Searching the MDL Available Chemicals Directory

DiscoveryGate[SM]
Version 1.4 SP2
Participant's Guide

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Searching the MDL Available Chemicals Directory

Key points

- This module focuses on the content of the MDL Available Chemicals Directory, the largest structure-searchable database of commercially available chemicals.
- You will be using the MDL Database Browser, a component of DiscoveryGate, to search the database.

Notes

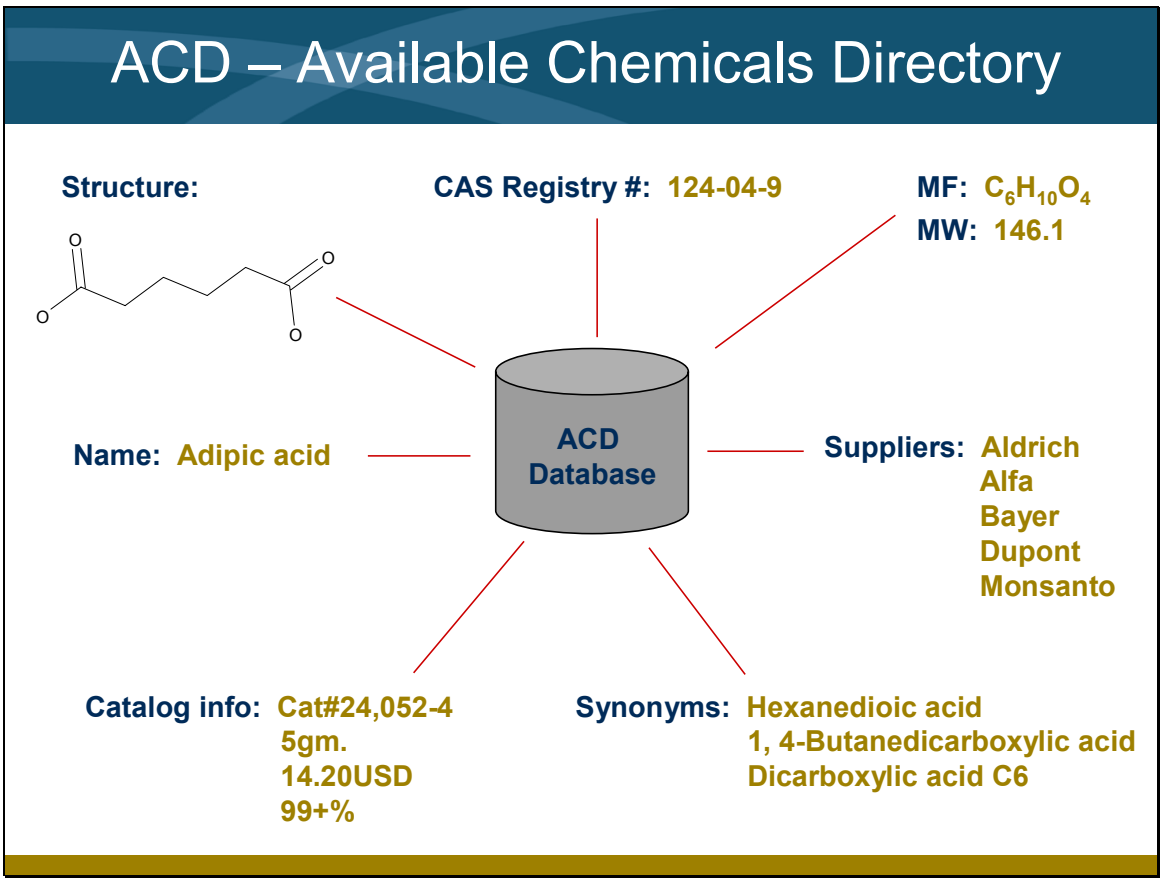
Module objectives

- Retrieve compounds based on associated data
- Retrieve compounds based on structural features
- Display catalog, pricing, and supplier information
- Sort search results
- Create a report

Key points

- You will learn some basic search techniques for retrieving compounds based on associated data and structural features.
- After you have completed a search, you will be able to collect information, create a report, and print it.

Notes

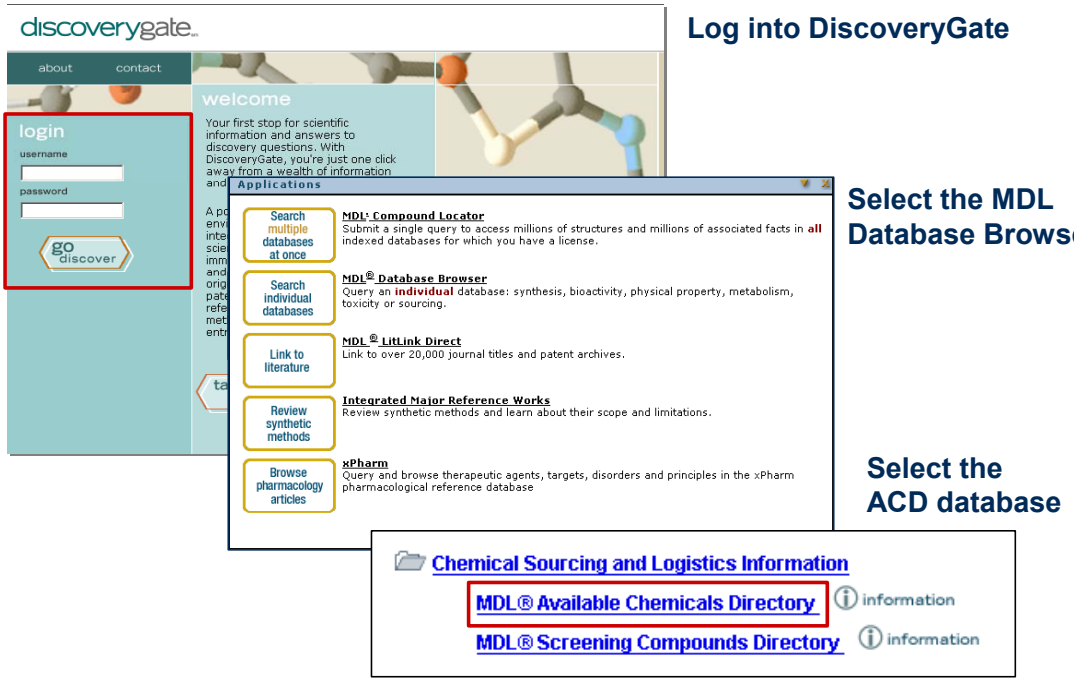


Key points

- The MDL Available Chemicals Directory provides access to pricing and supplier information for nearly 400,000 research-grade and bulk chemicals.
- The ACD database includes information on product purities, forms, grades, available quantities, and prices, along with supplier and distributor contact information.

Notes

Launch the application and database



Log into DiscoveryGate

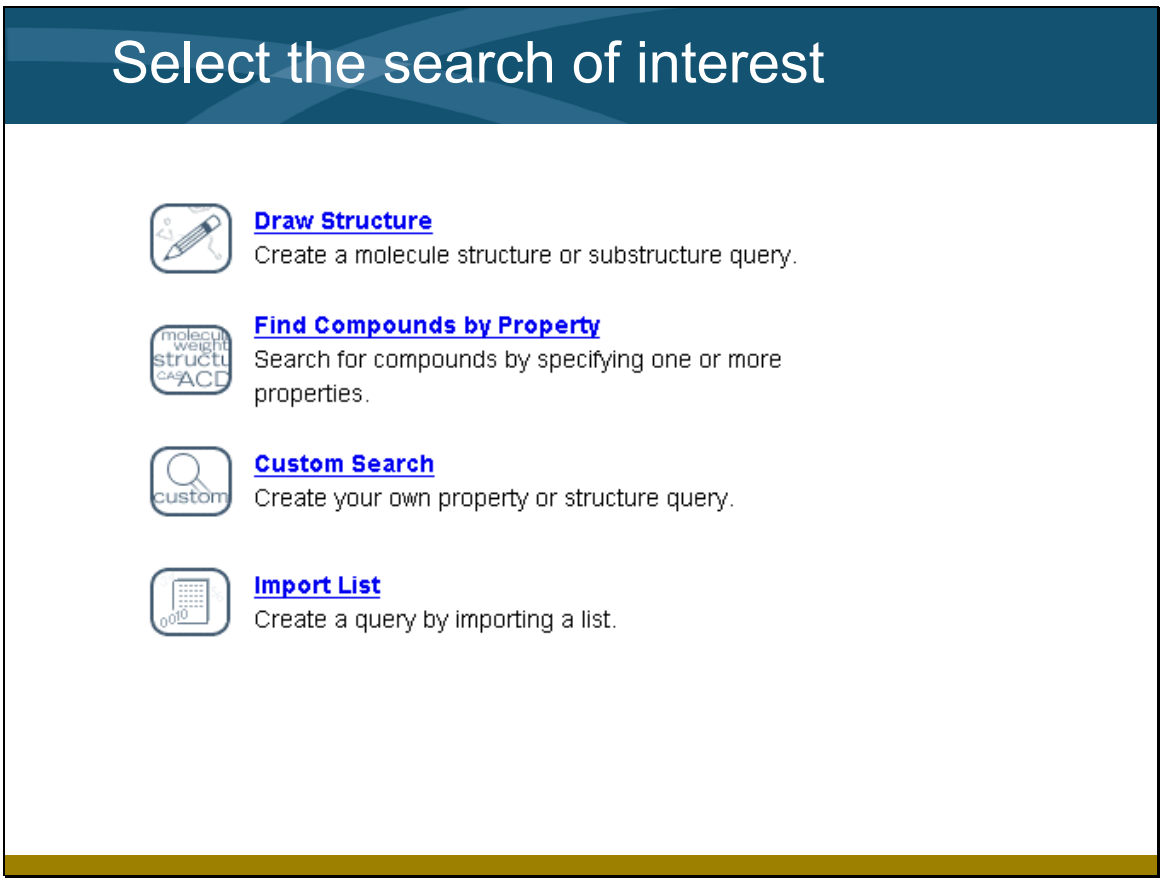
Select the MDL Database Browser

Select the ACD database

Key points

- To begin, you will launch your internet browser and enter the URL for Discoverygate: www.discoverygate.com
- Log into DiscoveryGate using your user name and password, and enter a company number if prompted. Then click go discover.
- On the DiscoveryGate home page, click MDL Database Browser to launch the application. A list of licensed databases for your site will be displayed.
- Click MDL Available Chemicals Directory to choose the ACD database.

Notes



Key points

- You will be presented with the search options shown above.
- The next section will discuss searching using compound properties.

Notes

Demonstration: Choose the ACD database

Login to DiscoveryGate. Then launch the MDL Database Browser and choose the ACD database.

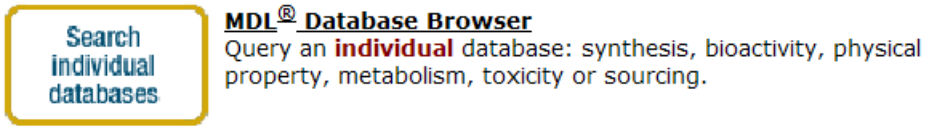
Login to DiscoveryGate

1. Launch your web browser.
2. Enter the URL, **www.discoverygate.com**.
3. Enter your user name and password, including the company number, if prompted.

4. Click **go discover**.

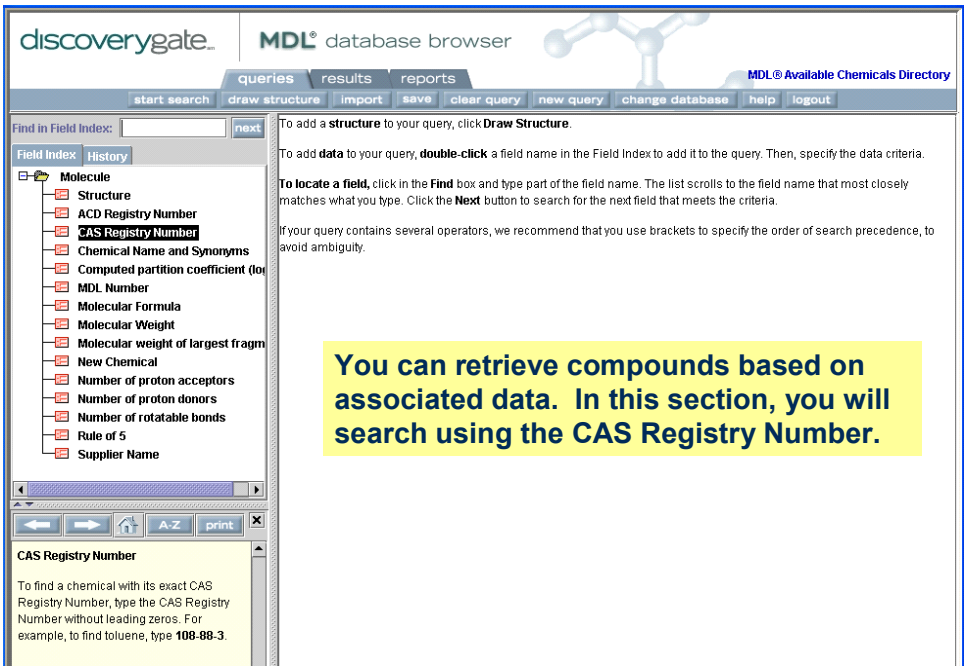
Launch the MDL Database Browser and choose ACD

1. From the DiscoveryGate home page, click **MDL Database Browser**.



2. From the list of databases, click **MDL Available Chemicals Directory**.

Property searching

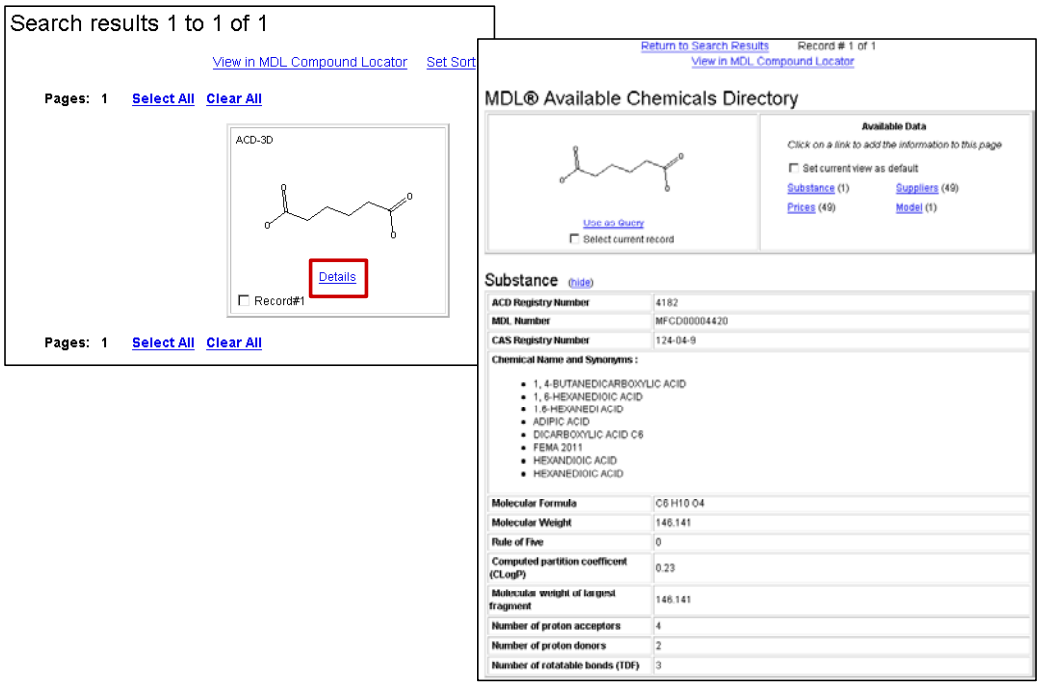


Key points

- When you click Find Compounds by Property, you are taken to the queries page shown here.
- The data fields in the ACD database are listed on the Field Index tab. You can search using any field.
- When you click a field name, a description of that field appears in the help pane below the field index.
- You will be conducting a search using the CAS Registry Number for a compound.

Notes

Search results

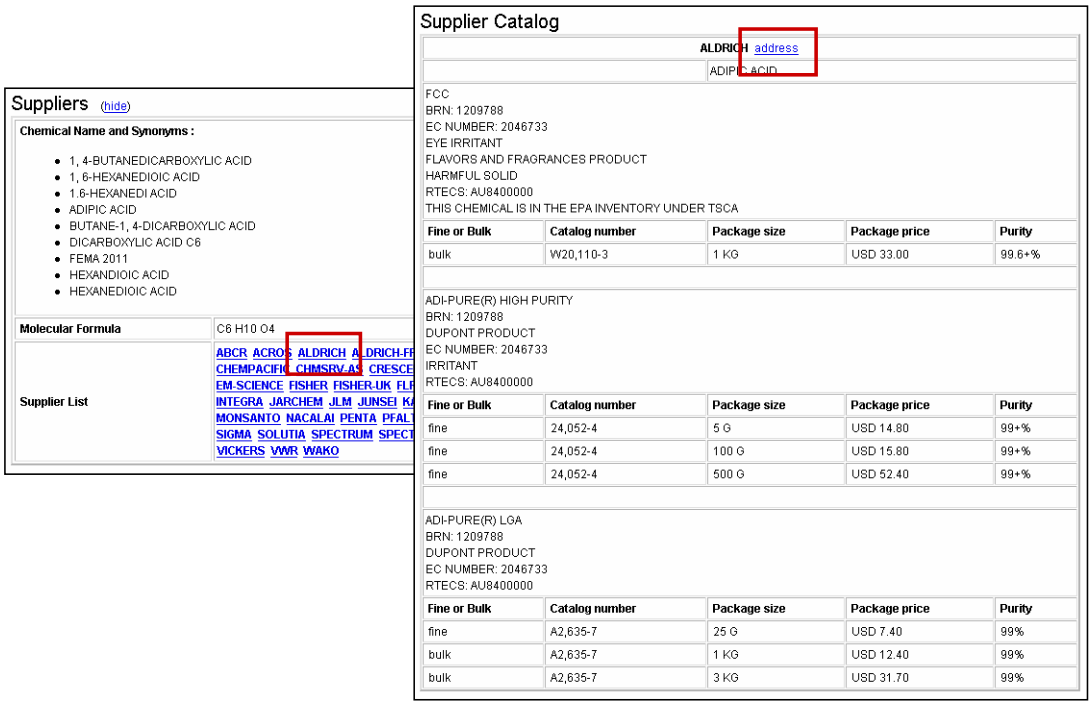


Key points

- When the search is complete, you will see the search results presented on the results page. The results are initially displayed as a structure grid.
- In this example, only one compound was retrieved.
- By clicking the Details link, you will see the complete Substance data for the compound.
- Under Available Data are links for Prices, Suppliers, and Model.

Notes

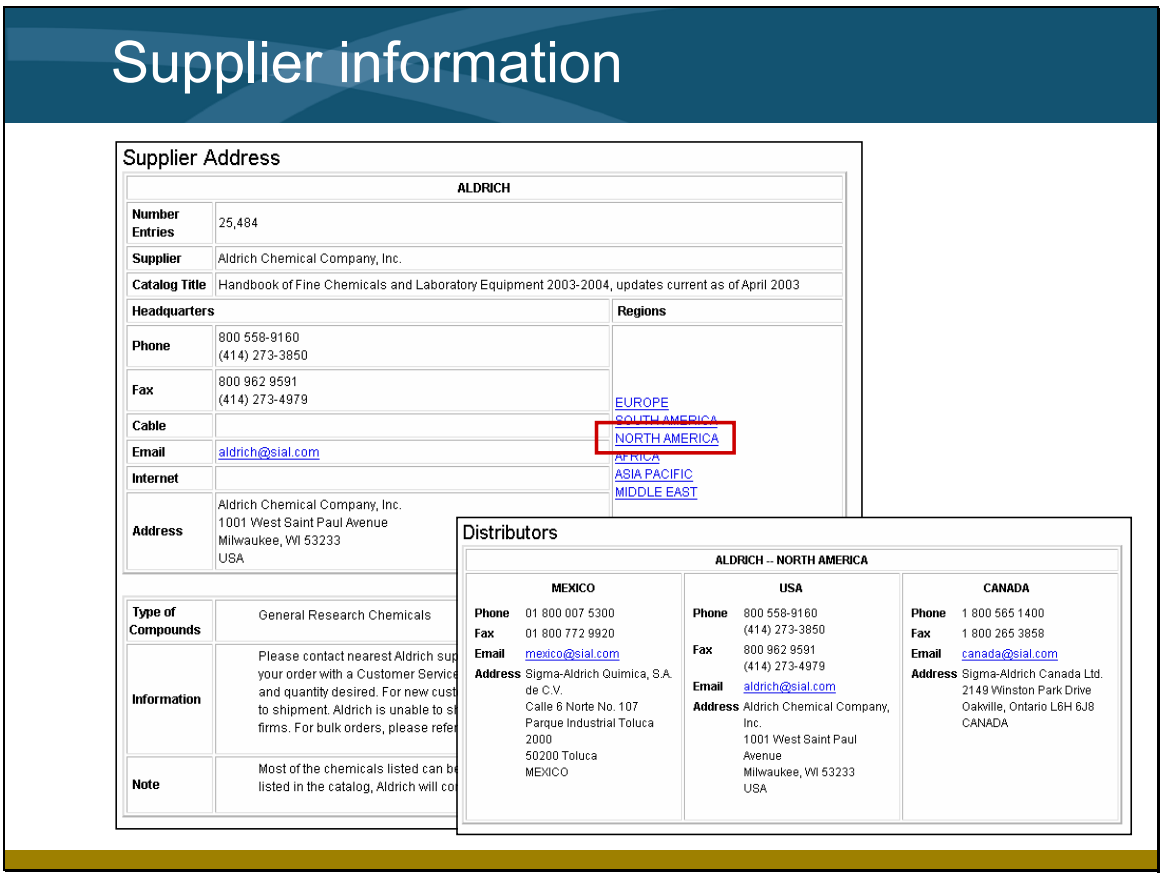
Catalog information



Key points

- By clicking the Suppliers link, a complete list of suppliers for the compound is added to the results page.
- By clicking any of the suppliers on the list, you will see the catalog data for that supplier.
- To see the supplier address, click the address link next to the supplier name.

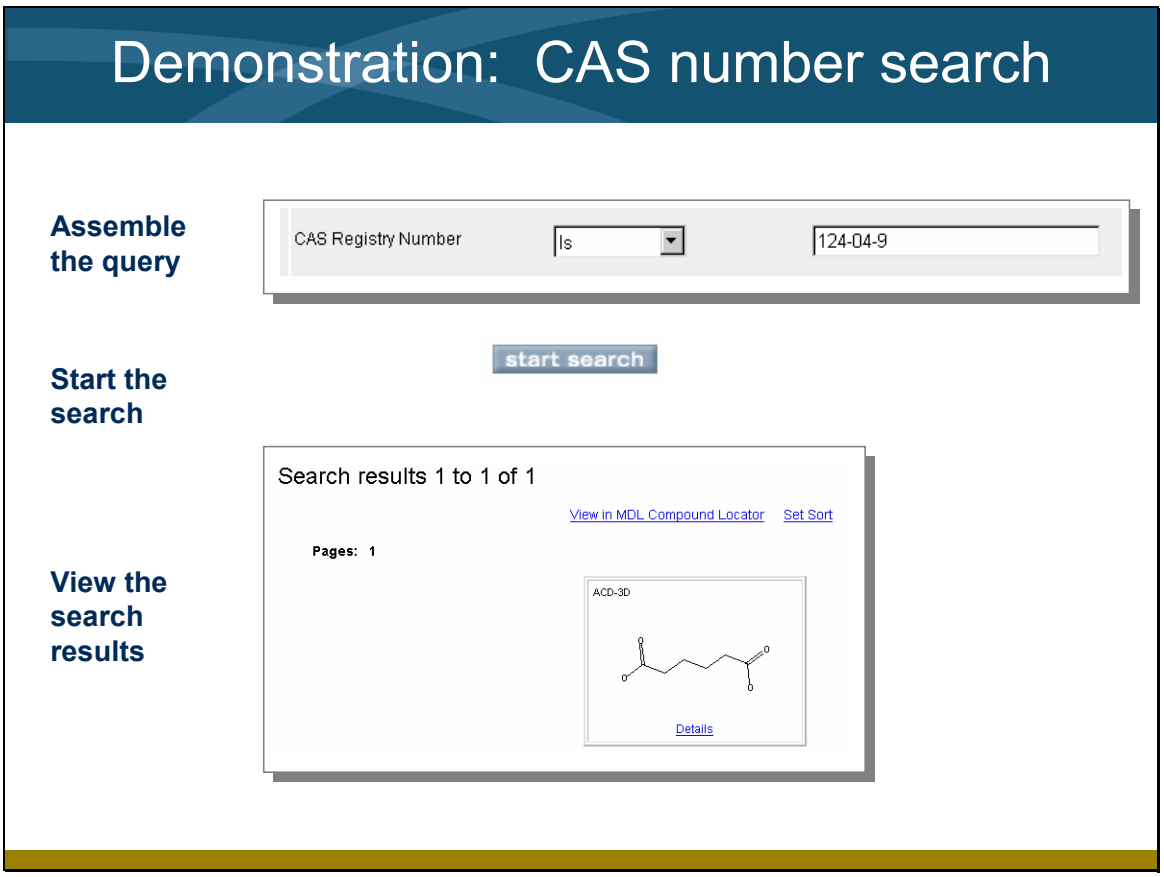
Notes



Key points

- The supplier address may contain other links for contacting the supplier by email or distributor information by region.

Notes



Key points

- In this demonstration, you will search for a compound using its CAS Registry Number.
- When the search is complete, you will examine the catalog data for a specific supplier.

Notes

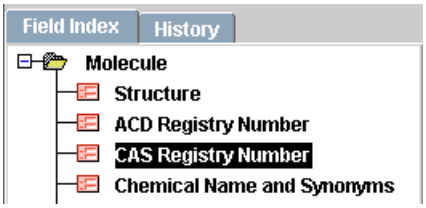
Demonstration: Search by CAS Number

Retrieve adipic acid using its CAS registry number, 124-04-9. View the catalog data and supplier information for Aldrich.

Assemble the query

1. Click **Find Compounds by Property**.

2. On the Field Index tab, double-click the **CAS Registry Number** field.

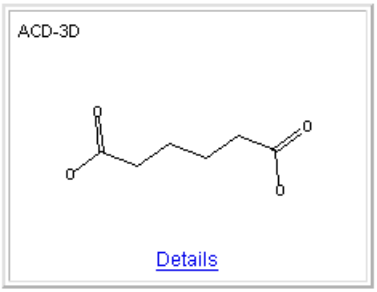


The query field for CAS Registry Number appears in the pane on the right. You will use the default data operator, Contains.

3. Enter **124-04-9** in the target box.

4. Click **start search**. The search results are displayed on the Results tab.

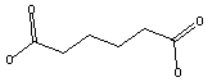
View in MDL Compound Locator Set Sort



View compound data

1. Click the **Details** link below the compound structure. The default Substance data is displayed.

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 (49)

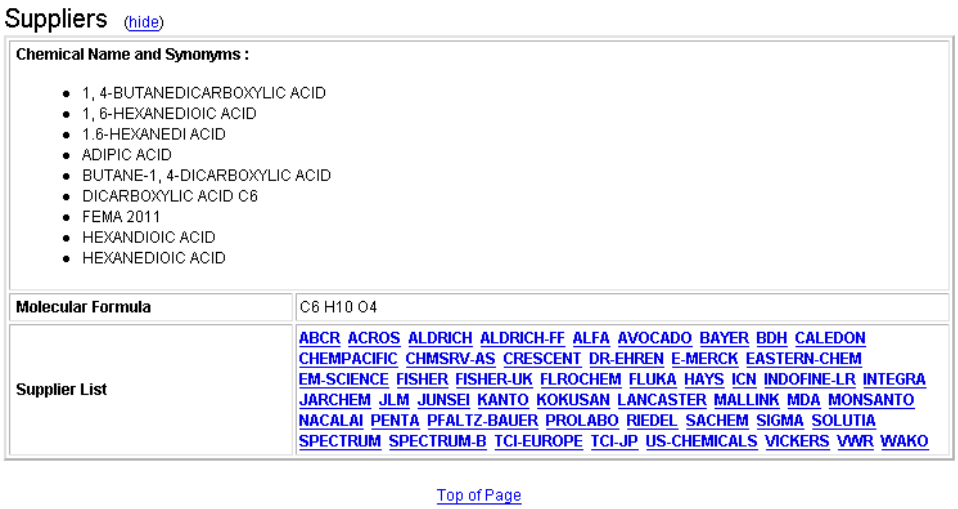
Prices (49) Model (1)

Substance (hide)

ACD Registry Number	4180
MDL Number	MFCD00004420
CAS Registry Number	124-04-9
Chemical Name and Synonyms : • 1, 4-BUTANEDICARBOXYLIC ACID • 1, 6-HEXANEDIOIC ACID • 1.6-HEXANEDI ACID • ADIPIC ACID • BUTANE-1, 4-DICARBOXYLIC ACID • DICARBOXYLIC ACID C6 • FEMA 2011 • HEXANDIOIC ACID • HEXANEDIOIC ACID	
Molecular Formula	C6 H10 O4
Molecular Weight	146.141
Number of proton acceptors	4
Number of proton donors	2
Molecular weight of largest fragment	146.141
Rule of 5	0
Number of rotatable bonds	3
Computed partition coefficent (logp)	0.23

View suppliers

1. Under Available Data, click **Suppliers**. The list of suppliers is added to the data display.



Suppliers (hide)

Chemical Name and Synonyms :

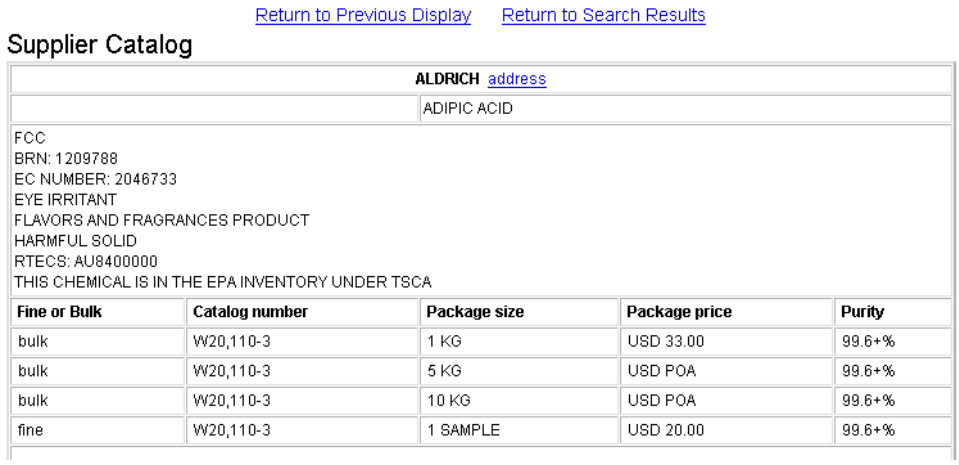
- 1, 4-BUTANEDICARBOXYLIC ACID
- 1, 6-HEXANEDIOIC ACID
- 1.6-HEXANEDI ACID
- ADIPIC ACID
- BUTANE-1, 4-DICARBOXYLIC ACID
- DICARBOXYLIC ACID C6
- FEMA 2011
- HEXANDIOIC ACID
- HEXANEDIOIC ACID

Molecular Formula	C6 H10 O4
Supplier List	ABCR ACROS ALDRICH ALDRICH-FF ALFA AVOCADO BAYER BDH CALEDON CHEMPACIFIC CHMSRV-AS CRESCENT DR-EHREN E-MERCK EASTERN-CHEM EM-SCIENCE FISHER FISHER-UK FLROCHEM FLUKA HAYS ICN INDOFINE-LR INTEGRA JARCHEM JLM JUNSEI KANTO KOKUSAN LANCASTER MALLINK MDA MONSANTO NACALAI PENTA PFALTZ-BAUER PROLABO RIEDEL SACHEM SIGMA SOLUTIA SPECTRUM SPECTRUM-B TCI-EUROPE TCI-JP US-CHEMICALS VICKERS VWR WAKO

Top of Page

View catalog data for Aldrich

1. From the Supplier List, click **ALDRICH**. The catalog data for Aldrich appears.



Return to Previous Display Return to Search Results

Supplier Catalog

ALDRICH address

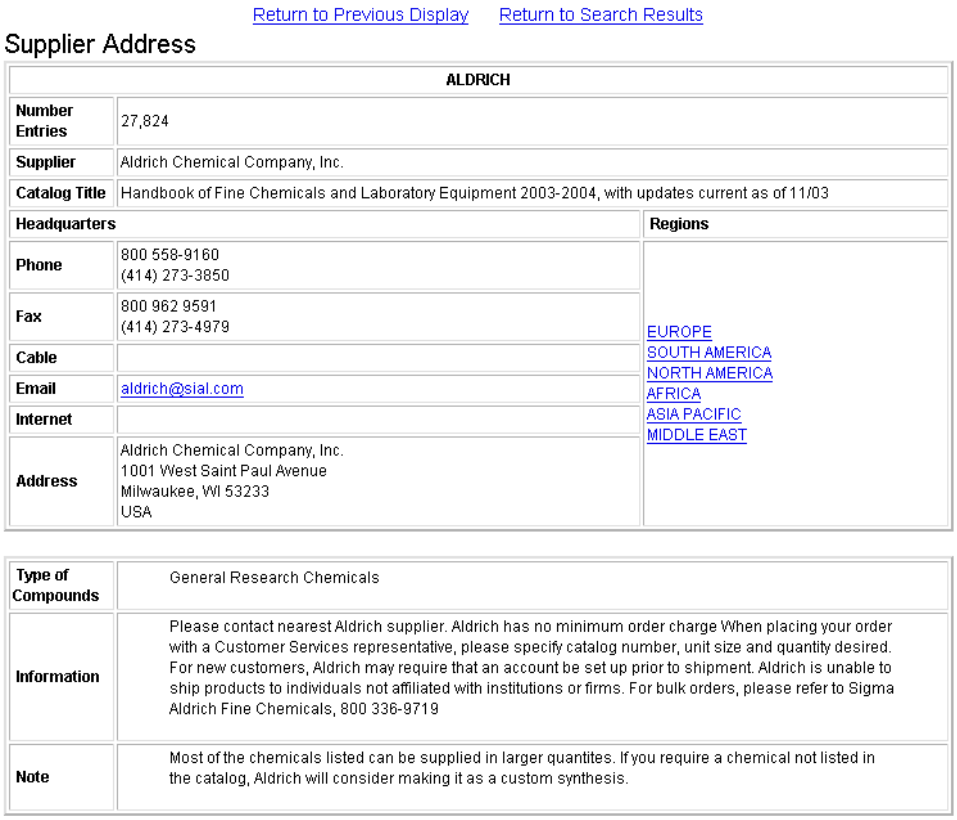
ADIPIC ACID

FCC
BRN: 1209788
EC NUMBER: 2046733
EYE IRRITANT
FLAVORS AND FRAGRANCES PRODUCT
HARMFUL SOLID
RTECS: AU8400000
THIS CHEMICAL IS IN THE EPA INVENTORY UNDER TSCA

Fine or Bulk	Catalog number	Package size	Package price	Purity
bulk	W20,110-3	1 KG	USD 33.00	99.6+%
bulk	W20,110-3	5 KG	USD POA	99.6+%
bulk	W20,110-3	10 KG	USD POA	99.6+%
fine	W20,110-3	1 SAMPLE	USD 20.00	99.6+%

View address information for Aldrich

1. Click the **address** link next to ALDRICH. The address information appears.



Return to Previous Display Return to Search Results

Supplier Address

ALDRICH		
Number Entries	27,824	
Supplier	Aldrich Chemical Company, Inc.	
Catalog Title	Handbook of Fine Chemicals and Laboratory Equipment 2003-2004, with updates current as of 11/03	
Headquarters		**Regions**
Phone	800 558-9160 (414) 273-3850	EUROPE SOUTH AMERICA NORTH AMERICA AFRICA ASIA PACIFIC MIDDLE EAST
Fax	800 962 9591 (414) 273-4979	
Cable		
Email	aldrich@sial.com	
Internet		
Address	Aldrich Chemical Company, Inc. 1001 West Saint Paul Avenue Milwaukee, WI 53233 USA	

Type of Compounds	General Research Chemicals
Information	Please contact nearest Aldrich supplier. Aldrich has no minimum order charge When placing your order with a Customer Services representative, please specify catalog number, unit size and quantity desired. For new customers, Aldrich may require that an account be set up prior to shipment. Aldrich is unable to ship products to individuals not affiliated with institutions or firms. For bulk orders, please refer to Sigma Aldrich Fine Chemicals, 800 336-9719
Note	Most of the chemicals listed can be supplied in larger quantites. If you require a chemical not listed in the catalog, Aldrich will consider making it as a custom synthesis.

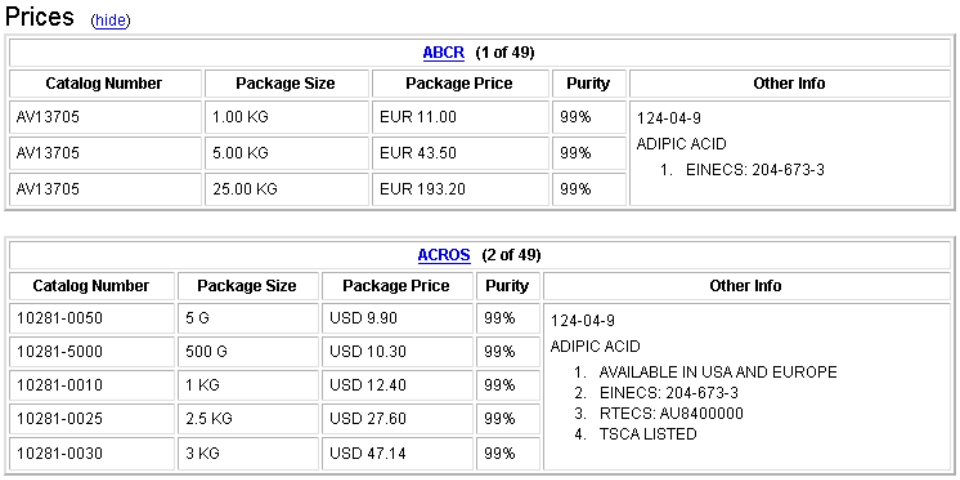
View prices from multiple suppliers

1. Click **Return to Previous Display**. The catalog data is displayed.

2. Click **Return to Previous Display**. The details page for adipic acid is displayed.

3. Click **Top of Page**.

4. Under Available Data, click **Prices**. The price information from all available suppliers is added to the details page. In this case, there are 49 records.



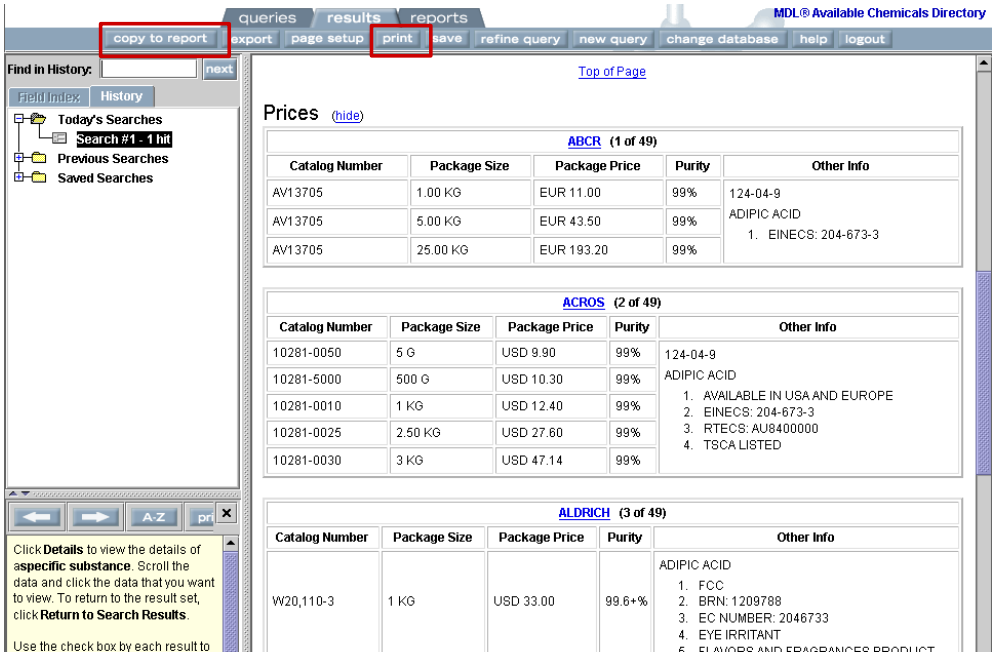
Prices (hide)

ABCR (1 of 49)				
Catalog Number	**Package Size**	**Package Price**	**Purity**	**Other Info**
AV13705	1.00 KG	EUR 11.00	99%	124-04-9 ADIPIC ACID 1. EINECS: 204-673-3
AV13705	5.00 KG	EUR 43.50	99%	
AV13705	25.00 KG	EUR 193.20	99%	

ACROS (2 of 49)				
Catalog Number	**Package Size**	**Package Price**	**Purity**	**Other Info**
10281-0050	5 G	USD 9.90	99%	124-04-9 ADIPIC ACID 1. AVAILABLE IN USA AND EUROPE 2. EINECS: 204-673-3 3. RTECS: AU8400000 4. TSCA LISTED
10281-5000	500 G	USD 10.30	99%	
10281-0010	1 KG	USD 12.40	99%	
10281-0025	2.5 KG	USD 27.60	99%	
10281-0030	3 KG	USD 47.14	99%	

5. Click **hide** next to Suppliers to remove the supplier list from the details page.

Saving, printing, and copying results



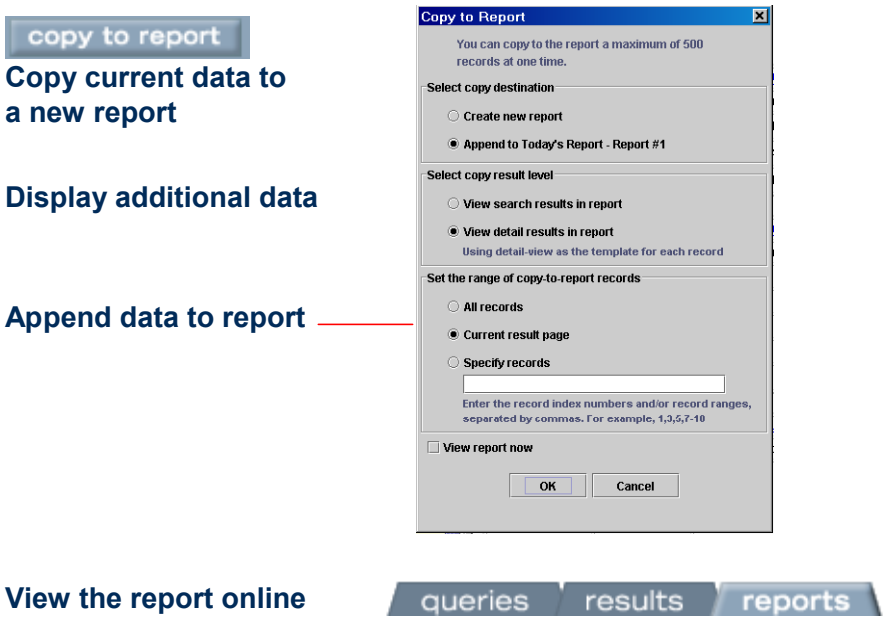
You can print the information directly or copy it to a report.

Key points

- When the search is complete, the results are displayed on the results page.
- You can print directly from the results page by clicking print on the top menu bar.
- Or, you can copy the information to a report by clicking copy to report.
- By displaying additional information and then clicking copy to report, you can append the new information to the current report, or create a new report.
- You can view your report by clicking the reports tab.

Notes

Demonstration: Creating a report



Key points

- In this demonstration, you will copy to a report (and append as needed) the substance data, catalog data, and supplier address, and then view the report.

Notes

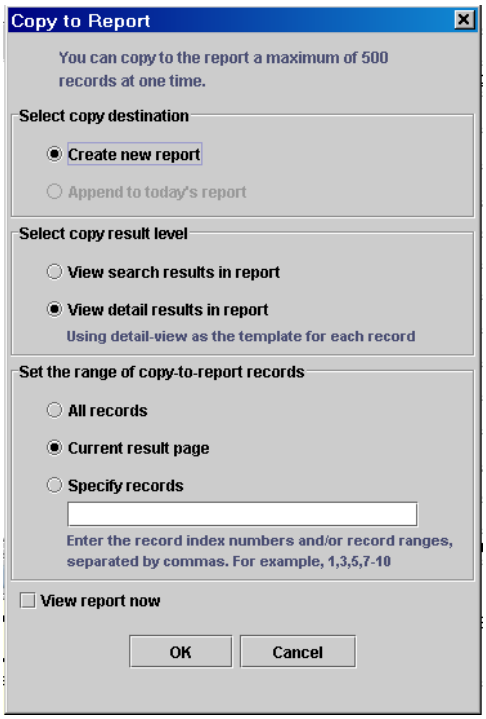
Demonstration: Create a report

Copy supplier and price information to a report and view it online.

Create a report

1. With the Substance and Prices information displayed on the details page, click **copy to report** on the top menu bar.

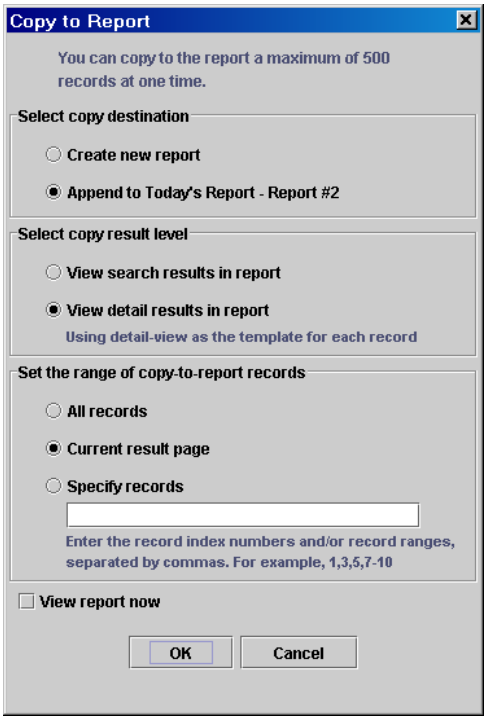
2. Click **OK** to create a new report.



3. Click the Suppliers link. Click the link for **ALDRICH** to display the catalog data from Aldrich only.

4. Click **copy to report**.

5. Click **OK** to append the catalog data to the current report.



6. Click the **address** link next to ALDRICH.

7. Click **copy to report**.

8. Click **OK** to append to the address information to the current report.

View the report

1. Click the **reports** tab to view the report. To print the report, click the **print** button on the top menu bar.

Skills summary

In this section, you learned how to:

- Conduct a property search
- View catalog information
- View supplier information
- Create a report

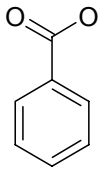
Key points

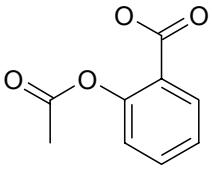
- In this section, we used the CAS Registry Number as the field to search. You can use the same search technique to search any of the property fields in the ACD database.
- You viewed the details for the compound of interest, and learned how to add and hide additional information on the page (Suppliers, Prices).
- Using page links, you were able to view catalog data for a specific supplier, and the supplier's address.
- You learned how to copy the displayed information to a report, including how to append information to an existing report.

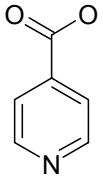
Notes

Structure searching

Exact	Substructure	Similarity
Retrieves exact match of the structure query. Alternatively, select: Include Isomers Include Tautomers Include Salts	Retrieves molecules that contain the embedded substructure. All open valences are sites for possible substitution. Query features can be added to specify allowed structural variations.	Retrieves molecules that have general features in common. Can retrieve molecules not retrieved by a substructure search.







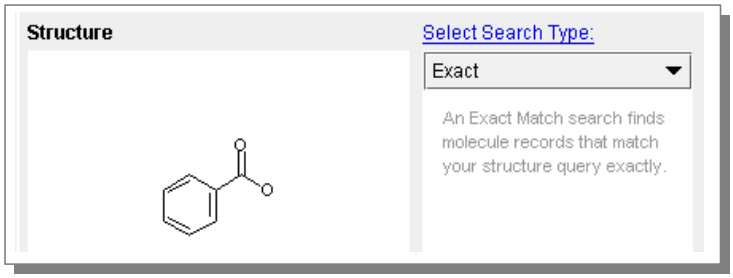
Key points

- When searching by structure, you have the search options listed above.
- To retrieve an exact match of your query structure, choose Exact. To allow specific variations, you can instead choose Include Isomers, Include Tautomers, or Include Salts.
- To find a class of compounds that contain a substructure of interest, choose Substructure. All of the molecules retrieved will contain your query as a substructure.
- To find compounds that are structurally similar to your query, but do not necessarily contain all of the same components, choose Similarity.

Notes

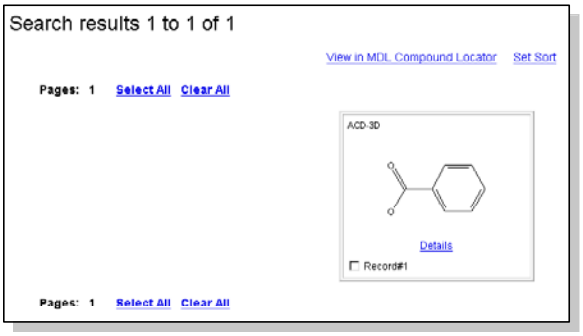
Demonstration: Exact search

Draw the query and select the search type



Start the search

View the search results



Key points

- In this demonstration, you retrieve benzoic acid from the database using the exact structure as a query.
- You will draw the query in MDL Draw, and then transfer it to the queries page in MDL Database Browser.
- The search type is Exact.

Notes

Demonstration: Exact match search

Conduct an exact match search for benzoic acid. View the compound details.

Choose the Structure field

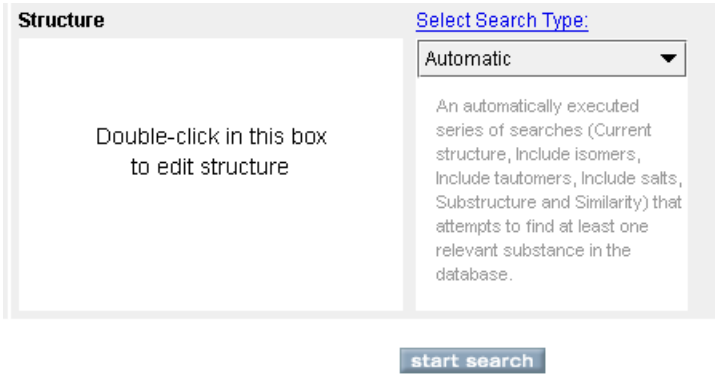
1. Click the **queries** tab. Then click **clear query**. Go to Step 2.

   – Or –

   Click **new query** in the top menu bar. Then click **Draw Structure**. Go to "Draw the structure query" below for continuing instructions.

2. On the Field Index tab, double-click **Structure**.

3. In the query pane, double-click the Structure box.



   The MDL Draw window opens.

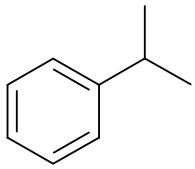
Draw the structure query

1. In MDL Draw, click the **benzene ring** template in the top tool bar.

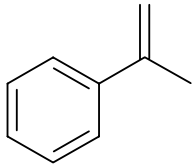
2. Click the drawing area. A benzene ring appears.

3. Click the **All-Purpose Drawing Tool** on the side tool bar.

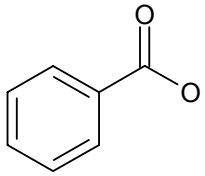
4. Drag from the atom sites to draw the bonds in the carbonyl group.



5. Click one of the single bonds to change it to a double-bond.



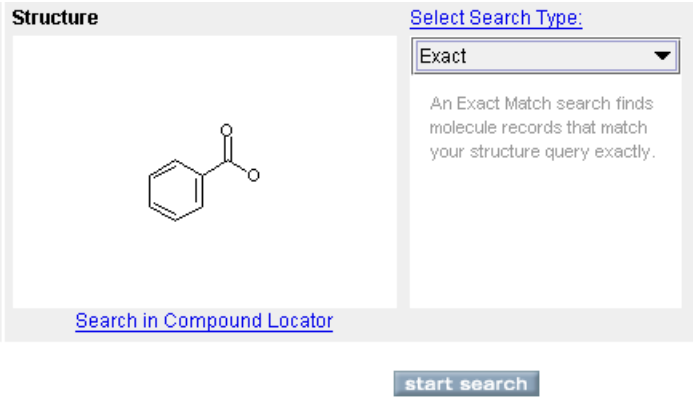
6. Right-click a terminal atom and choose **Atom Symbol**. Click **O** to signify oxygen. Repeat to place the other oxygen atom.



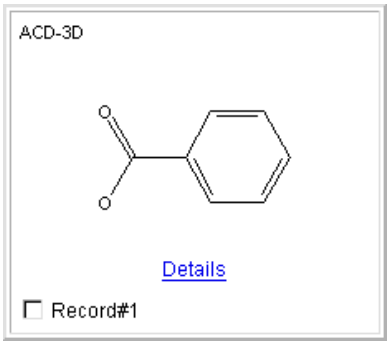
7. Click **Done** to transfer the structure to the structure query box.

Conduct an exact match search

1. Choose **Exact** as the search type.



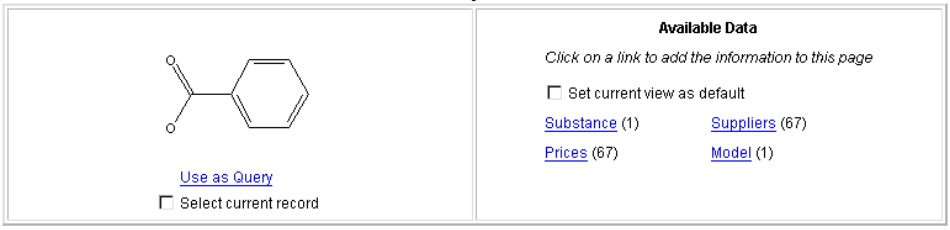
2. Click **start search**. The search results are displayed on the Results page.



View compound details

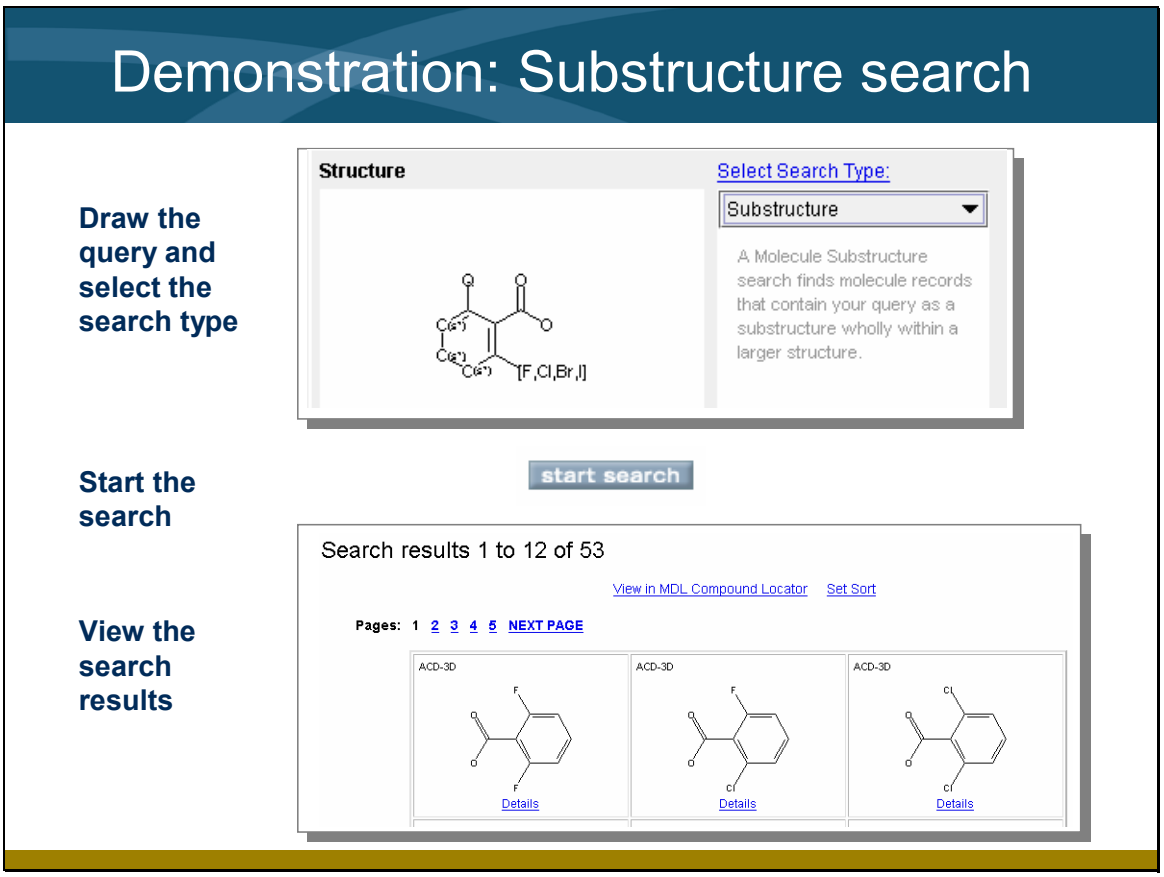
1. Click the **Details** link.

MDL® Available Chemicals Directory



Substance (hide)

ACD Registry Number	2286
MDL Number	MFCD00002398
CAS Registry Number	65-85-0
Chemical Name and Synonyms : • 'LGC' (2405) • 'LGC' (2606) • 'LGC' (4003) • ACIDUM BENZOICUM • BENZENE CARBOXYLIC ACID • BENZOIC ACID • CARBOXYBENZENE • DRACYLIC ACID • FEMA 2131 • PHENYLFORMIC ACID	
Molecular Formula	C7 H6 O2
Molecular Weight	122.122
Rule of Five	0
Computed partition coefficent (CLogP)	1.87
Molecular weight of largest fragment	122.122
Number of proton acceptors	2
Number of proton donors	1
Number of rotatable bonds (TDF)	0



Key points

- In this demonstration, you will retrieve compounds that contain benzoic acid as a substructure.
- You will add query features in MDL Draw that specify halogen substitution at the 2-position, any heteroatom at the 6-position, and prevent any other substitution on the ring.
- The search type is Substructure.

Notes

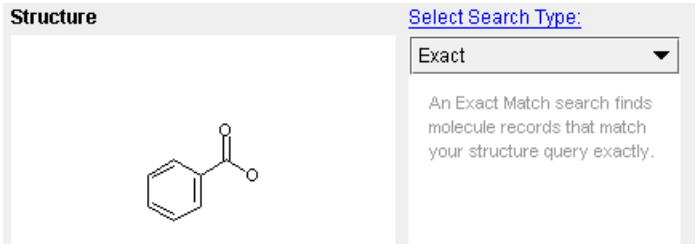
Demonstration: Substructure search

Conduct a substructure search to retrieve benzoic acids with a halogen at the 2-position and any heteroatom at the 6-position.

Refine the structure query

refine query

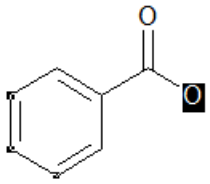
1. Click **refine query** on the top menu bar. The previous query is displayed.



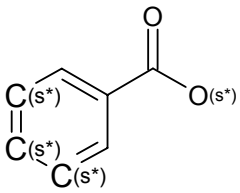
2. Double-click the structure query. The structure appears in the MDL Draw window for modification.

Prevent unwanted substitution

1. In MDL Draw, click the **All-Purpose Drawing** tool. Then shift-click to select the atom sites where you do not want substitution to appear.

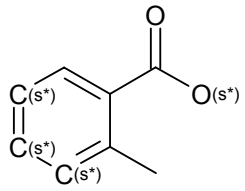


2. Right-click one of the selected atoms, and choose **Number of non-hydrogen substituents**. Then choose **As drawn**.



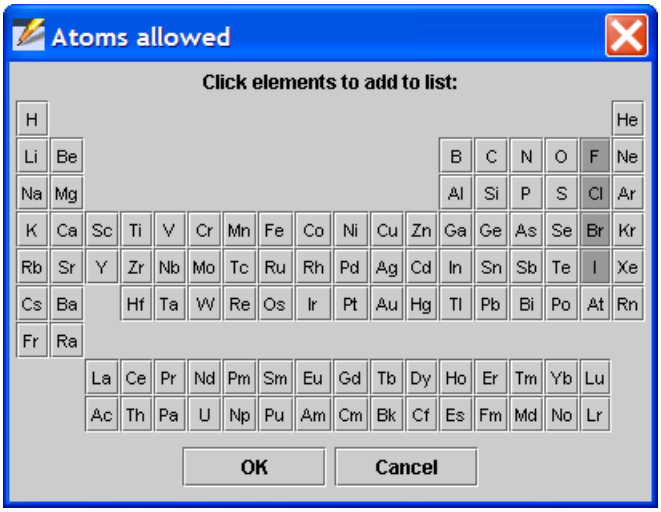
Specify a list of allowed atoms

1. Drag from the 2-position to draw a single bond.

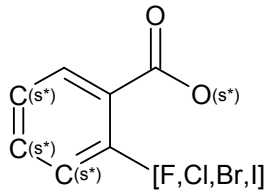


2. Right-click the terminal atom, and choose **Allow these atoms > Atom List**.

3. Click the atom symbols **F**, **Cl**, **Br**, **I**.

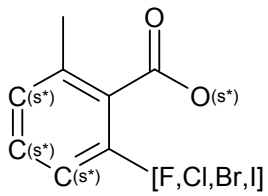


4. Click **OK**.

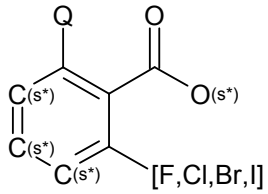


Specify heteroatom substitution

1. Drag from the 6-position to draw a single bond.



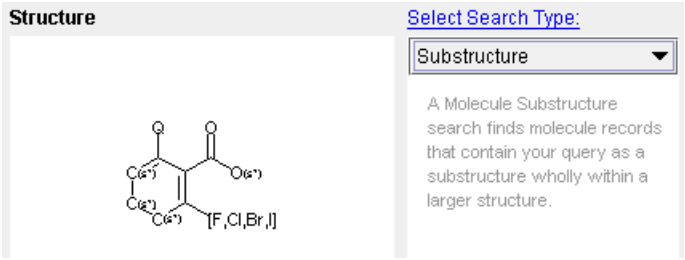
2. Right-click the terminal atom, and choose **Allow these atoms > Any atom except H or C (Q)**.



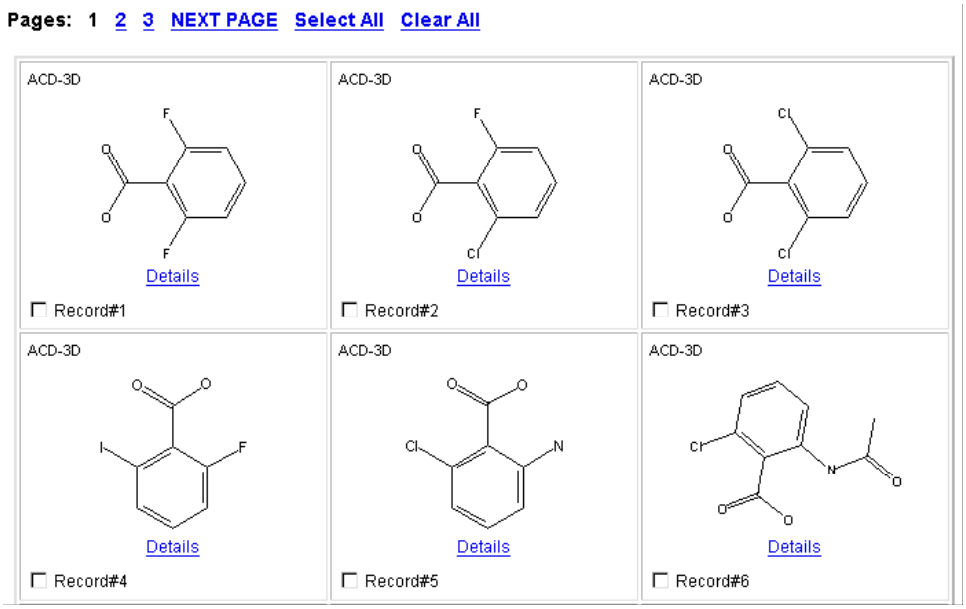
3. Click **Done** to transfer the modified structure to the structure query box.

Conduct a substructure search

1. Choose **Substructure** as the search type.



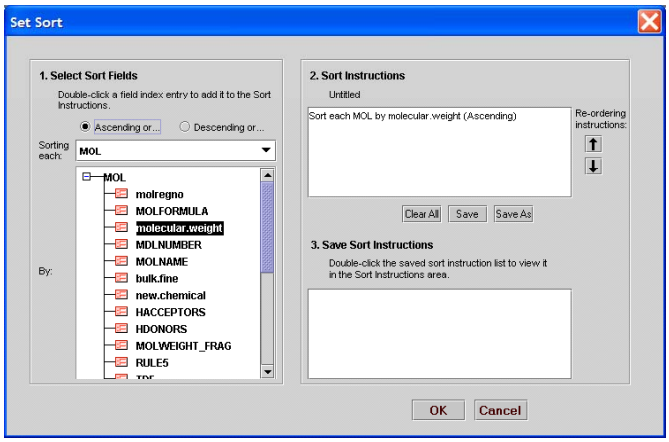
2. Click **start search**. The search results are displayed on the Results page.



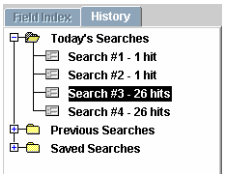
3. Click the links for pages **2** and **3** to see all of the compounds retrieved.

Demonstration: Sorting results

Specify sorting instructions



Retrieve previous (unsorted) results



Key points

- Using the results of the substructure search, you will sort the compounds by ascending molecular weight.
- After viewing the sorted search results, you will retrieve the previous (unsorted) search results by using the list of Today's Searches on the History tab.

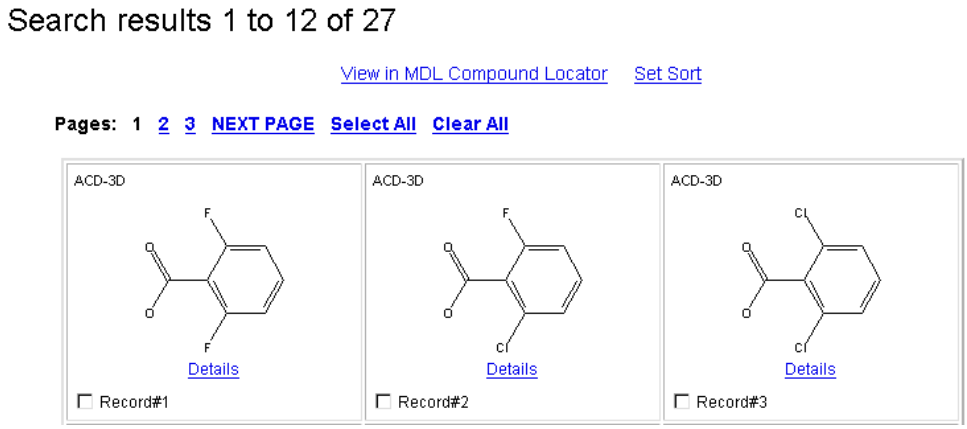
Notes

Demonstration: Sorting search results

Sort the search results by ascending molecular weight. Then redisplay the unsorted search results.

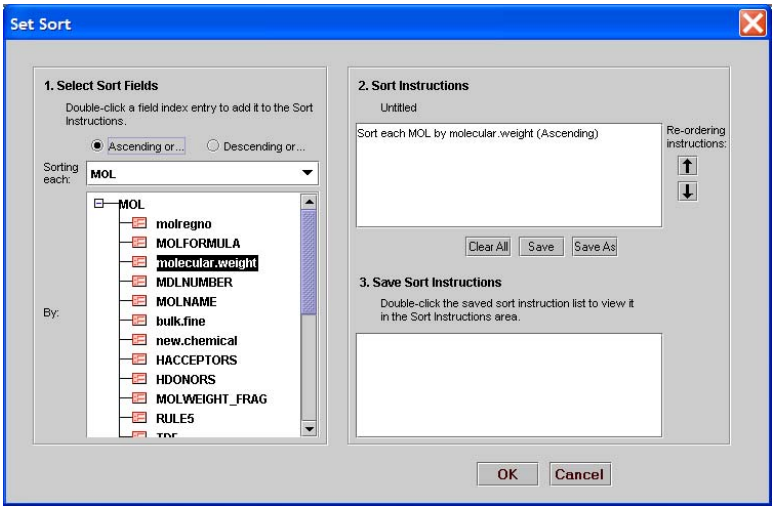
Specify sort instructions

1. Click the link for page **1** to return to the first page of search results.

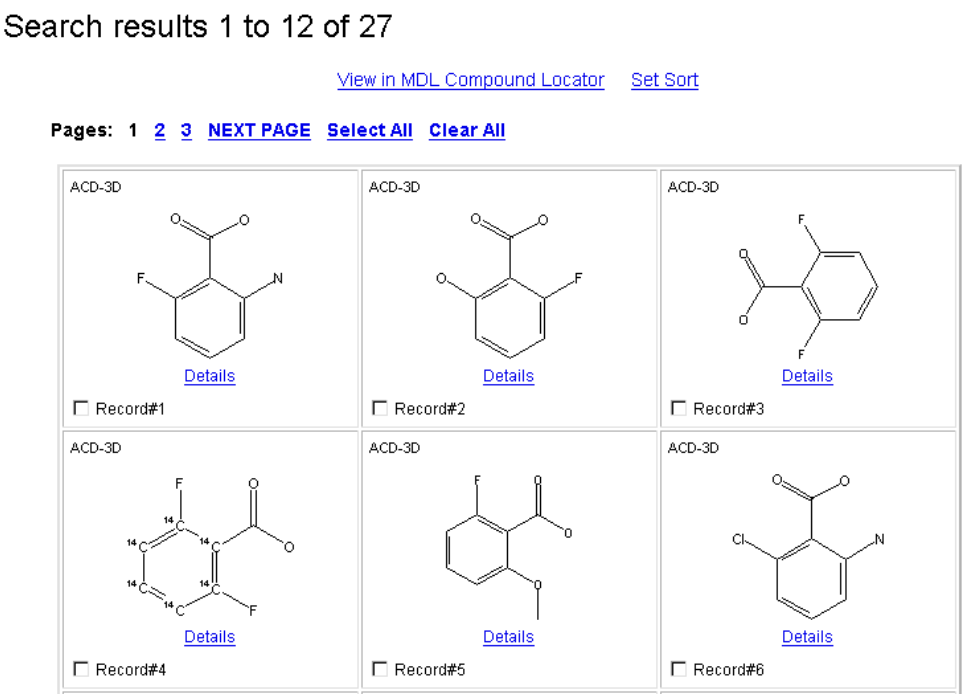


2. Above the structure grid, click **Set Sort**.

3. Double-click the **molecular.weight** field. The sort instructions appear in the Sort Instructions box.

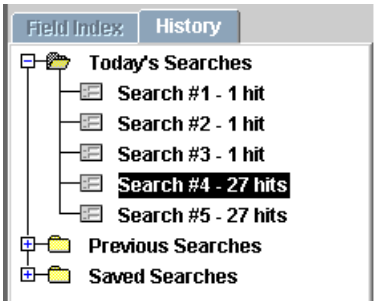


4. Click **OK**. The sorted search results are displayed in the structure grid.



Retrieve the previous search results

1. On the History tab, under Today's Searches, double-click the previous search results list (in this case, Search #4).



The previous (in this case, unsorted) search results are displayed.

Skills summary

In this section, you learned how to:

- Conduct an exact search
- Conduct a substructure search
- Sort search results
- Retrieve previous search results

Key points

- You learned the basic techniques for conducting a structure search. We conducted an exact search and a substructure search.
- We introduced some substructure query features that you can use to refine your search requirements. You can read more about this topic in a 23-page Request-A-Document available through the online help (click search types > Molecule Substructure from the help index).
- You learned how to sort search results and retrieve previous search results.

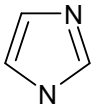
Notes

Workshop description

The following descriptions explain the goal of the workshop. If you like to figure things out on your own, use the descriptions to perform the necessary tasks. If you prefer step-by-step instructions, go to the page listed below the description.

Scenario

Search for compounds that contain the imidazole substructure and have a molecular weight less than 120.



View the details for a compound of interest. Create a new report that contains the substance data, catalog information for a specific supplier, and the supplier address.

Tasks

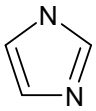
- **Specify the substructure search query.** Add the Structure field to your query. Draw the imidazole substructure. Choose Substructure as the search type.
- **Specify the molecular weight query.** Add the Molecular Weight field to your query. Choose < as the data operator, and enter 120 as the target value.
- **Conduct the combined search.** Verify that the logical operator is AND. Start the search.
- **View details for a particular compound.** After the search is complete, view the Details page for one of the compounds.
- **Create a report with the desired information.** Display the substance data, catalog information for a specific supplier, and the supplier address. Copy the information to a new report. View the report.

Specify the substructure search query

1. Click the **queries** tab. Click **clear query** on the top menu bar to clear the previous query, if any.

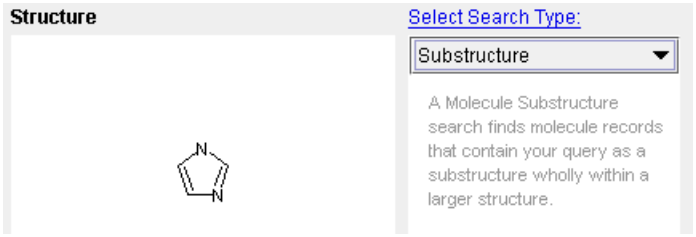
2. Double-click **Structure** from the Field Index. Then double-click the Structure box.

3. In MDL Draw, draw imidazole using the cyclopentadiene template and the **All-Purpose Drawing** tool.



4. Click **Done** to transfer the structure to the Queries page.

5. Choose **Substructure** as the search type.



Specify the molecular weight query

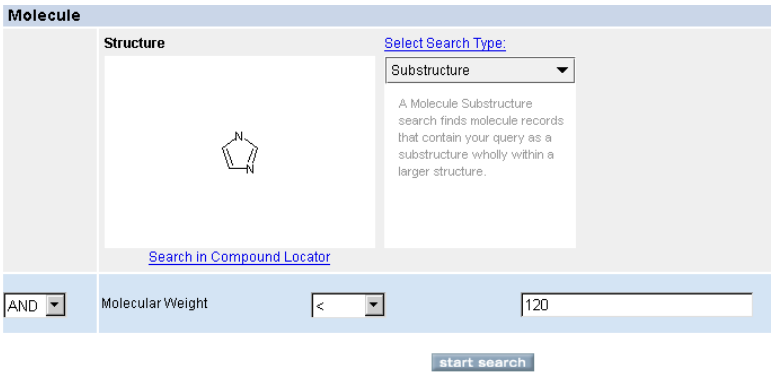
1. Double-click **Molecular Weight** from the Field Index.

2. Choose **<** as the data operator.

3. Enter **120** as the target value.

Conduct the combined search

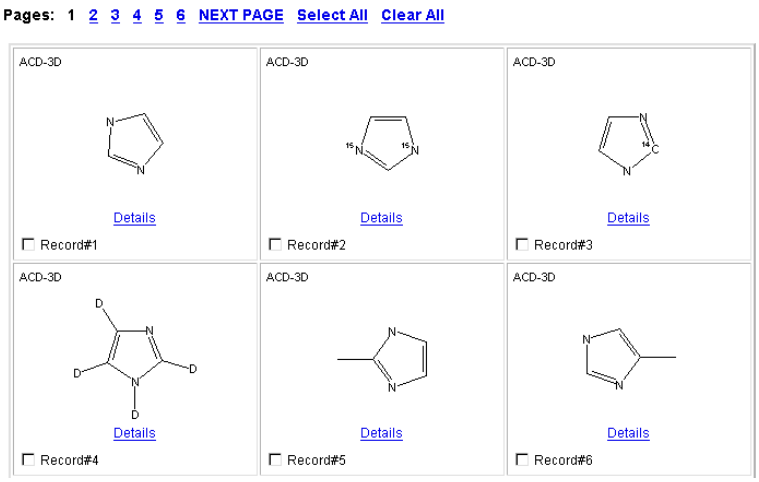
1. Verify that the logical operator between the structure query and the molecular weight query is set to AND.



2. Click **start search**.

View details for a particular compound

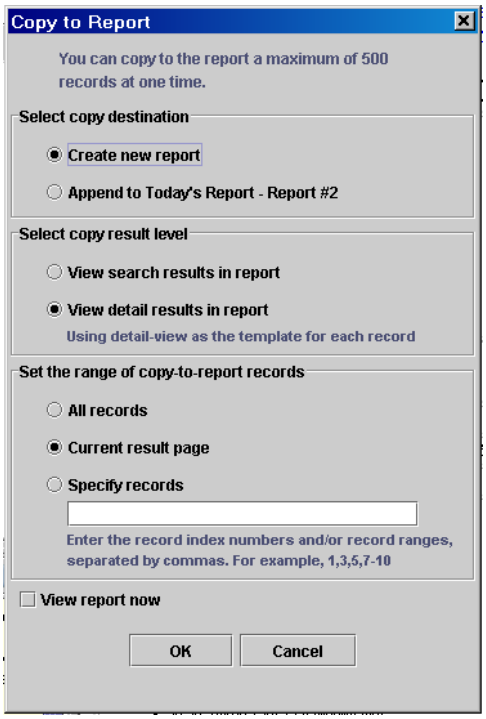
When the search is complete, the search results are displayed in the structure grid.



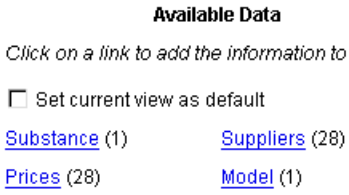
1. Click **Details** below a structure of interest. The Substance data is displayed by default.

Create a report with the desired information

1. Click **copy to report** on the top menu bar. Click the radio button for **Create new report**, if needed. Click **OK**.

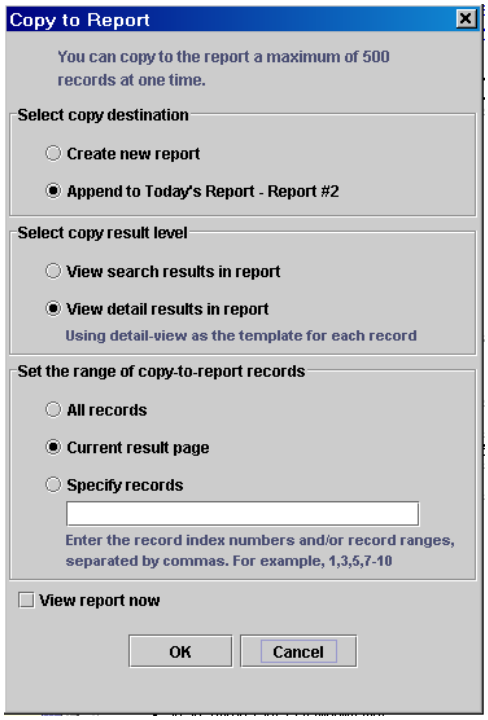


2. Under Available Data, click **Suppliers**.



3. From the list of suppliers, click a supplier of interest. The catalog data for that supplier is displayed.

4. Click **copy to report**. Click **OK** to append the catalog data to the current report.



5. Click **address** next to the supplier name. The address information is displayed.

6. Click **copy to report**. Click **OK** to append the catalog data to the current report.