

DiscoveryGate®

Quick Start Guide



Platform with Content and Services

**Primary Literature:
Journals and
Patents**



**Secondary
Databases**

Pharmacology, synthetic
methodology, bioactivity,
sourcing, ADME/T



**Single search
across a huge
chemical
database**



**Powerful
administration
environment
and software
deployment**



**Authoritative
Major Reference
Works**



**We handle
maintenance,
security and
support - so you
can focus on
research**



Integration, indexing and linking

Information access when you want

Information from wherever you want

Searching a database

The screenshot shows the DiscoveryGate search interface. At the top, there is a navigation bar with links: start search, import, save, clear form, help, and logout. Below this, the 'Database' dropdown menu is set to 'MDL Compound Index' (callout 1). To the right, the 'MolStructure' box contains the text 'Double-click in this box to edit structure' (callout 2). Below the 'MolStructure' box, there is a search query builder showing 'AND' and 'Molecular Weight' with an equals sign and an empty input field. A 'start search' button is located below the query builder. On the left side, the 'Field Index' tree is visible, with 'Molecular Formula' selected (callout 4). At the bottom left, there are navigation buttons: back, forward, home, and A-Z (callout 5). A footer note says 'Click here for more information about the MDL Compound Index.'

1. Select database:

Select the database you want to search by selecting from the **Database** drop down menu. A list of database names appears. Make your selection. A screen with preset fields appropriate for your database selection appears.

2. Draw a structure:

Double-click in the **Molstructure** (or **RxnStructure**) box to launch the MDL Draw structure drawing tool.

3. Locate a property field:

Type the first few letters of the property field that you are looking for, for example **carcinogen**. The field will be located and highlighted in the **Field Index** tree.

4. Select a property:

Double click on any property in the **Field Index** to add that field to your query.

5. Find help:

Context-sensitive help appears for all features.

Drawing a structure

1 File Chemistry Help

Done Clear All Undo Redo

3

5

2

4 Home A-Z P

Tooltips and Hints

[Quick Start](#)

Key differences from [CrossFire](#) and [M](#)

Use the **Properties tool** to add [gu](#) for more effective searching.

1. Open existing structure file

Choose **File>Open** to import an existing structure in **.mol**, **.skc** and **.smi** formats.

2. Select a tool:

A variety of drawing tools are provided. The lasso tool allows you to select all or part of the structure. The 'all purpose' drawing tool lets you draw bonds, rings, chains, specify atoms and do other tasks.

3. Use pre-defined templates

Select ring templates and click in the palette to add that ring. You can add a frequently-drawn structure by selecting it with the lasso tool and dragging it onto the template bar.

4. Find Help

Each tool and button has its own tool tip and hints for use.

5. Transfer structures to query

Once you have drawn your structure or reaction, click **Done** to transfer it back to the DiscoveryGate query page.

Browsing results in Compound Index

4

queries

results

reports

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

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

1

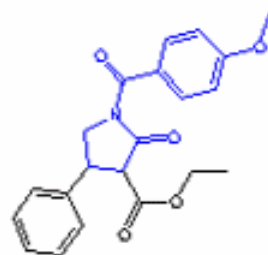
[Create List](#)[View selected records in another database](#)

5

Next

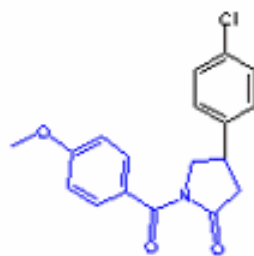
Pages: 1 [Next](#) [Select All](#) [Clear All](#)

1

 Record#1[3d Configuration](#)[Chemical](#)[Commercially Available](#)[Literature Reference](#)[Name](#)[Pharmacological](#)[Preparation](#)[Toxicity](#)

3

2

 Record#2[3d Configuration](#)[Chemical](#)[Commercially Available](#)[Literature Reference](#)[Name](#)[Pharmacological](#)[Preparation](#)[Toxicity](#)**1. Results view:**

View results as structures only (Grid View), structures and properties (Properties View), or structures and corresponding databases (Database View).

2. Results list:

Original Query structure is highlighted within displayed results. To see results from one or more than one structure, tick the **Record #** box before you click the property or database you want to view.

3. See the data:

Click the property name (or database name, depending on your view) to see the data

4. Create report or export data:

Export structures and data to an SDF file, RDF file or tab-delimited file. Create an HTML report file to include in your notebook or share with colleagues.

5. Create a list:

Click **Create List** to save all (or a subset) of your results to a list in the History tree.

Browsing results from individual databases

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

Database:

MDL® Available Chemic... ?

Find in History: Next

Full Index History

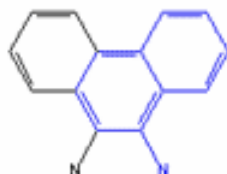
1

- Today's Searches
 - Search #1
 - Search #2
- Previous Searches
- Saved Searches
- Temporary Lists

[Get Count](#)Also found in: [CIRX](#) [DWPI](#) [NCI](#) [OHS MSDS](#) [Patent Chemistry](#)

3

MDL® Available Chemicals Directory

[Use as Query](#) Select current record

Available

Click on a link to add the

 Set current view as default[Substance](#) (1)[Prices](#) (2)

2

Substance [\(hide\)](#)

ACD Registry Number	1148
MDL Number	MFC00001178
CAS Registry Number	53348-04-2

Chemical Name and Synonyms :

- 9,10-DIAMINOPHENANTHRENE
- 9,10-PHENANTHRENE-DIAMINE

1. History tree:

View previous or saved searches and your saved lists in the **History tree**.

All searches are saved for your session.

2. Browse available data:

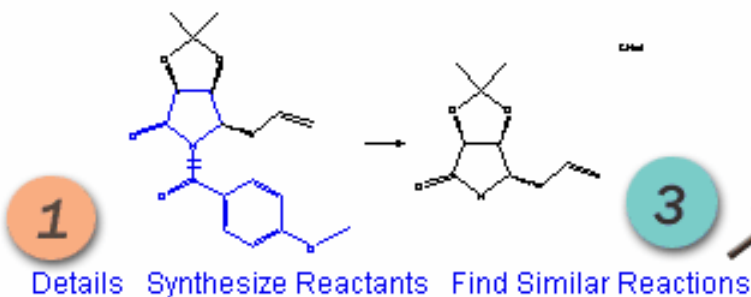
Available data in the current database is easily accessible via links in the Available Data box. Substance data is displayed by default. Click on the appropriate hyperlinks to expand (or hide) viewable data.

3. See related information in other databases:

To see data for structures contained in other indexed databases click the appropriate **Also Found In** link.

Exploring reactions

ChemInform Reaction Library

 Record#1

2

Database: Synthetic Methodology Information

Find in Row Tree: Next

Row Tree History

- Substance cird296:169242
- Reaction cird296:223609
- Substance cird296:169248
- Reaction cird296:223608
- Substance cird296:169238
- Reaction cird296:223606**
- Substance cird296:169236
- Substance cird296:509
- Substance cird296:3
- Substance cird296:358

Synthetic Scheme for Substance cird296:169242

[Details](#) for Reaction cird296:223609

[Details](#) for Reaction cird296:223608

[Details](#) for Reaction cird296:223606

MDL Database Browser

Please select reaction to search

Please select target application

- Integrated Major Reference Works
- Integrated Major Reference Works
- Beilstein - MDL Database Browser
- Patent - MDL Database Browser
- Gmelin - MDL Database Browser
- Synthetic Methodology - MDL Database Browser

1. See reaction details:

From your initial result set, you can view **Details** about the reaction, including reaction schemes, yield and more. Link from any bibliographic reference to the corresponding full text article or patent.

2. View full synthesis schemes:

Select **Synthesize Reactants** to create an entire synthesis scheme. Full details are available for synthetic scheme.

3. Find similar reactions:

Use **Find Similar Reactions** to locate reactions in Broad, Medium, or Narrow classifications, depending on your similarity preferences. All reaction sources on DiscoveryGate, including the Integrated Major Reference Works, and the MDL Patent Chemistry Database are classified and interlinked.

Exporting Data

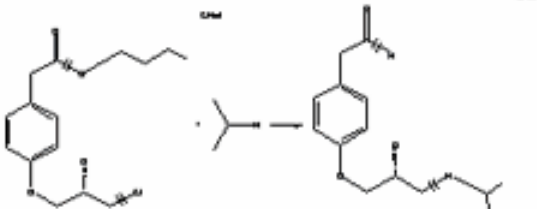
1 queries results reports rxn schemes

export page setup print save refine query lists help logout Synthet

[View selected records in another database](#)

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

Cheminform Reaction Library



[Details](#) [Synthesize Reactants](#) [Find Similar Reactions](#)

2 Export D

3

find: Next

Database Fields

- FOON
 - FOONSTRUCTURE
 - FOONREGNO
 - FOONCENTERSIMILARITY
 - FOONSTRUCTURESIMILAR
 - VARIATION
 - reactant_link
 - product_link
 - regno
 - product_no
 - MOL
 - MOLREGNO
 - MOLFORMULA**
 - MOLSTRUCTURE

Exporting Fields

- FOON
 - FOONSTRUCTURE
 - product_link
 - MOL
 - MOLFORMULA**

Export SDF ...
Export RDF ...
Export TAB ...
Help
Cancel

Add Remove ↑ ↓

1. Export selection:

From your result set, check all the structures or reactions you wish to export and then click **Export**. The export limit is 500 structures.

2. Select the fields to export:

Choose the type of data you want to export. For example, reaction structures and product molecular formulas. Choose the data to export by clicking the field name in the **Database Fields** tree and then clicking **Add**. The fields you choose will be visible in the **Exporting Fields** tree.

3. Choose your export format:

Export an **SD** (Structure Data) file, **RD** (Reaction Data) file or tab-delimited file by clicking on the appropriate button.

For more information, visit
www.discoverygate.com