers:** Search for all tautomers, and also for structures with different charges and different isotopes.
- ❑ **Include Salts:** Search for substances that include different salts.
- ❑ **Substructure:** Search for substances that contain your query wholly embedded within them.
- ❑ **Similarity:** Search for substances that are structurally similar to your query.

View the retrieved compound

DiscoveryGate® | MDL® Database Browser

queries results reports

copy to report export page setup print save refine query lists help logout MDL® Compound Index Version

Database: MDL® Compound Index ?

Find in History: Next

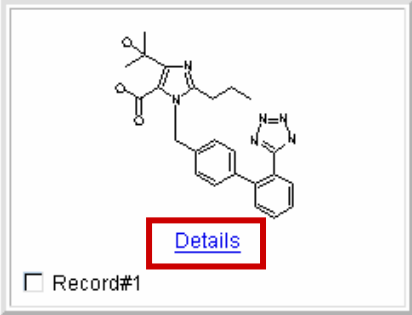
Field Index History

- Today's Searches
 - Search #1
- Previous Searches
- Saved Searches
- Temporary Lists

Grid View Database View Properties View Create List

View selected records in another database

Pages: 1 Select All Clear All Total Records: 1



Record#1

Pages: 1 Select All Clear All Total Records: 1

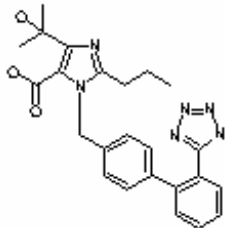
Grid View Database View Properties View Create List

View selected records in another database

View the detailed information

[Return to Search Results](#) [View selected records in another database](#) Record # 1 **Total Records: 1**

Also found in: [ACD](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [MDDR](#) [Metabolite](#) [Patent Chemistry](#)



[Use as Query](#)

 Select current record

Torsional degree of freedom	5
clogP (Syracuse Res. Center)	3.63
Molecular Formula	C24 H26 N6 O3
Mol. Weight/Largest Fragment	446.508
Proton Acceptors (O+N)	9
Molecular Weight	446.508
Total Polar Surface Area	129.81
Rule of Five	0
Proton Donors	3

[Return to Search Results](#) [View selected records in another database](#) Record # 1 **Total Records: 1**

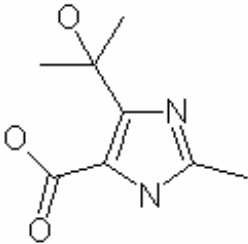
Also found in: [ACD](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [MDDR](#) [Metabolite](#) [Patent Chemistry](#)

Information for this compound can also be found in these databases.

Conduct a substructure search

Determine other known 2-alkyl-, 4-carboxy-, 5-alkylhydroxy-imidazole derivatives.

Structure



Select Search Type:

Substructure ▼

A Molecule Substructure search finds molecule records that contain your query as a substructure wholly within a larger structure.

Query Highlighting.

Substructure search rules:

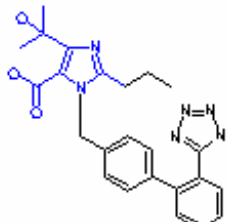
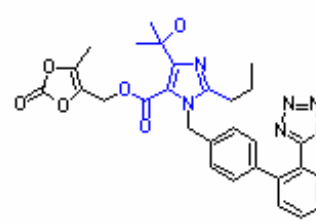
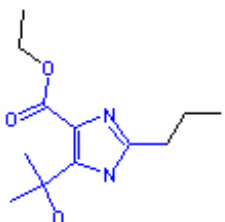
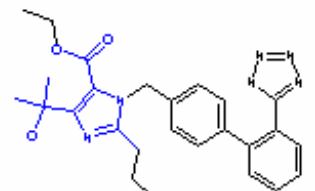
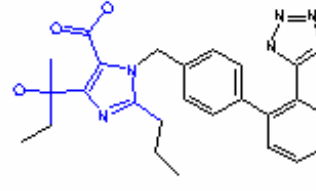
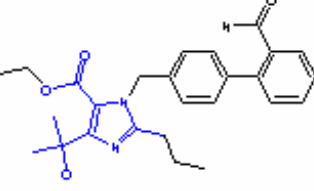
- The core structure must be embedded in all compounds retrieve
- Substitution can occur at any open valence

Substructure results – Grid View

Grid View [Database View](#) [Properties View](#) [Create List](#)

[View selected records in another database](#)

Pages: 1 [Next](#) [Select All](#) [Clear All](#) Total Records: [Get Count](#) → Total Records: 170

 Details <input type="checkbox"/> Record#1	 Details <input type="checkbox"/> Record#2	 Details <input type="checkbox"/> Record#3
 Details <input type="checkbox"/> Record#4	 Details <input type="checkbox"/> Record#5	 Details <input type="checkbox"/> Record#6

Database View

[Grid View](#) [Database View](#) [Properties View](#) [Create List](#)

[View selected records in another database](#)

Pages: [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#) [10](#) [▶](#) [Next](#) [Next 10](#) [Select All](#) [Clear All](#) **Total Records: 158**

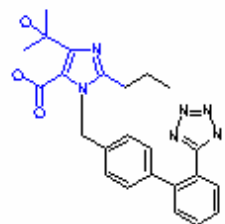
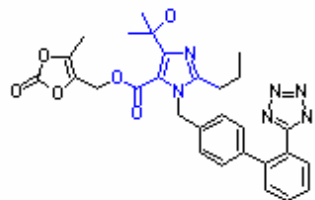
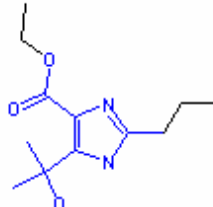
1	 <input type="checkbox"/> Record#1	ACD DWPI MDDR Patent Chemistry CMC Index Chemicus Metabolite
2	 <input type="checkbox"/> Record#2	ACD DWPI Index Chemicus MDDR Metabolite

Properties View

[Grid View](#) [Database View](#) [Properties View](#) [Create List](#)

[View selected records in another database](#)

Pages: [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#) [10](#) [▶](#) [Next](#) [Next 10](#) [Select All](#) [Clear All](#) **Total Records: 170**

1	 <input type="checkbox"/> Record#1	3d Configuration ADME Agrochemical Analytical Chemical Commercially Available Literature Reference Metabolism Name Pharmacological Physical Chemical Preparation
2	 <input type="checkbox"/> Record#2	3d Configuration ADME Agrochemical Chemical Commercially Available Literature Reference Metabolism Name Pharmacological Preparation Toxicity
3	 <input type="checkbox"/> Record#3	Chemical Literature Reference Name

Viewing compounds by property

View in another database

Select the records that you want to view:

All Records

Current Page

Specify Record Numbers

1

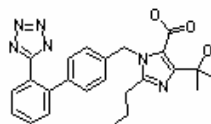
The numbers in the box (if present) correspond to those records that are already selected by you. To specify other records, enter the record numbers and/or record ranges, separated by commas. For example, 1,3,4,7-10. If you specify a large number of records, performance might be slow.

[Return to MDL® Compound Index](#)

[DWPI](#) [MDDR](#) [Metabolite](#) [Toxicity](#)

Record # 1 → **Total Records: 41**

MDL® Comprehensive Medicinal Chemistry



Available Data

Click on a link to add the information to this page

Set current view as default

[Substance](#) (1)

[Model](#) (1)

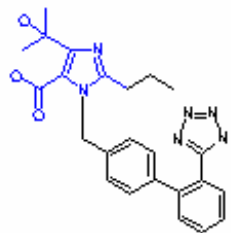
[Literature](#) (1)

Substance [\(hide\)](#)

MDL Number	MCMC00010881		
CAS Registry Number	144689-24-7		
Source	Sankyo Co., Japan		
Generic Name	• OLMESARTAN [USAN]		
Class	Antihypertensive		
LogP	3.63	Comment	
pKa		Comment	
Formula	C24 H26 N6 O3		
Molecular Weight	446.508		

Viewing data for a single record

1



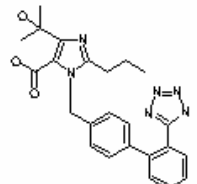
Record#1

[3d Configuration](#) [ADME](#)
[Agrochemical](#) [Analytical](#)
[Chemical](#)
[Literature Re](#)
[Name](#)
[Physical Che](#)

[Return to MDL® Compound Index](#)
[CMC](#) [DWPI](#) [Index Chemicus](#) [MDDR](#) [Metabolite](#) [Patent Chemistry](#)

Record # 1 ➔ **Total Records:** 7

MDL® Available Chemicals Directory



Available Data
Click on a link to add the information to this page

Set current view as default

[Substance](#) (1) [Suppliers](#) (2)
[Prices](#) (2) [Model](#) (1)

Substance [\(hide\)](#)

ACD Registry Number	142813
MDL Number	MFCD00914967
CAS Registry Number	144689-24-7 144689-63-4
Chemical Name and Synonyms :	<ul style="list-style-type: none">• OLMESARTAN
Molecular Formula	C24 H26 N6 O3
Molecular Weight	446.508
Rule of Five	0
Computed partition coefficient (CLogP)	3.63
Molecular weight of largest fragment	446.508
Number of proton acceptors	9
Number of proton donors	3
Number of rotatable bonds (TDF)	5

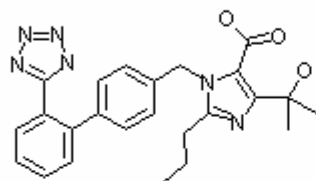
ACD database information

[Return to MDL® Compound Index](#)

[ACD](#) [DWPI](#) [Index Chemicus](#) [MDDR](#) [Metabolite](#) [Patent Chemistry](#)

← Record # 2 → **Total Records: 7**

MDL® Comprehensive Medicinal Chemistry



Available Data

Click on a link to add the information to this page

Set current view as default

[Substance](#) (1)

[Model](#) (1)

[Literature](#) (1)

Substance [\(hide\)](#)

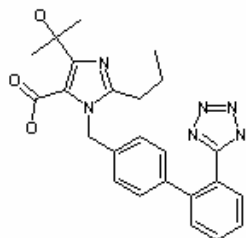
MDL Number	MCMC00010881		
CAS Registry Number	144689-24-7		
Source	Sankyo Co., Japan		
Generic Name	● OLMESARTAN [USAN]		
Class	Antihypertensive		
LogP	3.63	Comment	
pKa		Comment	
Formula	C ₂₄ H ₂₆ N ₆ O ₃		
Molecular Weight	446.508		

[Return to MDL@ Compound Index](#)

[ACD](#) [CMC](#) [Index Chemicus](#) [MDDR](#) [Metabolite](#) [Patent Chemistry](#)

← Record # 3 → **Total Records: 7**

Derwent World Patents Index®



DCR:	121764-0-0-0
Name:	OLMESARTAN
Molecular Formula:	C ₂₄ H ₂₆ N ₆ O ₃
Molecular Weight:	446.508
Description:	The active form of CS-866
Description:	5-(1-Hydroxy-1-methyl-ethyl)-2-propyl-3-[2'-(1H-tetrazol-5-yl)-biphenyl-4-ylmethyl]-3H-imidazole-4-carboxylic acid
No. of refs:	29

Patent references in Derwent World Patents Index®

[2003-015683](#)

New method for determining and utilizing the circulating blood of a living being over a range of shear rates, useful for e.g. the treatment of peripheral arterial disease

Derwent Classification

(A96) Medical, dental, veterinary, cosmetic.

(B07) General - tablets, dispensers, catheters (excluding drainage and angioplasty), encapsulation etc, but not systems for administration of blood or saline or IV feeding etc.

(C07) Apparatus, formulation, general. including veterinary syringes, general formulations where the active compound is not central to the invention (e.g. wettable powders) and analysis.

Compound Index Classification

Agrochemical

Analytical > Separation Methods

Literature Reference > Patent

Literature Reference > Patent > Analysis and Purification

Literature Reference > Patent > Pharmaceutical/Agrochemical

Literature Reference > Patent > Therapeutic Effect

Pharmacological

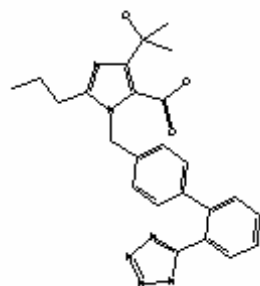
Index Chemicus

[Return to MDL® Compound Index](#)

[ACD](#) [CMC](#) [DWPI](#) [MDDR](#) [Metabolite](#) [Patent Chemistry](#)

← Record # 4 → **Total Records: 7**

Index Chemicus®



Compound Number:	538321-072
Molecular Formula:	C ₂₄ H ₂₆ N ₆ O ₃
Molecular Weight:	446.513

ISI Index Chemicus(R) citation details

Abstract Number: [538321](#)

Compounds abstracted: 126

Title

NONPEPTIDE ANGIOTENSIN-II RECEPTOR ANTAGONISTS - SYNTHESIS, BIOLOGICAL-ACTIVITIES, AND STRUCTURE - ACTIVITY RELATIONSHIPS OF IMIDAZOLE-5-CARBOXYLIC ACIDS BEARING ALKYL, ALKENYL, AND HYDROXYALKYL SUBSTITUENTS AT THE 4-POSITION AND THEIR RELATED-COMPOUNDS.

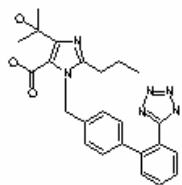
MDDR

[Return to MDL® Compound Index](#)

[ACD](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [Metabolite](#) [Patent Chemistry](#)

← Record # 5 → Total Records: 7

MDL® Drug Data Report



Available Data

Click on a link to add the information to this page

Set current view as default

[Substance](#) (1)

[Model](#) (1)

[Biology](#) (1)

[Identification](#) (1)

[Literature and Patent](#) (1)

Substance [\(hide\)](#)

External Registration Number	188868
Prous Entry Number	188868
Preview Number	
CAS Registry Number	144689-24-7
Derivative	
Chemical Name :	<ul style="list-style-type: none">4-(1-HYDROXY-1-METHYLETHYL)-2-PROPYL-1-[2'-(1H-TETRAZOL-5-YL)BIPHENYL-4-YLMETHYL]IMIDAZOLE-5-CARBOXYLIC ACID
Generic Name	OLMESARTAN < USAN >
Formula	C24 H26 N6 O3
Molecular Weight	446.508
Development Phase:	Launched
Year	
Active Investigation	
Index	Activity
16000	ANTI GLAUCOMA
31000	ANTI HYPERTENSIVE
31432	ANGIOTENSIN II AT1 ANTAGONIST

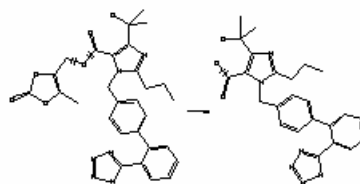
Metabolite

[Return to MDL® Compound Index](#)

[ACD](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [MDDR](#) [Patent Chemistry](#)

← Record # 6 → Total Records: 7

MDL® Metabolite Database



Available Data

Click on a link to add the information to this page

Set current view as default

View results as **transformations:**

[Transformation](#) (1)
[Reference](#) (1)
[Species](#) (1)
[Enzyme](#) (1)

View results as **molecules:**

[Parent](#) (1)
[Species](#) (1)
[Substrate](#) (1)
[Metabolite](#) (1)

Transformation Results -- Transformation [\(hide\)](#)

MDL number	RMTB00058294
Path	MTB9122-A
Step	1 Step
Scheme	MTB9122
Chemical Name and Synonyms : <ul style="list-style-type: none">• CS-866• (5-Methyl-2-oxo-1,3-dioxol-4-yl)methyl 4-(hydroxy-1-methylethyl)-2-propyl-1-((2-(1H-tetrazol-5-yl)-1,1'-biphenyl-4-yl)methyl)-1H-imidazole-5-carboxylate	
Reaction Class : <ul style="list-style-type: none">• Hydrolysis• O-Dealkylation	

Choose data fields

The screenshot displays the DiscoveryGate MDL Database Browser interface. On the left, a 'Field Index' sidebar is highlighted with a red border, listing various data fields. 'Molecular Weight' is selected and highlighted in orange. The main area shows a search form with 'molstructure' selected as the search type. A custom search form is visible, consisting of a dropdown menu set to 'AND', the text 'Molecular Weight', an equals sign dropdown, and an empty input field. Below the form are buttons for 'start search', 'show brackets', and 'save form'. The top navigation bar includes 'queries', 'results', and 'reports' tabs, along with 'start search', 'import', 'save', 'clear form', 'help', and 'logout' options. The right side of the top bar shows 'MDL® Compound Index' and 'Version'.

Database: MDL® Compound Index

Find in Field Index: [] Next

Field Index History

- Molecular Formula
- Molecular Weight**
- cdbrigno
- molstructure
- Pharmacological
- Physical Chemical
- Preparation
- Safety
- Analytical
- Structure based
- Toxicity
- ADME
- Chemical
- Commercially Available
- Name
- Literature Reference
- Agrochemical
- Metabolism
- 3d Configuration

molstructure

Select Search Type: Automatic

Double-click in this box to edit structure

An automatically executed series of searches (Current structure, Include isomers, Include tautomers, Include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.

Query Highlighting.

AND Molecular Weight = []

start search

show brackets save form

Reset Delete Duplicate Info

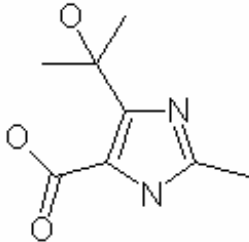
Delete Duplicate Info

Double-click a data field to create a custom form.

Structure/Data search

Enter the core structural fragment

molstructure



Select Search Type:
Automatic

An automatically executed series of searches (Current structure, Include isomers, Include tautomers, Include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.

Query Highlighting.

[Reset](#)
[Delete](#)
[Duplicate](#)
[Info](#)

AND Molecular Weight < 350

[Delete](#)
[Duplicate](#)
[Info](#)

start search

show brackets save form

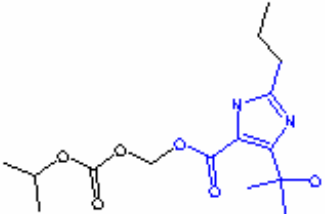
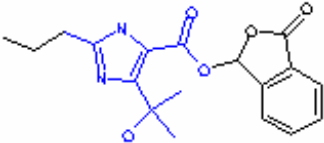
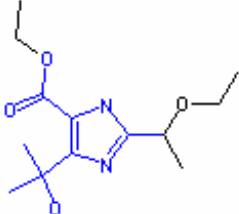
Enter data and specify an operator

Structure/Data results

Grid View [Database View](#) [Properties View](#) [Create List](#)

[View selected records in another database](#)

Pages: 1 **2** ▶ [Next](#) [Select All](#) [Clear All](#) **Total Records: 18**

 Details <input type="checkbox"/> Record#1	 Details <input type="checkbox"/> Record#2	 Details <input type="checkbox"/> Record#3
---	--	---

Substructure search results – 170 compounds.

Substructure search with data constraint results – 18 compounds.

Data searching

In this section, you will learn how to:

- ❑ Search individual databases
- ❑ Select the data fields that you want to search
- ❑ Use the Data Lookup table to build your query
- ❑ Save the modified query form as your default form for the current database
- ❑ Use predefined search forms
- ❑ Display hidden data in Details view
- ❑ Create a report

Selecting an individual database

The screenshot displays the DiscoveryGate MDL Database Browser interface. On the left, a vertical list of databases is shown, with 'MDL@ Compound Index' selected and highlighted in blue. A red box highlights this list. The main area on the right is titled 'MolStructure' and contains a search form. The 'Select Search Type:' dropdown is set to 'Automatic'. Below this, there is a text box with the instruction 'Double-click in this box to edit structure'. A search query is entered as 'Molecular Weight =', followed by an empty input field. The 'start search' button is visible. At the bottom, there are buttons for 'show brackets' and 'save form'. On the far right, there are links for 'Reset', 'Delete', 'Duplicate', and 'Info'.

Select an individual database from the drop-down list

Default forms

MDL® Available Chemicals Directory

Molecule

Structure [Select Search Type:](#)
Automatic

Double-click in this box to edit structure

An automatically executed series of searches (Current structure, include isomers, include tautomers, include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.

[Reset](#)
[Delete](#)
[Duplicate](#)
[Info](#)

Query Highlighting.

Each database has a defined default form.

MDL® Metabolite Database

Parent Molecule

Structure [Select Search Type:](#)
Automatic

Double-click in this box to edit structure

An automatically executed series of searches (Current structure, include isomers, include tautomers, include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.

[Reset](#)
[Delete](#)
[Duplicate](#)
[Info](#)

AND	Catalog Number	Contains
AND	Chemical Name and Synonyms	Contains
AND	CAS Registry Number	Is
AND	MDL Number	Contains
AND	Supplier Name	Contains

MDL® Patent Chemistry Database

Transformation

AND	Route	Contains
AND	Species	Contains
AND	Journal Author	Contains
AND	Journal Name	Contains
AND	Journal Year	=

Structure

Find this compound and its properties

Double-click in this box to edit structure

Query Highlighting

Search Stereoinformation: As drawn

Substitution as drawn, exclude tautomers
 Substitution as drawn, include tautomers
 Unlimited substitution on all atoms, exclude tautomers

Allow:

- Multi-component substances
- Ring closure through substitution
- Isotopes Charges Radicals
- Keep fragments separate

[Reset](#)
[Delete](#)
[Info](#)

Patent Inventors (Authors)

AND	Inventor (Author)	Contains	<input type="text"/>	Delete Duplicate Info
Data Lookup...				

Publication/Application Data

AND	Patent Number	Contains	<input type="text"/>	Delete Duplicate Info
Data Lookup...				
AND	Patent Country Code	Contains	<input type="text"/>	Delete Duplicate Info
Data Lookup...				

Substance Characterization

AND	CAS Registry Number	Is	<input type="text"/>	Delete Duplicate Info
Data Lookup...				
AND	Chemical Name	Contains	<input type="text"/>	Delete Duplicate Info
Data Lookup...				

Predefined search forms

In addition to the default forms, the CrossFire Beilstein, CrossFire Gmelin, and the MDL Patent Chemistry databases have a series of predefined forms.

Database: CrossFire Beilstein

Find in Field Index: Next

Field Index History

- Structure
- Easy Data Search (highlighted with a red box)
 - Bibliographic Data
 - Substance Identification Data
 - Molecular Formula Search
 - Reaction Data
 - Physical Data
 - Spectroscopic Data
 - Pharmacological Data
 - Ecotoxicological Data
 - Solubility Data
- Basic Indexes
- Bibliographic Information
- Substance Identification
- Chemical Properties
- Physical Properties
- Pharmacological and Ecological Data

Database: CrossFire Gmelin

Find in Field Index: Next

Field Index History

- Structure
- Easy Data Search (highlighted with a red box)
 - Bibliographic Data
 - Substance Identification Data
 - Molecular Formula Search
 - Reaction Data
 - Physical Data
 - Spectroscopic Data
 - Solubility Data
 - Alloy Search
 - Crystal Structure Data
 - Electrical Data
 - Electrolytic / Electrochemical Data
 - Magnetic Data
 - Mechanical Data
 - Molecular Data
 - Thermal Data
- Basic Indexes
- Bibliographic Information
- Substance Characterization
- General Information

Database: MDL Patent Chemistry Database

Find in Field Index: Next

Field Index History

- Structure
- Easy Data Search (highlighted with a red box)
 - Bibliographic Data
 - Patent Data
 - Substance Identification Data
 - Molecular Formula Search
 - Reaction Data
 - Physical Data
 - Spectroscopic Data
 - Bioactivity data
 - Application data
 - Composition
- Citations
- Substances
- Reactions

Data search features

Data field

The screenshot shows a search interface for 'Substance' with five search criteria: Beilstein Registry Number, CAS Registry Number, Chemical Name, Molecular Formula, and Molecular Weight. Each criterion has a dropdown menu for operators and a text input field. The 'Chemical Name' dropdown is open, showing options like 'Is', 'Contains', 'Starts With', 'Ends With', and 'Is'. The 'Data Lookup...' link for the 'Chemical Name' field is circled in red. A 'start search' button is at the bottom. A 'Show Brackets' link is at the bottom left. A 'Delete Duplicate Info' link is at the top right. A 'Data field index controls' label points to the right side of the interface.

Operator	Data Field	Operator	Input Field	Controls
	Beilstein Registry Number	=		Delete Duplicate Info
OR	CAS Registry Number	Contains	Data Lookup...	Delete Duplicate Info
OR	Chemical Name	Is	Data Lookup...	Delete Duplicate Info
OR	Molecular Formula		Data Lookup...	Delete Duplicate Info
OR	Molecular Weight	=		Delete Duplicate Info

Data field index controls

Operators used to connect multiple search criteria

Operators used with text and/or numeric search entries

Data operators and wildcards

Operators	Use to retrieve records that:
AND	satisfy both criteria
OR	satisfy either criterion
NOT	do not satisfy the criterion
=	satisfy the exact entry
<	are less than the specified entry
<=	are less than or equal to the specified entry
>	are greater than the specified entry
>=	are greater than or equal to the specified entry
<>	are not included as an entry
Is	have the exact entry
Starts with	begin with the entry
Ends with	end with the entry
Contains	have the term contained within
Wildcards	Use in text string to represent
?	One character
??	Two characters

Search for a specific compound

Conduct two different data searches to retrieve the compound acyclovir (CAS number 59277-89-3) from the CrossFire Beilstein database.

Structure

Find this compound and its properties

Double-click in this box to edit structure

Query Highlighting

Substitution as drawn, exclude tautomers
 Substitution as drawn, include tautomers
 Unlimited substitution on all atoms, exclude tautomers

Allow:

Multi-component substances
 Ring closure through substitution
 Isotopes Charges Radicals
 Keep fragments separate

Search Stereoinformation

[Reset](#)
[Delete](#)
[Info](#)

Substance Identification

<input type="text" value="AND"/>	Beilstein Registry Number	=	<input type="text"/>	Delete Duplicate Info
<input type="text" value="AND"/>	CAS Registry Number	1	Is <input type="text"/>	Delete Duplicate Info
<input type="text" value="AND"/>	Chemical Name	2	Contains <input type="text"/>	Delete Duplicate Info
<input type="text" value="AND"/>	Molecular Formula	Contains	<input type="text"/>	Delete Duplicate Info
<input type="text" value="AND"/>	Molecular Weight	=	<input type="text"/>	Delete Duplicate Info

Note: In the Substance Identification table, the '1' and '2' in the second and third rows are circled in orange. The 'Data Lookup...' buttons in the second and third rows are highlighted with a red box.

Data Lookup

Chemical Name search

Data Look up - Chemical Name

Find: acyclovir **Find**

Frequency: Values:

6	acyclovir	Start
1	acyclovir β -glucoside	
1	acyclovir (na salt)	↑
1	acyclovir carboxyphosphonate ammonium	
1	acyclovir diphosphate	↓
1	acyclovir diphosphate dimyristoylglyce	
1	acyclovir elaidate	
1	acyclovir ethoxycarbonylphosphonate an	End

Double-click the values you want to add to your query:

Your Query: acyclovir **Clear**

Find any of these terms (OR operator) **OK**

Find all of these terms (AND operator)

Find all of these terms adjacent to one another in order **Cancel**

CAS number search

Data Look up - CAS Registry Number

Find: 59277-89-3 **Find**

Frequency: Values:

2	59277-89-3	Start
1	59277-90-6	
1	59277-91-7	↑
1	59277-92-8	
1	59277-93-9	↓
1	59277-94-0	
1	59277-95-1	
1	59277-96-2	End

Double-click the values you want to add to your query:

Your Query: 59277-89-3 **Clear**

Find any of these terms (OR operator) **OK**

Find all of these terms (AND operator)

Find all of these terms adjacent to one another in order **Cancel**

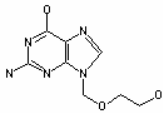
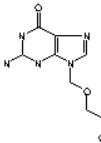
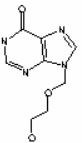
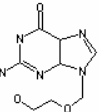
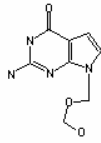
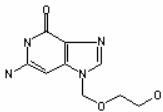
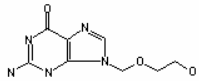
Data Lookup tables display the specified value and the number of occurrences found in the database.

Search results

Chemical Name search results

[View selected records in another database](#) [Create List](#)

Pages: 1 [Select All](#) [Clear All](#) Total Records: 7

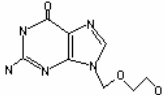
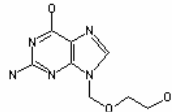
BRN: 4257573 BIO  Details Synthesize <input type="checkbox"/> Record#1	BRN: 6411198 BIO  Details Synthesize <input type="checkbox"/> Record#2	BRN: 6514132 BIO  Details Synthesize <input type="checkbox"/> Record#3
BRN: 6603483  Details Synthesize <input type="checkbox"/> Record#4	BRN: 7430620 BIO  Details Synthesize <input type="checkbox"/> Record#5	BRN: 8626446  Details Synthesize <input type="checkbox"/> Record#6
BRN: 9132217 BIO  Details Synthesize <input type="checkbox"/> Record#7		

The “BIO” label indicates that the compound has pharmacological or toxicological data associated with it.

CAS number search results

[View selected records in another database](#) [Create List](#)


Pages: 1 [Select All](#) [Clear All](#) Total Records: 2

BRN: 1219402 BIO  Details Synthesize <input type="checkbox"/> Record#1	BRN: 4257573 BIO  Details Synthesize <input type="checkbox"/> Record#2
---	---

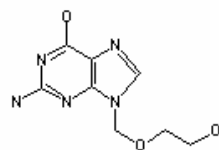
Link to additional data

[Return to Search Results](#)

[View selected records in another database](#)

Record # 1 of 7 

CrossFire Beilstein Substance 4257573



[Use as Query](#) [Synthesize](#)

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

[Liquid/Liquid Systems \(MCS\)](#) (1)

[NMR Spectroscopy](#) (1)

[Pharmacological Data](#) (9)

[Substance Identification](#) (1)

[Melting Point](#) (1)

[Partition octan-1-ol/water \(MCS\)](#) (1)

[Related Structure](#) (1)

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

Click a link to obtain specific data for the retrieved compound.

Substance Identification [\(hide\)](#)

Substance Identification record 1 of 1

Beilstein Registry Number	4257573
Beilstein Preferred RN	59277-89-3
CAS Registry Number	59277-89-3
Chemical Name	acyclovir
Autoname	2-amino-9-(2-hydroxy-ethoxymethyl)-9H-purin-6-ol
Fragment Molecular Formula	Molecular Weight 225.21
Molecular Formula	C8H11N5O3
Lawson Number	30725, 689, 514
Type of Substance	heterocyclic
Constitution ID	3789454
Tautomer ID	1194427
Beilstein Reference	6-26
Entry Date	1992/07/20
Update Date	2002/04/29

Click to link to reactions or citations for this substance.

Available data

Displays or hides the data

Links to the literature reference

Pharmacological Data (hide)	
Pharmacological Data record 1 of 9	
Citation Pointer	5960932
Pharmacological Data Citations	<ul style="list-style-type: none">Journal; Sato, Yoshiko; Maruyama, Tokumi; CPBTAL; Chem. Pharm. Bull.; EN; 43; 1; 1995; 91-95;
Entry Date	1995/12/31
Comment	antiviral activity against HSV-1 in Vero cell (EC50: 0.41 µg/ml) and HSV-2 in Vero cell (0.18 µg/ml)
Pharmacological Data record 2 of 9	
Citation Pointer	5911291
Pharmacological Data Citations	<ul style="list-style-type: none">Journal; Winkelmann, E.; Winkler, I.; Rolly, H.; Roesner, M.; Jaehne, G.; ARZNAD; Arzneim. Forsch.; EN; 38; 11; 1988; 1545-1548;
Entry Date	1988/06/27
Comment	Chemotherapeutic activity against Herpes simplex (HSV-1) infection in mouse i.p.
Pharmacological Data record 3 of 9	
Citation Pointer	5904365
Pharmacological Data Citations	<ul style="list-style-type: none">Journal; El-Kousy, S.; Pedersen, E. B.; Nielsen, C.; MOCMB7; Monatsh. Chem.; EN; 125; 6/7; 1994; 713-722;
Entry Date	1994/12/31
Comment	activity against Herpes Simplex Virus, type 1, strain McIntyre, in SIRC cells: ED 50 = 0.5 µM; cytotoxicity against normal uninfected SIRC cells: CD 50 = >50 µM

Search the MDL Toxicity database

Conduct a search, using the MDL Toxicity database to retrieve compounds that have tumorigenicity data associated with fatty liver degeneration.

MDL® Toxicity Database

Database: MDL® Toxicity Database ?

Find in Field Index: Next

Field Index History

- Chemical
 - Structure
 - Beilstein Handbook Registry
 - Beilstein Registry Number
 - CAS Registry Number
 - Chemical Carcinogenesis(CCRIS)
 - Chemical Name and Synonyms
 - GENETOX Number
 - IARC Cancer Reviews
 - MDL Number
 - Molecular Formula
 - Molecular Weight
 - RTECS Registry Number
 - Threshold Limit Value
 - Toxicology Reviews
- Acute Toxicity
- Mutagenicity
- Irritation
- Tumorigenicity
- Reproductive Effects
- Other Multiple Dose

CHEMICAL

Structure [Select Search Type:](#)

Automatic

Double-click in this box to edit structure

An automatically executed series of searches (Current structure, Include isomers, Include tautomers, Include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.

Query Highlighting.

[Reset](#)
[Delete](#)
[Duplicate](#)
[Info](#)

AND Chemical Name and Synonyms Contains

[Delete](#)
[Duplicate](#)
[Info](#)

AND CAS Registry Number Is

[Delete](#)
[Duplicate](#)
[Info](#)

Acute Toxicity

AND Dosage = mg/kg

[Delete](#)
[Duplicate](#)
[Info](#)

AND Endpoint Contains

[Data Lookup...](#)
[Delete](#)
[Duplicate](#)
[Info](#)

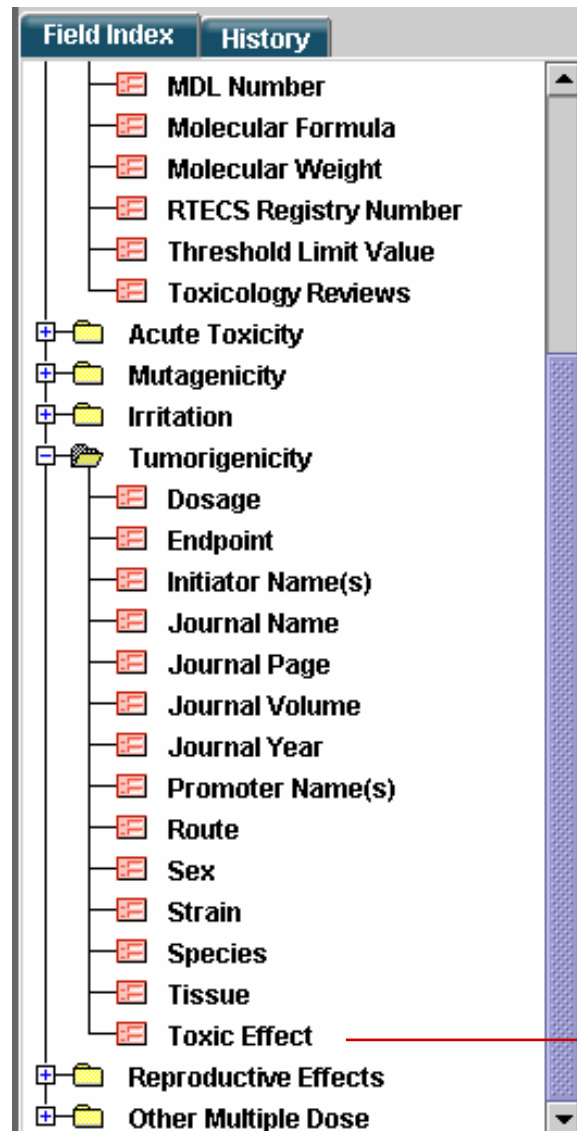
AND Species Contains

[Data Lookup...](#)
[Delete](#)
[Duplicate](#)
[Info](#)

start search

show brackets save form sort results

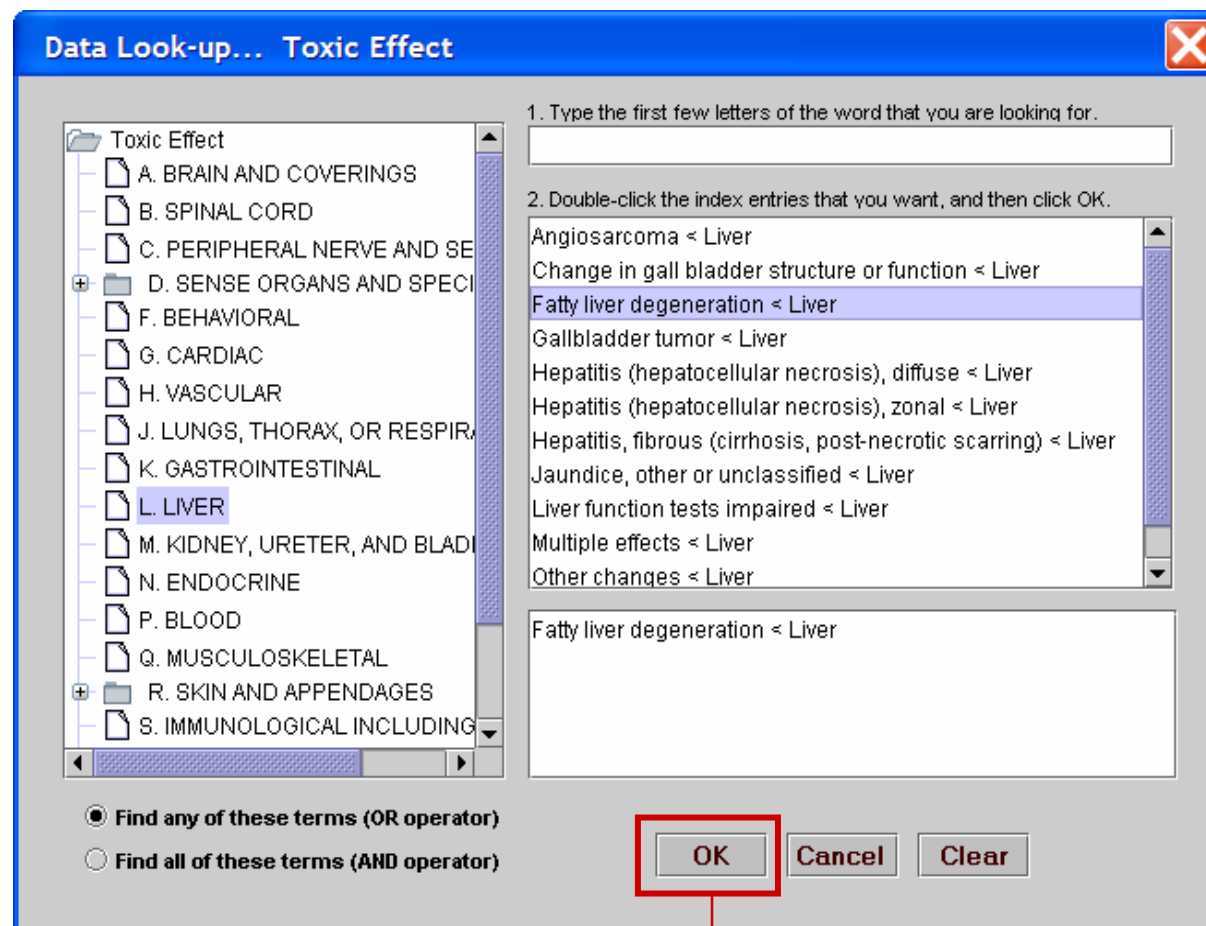
Create a custom form



The query form titled 'Tumorigenicity' shows a search criteria entry: 'AND' (operator), 'Toxic Effect' (field), 'Contains' (operator), and an empty text input field. A 'Data Lookup...' link is next to the input field. A 'start search' button is at the bottom.

Double-click to add field to query form

Enter the 'toxic effect' data constraint



Saving a form

CHEMICAL

Structure [Select Search Type:](#)
Automatic
An automatically executed series of searches (Current structure, Include isomers, Include tautomers, Include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.
 Query Highlighting.

Double-click in this box to edit structure

[Reset](#)
[Delete](#)
[Duplicate](#)
[Info](#)

AND Chemical Name and Synonyms Contains [Delete](#)
[Duplicate](#)
[Info](#)

AND CAS Registry Number

Acute Toxicity

AND Dosage

AND Endpoint

AND Species Contains [Data Lookup...](#) [Delete](#)
[Duplicate](#)
[Info](#)


Tumorigenicity

AND Toxic Effect Contains [Data Lookup...](#) [Delete](#)
[Duplicate](#)
[Info](#)

start search

show brackets **save form** sort results

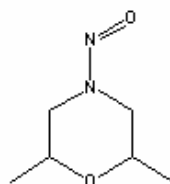
Save Form

 The current query will now become the default query for this data source and overwrite your existed default query form. Do you want to proceed?

OK Cancel

Tumorigenicity data

MDL® Toxicity Database



[Use as Query](#)

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

[Chemical](#) (1)

[Acute Toxicity](#) (4)

[Mutagenicity](#) (35)

[Tumorigenicity](#) (35)

[Review](#) (1)

[Model](#) (1)

Tumorigenicity [\(hide\)](#)

Full Citation 1 of 35

[Journal of the National Cancer Institute 64,529,1980](#)

Source ID : QE2150000	Source : RTECS
Chemical Name	MORPHOLINE, 2,6-DIMETHYL-N-NITROSO-
Species	guinea pig
Route	ORAL
Dosage	400 MG/KG/23W-I
Endpoint :	TD
Endpoint (Incidence) :	(Carcinogen, Carcinogen+Inhibitor, %Diff., Significance)
Endpoint (Multiplicity) :	
Endpoint (Latency) :	(Carcinogen, Carcinogen+Inhibitor, Significance)

Toxic Effects :

- Carcinogenic by RTECS criteria < Tumorigenic
- Fatty liver degeneration < Liver
- Tumors < Liver

Creating a report

The screenshot shows a software interface with a menu bar containing 'queries', 'results', and 'reports'. Under the 'reports' menu, the 'copy to report' option is highlighted with a red box. A 'Copy to Report' dialog box is open, featuring a blue title bar with a close button (X). The dialog contains the following text and options:

You can copy to the report a maximum of 500 records at one time.

Select copy destination

- Create new report
- Append to today's report

Select copy result level

- View search results in report
- View detail results in report
Using detail-view as the template for each record

Set the range of copy-to-report records

- All records
- Current Page
- Specify Record Numbers

Enter the record index numbers and/or record ranges, separated by commas. For example, 1,3,5,7-10

View report now

OK Cancel

Reports tab

DiscoveryGate® | MDL® Database Browser

queries results **reports**

export page setup print save refine query help logout MDL® Toxicity Database

Database: MDL® Toxicity Database ?

Find in Outline: Next

Outline History

Today's Report - Report #1

Section 1

Tumorigenicity

Full Citation 1 of 35

Journal of the National Cancer Institute 64,529,1980

Source ID : QE2150000	Source : RTECS
Chemical Name	MORPHOLINE, 2,6-DIMETHYL-N-NITROSO-
Species	guinea pig
Route	ORAL
Dosage	400 MG/KG/23W-I
Endpoint :	TD
Endpoint (Incidence) :	(Carcinogen, Carcinogen+Inhibitor, %Diff., Significance)
Endpoint (Multiplicity) :	
Endpoint (Latency) :	(Carcinogen, Carcinogen+Inhibitor, Significance)

Toxic Effects :

- Carcinogenic by RTECS criteria < Tumorigenic
- Fatty liver degeneration < Liver
- Tumors < Liver

Manually add a data field

The screenshot displays the DiscoveryGate MDL Database Browser interface. The top navigation bar includes tabs for 'queries', 'results', 'reports', and 'rxn schemes'. Below this, there are links for 'start search', 'import', 'save', 'clear form', 'help', and 'logout'. The main header identifies the database as 'Synthetic Methodology Information' and shows the 'Version'.

On the left side, there is a 'Field Index' section. A red box highlights the 'Find in Field Index' search bar, which contains the text 'conditions' and a 'Next' button. Below this, a tree view shows the hierarchy of fields. The 'Reaction' folder is expanded, and the 'Conditions' field is highlighted with a red box. A red arrow points from this 'Conditions' field to the search form on the right.

The search form on the right is titled 'Reaction' and contains a 'Structure' section with a 'Select Search Type' dropdown set to 'Reaction Automatic'. Below this, there are several search criteria rows, each with a logical operator, a field name, a comparison operator, a value, and a unit dropdown. The criteria are:

- AND Percent Yield = %
- AND Author Contains [Data Lookup...]
- AND Journal Contains J Am Chem Soc [Data Lookup...]
- AND Year =
- OR Journal Contains Tetrahedron Lett [Data Lookup...]
- AND Conditions Contains Hydrogenations [Data Lookup...]

Each row includes 'Delete', 'Duplicate', and 'Info' links. The 'Conditions' field is currently empty in the search form.

Use the Field Index to find the data field. Double-click to add it to the form.

Setting parenthetical statements

Initial search

AND	[Journal	Contains	J Am Chem Soc Data Lookup...		Delete Duplicate Info
AND		Year	=			Delete Duplicate Info
OR		Journal	Contains	Tetrahedron Lett Data Lookup...]	Delete Duplicate Info
Reaction						
AND		Conditions	Contains	Hydrogenations Data Lookup...		Delete Duplicate Info

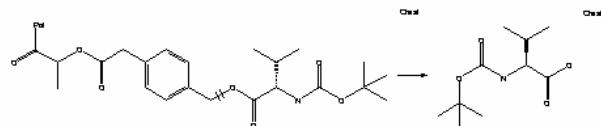
Modified search

AND	[Journal	Contains	J Am Chem Soc Data Lookup...		Delete Duplicate Info
OR		Journal	Contains	Tetrahedron Lett Data Lookup...]	Delete Duplicate Info
AND		Year	>	2000		Delete Duplicate Info
Reaction						
AND		Conditions	Contains	Hydrogenations Data Lookup...		Delete Duplicate Info

Manually adjust fields to create the correct parenthetical statements.

Search results

MDL® Solid-Phase Organic Reactions



[Use as Query](#)

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

[Reaction Details](#) (4)

[Reactant](#) (1)

[Product](#) (1)

Reaction Details [\(hide\)](#)

RSPO69000650 **Reaction Variation 1 of 4**

Product no.	% Yield	Grade	%cs	%ds	%de	%ee	Reactant no.	Reactant Grade
1	50	(S)-isomer	100				1	(S)-isomer

Step no.	Catalysts and Solvents	Catalyst ID click ID for details	Solvent ID click ID for details
1	H2 Pd(O-Ac)2 (cat) DMF	18137 48	9

Detailed Data	Conditions References	Solid Support Protecting Group	External Registry No.	Path	Step
			698000501	I	4 OF 4

[TAM, J. P.; TJOENG, F. S.; MERRIFIELD, R. E.; J Am Chem Soc \[JACSAT\] 1980, 102 \(19\), 6117-6127.](#)
[TAM, J. P.; TJOENG, F. S.; MERRIFIELD, R. E.; Tetrahedron Lett \[TELEAY\] 1979, 51, 4935-4938.](#)
[WHITNEY, D. B.; TAM, J. P.; MERRIFIELD, R. E.; Tetrahedron \[TETRAH\] 1984, 40 \(21\), 4237-4244.](#)

Conditions

Step	1
Hours	17
Temp (C)	50
Conditions	Hydrogenations Transition Metal Salts Thermal

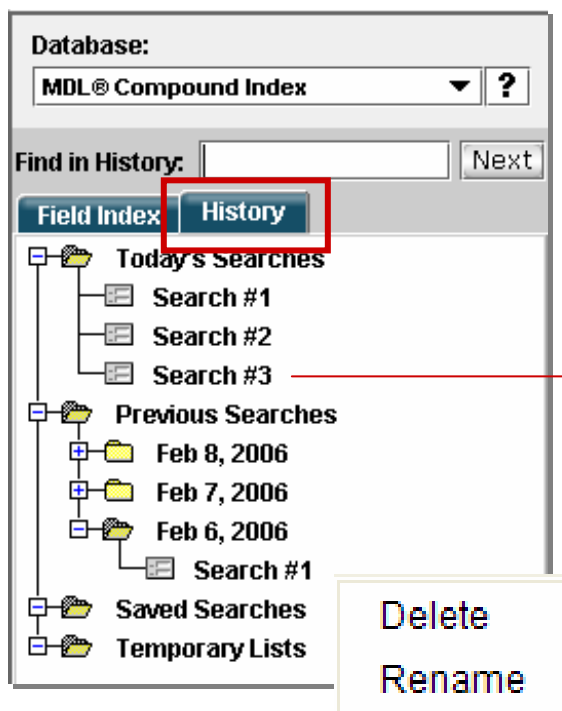
Manipulating search results

In this section, you will learn how to:

- ❑ Work with the History tab
- ❑ Create a temporary list
- ❑ Save a permanent list
- ❑ Combine temporary lists
- ❑ Export results

Working with the History tab

The History tab is unique to the database you are using.



Using the "results" tab,
double-click to open

Right-click a list to
Delete or Rename

Create a temporary list

The screenshot displays the DiscoveryGate MDL Database Browser interface. The main window shows search results for the MDL Compound Index database. A 'Create List' dialog box is open, allowing the user to select records to store in the results set. The dialog box has three radio button options: 'All Records' (selected), 'Current Page', and 'Specify Record Numbers'. Below these options is a text input field for record numbers and a 'Description' field containing the text 'Structure and MW<350'. The dialog box also includes 'OK' and 'Cancel' buttons.

The background interface includes a navigation bar with 'queries', 'results', and 'reports' tabs. Below this is a menu with options like 'copy to report', 'export', 'page setup', 'print', 'save', 'refine query', 'lists', 'help', and 'logout'. The main content area shows 'Grid View', 'Database View', and 'Properties View' options, along with a 'View selected records in another database' link. A 'Total Records: 18' indicator is visible. A search history window is also open, showing a tree view of searches, with a new entry 'L1 Structure and MW<350' highlighted under 'Temporary Lists'.

Red arrows indicate the flow of information: one arrow points from the 'Create List' button in the top right to the dialog box, and another arrow points from the 'L1 Structure and MW<350' entry in the search history window to the 'Description' field in the dialog box.

Create a permanent list

The screenshot displays the DiscoveryGate MDL Database Browser interface. The main window has tabs for 'queries', 'results', and 'reports'. A red box highlights the 'save' button in the top navigation bar. A red arrow points from this button to a 'Save As' dialog box. The dialog box has a 'File name:' field containing 'Structure SSS' and 'OK' and 'Cancel' buttons. Below the dialog box, a chemical structure is visible. In the bottom right corner, a separate window shows the search history tree. A red arrow points from the 'Structure SSS' entry in this tree back to the 'save' button in the main interface. The search history tree includes categories like 'Today's Searches', 'Previous Searches', and 'Saved Searches', with 'Structure SSS' listed under 'Saved Searches'.

DiscoveryGate® | MDL® Database Browser

queries results reports

copy to report export page setup print save refine query lists help logout MDL® Compound Index Version

Database: MDL® Compound Index ?

Find in History: [] Next

Grid View Database View Properties View

View selected records in another database

Save As

File name: Structure SSS

OK Cancel

Total Records: Get Count

Database: MDL® Compound Index ?

Find in History: [] Next

Field Index History

- Today's Searches
 - Search #1
 - Search #2
 - Search #3
- Previous Searches
 - Feb 8, 2006
 - Feb 7, 2006
 - Feb 6, 2006
- Saved Searches
 - Search #1
 - Structure SSS
- Temporary Lists

Export a list

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queries results reports

copy to report export page setup print save refine query lists help logout

Set the Range of Export Records - Compound Index

You can export a maximum of 500 records at one time.

All Records

Current Page

Specify Record Numbers

1-5

Enter the record index numbers and/or record separated by commas. For example, 1,3,5,7-10

OK Cancel

Export Database Results

Find: [] Next

Database Fields

- MOL
 - MOLSTRUCTURE
 - cdbregno
 - Molecular Formula
 - Molecular Weight
 - Rule of Five
 - clogP (Syracuse Res. Cente
 - Torsional degree of freedom
 - Proton Acceptors (O+N)
 - Proton Donors
 - Mol. Weight:Largest Fragme
 - Total Polar Surface Area

Add

Exporting Fields

- MOL
 - MOLSTRUCTURE
 - Molecular Weight
 - Molecular Formula

Remove

↑ ↓

Export SDfile ...

Export TAB ...

Export format selections and the exported lists are supported by the database.

Export formats

You can export results, both structures and data, in the following formats:

.sdf	<ul style="list-style-type: none">▪ This is a flat file format and can store structures, but not reactions.▪ This format is suitable for files to be exported to ISIS for Excel and to ISIS/Base databases.▪ The “results” tab needs to be active.
.rdf	<ul style="list-style-type: none">▪ This is a hierarchical file format and can store reactions.▪ This format is suitable for files to be exported to ISIS/Base databases.▪ The “results” tab needs to be active.
.tab	<ul style="list-style-type: none">▪ This format is suitable for files to be exported to ISIS for Excel.▪ The “results” tab needs to be active.▪ You require Chime software to view the structures.



Searching for reactions



Reaction Query

The screenshot shows the MDL Draw for Database Browser interface. The main window displays a chemical structure of a benzothienopyridine derivative. A carbon atom in the benzene ring is highlighted with a red box and labeled **C[RC]**. A sulfur atom in the thiophene ring is labeled **S**. The software's menu bar includes File, Edit, Chemistry, and Help. Below the menu bar is a toolbar with various drawing tools. On the left side, there is a vertical toolbar with icons for selection, zoom, and other functions. Two context menus are open: one for the **C[RC]** atom and one for the **S** atom. The **C[RC]** menu is open to the 'Atom role in product' option, and the **S** menu is open to the 'Bond role in product' option.

Bond Property	
Bond order	▶
Stereobond	▶
Query bond type	▶
Chain or ring bond	▶
Bond role in product	▶ Breaks in reaction
Remove properties	▶ Forms in reaction
	Changes ▶
	Must NOT change
	Off

Bond Role in Product – Bond must form in reaction.

Must change in reaction – the selected atom must be part of the reaction.

Isotope	▶
Valence...	▶
Radical	▶
Additional substituents...	▶
Hydrogen count	▶
Chain or ring atom	▶
Allow these atoms	▶
Prohibit these atoms	▶
Beilstein generic group	▶
Atom role in product	▶ Must change in reaction
Stereoconfiguration at atom	▶ Must NOT change in reaction
Remove Properties	Off

Query

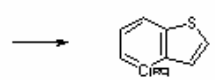
L[®] Database Browser

queries results reports rxn schemes

start search import save clear form help logout **CrossFire Beilstein** Version

Reaction

Find this reaction and its conditions



Substitution as drawn, exclude tautomers
 Substitution as drawn, include tautomers
 Unlimited substitution on

Allow: Multi-component Ring closure through Isotopes Charge Ignore atom mapping Keep fragments separate

Query Highlighting

Search Stereoinformation

start search

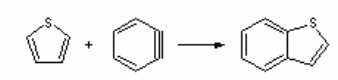
show brackets save form

Results

Pages: 1 [Select All](#) [Clear All](#) Total Records: 4

Record#1

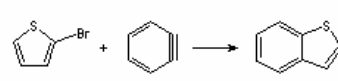
Reaction ID: 1503815



[Details](#) [Synthesize Reactant\(s\)](#) [Find Similar Reactions](#)

Record#2

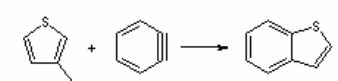
Reaction ID: 1519346



[Details](#) [Synthesize Reactant\(s\)](#) [Find Similar Reactions](#)

Record#3

Reaction ID: 1741026



[Details](#) [Synthesize Reactant\(s\)](#) [Find Similar Reactions](#)

Record#4

Return to Query Tab

Choose Find Citations

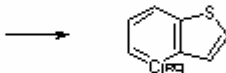
queries results reports rxn schemes

search import save clear form help logout

CrossFire Beilstein Version

Reaction

Find citations of this reaction



Query Highlighting

Substitution as drawn, exclude tautomers
 Substitution as drawn, include tautomers
 Unlimited substitution on all atoms, exclude tautomers

Allow: Multi-component substances
 Ring closure through substitution
 Isotopes Charges Radicals
 Ignore atom mapping
 Keep fragments separate

Search Stereoinformation: As drawn

[Reset](#)
[Delete](#)
[Info](#)

start search

show brackets save form

Citations

Database Browser

queries results reports rxn schemes

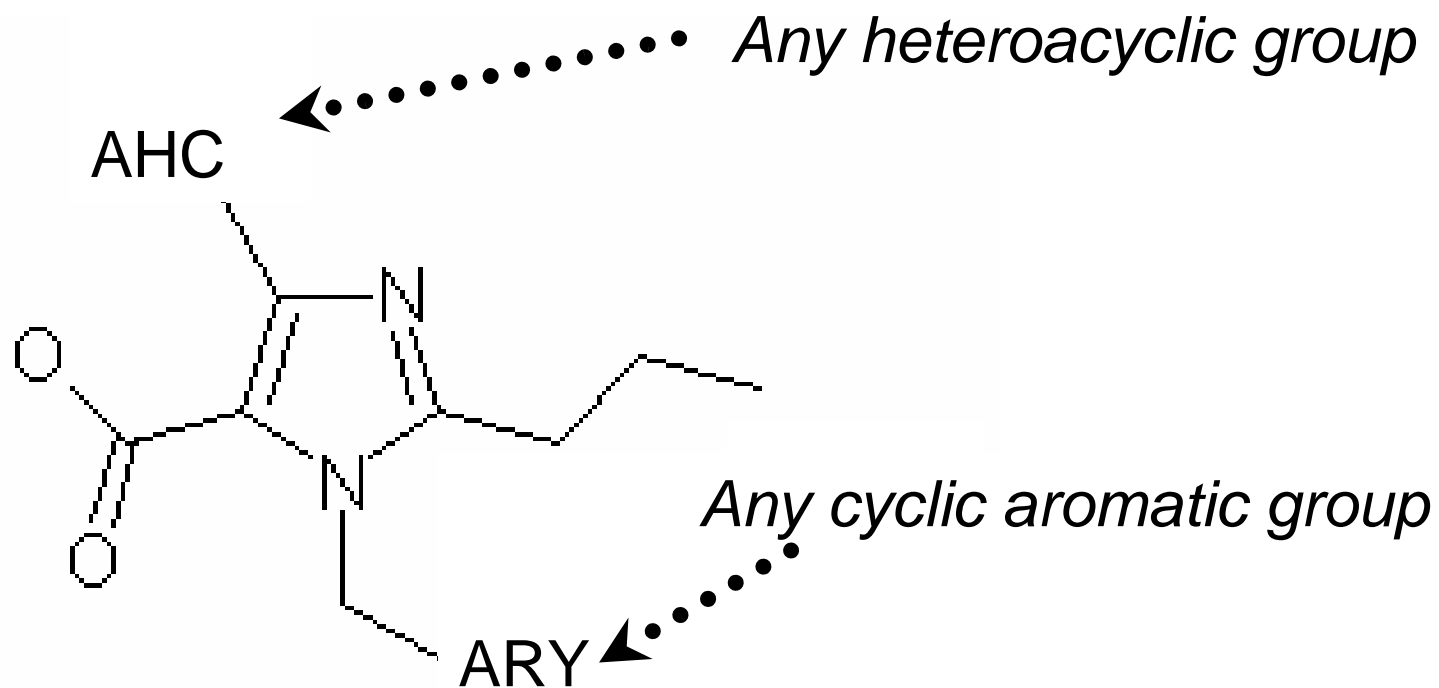
export selected citations page setup print save refine query lists help logout

Pages: 1 [Select All](#) [Clear All](#) Total Records: 2
[Select all citations / Deselect all citations](#)

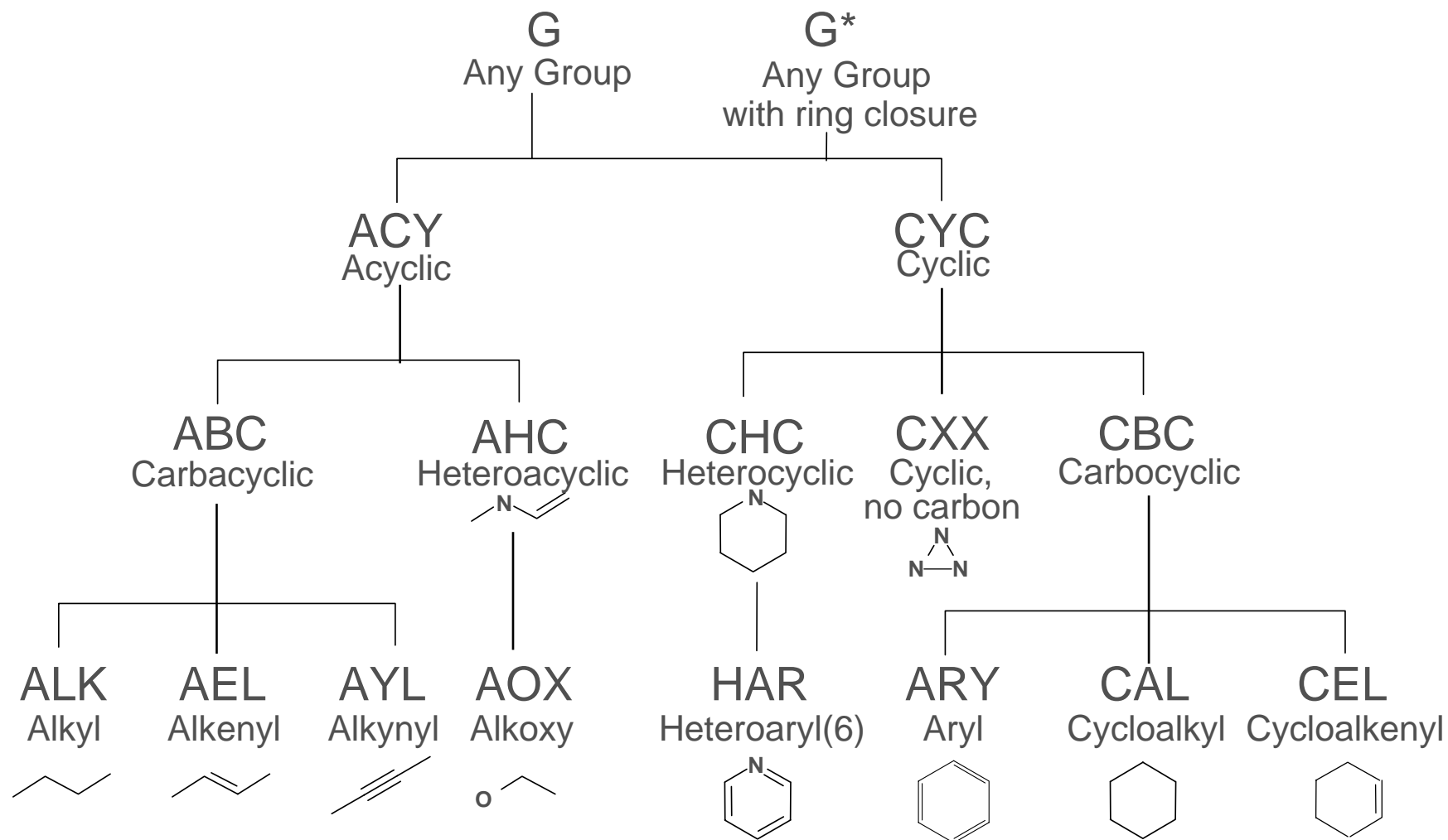
Journal; Mazza, Dario Del; Reinecke, Manfred G.; JCCCAT; J. Chem. Soc. Chem. Commun.; EN; 3; 1981; 124-125	Details
Record 1 <input type="checkbox"/> Export citation <input type="checkbox"/>	
Journal; Yu, Sara Y.; Li, Wei; Iglesia, Enrique; JCTLA5; J. Catal.; EN; 187; 2; 1999; 257 - 261	Details
Record 2 <input type="checkbox"/> Export citation <input type="checkbox"/>	

Pages: 1 [Select All](#) [Clear All](#) Total Records: 2

Query



Beilstein generic groups



Add Beilstein Generic Group

Right-click the atom
with the **select** tool

The image shows a chemical structure with a right-click context menu open over a carbon atom. The menu includes options like 'Atom Property', 'Charge...', 'Isotope', 'Valence...', 'Radical', 'Additional substituents...', 'Hydrogen count', 'Chain or ring atom', 'Allow these atoms', 'Prohibit these atoms', 'Beilstein generic group', 'Remove Properties', 'Copy', 'Cut', 'Duplicate', and 'Bond Properties'. The 'Beilstein generic group' option is expanded, showing 'Any group...', 'Acyclic group', 'Cyclic group', and 'Off'. The 'Cyclic group' option is further expanded to show 'Carbon atoms only...', 'Carbon and/or hetero atoms...', and 'Any acyclic group...'. A dialog box titled 'Carbon and/or hetero atoms...' is also visible, containing a table of Beilstein generic groups.

Off	AHC	Any heteroacyclic group	AHH	Any heteroacyclic group, or H
	AOX	Alkoxy group	AOH	Alkoxy group, or H

Add Beilstein Generic Group

AHC

Atom Property

- Atom symbol...
- Charge...
- Isotope
- Valence...
- Radical
- Additional substituents...
- Hydrogen count
- Chain or ring atom
- Allow these atoms
- Prohibit these atoms
- Beilstein generic group
 - Any group...
 - Acyclic group
 - Cyclic group
 - Carbon atoms only...
 - Carbon and/or hetero atoms...
 - Hetero atoms only...
 - Any cyclic group...
 - Off
- Remove Properties
- Copy
- Cut
- Duplicate
- Bond Properties

Off	CBC	Any carbocyclic group	CBH	Any carbocyclic group, or H
	CAL	Any cycloalkyl group	CAH	Any cycloalkyl group, or H
	CEL	Any cycloalkenyl group	CEH	Any cycloalkenyl group, or H
	ARY	Aryl group	ARH	Aryl group, or H

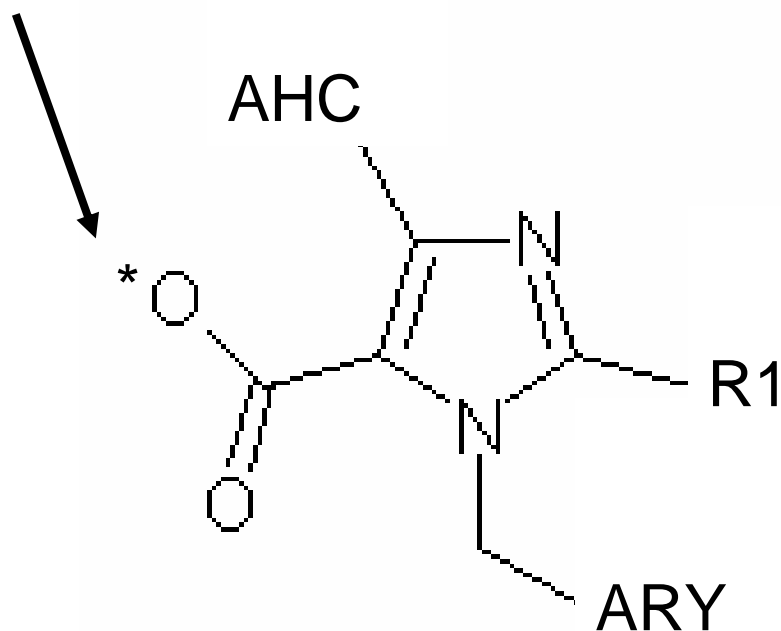
ARY

Right-click the atom with the *select* tool

Force Substitution

Right-click the atom
using the **select** tool

Choose **Additional
substituents>Any#**



Atom Property
Atom symbol...
Charge...
Isotope ▶
Valence...
Radical ▶
Additional substituents...
Hydrogen count ▶
Chain or ring atom ▶
Allow these atoms ▶
Prohibit these atoms ▶
Beilstein generic group ▶
Remove Properties
Copy
Cut
Duplicate

Additional substit... [X]

Any#	1	2	3	4	5
Off	6	7	8	9	10
	11	12	13	14	15



Click Details or Synthesize

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copy to report export records export selected citations page setup print save refine query lists help logout

Database: CrossFire Beilstein

Find in History: [] Next

Field Index History

Today's Searches

- Search #1
- Search #2
- Search #3
- Search #4
- Search #5
- Search #6
- Search #7
- Search #8

Previous Searches

Saved Searches

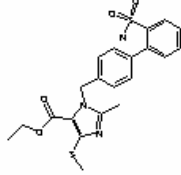
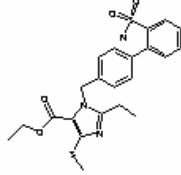
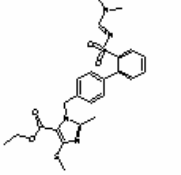
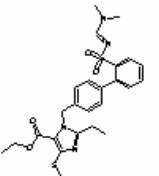
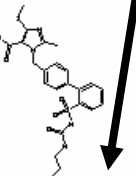
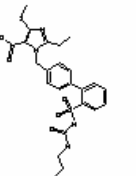
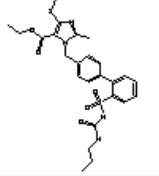
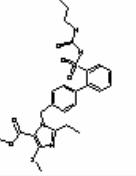
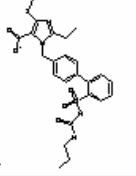
Temporary Lists

View selected records in another database

Create List

Pages: 1 2 Next Select All Clear All

Total Records: 22

BRN: 7394079  Details Synthesize <input type="checkbox"/> Record#1	BRN: 7395096  Details Synthesize <input type="checkbox"/> Record#2	BRN: 7397781  Details Synthesize <input type="checkbox"/> Record#3
BRN: 7398171  Details Synthesize <input type="checkbox"/> Record#4	BRN: 7399224  Details Synthesize <input type="checkbox"/> Record#5	BRN: 7399670 BIO  Details Synthesize <input type="checkbox"/> Record#6
BRN: 7399983 	BRN: 7400295 	BRN: 7406746 BIO 

Browsing Database Results in the Grid View

Click [Details](#) to view the details of a specific substance or reaction. Scroll the data and click the data links that you want to view. To return to the result set, click [Return to Search Results](#).

Use the check box by each result to select those results that you want to copy to a report, export, view in another database, or include in a

Applet WebClientApplet started

Internet

BIO
denotes
bioactivity
data is
available

Click on the “+” to uncover the retrosynthetic pathway

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queries results reports rxn schemes

copy to report export selected citations page setup print save refine query help logout CrossFire Beilstein

Database: CrossFire Beilstein

Find in Rxn Tree: Next

Rxn Tree History

- Substance 7399224
 - Reaction 4372587
 - Substance 7399983
 - Reaction 4336261
 - Substance 1098489
 - Substance 7394079
 - Reaction 4371895
 - Substance 7397781

Synthetic Scheme for Substance 7399224

Details for Reaction 4372587

Details for Reaction 4336261

Details for Reaction 4371895

The Rxn Schemes tab displays a hierarchy of reaction pathways beginning with the final product. To **expand the reaction tree**, click the **+ sign** in front of a substance or a reaction folder. As you expand the reaction tree, you see the **full synthetic scheme** appear in the workspace on the right.

Click **Details** below a reaction step to view **reaction conditions** and **citation information**.

Applet WebClientApplet started

Internet

Click to view reaction details

View reaction details

Click **Results Tab** to return to previous page

https://www.discoverygate.com - MDL Database Browser - Microsoft Inter

DiscoveryGate® | MDL® Database Browser

queries

results

reports

rxn schemes

copy to report export selected citations page setup print save refine query help logout

CrossFire Beilstein

Database:

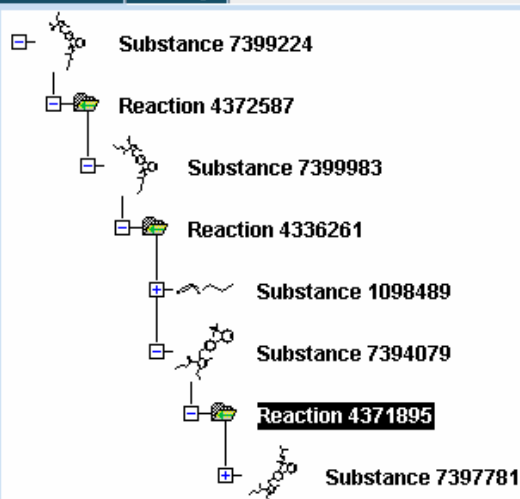
CrossFire Beilstein

Find in Rxn Tree:

Next

Rxn Tree

History



← → A-Z Print

The **Rxn Schemes** tab displays a hierarchy of reaction pathways beginning with the final product. To **expand the reaction tree**, click the **+** sign in front of a substance or a reaction folder. As you expand the reaction tree, you see the **full synthetic scheme** appear in the workspace on the right.

Click **Details** below a reaction step to view **reaction conditions** and **citation information**.

Reaction record 1 of 1

Reaction ID	4372587	
Reactant	Reactant BRN	7399983
	Reactant	C25H30N4O5S2
Product	Product BRN	7399224
	Product	C23H26N4O5S2
No of Reaction Details	1	
Reaction Entry Date	1995/12/31	
Reaction Update Date	1995/12/31	

[Top of Page](#)

Reaction Details

Reaction Details record 1 of 1

Citation Pointer	• 5999345	
Reaction Detail ID	4372587.1	
Reaction Classification	• Preparation	
Stage	Reagent	2N NaOH
	Solvent	ethanol
	Time	36 hour(s)
	Other Conditions	Ambient temperature
Entry Date	1995/12/31	
Comment	• Yield given	
Reaction Details Citations	Export	
	<input type="checkbox"/>	Journal; Deprez, Pierre; Guillaume, Jacques; Becker, Reinhard; Corbier, Alain; Didierlaurent, Stanislas; et al.; JMCMAR; J. Med. Chem.; EN; 38; 13; 1995; 2357-2377;

[Top of Page](#)

DiscoveryGate

- ❑ We covered a lot of material!
- ❑ DiscoveryGate is an extremely valuable tool.
- ❑ Beilstein is the largest and most powerful source of data on DiscoveryGate for organic chemists. The additional databases create a very strong single repository of data.

- ❑ Thank you for your time and attention