

Introduction to DiscoveryGate

using DiscoveryGate v2.5

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Symyx

Course Objectives

- In this workshop, you will learn how to:
 - Log into DiscoveryGate
 - Change Personal Settings for DiscoveryGate
 - Conduct structure and data searches using the Database Browser and individual databases
 - View the search results using the Grid, Database, and Properties views
 - Save search results as Temporary and Permanent lists, and Combine lists
 - Create Reports
 - Modify Query Forms and Save as Default Forms
 - Introduce Synthetic Methods

What is DiscoveryGate?

- **An online content platform (www.discoverygate.com)**
- **For accessing a collection of reference databases**
 - Symyx scientific content
 - 3rd Party databases
- **Which are integrated and cross-indexed**
 - **Symyx Compound Index** – 27 million unique chemical structures
 - Compiled from compounds covered in the underlying databases
 - Every search retrieves relevant records from all databases
- **Augmented by direct retrieval of the original publications**
 - Abstracts, papers and patents
 - Delivered directly to the user's desktop
 - Using out-of-box citation service or commercial OpenURL services

DiscoveryGate – Delivers Lots of Individual Databases

Chemistry Reference

CrossFire Beilstein (Elsevier)
CrossFire Gmelin (Elsevier)
OHS Pure Substance MSDS
Index Chemicus (Thomson)

Bioactivity

MDDR (Drug Data Report)
Symyx Metabolite Database
Symyx Toxicity Database
National Cancer Institute Database
Symyx Comp. Medicinal Chemistry
PubChem (NIH)
PharmaPendium (Elsevier)

Synthetic Methodology

ChemInform Reaction Library (FIZ Chemie)
Current Synth Methodology (FIZ Chemie)
Derwent J. of Synth. Methods (Thomson)
OrgSyn Database (OrgSyn)
Symyx Solid Phase Org Rxns (FIZ Chemie)
ISI Current Chemical Reactions (Thomson)
Integrated Major Ref Works
(Elsevier; Springer; InfoChem)

Patent Sources

Patent Chemistry Database (Elsevier)
Derwent World Patent Index (Thomson)

Sourcing Databases

Symyx Available Chemicals Directory
Symyx Screening Compounds Directory

Login to DiscoveryGate

DiscoveryGate®

... Find the information you need

User Login

Username

Password

Go

[Forgot your password?](#)

Flat fee usage


Easy access to chemical , pharmacological and biological information - use it as much as you want, when you want and from anywhere.


Search 25 million indexed chemical structures with a single query. Exploit our collection of over 17 million chemical transformations. Drill down to more than 500 million observed properties.


[More Information](#)

No License?

[30 Day evaluation](#) | [Buy Online](#) | [Contact Us](#)

 DiscoveryGate supports MAC OS X

 **Videos** | [DiscoveryGate](#) | [Symyx Draw](#) | [Video Library](#)



when you need it and from anywhere you need it....

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DiscoveryGate Home Page


The screenshot shows the DiscoveryGate Home Page. At the top left is the DiscoveryGate logo. To its right is a 'Quick Start Guide' link with the text 'Useful information to get you started'. Further right are navigation tabs for 'DiscoveryGate', 'Brenda's Settings', and 'Company Settings'. Below these is a dark blue navigation bar with links for 'Home', 'Support', and 'Logout brenda.waller@symyx.com'. A secondary bar contains 'Tour DiscoveryGate' and 'Download Software' buttons.

The main content area is divided into several sections:

- How Do I?:** Contains an 'Online Guide' (with a question mark icon) and 'Learning Videos' (with a film strip icon). The 'Online Guide' section includes the text 'Quickly view steps to complete common tasks. Query, browse and filter data with ease...' and a list of links: 'Molecule search', 'Reaction search', 'Data search', 'Create a report', 'PharmaPendium search', 'xPharm search', 'Access Beilstein from Scopus', and 'Full video library'.
- QuickSearch:** A search interface with the text 'Search all databases for which you have a license.' and a link 'If you see a gray box below, click here.' Below this is a large empty box with the text 'Double-click to draw structure'. At the bottom, it says '2. Select a Search Type:' followed by a dropdown menu set to 'Exact', a question mark button, and a 'start search' button.
- Applications:** A list of application categories, each with an icon and a brief description:
 - Search Databases:** Synthesis, bioactivity, physical properties, metabolism, toxicity or sourcing.
 - Integrated Major Reference Works:** Review synthetic methods and learn about their scope and limitations.
 - PharmaPendium:** Browse adverse effects and regulatory information for marketed drugs.
 - xPharm:** No Longer Hosted on DiscoveryGate. This link will direct to the new service.
- Right-hand navigation:** Three buttons: 'FDC Reports - The Pink Sheet', 'My Company Links', and 'My Company Alerts'.
- Bottom-left navigation:** 'Administrator Quick Links' and 'What Is New?' buttons.

The footer contains copyright information: '© Elsevier MDL | Terms: rev.22-Aug-2007' on the left, and 'System Requirements | Layout: Standard view | Symyx Training' on the right.

Personal Settings Tab

DiscoveryGate®  **Quick Start Guide**
Useful information to get you started

DiscoveryGate | **Brenda's Settings** | Company Settings

Edit your personal DiscoveryGate settings Home | Support | Logout [brenda.waller@symyx.com](#)

Security Settings

Ask for my company ID the next time I log in

Old Password

New Password

Confirm Password

Update

Database Browser Settings

Select default database
MDL® Compound Index

Select default view of Compound Index search results

Grid View

Database View

Properties View

Display hover help for database contents

Update

Autoupdate Configuration

Select a radio box and click update

Enable Autoupdate

Disable Autoupdate

Update

My Gatelet Settings

Administrator Quick Links

Applications

My Company Bulletins

Embase

FDC Reports - The Pink Sheet

How do I?

What Is New?

QuickSearch

My Company Web Sites

Update

Software Downloads

You must have administrative privileges on your computer in order to install the DiscoveryGate software.

[Click to install software](#)

If you need assistance, please click on the support link..

My Layout Settings

Select a radio box and click update

[Express View](#)

[Standard view](#)

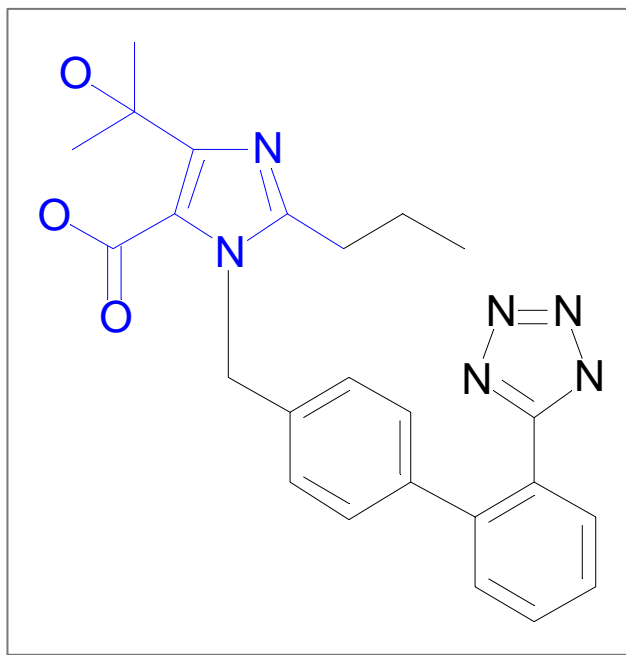
Update

Structure Searching

- In this module, you will learn how to:
 - Conduct an Exact Match and Substructure Search using the Database Browser
 - View Search Results using the Grid, Database, and Properties Views
 - Conduct a Combination Structure and Data Search

Search Scenario

Olemesartan 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 displays the Symyx software interface. The top menu bar includes 'File', 'Edit', 'Chemistry', and 'Help'. Below the menu is a toolbar with various drawing tools. The 'Done' button is highlighted with a red box. The 'All-Purpose Drawing Tool' help panel is open on the right, providing instructions for drawing atoms, bonds, chains, adjusting bond angles, changing bond order, pulling out rings, and changing atom or bond properties. The main workspace shows a complex chemical structure, which is a substituted benzimidazole derivative. The 'All-Purpose Drawing Tool' icon in the toolbar is also highlighted with a red box.

File **Edit** **Chemistry** **Help**

Done Clear All Undo Redo

All-Purpose Drawing Tool

Use this tool to draw an **entire structure without switching tools**. You can also edit structures with this tool.

You can:

- * **Draw an atom:** Click the screen and type the symbol.
- * **Draw a bond:** Press and drag an atom, or press and drag on the screen.
- * **Draw a chain of atoms:** Press and drag an atom, or press and drag on the screen.
- * **Adjust the bond angle:** Click the Lasso Tool or Select Tool . Then, click the atom at the end of the bond and rotate the bond.
- * **Change bond order:** Click a bond repeatedly to switch between single, double, and triple bonds.
- * **Pull out a ring:** Click a bond, then press and drag.
- * **Change atom or bond properties:** Select **one or more** atoms or bonds (using the Shift key), then right-mouse click.
- * **Change the atom symbol:** Right-click the atom. Choose **Atom symbol...** from the menu that appears. Select the atom symbol that you

+

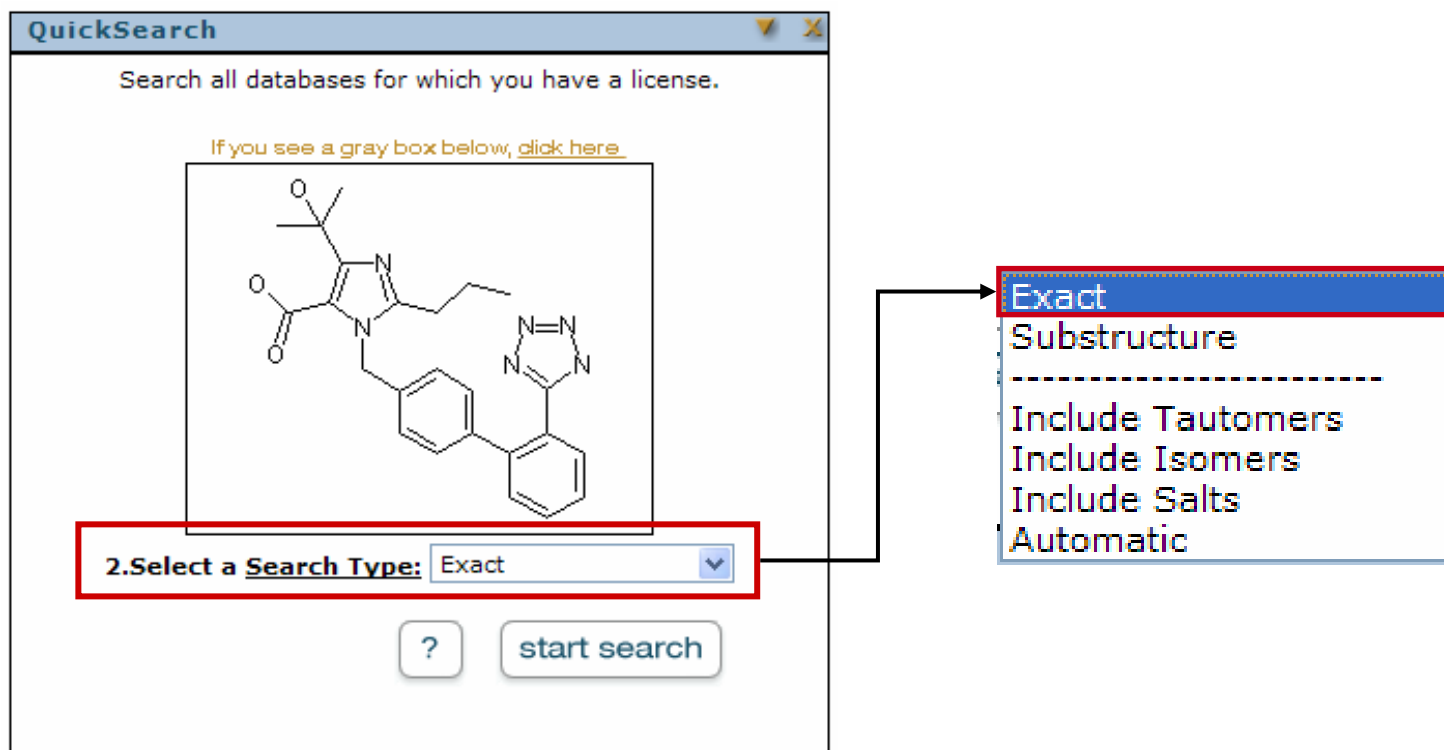
1.

R1

R1=

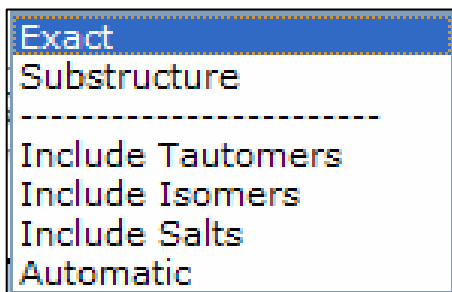
Conduct an Exact Match Search

QuickSearch is a shortcut to the molecule searching functionality.



The screenshot shows the QuickSearch interface. At the top, it says "Search all databases for which you have a license." Below that, there is a link: "If you see a gray box below, click here." In the center, there is a chemical structure of a complex molecule. Below the structure, there is a dropdown menu labeled "2. Select a Search Type:" with "Exact" selected. A red box highlights the dropdown menu, and an arrow points to a larger view of the dropdown options: "Exact", "Substructure", a dashed line, "Include Tautomers", "Include Isomers", "Include Salts", and "Automatic". Below the dropdown menu, there are two buttons: a question mark "?" and "start search".

Structure 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 records export selected citations page setup print save refine query lists help logout MDL® Compound Index

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

[Details](#)

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

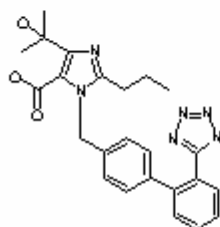
[Return to Search Results](#)

[View selected records in another database](#)

Record # 1 **Total Records:** 1

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

[Select](#) / [deselect](#) all citations from this page.



[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

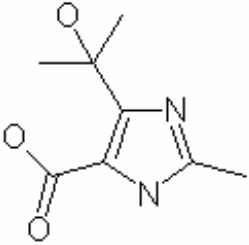
Also found in: [ACD](#) [Beilstein](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [MDDR](#) [MetaCore](#) [MetaDrug](#) [Metabolite](#) [Patent Chemistry](#)

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.

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

save form

start search

Substructure search rules:

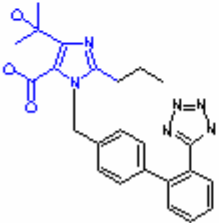
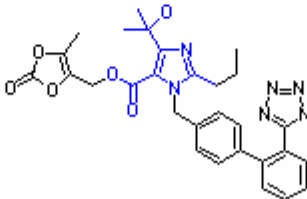
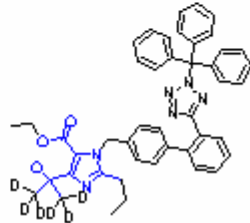
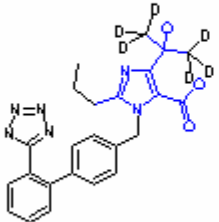
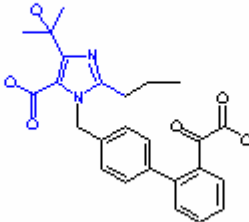
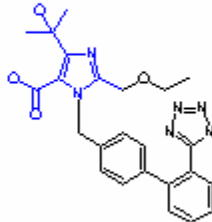
- The core structure must be embedded in all compounds retrieve
- Substitution can occur at any open valence

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](#)

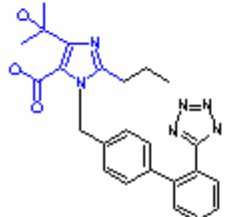
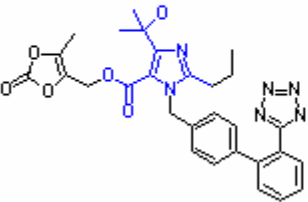
 Details <input type="checkbox"/> Record#1	 Details <input type="checkbox"/> Record#2	 Details <input type="checkbox"/> Record#3
 Details <input type="checkbox"/> Record#4	 Details <input type="checkbox"/> Record#5	 Details <input type="checkbox"/> Record#6

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: 248**

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

Viewing Compounds by Database

View in another database ✕

Select the records that you want to view:

All Records

Current Page

Specify Record Numbers

1

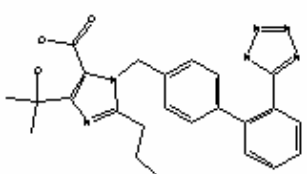
The numbers in the box (if present) correspond to those records that are already selected by checkboxes. To specify other records, enter the record index numbers and/or record ranges, separated by commas. For example, 1,3,4,7-10. If you specify a large number of records, performance might be slow.

OK Cancel

[Return to MDL® Compound Index](#) Record # 1 ➔ Total Records: 6

MDL® Available Chemicals Directory

[Select](#) / [deselect](#) all citations from this page.

CC1(C)C(=O)C2=C(C1)C(=O)C(C2)CC3=CC=C(C=C3)C4=CC=CC=C4

Available Data

Click on a link to add the information to this page

Set current view as default

[Substance](#) (1) [Suppliers](#) (12)

[Prices](#) (12) [Model](#) (1)

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: 248
1	 <input type="checkbox"/> Record#1	3d Configuration ADME Agrochemical Analytical Chemical Commercially Available Information Source Metabolism Name Pharmacological Physical Chemical Preparation
2	 <input type="checkbox"/> Record#2	3d Configuration ADME Adverse Effects Agrochemical Analytical Chemical Commercially Available Information Source Metabolism Name Pharmacological Physical Chemical Preparation Toxicity

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) those records that are already selected. To specify other records, enter the numbers and/or record ranges, separated by commas. For example, 1,3,4,7-10. If you specify records, performance might be slow.

OK

[Return to MDL® Compound Index](#)

[Beilstein](#) [DWPI](#) [MDDR](#) [Patent Chemistry](#) [PharmaPendium](#) [Toxicity](#)

← Record # 18 → **Total Records: 61**

MDL® Comprehensive Medicinal Chemistry

[Select / deselect](#) all citations from this page.

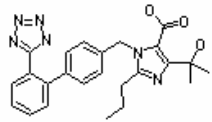
Available Data

Click on a link to add the information to this page

Set current view as default

[Substance](#) (1) [Model](#) (1)

[Literature](#) (1)

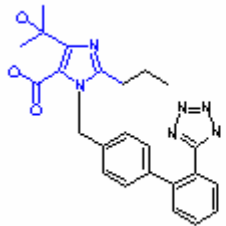


Substance [\(hide\)](#)

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

Viewing Data for a Single Record

1



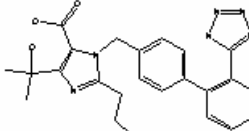
Record#1

[3d Configuration](#) [ADME](#)
[Agrochemical](#) [Analytical](#)
[Chemical](#)
[Information](#)
[Name](#)
[Physical](#)

[Return to MDL® Compound Index](#)
[Beilstein](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [MDDR](#) [Metabolite](#) [Patent Chemistry](#)
Record # 1 ➔ **Total Records:** 8

MDL® Available Chemicals Directory

[Select](#) / [deselect](#) all citations from this page.



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

Set current view as default

[Substance](#) (1) [Suppliers](#) (12)
[Prices](#) (12) [Model](#) (1)

Substance [\(hide\)](#)

ACD Registry Number	153440
Availability	Large and small quantities
MDL Number	MFCD00914967
CAS Registry Number	144689-24-7
Chemical Name and Synonyms :	
• OLMESARTAN	
Molecular Formula	C24 H26 N6 O3
Molecular Weight	446.508
Rule of Five	0
Computed partition coefficient (CLogP)	3.63

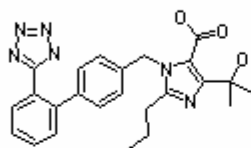
[Return to MDL® Compound Index](#)

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

← Record # 3 → **Total Records: 8**

MDL® Comprehensive Medicinal Chemistry

[Select](#) / [deselect](#) all citations from this page.



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 [U]		
Class	Antihypertensive		
LogP	3.63	Comment	
pKa		Comment	
Formula	C24 H26 N6 O3		
Molecular Weight	446.508		

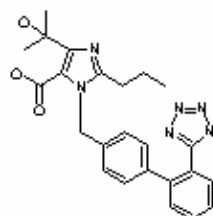
[Return to MDL® Compound Index](#)

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

← Record # 6 → **Total Records:** 8

MDL® Drug Data Report

[Select](#) / [deselect](#) all citations from this page.



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

Metabolite

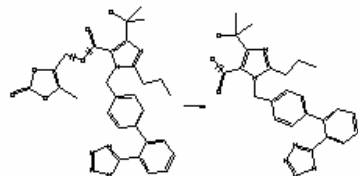
[Return to MDL® Compound Index](#)

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

← Record # 7 → **Total Records: 8**

MDL® Metabolite Database

[Select](#) / [deselect](#) all citations from this page.



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](#) (3)
[Species](#) (3)
[Enzyme](#) (3)

View results as **molecules:**

[Parent](#) (1)
[Species](#) (3)
[Substrate](#) (1)
[Metabolite](#) (1)

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

MDL number	RMTB00058294
Path	MTB9122-A
Step	1 Step
Scheme	MTB9122

Chemical Name and Synonyms :

- CS-866
- (5-Methyl-2-oxo-1,3-dioxol-4-yl)methyl 4-(1-hydroxy-1-methylethyl)-2-propyl-1-((2-(1H-tetrazol-5-yl)-1,1'-biphenyl-4-yl)methyl)-1H-imidazole-5-carboxylate
- Olmesartan medoxomil
- CS 866
- 5-Methyl-2-oxo-1,3-dioxol-4-ylmethyl 4-(1-hydroxy-1-methylethyl)-2-propyl-1-((2-(1H-tetrazol-5-yl)biphenyl-4-yl)methyl)imidazole-5-carboxylate

Adding a Data Criterion to Your Structure Search

DiscoveryGate® | MDL® Database Browser

queries results reports

start search import save clear form help logout MDL® Compound Index Version

Database: MDL® Compound Index

Find in Field Index: Next

Field Index History

- Molecular Formula
- Molecular Weight**
- cdbregno
- molstructure**
- Adverse Effects
- Pharmacological
- Physical Chemical
- Preparation
- Safety
- Analytical
- Structure based
- Toxicity
- ADME
- Chemical
- Commercially Available
- Ecological
- Name
- Information Source
- Agrochemical
- Metabolism
- 3d Configuration

molstructure

Select Search Type: Substructure

Double-click in this box to edit structure

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

Query Highlighting.

Reset Delete Duplicate Info

AND Molecular Weight =

Delete Duplicate Info

start search

show brackets **save form**

Completed Search Form

Enter the core structural fragment

The screenshot shows a search form with the following elements:

- molstructure**: A text area containing a chemical structure of a substituted imidazole ring.
- Select Search Type:** A dropdown menu set to "Substructure". Below it is a description: "A Molecule Substructure search finds molecule records that contain your query as a substructure wholly within a larger structure." and a checked checkbox for "Query Highlighting".
- Buttons:** "Reset", "Delete", "Duplicate", and "Info" are located to the right of the search type dropdown.
- AND**: A dropdown menu set to "AND".
- Molecular Weight**: A text field containing the value "350".
- Operator**: A dropdown menu set to "<".
- start search**: A button to execute the search.
- show brackets** and **save form**: Buttons at the bottom left.

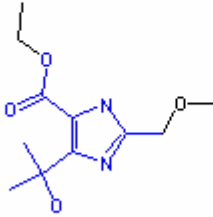
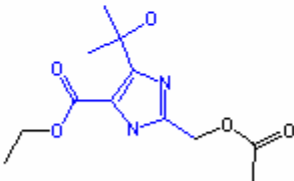
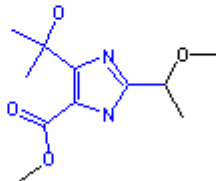
Enter data and specify an operator

Results of the Structure and Data Search

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

[View selected records in another database](#)

Pages: 1 **2** 3 [Next](#) [Select All](#) [Clear All](#) **Total Records: 26**

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

Substructure search results – 248 compounds

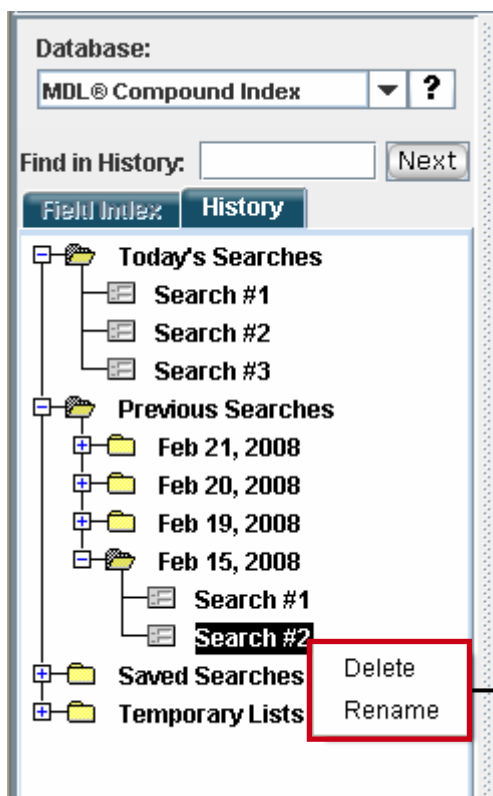
Substructure search with data constraint results – 26 compounds

Manipulating Search Results

- In this module, 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

DiscoveryGate® | MDL® Database Browser

queries results reports

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

Database: MDL® Compound Index ?

Find in History: [] Next

Field Index History

Today's Searches

- Search #1
- Search #2
- Search #3

Previous Searches

- Feb 21, 2008
- Feb 20, 2008
- Feb 19, 2008
- Feb 15, 2008

Saved Searches

Temporary Lists

Grid View Database View Properties View

View selected records in another database

Pages: 1 Next Select All Clear All

Database: MDL® Compound Index ?

Find in History: [] Next

Field Index History

Today's Searches

- Search #1
- Search #2
- Search #3

Previous Searches

- Feb 21, 2008
- Feb 20, 2008
- Feb 19, 2008
- Feb 15, 2008

Saved Searches

Temporary Lists

L1 Structure and MW<350

Record#2

Record#5

Record#6

Create List

Select the records that you want to store in the results set:

- 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

Description: Structure and MW<350

Your results set is stored in the History tab, Temporary Lists folder. Edit the description there by right-clicking it.

OK Cancel

Create a Permanent List

The screenshot displays the DiscoveryGate MDL Database Browser interface. At the top, there are tabs for 'queries', 'results', and 'reports'. Below these, a navigation bar includes options like 'copy to report', 'export records', 'export selected citations', 'page setup', 'print', 'save', 'refine query', 'lists', 'help', and 'logout'. The 'save' button is highlighted with a red box. A 'Save As' dialog box is open, showing 'File name: Structure SSS' in a text field, also highlighted with a red box. The dialog has 'OK' and 'Cancel' buttons. In the background, the 'results' tab is active, showing a search history on the left and a list of records on the right. The 'save' button in the navigation bar is connected by a line to the 'Save As' dialog. The 'Save As' dialog is also connected by a line to the 'Structure SSS' entry in the search history on the right, which is also highlighted with a red box. The search history on the right shows 'Today's Searches' (Search #1, Search #2, Search #3) and 'Previous Searches' (Feb 21, 2008, Feb 20, 2008, Feb 19, 2008, Feb 15, 2008). Below these is a 'Saved Searches' folder containing 'Structure SSS' and 'Temporary Lists' containing 'L1 Structure and MW<350'. The 'Structure SSS' entry is highlighted with a red box. The 'save' button in the navigation bar is also connected by a line to the 'Structure SSS' entry in the search history.

Combining Lists

DiscoveryGate® | MDL® Database Browser

queries

results

reports

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

Combine Lists

Result Set 1

Temporary Lists

- L1 Structure and MW<350
- L2 Structure SSS

- AND OR NOT

Result Set 2

Temporary Lists

- L1 Structure and MW<350
- L2 Structure SSS

Apply

Cancel

Description:

Structure and MW > 350

Your resulting list is stored in the History tab, Temporary Lists folder. Edit the description there by right-clicking it.

Lists

Which list operation do you want to perform?

- Import a list
- Export a list
- Combine two lists with an And/Or/Not operator

OK

Cancel

Database:

MDL® Compound Index

Find in History: Next

Field Index

History

- Today's Searches
- Previous Searches
- Saved Searches
- Temporary Lists
 - L1 Structure and MW<350
 - L2 Structure SSS
 - L3 (L2 NOT L1) Structure and M

Export a List

DiscoveryGate® | MDL® Database Browser

queries results reports

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

Database: MDL® Compound Index

Grid View Database View Properties View

[View selected records in another database](#)

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 ranges, 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

Exporting Fields

- MOL
 - MOLSTRUCTURE
 - Molecular Weight
 - Molecular Formula

Export SDfile ...

Export TAB ...

Cancel

Add Remove ↑ ↓

Include highlighting information

Export format selection 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.

Data Searching

- In this module, you will learn how to:
 - Search Individual Databases
 - Select your Preferred Data Fields
 - Save the Modified Query Form as Your Default Form for the Current Database
 - Display Hidden Data in Details View
 - Create a Report

Selecting an Individual Database

DiscoveryGate® | MDL® Database Browser

queries results reports

start search import save clear form help logout

MDL® Compound Index Version

Database:

- MDL® Compound Index
- CrossFire Beilstein
- CrossFire Gmelin
- MDL® Compound Index
- Bioactivity Information
- MDL® Comprehensive Medicinal Chemistry
- MDL® Drug Data Report
- National Cancer Institute Database
- MDL® Metabolite Database
- MDL® Toxicity Database
- Chemical Sourcing and Logistics Information
- MDL® Available Chemicals Directory
- MDL® Screening Compounds Directory
- Patent Information
- MDL® Patent Chemistry Database
- Synthetic Methodology Information
- ChemInform Reaction Library
- Current Synthetic Methodology
- Derwent Journal of Synthetic Methodology
- ORGSYN Database
- MDL® Reference Library of Synthetic Organic Chemistry
- MDL® Solid-Phase Organic Reactions
- 3d Configuration

molstructure

Select Search Type:

Substructure

Double-click in this box to edit structure

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

Query Highlighting.

AND Molecular Weight =

start search

show brackets save form

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

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

Select an individual database from the drop-down list

Using 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.

Query Highlighting

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

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

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](#)

Transformation

AND	Route	Contains		Data Lookup... Delete Duplicate Info
AND	Species	Contains		Data Lookup... Delete Duplicate Info
AND	Journal Author	Contains		Delete Duplicate Info
AND	Journal Name	Contains		Data Lookup... Delete Duplicate Info
AND	Journal Year	=		Delete Duplicate Info

Predefined Search Forms

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

Database: MDL Patent Chemistry Database

Find in Field Index: Next

Field Index History

- Structure
- Easy Data Search**
- Bibliographic Data
- Patent Data
- Substance Identification Data
- Molecular Formula Search
- Reaction Data
- Physical Data
- Spectroscopic Data
- Bioactivity data
- Application data
- Composition
- Citations
- Substances
- Reactions

Database: CrossFire Beilstein

Find in Field Index: Next

Field Index History

- Structure
- Easy Data Search**
- 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**
- 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

Data Search Features

Data field

Substance				
	Beilstein Registry Number	=	<input type="text"/>	Delete Duplicate Info
OR	CAS Registry Number	Contains	<input type="text"/> Data Lookup...	Delete Duplicate Info
OR	Chemical Name	Is	<input type="text"/> Data Lookup...	Delete Duplicate Info
OR	Molecular Formula	Is	<input type="text"/> Data Lookup...	Delete Duplicate Info
OR	Molecular Weight	=	<input type="text"/>	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 ACD database.

Molecule				
Structure		Select Search Type:		
Double-click in this box to edit structure		Substructure		Reset Delete Duplicate Info
A Molecule Substructure search finds molecule records that contain your query as a substructure wholly within a larger structure.		<input checked="" type="checkbox"/> Query Highlighting.		
AND	Catalog Number	Contains	<input type="text"/>	Delete Duplicate Info
AND	Chemical Name and Synonyms	Contains	<input type="text"/>	Delete Duplicate Info
AND	CAS Registry Number	Is	<input type="text"/>	Delete Duplicate Info
AND	MDL Number	Contains	<input type="text"/>	Delete Duplicate Info
AND	Supplier Name	Contains	<input type="text"/>	Delete Duplicate Info

Search Results

Chemical Name search results

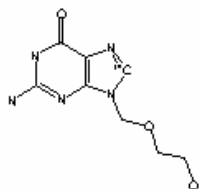
[View selected records in another database](#)

[Sort Results](#) [Create List](#)

Pages: 1 **2** [Next](#) [Select All](#) [Clear All](#)

Total Records: 23

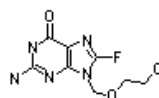
MDL® Available Chemicals Directory



[Details](#)

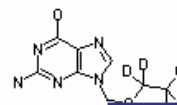
Record#1

MDL® Available Chemicals Directory



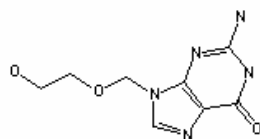
[Details](#)

MDL® Available Chemicals Directory



[Details](#)

MDL® Available Chemicals Directory



[Details](#)

Record#4

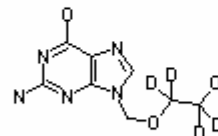
[View selected records in another database](#)

[Sort Results](#) [Create List](#)

Pages: 1 [Select All](#) [Clear All](#)

Total Records: 2

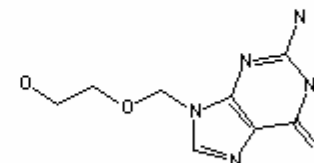
MDL® Available Chemicals Directory



[Details](#)

Record#1

MDL® Available Chemicals Directory



[Details](#)

Record#2

CAS number search results

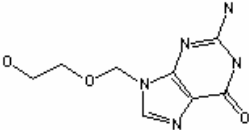
Link to Additional Data

[Return to Search Results](#) [View selected records in another database](#) ← Record # 4 → **Total Records: 23**

Also found in: [CCR](#) [CIRX](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [MDDR](#) [Metabolite](#) [OHS MSDS](#) [PharmaPendium](#) [SCD](#) [SPORE](#) [Toxicity](#) [Patent Chemistry](#) [Beilstein](#)

MDL® Available Chemicals Directory

[Select / deselect](#) all citations from this page.



[Use as Query](#)

 Select current record

Available Data

Click on a link to add the information to this page

 Set current view as default

[Substance](#) (1) [Suppliers](#) (64)
[Prices](#) (64) [Model](#) (1)

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

View Supplier Information

Displays or hides the data

Suppliers [\(hide\)](#)

Chemical Name and Synonyms :

- 2-AMINO-9-(2-HYDROXY-ETHOXYMETHYL)-1,9-DIHYDRO-PURIN-6-ONE
- 9-(2'-HYDROXYETHOXYMETHYL)-GUANINE
- 9-(2-HYDROXYETHOXY)METHYLGUANINE
- ACICLOVIR
- ACV
- ACYCLOGUANOSINE
- ACYCLOVIR
- ACYCLOVIR SUBST
- AKOS NCG1-0055
- ZOVIRAX

Molecular Formula	C8 H11 N5 O3
Supplier List	AAGAMI AAKASH-API AAKASH-CHEM AAKASH-PHARM ABCHEM-INC ACETO ACP-SCI ADVTECHIND AKOS AKSCI ALLTECH AMPLACHEM ANDACHEM APAC APIN-NP APOLLO-INTER ARKPHARMINC BEPHARM BETAPHARM-CN BETAPHARMA BOSCHESCI CALBIO CALBIO-ST CGENETECH CHEMICEU CHEMPACIFIC CHIMEX CRESCENT DR-EHREN FINECHEMIE FWDCHEM GEORGE-UHE HAISOPHARM HALLOCHEM IBSCREEN-BB KEMPROTEC LACHEM-BRNO LKT-LABS LKT-LABS-SPC MCTONY MOLEKULA MORAVEK MPBIO OCHEMINC PHARMACN PIPHARM RADIAN RECORDATI SEQUOIA SIGMA SINOVA SPECBIOCHEM SPECTRUM SPECTRUM-B SPECTRUM-USP TOCRIS-UK TOCRIS-US TORONTO VWR WAKO WATERSTONE WILSHIRE ZERENEX ZHONGSHUO

[Top of Page](#)

Search the Toxicity Database

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

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:](#)
Substructure

Double-click in this box to edit structure

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

 Query Highlighting.

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

AND	Chemical Name and Synonyms	Contains	<input type="text"/>	Delete Duplicate Info
AND	CAS Registry Number	Is	<input type="text"/>	Delete Duplicate Info
Acute Toxicity				
AND	Dosage	=	<input type="text"/> mg/kg	Delete Duplicate Info
AND	Endpoint	Contains	<input type="text"/> Data Lookup...	Delete Duplicate Info
AND	Species	Contains	<input type="text"/> Data Lookup...	Delete Duplicate Info

Create a Custom Form

Field Index History

- MDL Number
- Molecular Formula
- Molecular Weight
- RTECS Registry Number
- Threshold Limit Value
- Toxicology Reviews
- Acute Toxicity
- Mutagenicity
- Irritation
- Tumorigenicity
 - Dosage
 - Endpoint
 - Initiator Name(s)
 - Journal Name
 - Journal Page
 - Journal Volume
 - Journal Year
 - Promoter Name(s)
 - Route
 - Sex
 - Strain
 - Species
 - Tissue
 - Toxic Effect
- Reproductive Effects
- Other Multiple Dose

Tumorigenicity

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

start search

Double-click to add field to query form

Enter the “Toxic Effect” Data Constraint

Data Look-up... Toxic Effect

1. Type the first few letters of the word that you are looking for.

2. Double-click the index entries that you want, and then click OK.

- Angiosarcoma < Liver
- Change in gall bladder structure or function < Liver
- Fatty liver degeneration < Liver**
- Gallbladder tumor < Liver
- Hepatitis (hepatocellular necrosis), diffuse < Liver
- Hepatitis (hepatocellular necrosis), zonal < Liver
- Hepatitis, fibrous (cirrhosis, post-necrotic scarring) < Liver
- Jaundice, other or unclassified < Liver
- Liver function tests impaired < Liver
- Multiple effects < Liver
- Other changes < Liver

Fatty liver degeneration < Liver

Find any of these terms (OR operator)
 Find all of these terms (AND operator)

OK Cancel Clear

Tumorigenicity

AND Toxic Effect Contains Fatty liver degeneration < Liver
[Data Lookup...](#)

start search

Saving a Form

CHEMICAL

Structure

Double-click in this box to edit 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.

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

Acute Toxicity

AND Chemical Name and Synonyms Co
AND CAS Registry Number Is

AND Dosage = [] mg/kg [Duplicate](#)
[Info](#)

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

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


Tumorigenicity

AND Toxic Effect Contains [Fatty liver degeneration < Liver] [Delete](#)
[Duplicate](#)
[Info](#)
[Data Lookup...](#)

start search

show brackets **save form** sort results

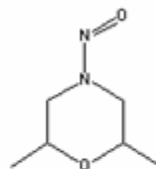
Save Form

 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



Copy to Report

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 Version

Database: MDL® Toxicity Database ?

Find in Outline: Next

Outline History

- Today's Report - Report #1
 - Section 1

Tumorigenicity

Full Citation 1 of 35

Export Journal of the National Cancer Institute 64,529,1980

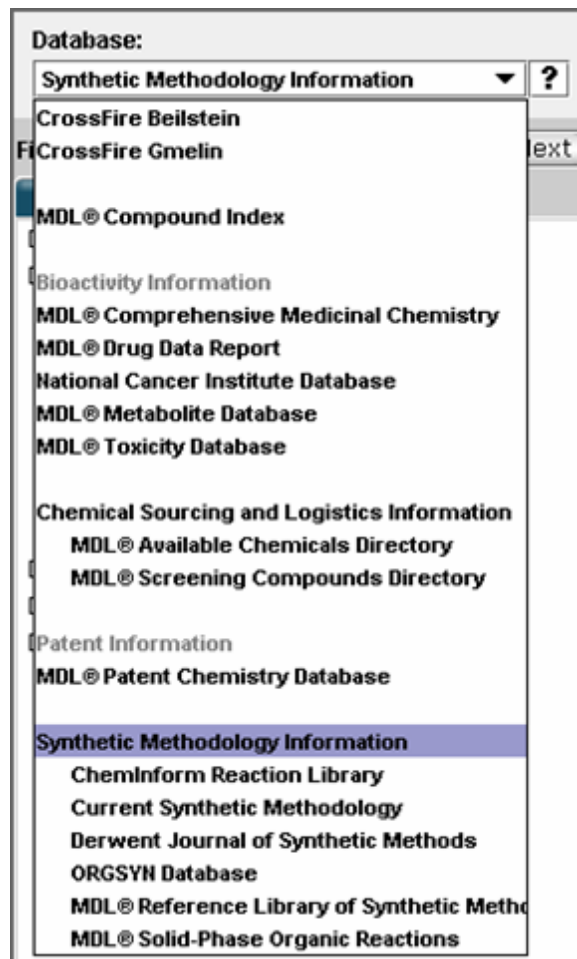
Source ID :	QE2150000	Source :	RTECS
Chemical Name	MORPHOLINE, 2,6-DIMETHYL-N-NITROSO-		
Species	guinea pig		
Route	ORAL		
Dosage	400 MG/KG/23W-I		
Endpoint :	TD		
Endpoint (Incidence) :	(Carcinogen, Carcinogen+Inhibitor, %Diff., Significance)		
Endpoint (Multiplicity) :			
Endpoint (Latency) :	(Carcinogen,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

Toxic Effects :

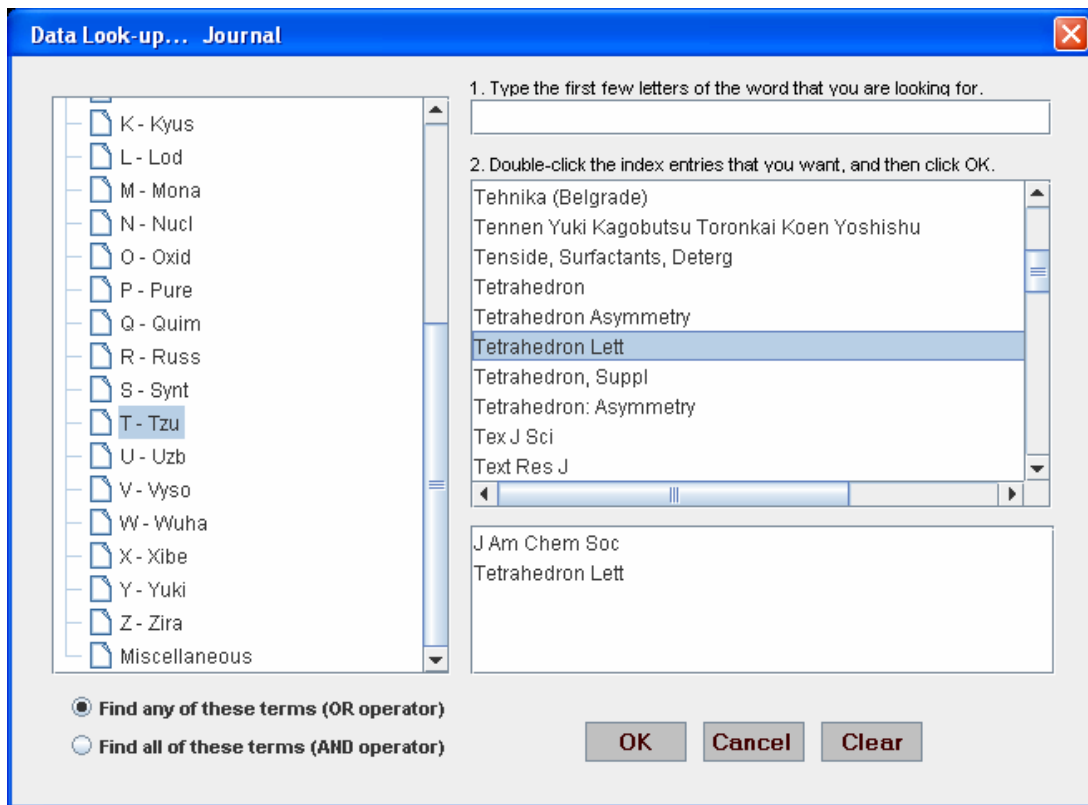
- Carcinogenic by RTECS criteria < Tumorigenic
- Fatty liver degeneration < Liver
- Tumors < Liver

Retrieving Reactions using a Data Query

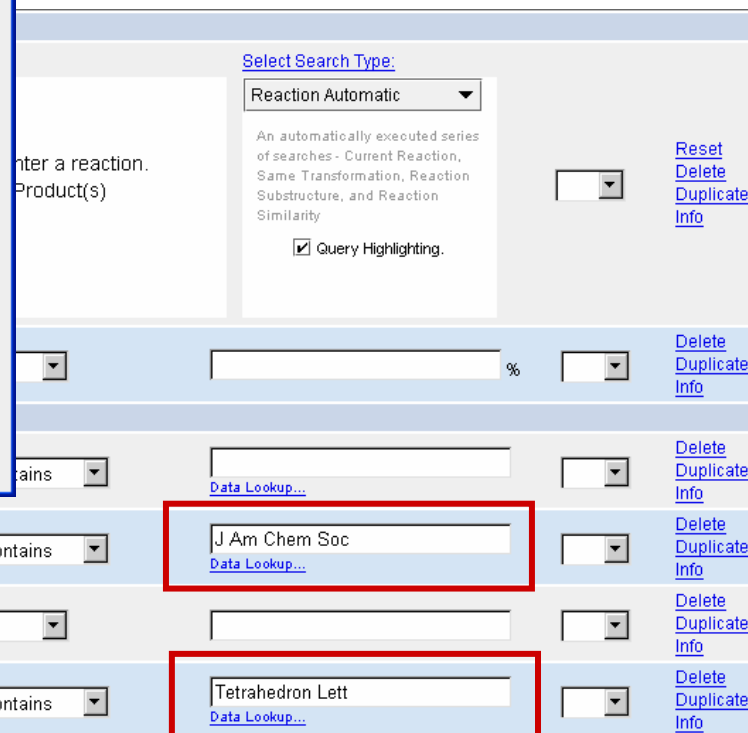
Conduct a search to retrieve hydrogenation reactions published in the Journal of the American Chemical Society or Tetrahedron Letters.



Additional Data Fields



When multiple selections are made in the Data Lookup dialog box additional fields are added to the form



Manually Add a Data Field

The screenshot displays the DiscoveryGate MDL Database Browser interface. On the left, the 'Field Index' tree is visible, with 'Conditions' highlighted in a red box. An arrow points from this box to the 'Reaction' section of the search form. The search form includes a 'Reaction' section with a 'Structure' field and a 'Select Search Type' dropdown set to 'Reaction Automatic'. Below this, there are several search criteria rows. The bottom row, which is also highlighted in a red box, shows the 'Conditions' field added to the search criteria. The criteria are: AND, Conditions, Contains, Hydrogenations, and a dropdown menu.

Database: Synthetic Methodology Information

Find in Field Index: conditions Next

Field Index History

- Reaction
 - Structure
 - Atmosphere
 - Conditions
 - Enantiomeric Excess
 - Percent Yield
 - Primary Reaction?
 - Reaction MDL Number
 - Systematic Classification
 - Temperature
 - Topics
 - Type
- Molecules
 - Reactant
 - Product
 - Catalyst
 - Solvent
 - Protecting Group
 - Solid Support
 - Polymer
- Citation
- Solid Phase
- Classification

Reaction

Structure

Select Search Type: Reaction Automatic

Double-click here to enter a reaction.
Reactant(s) --> Product(s)

AND Percent Yield = %

Citation

AND Author Contains Data Lookup..

AND Journal Contains J Am Chem Soc Data Lookup..

AND Year =

OR Journal Contains Tetrahedron Lett Data Lookup..

Reaction

AND Conditions Contains Hydrogenations Data Lookup..

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

Setting Search Logic

AND	[Journal	Contains	J Am Chem Soc		Delete Duplicate Info
AND		Year	=			Delete Duplicate Info
OR		Journal	Contains	Tetrahedron Lett)	Delete Duplicate Info
Reaction						
AND		Conditions	Contains	Hydrogenations		Delete Duplicate Info

Setting the parenthetical statement forces the search.

(Journal Contains J. Am.Chem.Soc. OR Journal Contains Tetrahedron Letters)
AND Conditions Contains Hydrogenations

Setting Parenthetical Statements

Initial search

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

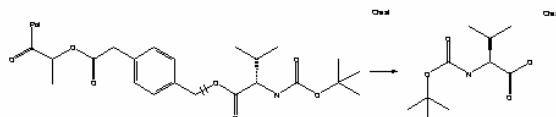
Modified search

AND	[Journal	Contains	J Am Chem Soc		Delete Duplicate Info
OR		Journal	Contains	Tetrahedron Lett]	Delete Duplicate Info
AND		Year	>	2000		Delete Duplicate Info
Reaction						
AND		Conditions	Contains	Hydrogenations		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. B., J Am Chem Soc \[JACSAT\] 1980, 102 \(19\), 6117-6127.](#)

[TAM, J. P.; TJOENG, F. S.; MERRIFIELD, R. B., Tetrahedron Lett \[TELEAY\] 1979, 51, 4935-4938.](#)

[WHITNEY, D. B.; TAM, J. P.; MERRIFIELD, R. B., Tetrahedron \[TETRAB\] 1984, 40 \(21\), 4237-4244.](#)

Conditions

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

Reaction Searching

- In this module, you will learn how to:
 - Conduct a Reaction Substructure Search
 - View Reactant and Product Data from Another Database
 - Link to Literature References
 - Find Similar Reactions

Synthetic Methodology Information

DiscoveryGate® | MDL® Database Browser

queries results reports rxn schemes

start search import save clear form help logout Synthetic Methodology Information Version

Database: Synthetic Methodology Information ?

Find in Field Index: Next

Field Index History

- Reaction
- Molecules
 - Reactant
 - Product
 - Catalyst
 - Solvent
 - Protecting Group
 - Solid Support
 - Polymer
- Citation
- Solid Phase
- Classification

Reaction

Structure

Select Search Type: Reaction Substructure

Double-click here to enter a reaction.
Reactant(s) --> Product(s)

Finds the reactions that contain the same structural fragments and reacting centers as your reaction.

Query Highlighting.

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

AND Percent Yield = % [Delete](#)
[Duplicate](#)
[Info](#)

Citation

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

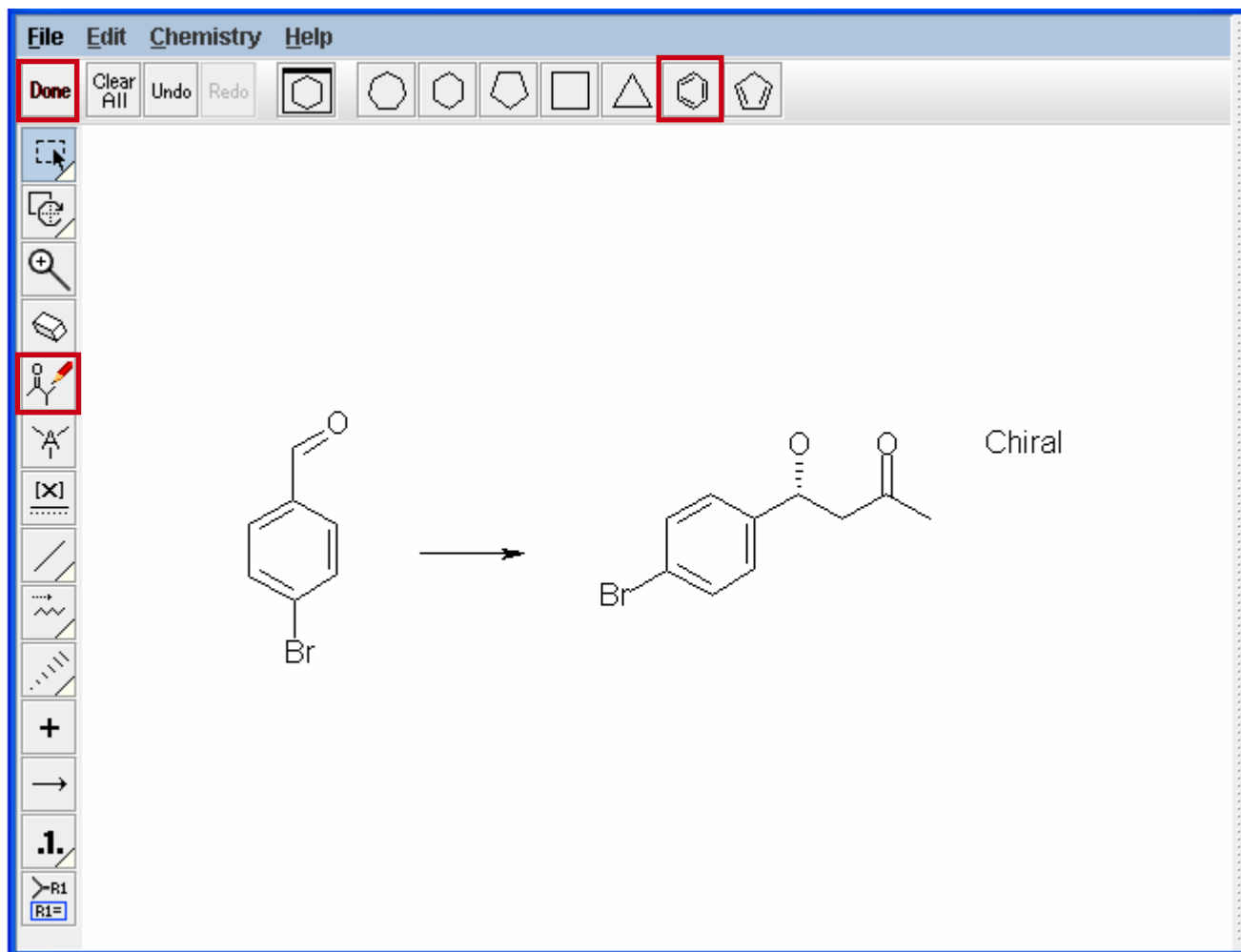
AND Journal Contains [Delete](#)
[Duplicate](#)
[Info](#)
[Data Lookup...](#)

AND Year = [Delete](#)
[Duplicate](#)
[Info](#)

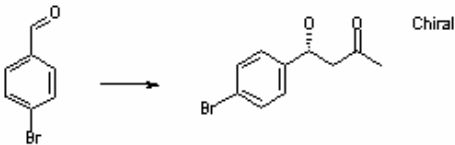
start search

show brackets save form sort results

Draw the Reaction Query in Symyx Draw



Conduct a Reaction Substructure Search

Reaction				
Structure		Select Search Type:		
		Reaction Substructure ▾		
		Finds the reactions that contain the same structural fragments and reacting centers as your reaction.	Reset Delete Duplicate Info	
		<input checked="" type="checkbox"/> Query Highlighting.		
AND ▾	Percent Yield	= ▾	<input type="text"/> %	Delete Duplicate Info
Citation				
AND ▾	Author	Contains ▾	<input type="text"/> Data Lookup...	Delete Duplicate Info
AND ▾	Journal	Contains ▾	<input type="text"/> Data Lookup...	Delete Duplicate Info
AND ▾	Year	= ▾	<input type="text"/>	Delete Duplicate Info
<input type="button" value="start search"/>				
<input type="button" value="show brackets"/> <input type="button" value="save form"/> <input type="button" value="sort results"/>				

Search Results

queries results reports rxn schemes

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

Synthetic Methodology Information

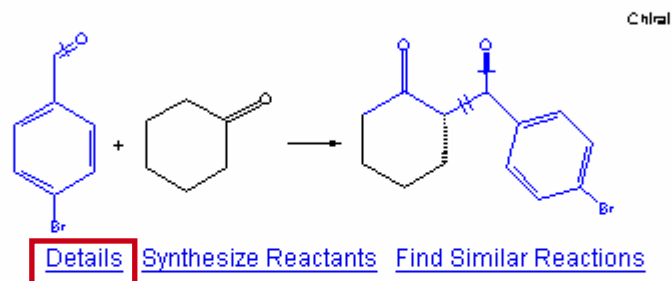
[View selected records in another database](#)

[Sort Results](#) [Create List](#)

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

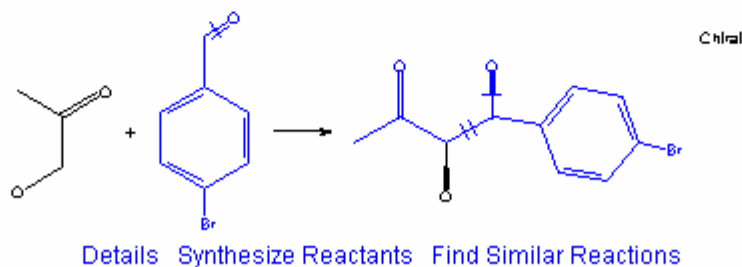
Total Records: 18

ChemInform Reaction Library



Record#1

ChemInform Reaction Library



Record#2

Details View

[Return to Search Results](#)

[View selected records in another database](#)

[Find Similar Reactions](#)

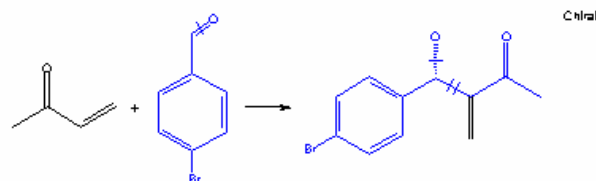
← Record # 12 → Total

Records: 18

Also found in: [ACD](#) [DWPI](#) [Index Chemicus](#) [NCI](#) [OHS MSDS](#) [PubChem](#) [SCD](#) [Toxicity](#) [Patent Chemistry](#) [Beilstein](#)

ChemInform Reaction Library

[Select / deselect](#) all citations from this page.



[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](#) (1)

[Reactant](#) (2)

[Product](#) (1)

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

RXCI03010134 Reaction Variation 1 of 1

Product no.	% Yield	Grade	%cs	%ds	%de	%ee	Reactant no.	Reactant Grade
1	31	(S)-isomer	100			27		

Step no.	Catalysts and Solvents	Catalyst ID click ID for details	Solvent ID click ID for details
1	COMPOUND182 [oxygen-bridged quinidine deriv.] (cat.) D-proline (cat.) DMF	667533 2806	38

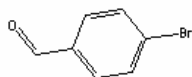
ACD Data for Reactant 1

[Return to Synthetic Methodology Information](#)

Record # 1 [→](#) Total Records: 3

MDL® Available Chemicals Directory

[Select](#) / [deselect](#) all citations from this page.



Available Data

Click on a link to add the information to this page

Set current view as default

[Substance](#) (1)

[Suppliers](#) (67)

[Prices](#) (67)

[Model](#) (1)

Substance [\(hide\)](#)

ACD Registry Number	3253
Availability	Large and small quantities
MDL Number	MFCD00003377
CAS Registry Number	1122-91-4
Chemical Name and Synonyms :	
<ul style="list-style-type: none">• 4-BBA• 4-BROMOBENZALDEHYDE• 4-BROMOBENZYLALDEHYDE• AKOS BBS-00003194• LABOTEST-BB LT00929178• LABOTEST-BB LT03333287• P-BROMOBENZALDEHYDE	
Molecular Formula	C7 H5 Br O
Molecular Weight	185.02
Rule of Five	0
Computed partition coefficient (CLogP)	2.6
Molecular weight of largest fragment	185.019
Number of proton acceptors	1
Number of proton donors	0
Number of rotatable bonds (TDF)	0

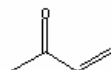
ACD Data for Reactant 2

[Return to Synthetic Methodology Information](#)

← Record # 2 → Total Records: 3

MDL® Available Chemicals Directory

[Select](#) / [deselect](#) all citations from this page.



Available Data

Click on a link to add the information to this page

Set current view as default

[Substance](#) (1)

[Suppliers](#) (35)

[Prices](#) (35)

[Model](#) (1)

Substance [\(hide\)](#)

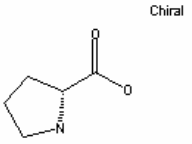
ACD Registry Number	8372
Availability	Large and small quantities
MDL Number	MFC000008777
CAS Registry Number	78-94-4
Chemical Name and Synonyms :	
<ul style="list-style-type: none">• 1-BUTEN-3-ONE• 3-BUTEN-2-ONE• METHYL VINYL KETONE• MVK• VINYL METHYL KETONE	
Molecular Formula	C4 H6 O
Molecular Weight	70.0904
Rule of Five	0
Computed partition coefficient (CLogP)	0.41
Molecular weight of largest fragment	70.09
Number of proton acceptors	1
Number of proton donors	0
Number of rotatable bonds (TDF)	0

ACD Data for Catalyst

[Return to Synthetic Methodology Information](#) ← Record # 3 **Total Records: 3**

MDL® Available Chemicals Directory

[Select / deselect](#) all citations from this page.



Chiral

Available Data

Click on a link to add the information to this page

Set current view as default

[Substance](#) (1) [Suppliers](#) (65)

[Prices](#) (65) [Model](#) (1)

Substance [\(hide\)](#)

ACD Registry Number	39629
Availability	Large and small quantities
MDL Number	MFCD00064317
CAS Registry Number	344-25-2

Chemical Name and Synonyms :

- (2R)-PYRROLIDINE-2-CARBOXYLIC ACID
- (R)-(+)-PROLINE
- (R)-PYRROLIDINE-2-CARBOXYLIC ACID
- D(+)-PROLINE
- D-2-PYRROLIDINECARBOXYLIC ACID
- D-PRO
- D-PROLINE
- D-PYRROLIDINE-2-CARBOXYLIC ACID
- H-D-PRO-OH
- H-D-PYRD(2)-OH
- PROLINE

Molecular Formula	C5 H9 N O2
Molecular Weight	115.131
Rule of Five	0
Computed partition coefficient (CLogP)	-2.15
Molecular weight of largest fragment	115.131
Number of proton acceptors	3
Number of proton donors	2

Link to Literature References

Detailed Data	Conditions References Scheme	External Registry No.	Path	Step
		1030803202	A	1 STEP

Export

[SHI, M.; JIANG, J.-K.; Tetrahedron: Asymmetry \[TASYE3\] 2002, 13 \(17\), 1941-1947.](#)



DiscoveryGate Literature Services

Document locations

Author: SHI, M.; JIANG, J.-K.
Journal: Tetrahedron: Asymmetry
Volume: 13
Issue: 17
Date: 2002
CODEN: TASYE3
Pages: 1941-1947

can be obtained from

[The publisher](#)
[Your librarian](#)

Find Similar Reactions

[Return to Search Results](#)

[View selected records in another database](#)

[Find Similar Reactions](#)

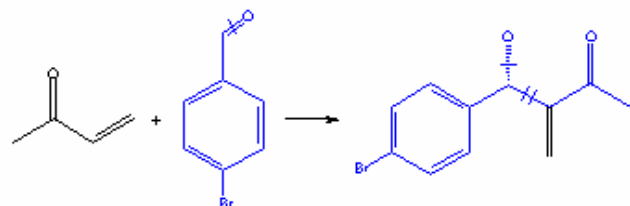
← Record # 12 →

Total Records: 18

Also found in: [ACD](#) [DWPI](#) [Index Chemicus](#) [NCI](#) [OHS MSDS](#) [PubChem](#) [SCD](#) [Toxicity](#) [Patent Chemistry](#) [Beilstein](#)

ChemInform Reaction Library

[Select](#) / [deselect](#) all citations from this page.



[Use as Query](#)

Select current record

Available Data

Click on a link to add the information to this page

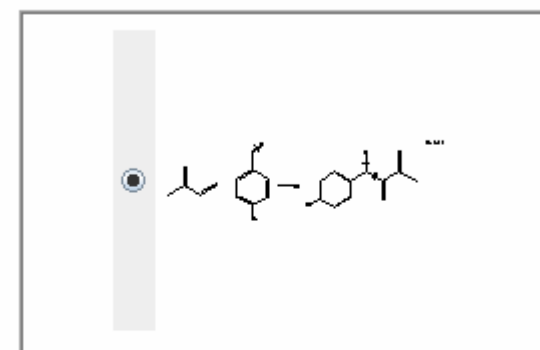
Set current view as default

[Reaction Details](#) (1)

[Reactant](#) (2)

[Product](#) (1)

Please select reaction to search



Please select target application

Beilstein - MDL Database Browser

Start Search

Cancel

Narrow Search Results

Reaction Classification Search Results

[Reaction Parent.Reaction code \(broad\) Parent.Reaction code \(broad\): 3488 Hits](#)

[Reaction Parent.Reaction code \(broad\) Parent.Reaction code \(medium\): 626 Hits](#)

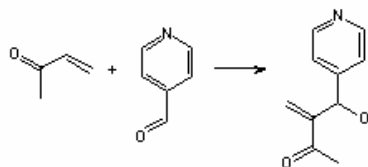
[Reaction Parent.Reaction code \(broad\) Parent.Reaction code \(narrow\): 143 Hits](#)

[Return to Reaction Classification Results](#)

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

Total Records: 143

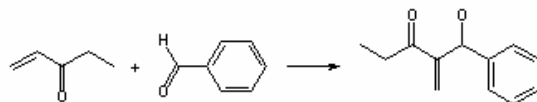
Reaction ID: 1524228



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

Record#1

Reaction ID: 2678985

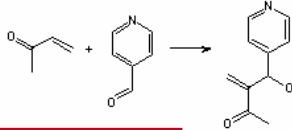


[Details](#) [Synthesize Reactant\(s\)](#) [Find Similar Reactions](#)

Record#2

Synthesize Reactant(s)

Reaction ID: 1524228



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

Record#1

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

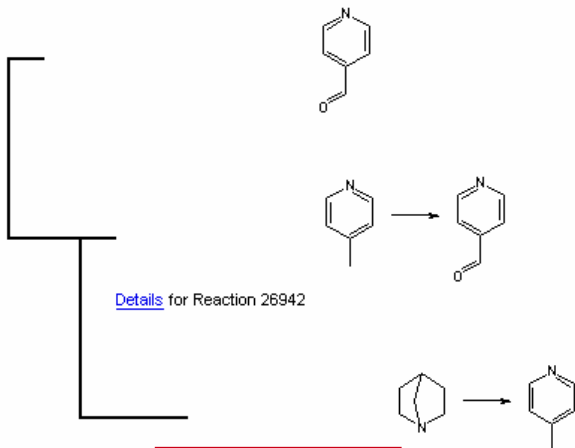
Database: CrossFire Beilstein

Find in Rxn Tree: Next

Rxn Tree History

- Substance 105342
 - Reaction 26942
 - Substance 104586
 - Reaction 16873**
 - Substance 102691
 - Reaction 21499
 - Reaction 21505
 - Reaction 21521
 - Reaction 22296
 - more

Synthetic Scheme for Substance 105342



[Details](#) for Reaction 26942

[Details](#) for Reaction 16873

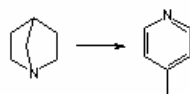
Reaction Details

[Return to Reaction Scheme](#)

[Find Similar Reactions](#)

CrossFire Beilstein Reaction 16873

[Select](#) / [deselect](#) all citations from this page.



[Use as Query](#)

Reaction

Reaction record 1 of 1		
Reaction ID	16873	
Reactant	Reactant BRN	102691
	Reactant	1-aza-bicyclo[2.2.1]heptane
Product	Product BRN	104586
	Product	4-methyl-pyridine
No of Reaction Details	2	
Reaction Entry Date	1988/06/27	
Reaction Update Date	1988/06/27	

[Top of Page](#)

Reaction Details

Reaction Details record 1 of 2		
Citation Pointer	<ul style="list-style-type: none">983616	
Reaction Detail ID	16873.2	
Reaction Classification	<ul style="list-style-type: none">Preparation	
Stage	Reagent	palladium/charcoal
	Temperature	330 C

Course Summary

- In this Workshop, we have covered how to:
 - Log into DiscoveryGate
 - Change Personal Settings for DiscoveryGate
 - Conduct structure and data searches using the Database Browser and individual databases
 - View the search results using the Grid, Database, and Properties views
 - Save search results as Temporary and Permanent lists, and Combine lists
 - Create Reports
 - Modify Query Forms and Save as Default Forms
 - Introduce Synthetic Methods

Support for DiscoveryGate

DiscoveryGate®



Quick Start Guide
Useful information to get you started

Terms of Use

My Support

DiscoveryGate > Issue support requests, learn about known limitations

Home

Support

Logout brenda.waller@symyx.com

DISCOVERYGATE SUPPORT

- Report Defects
- Request enhancements
- Obtain general Discovery Gate support

Where do we route your case?:

Operating System:

Web Browser:

Part of program you are having trouble with:

Note: To request a change to the IP range associated with your company, choose "Request change to IP range" in the select box below.

Report/Request:

Priority:

Comments:

Error Message:

Telephone contact number:

Done

Site Administrators

Your Company Administrators will be listed here

System Requirements

[Click here](#)

New Features, Fixes and Limitations

[DiscoveryGate 2.4](#)

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[MDL SCD Current List of Suppliers](#)
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