Factual Searching in CrossFire Beilstein

DiscoveryGate[SM]
Version 1.4
Participant's Guide

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Factual Searching in CrossFire Beilstein

Key points

- Welcome to the *Factual Searching in CrossFire Beilstein* module.
- In this module, you will search the Beilstein database through DiscoveryGate using the MDL Database Browser

Notes

Module objectives

- Conduct data searches to retrieve compounds based on their chemical name, CAS number, and physical or chemical properties
- Conduct searches using multiple data entries
- Conduct searches using data and structural entries
- Use predefined EDS forms and create custom forms to conduct the searches
- Review the search history, save a list, and create a report

Key points

- In this module, you will learn how to conduct data searches to retrieve compounds based on their chemical name, CAS number, and physical or chemical properties.
- You will learn how to use the predefined EDS forms, and create your own custom forms.

Notes

Search scenarios

Conduct a series of factual searches, in the CrossFire Beilstein database, to answer the following questions. In the process, you will learn how to use the MDL Database Browser in DiscoveryGate.

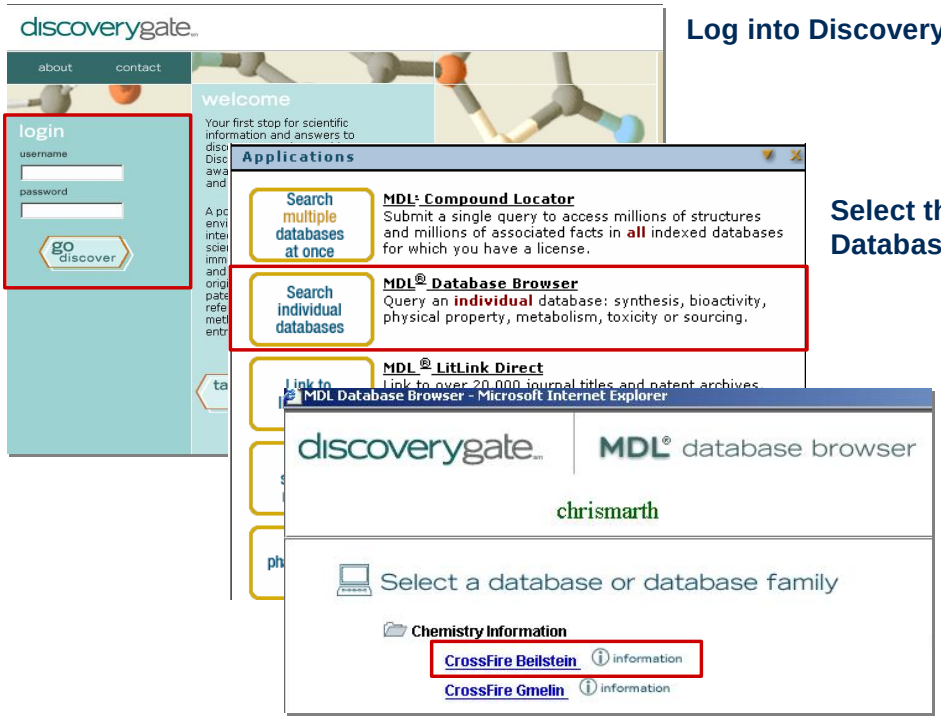
- How do I retrieve a compound from the database if I only have the chemical name or CAS number?
- How do I retrieve specific property data for a compound?
- How do I retrieve reactions without using a structural query?
- How do I conduct a search using a factual and structural entry?

Key points

- This module focuses on the capabilities of DiscoveryGate with respect to the individual capabilities of one of its main components, the MDL Database Browser.
- We will conduct a series of factual searches using the CrossFire Beilstein database.

Notes

Launch the application and database



Log into DiscoveryGate

Select the MDL Database Browser

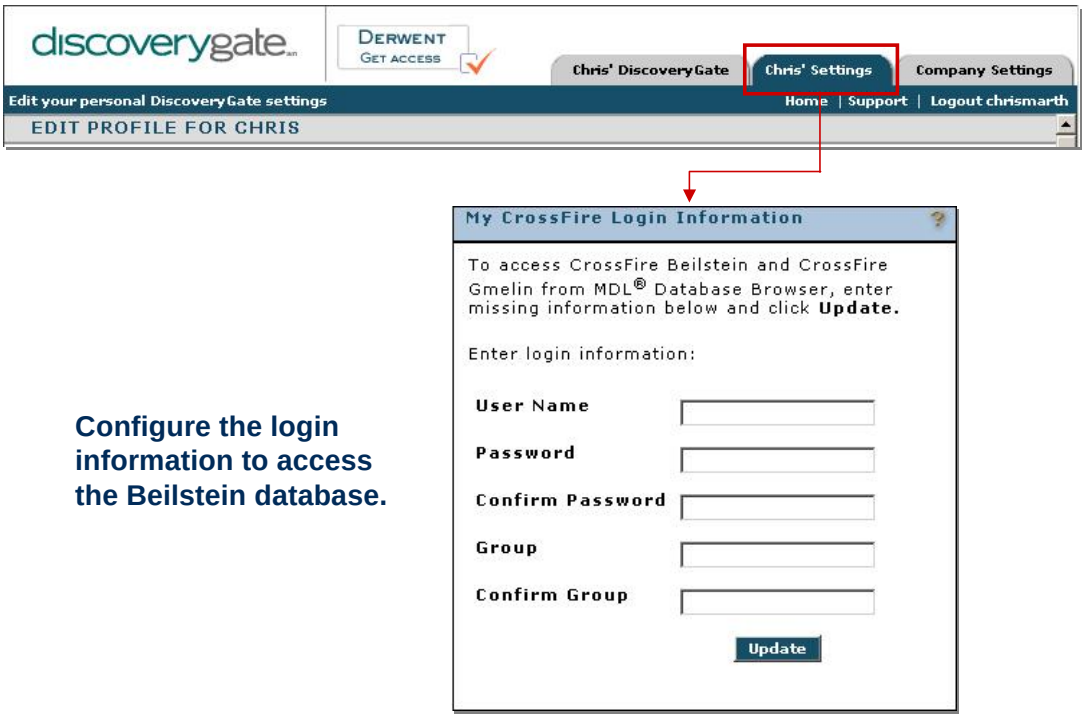
Select the CrossFire Beilstein database

Key points

- Launch the internet browser and enter the DiscoveryGate URL. To log in, enter your user name and password, and then click "go discover."
- DiscoveryGate uses the MDL Database Browser to search individual databases. Searching a specific database allows you to focus quickly on the information in a specific database and to search using data properties.

Notes

Configure CrossFire access information



Configure the login information to access the Beilstein database.

Key points

- To search the CrossFire Beilstein database, you will need to enter the CrossFire login information. If this is not configured, return to the main screen and click the Settings tab. Enter your user name, password, and group for CrossFire Beilstein.

Notes

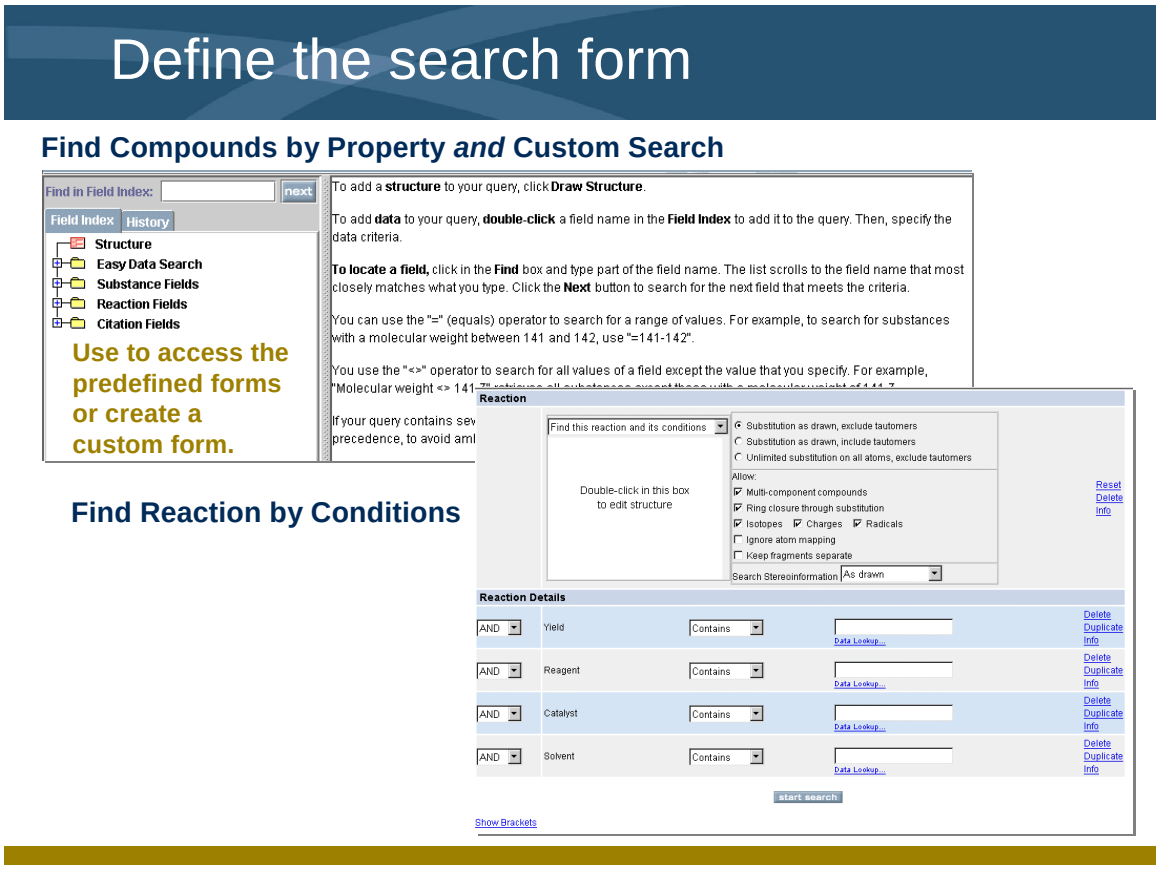
Select the Search of Interest

Key points

- The selections for data searching that we will use in this module are:
  - Find Compounds by Property
  - Find Reaction by Conditions
  - Custom Search

Notes

Define the search form

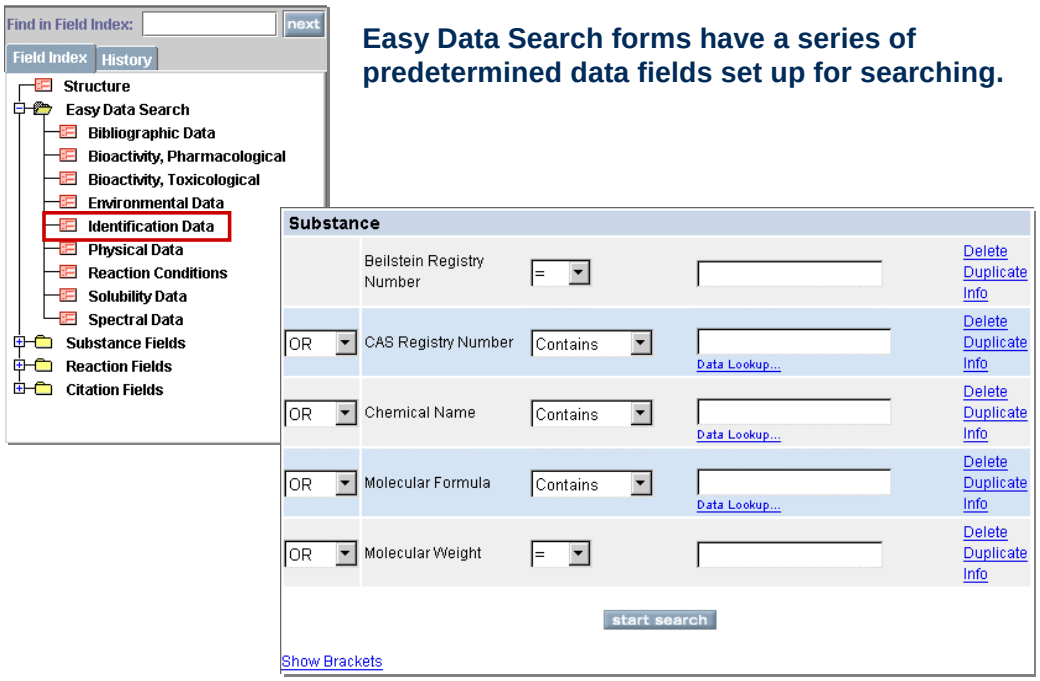


Key points

- The "Find Compounds by Property" option allows you to select predefined EDS forms or individual data fields to create a search to retrieve properties of interest.
- The "Find Reaction by Conditions" option allows you to select predefined EDS forms or individual data fields to create a search to retrieve types of reactions.
- The "Custom Search" option allows you to select individual data fields to create your own search combination.

Notes

Easy Data Search (EDS) forms



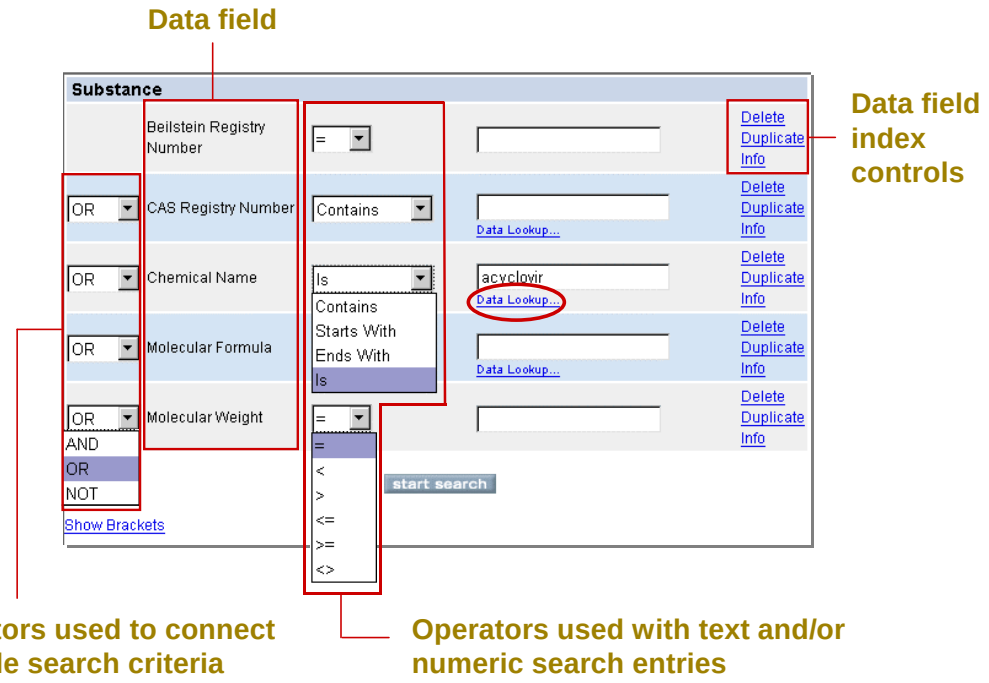
Easy Data Search forms have a series of predetermined data fields set up for searching.

Key points

- There is a section on the Field Index tab called Easy Data Search. This category contains a number of predefined forms that have common search criteria.
- The forms are organized by search area.

Notes

Factual search features



Key points

- The data fields on an EDS (Easy Data Search) form are predefined and are listed. The fields can be text or numeric fields.
- When using text or numeric fields, you can use any of the operators shown in the slide.
- In our example, you are interested in retrieving all compounds having the chemical name *acyclovir*. The Data Lookup feature allows you to view the contents of the database.

Notes

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 that 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

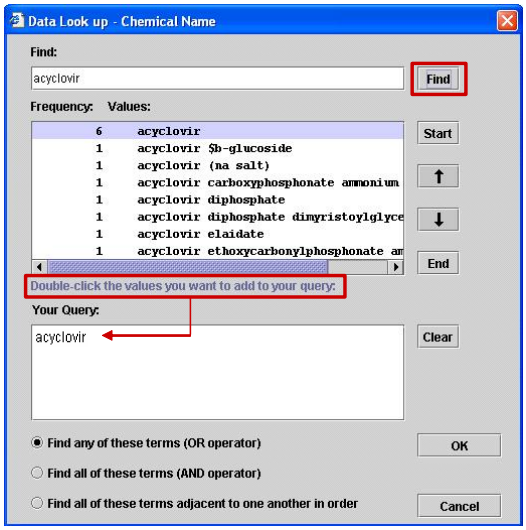
Key points

- When using multiple fields, you must use some of the data operators.

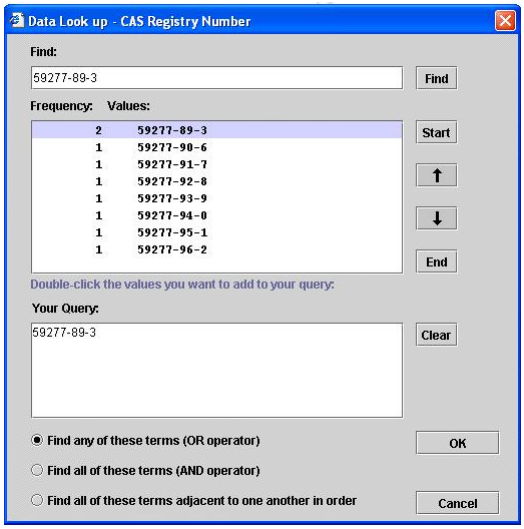
Notes

Data Lookup tables

Chemical Name search



CAS number search



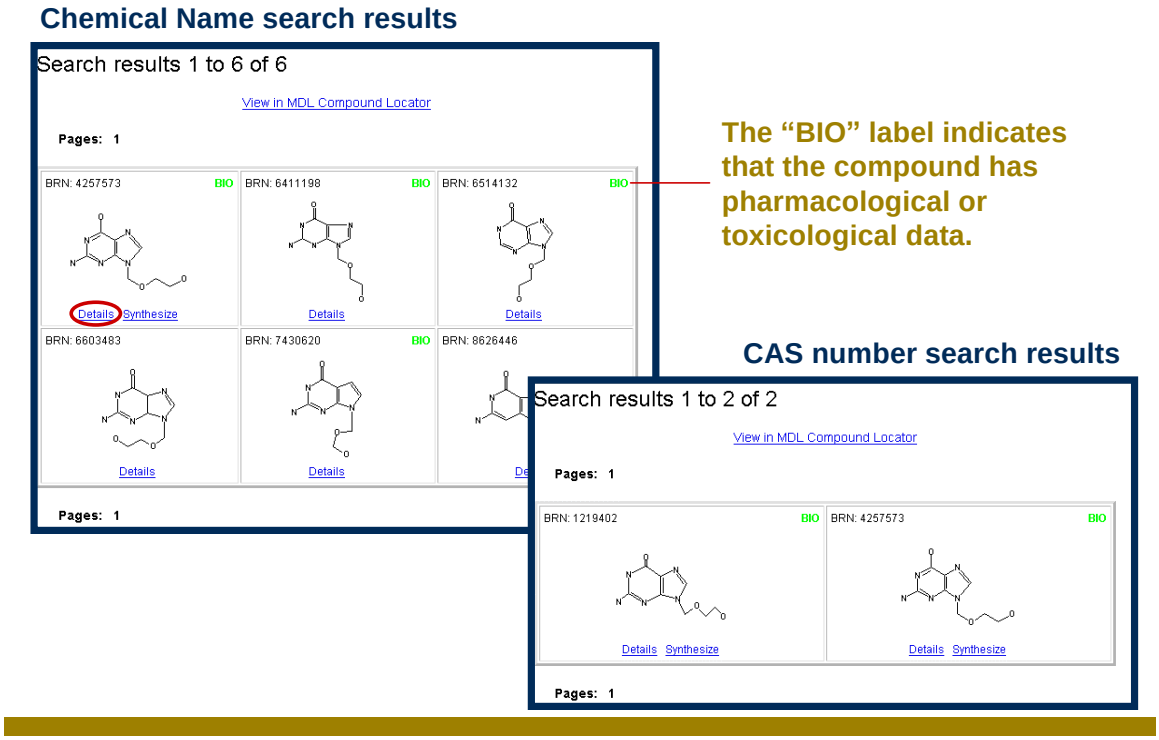
Data Lookup tables display the specified value and the number of occurrences found in the database.

Key points

- The Data Lookup feature indicates the number of occurrences for that data entry.
- By default, "Find any of these terms (OR operator)" is selected. This means that an OR operator will be used to connect each value you have selected.
- Select "Find all of these terms (AND operator)" to require that every value is present.
- Select "Find all of these terms adjacent to one another in order" to search for a string of values adjacent to one another.

Notes

Chemical name or CAS number results

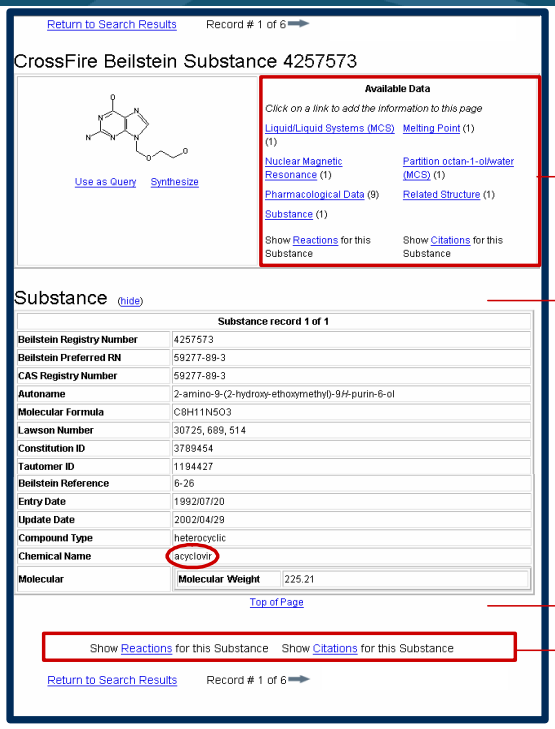


Key points

- Results are displayed on a separate form in a structural format. To obtain detailed data, click the "Details" link.
- In some of the result panels, you will notice the green BIO indicator. This label indicates that the compound has pharmacological or toxicological data associated with it.

Notes

Search details



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

Substance data

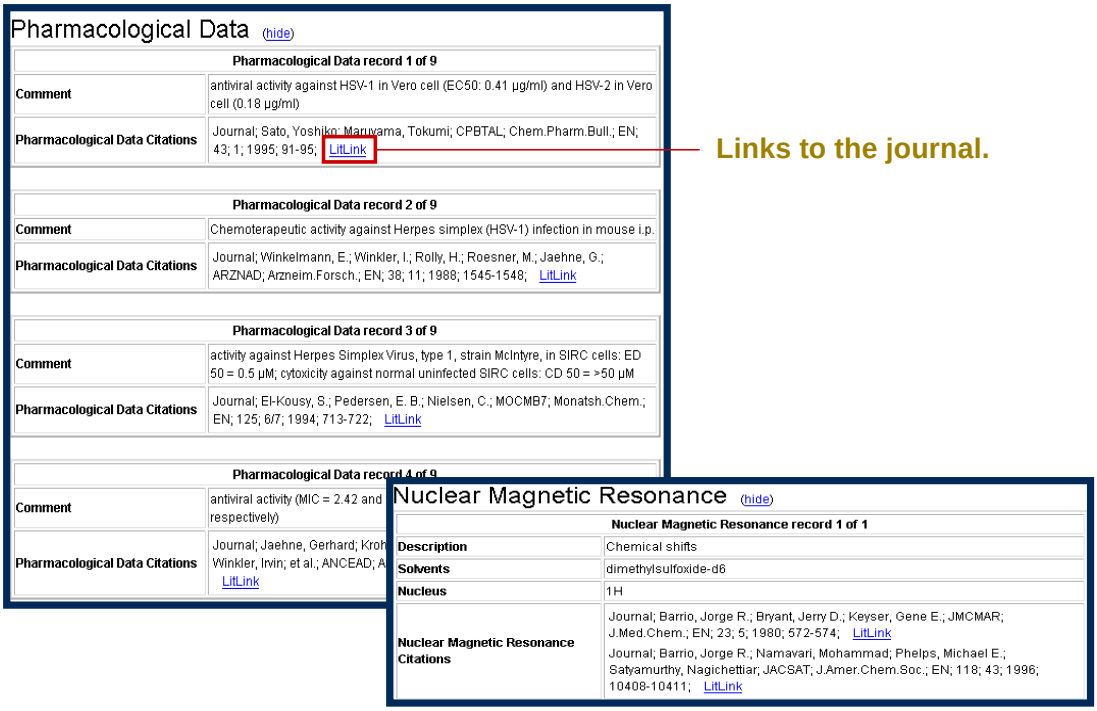
Click to link to reactions or citations for this substance

Key points

- The Substance data is shown, which includes identification information, such as registry numbers, molecular formula, CAS number, and chemical name.
- To obtain specific data for the compound, click a link in the Available Data box.
- If you would like to use this structure in a new query, click the "Use as Query" link.

Notes

Link to additional data



Key points

- Using MDL LitLink, you can obtain the original literature reference.
- When you are in LitLink, click the publication link to view the abstract.
- You must have the appropriate access rights in order to view the primary literature using LitLink.

Notes

Multiple search criteria

Conduct a search to retrieve substances with a melting point between 300 – 310, where the solvent used is water. Restrict the list to those compounds that display data for the density of the liquid.

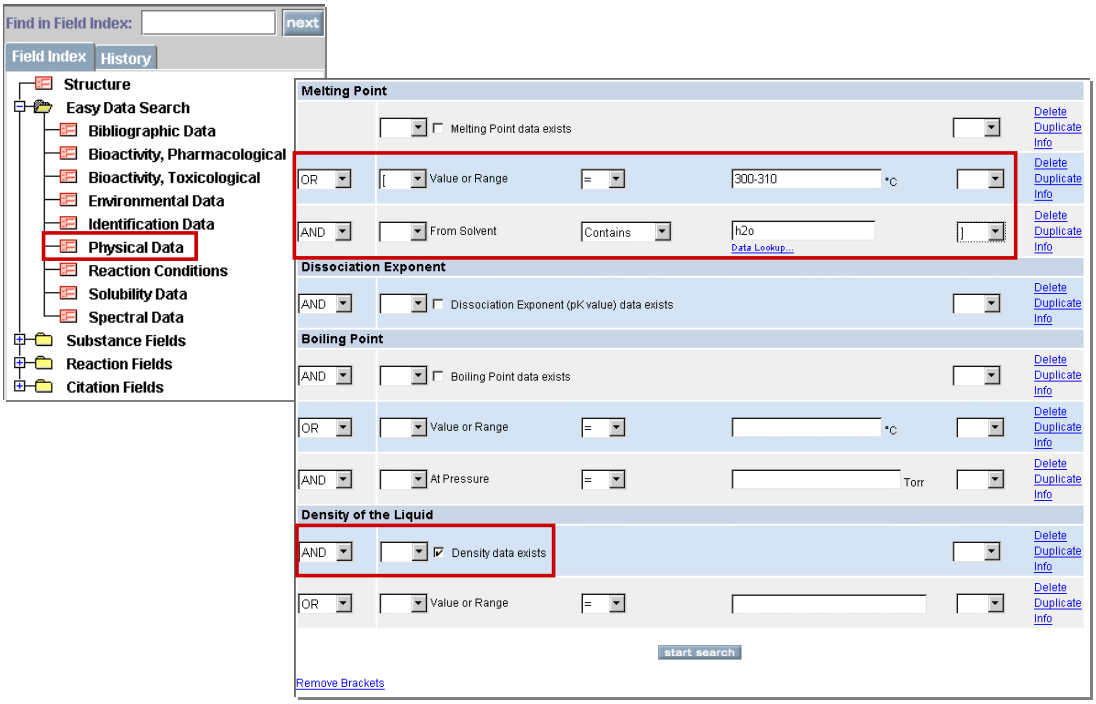
- use a predefined EDS search form
- use Available Data links to view retrieved data

Key points

- To search for compounds that have defined physical or chemical properties, use a multiple factual query.
- You want to retrieve substances with a melting point between 300-310, where the solvent used is water. A final requirement is to restrict the list to those compounds that display data for the density of the liquid.

Notes

Enter physical data search criteria

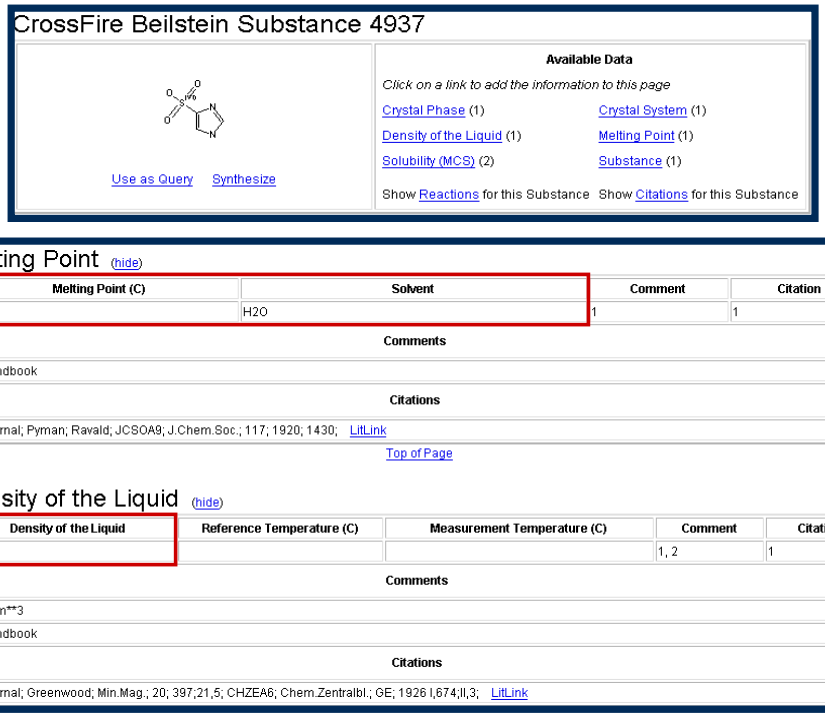


Key points

- This query form provides search criteria specific to fields related to physical data.
- You can search the database using fields with listed values.
- You can search some fields in the database without specifying a value. This technique is used to retrieve all records that have an entry in any subfield.
- Click the check mark next to the area of interest. This is a broad search for the occurrence of a fact in the database.

Notes

Physical data search results



CrossFire Beilstein Substance 4937

Use as Query Synthesize

Available Data

Click on a link to add the information to this page

Crystal Phase (1) Crystal System (1)
Density of the Liquid (1) Melting Point (1)
Solubility (MCS) (2) Substance (1)

Show Reactions for this Substance Show Citations for this Substance

Melting Point (hide)

Melting Point (C)	Solvent	Comment	Citation
307	H2O	1	1

Comments

1 Handbook

Citations

1 Journal; Pyman; Ravald; JCSOA9; J.Chem.Soc.; 117; 1920; 1430; LitLink

Top of Page

Density of the Liquid (hide)

Density of the Liquid	Reference Temperature (C)	Measurement Temperature (C)	Comment	Citation
1.838			1, 2	1

Comments

1 g/cm**3
2 Handbook

Citations

1 Journal; Greenwood; Min.Mag.; 20; 397;21,5; CHZEA6; Chem.Zentralbl.; GE; 1926 I,674;II,3; LitLink

Key points

- When used, the two connected search terms will only be retrieved as a hit if they are present in the same occurrence of a fact.

Notes

Custom form search for reactions

Conduct a search to retrieve hydrogenation reactions where Raney-Ni is used as a reagent or catalyst and acetic acid is used as a reagent.

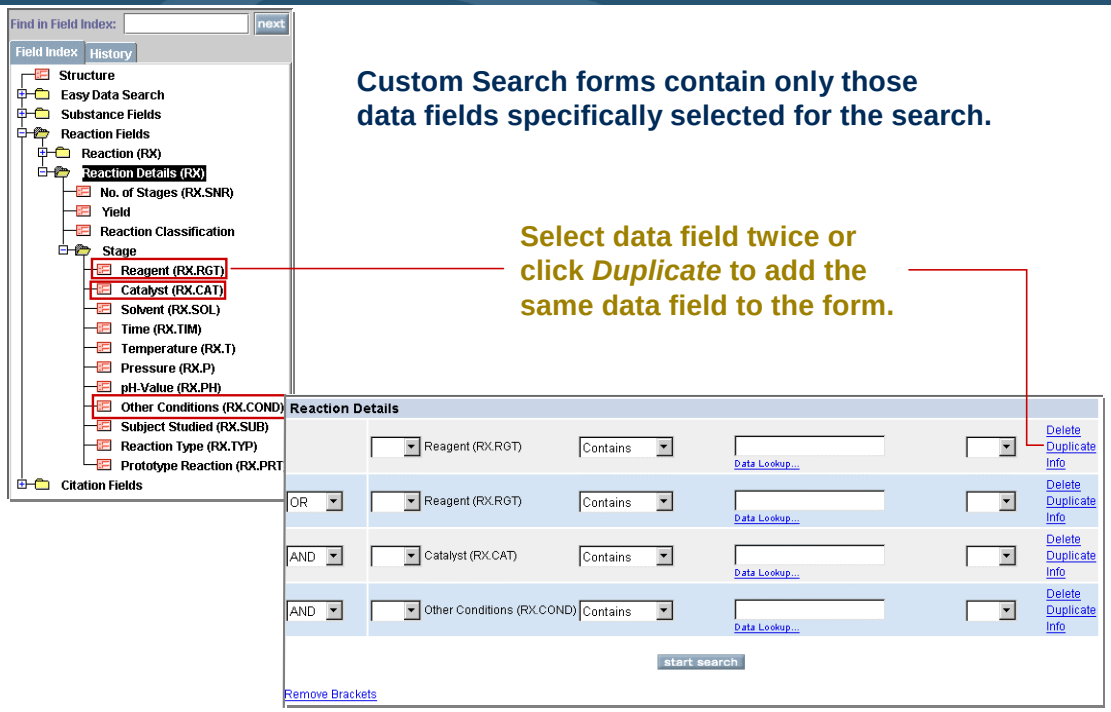
- create a Custom Search form
- use data operators and wildcards

Key points

- In this example, you are interested in retrieving hydrogenation reactions that use the Raney-Ni as a reagent or a catalyst, as well as acetic acid as a reagent.

Notes

Search for reactions

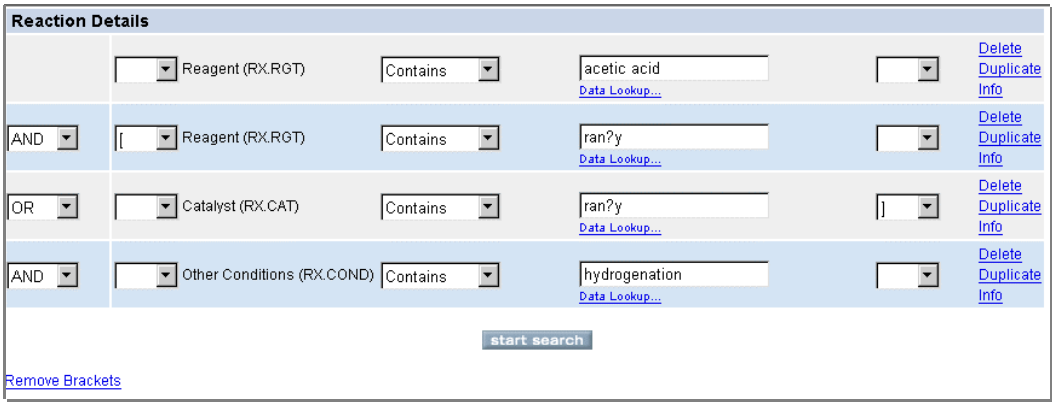


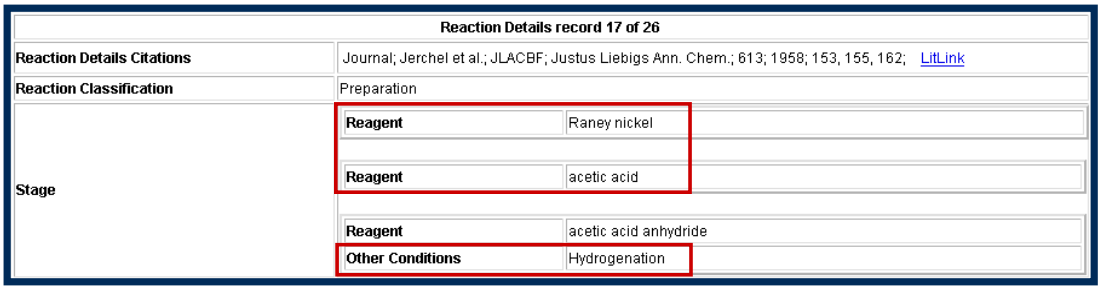
Key points

- Due to the inconsistencies of how authors report various reagents and catalysts in the literature, catalyst information can be stored in the catalyst and/or reagent field.
- To obtain a complete listing of information, you must search both data fields.

Notes

Reaction search query and results





Key points

- The substance, Raney Ni, occurs in the database using different entries. Use wildcards to include all occurrences of the catalyst and the reagent in the query.
- Use parentheses to force your search condition. You want to create an OR between the reagent and catalyst fields for Raney Ni.

Notes

Structure/data combination search

Conduct a search for the synthesis of para-halo-acetophenone compounds. Limit the list of reactions to those where methanol is used as the solvent.

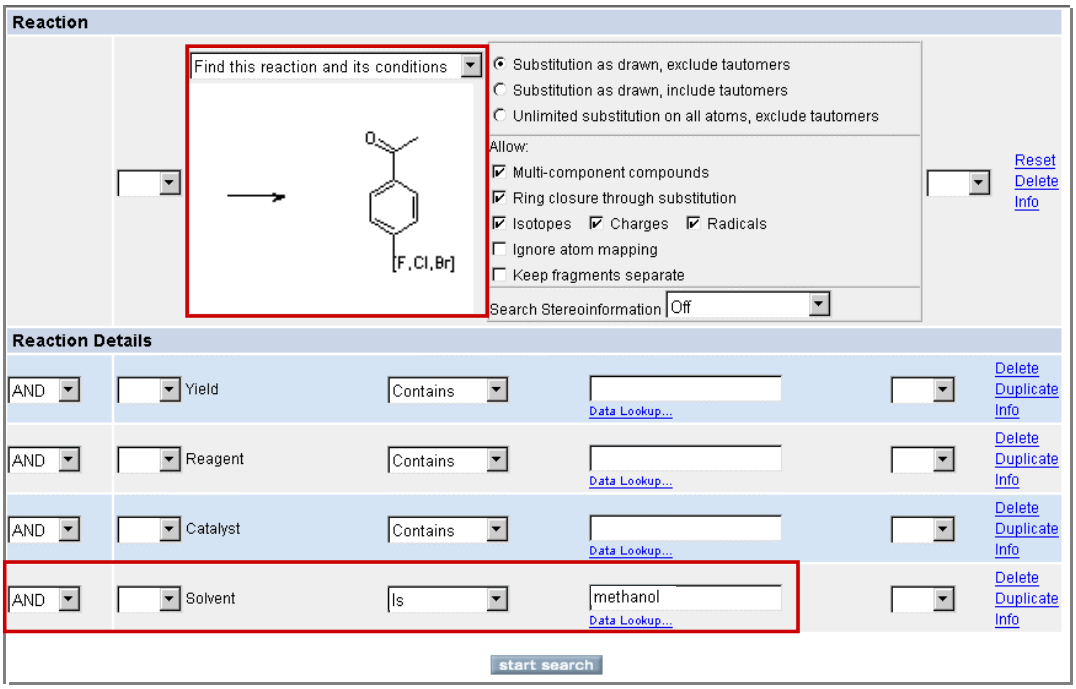
- use the Find Reaction by Conditions form
- combine structure and data components

Key points

- Factual searching is most effective when combined with a structure or reaction query.
- In the next example, we want to conduct a search for the synthesis of para-acetophenone compounds, limiting the list to only those reactions that use methanol as a solvent.

Notes

Find Reaction by Conditions

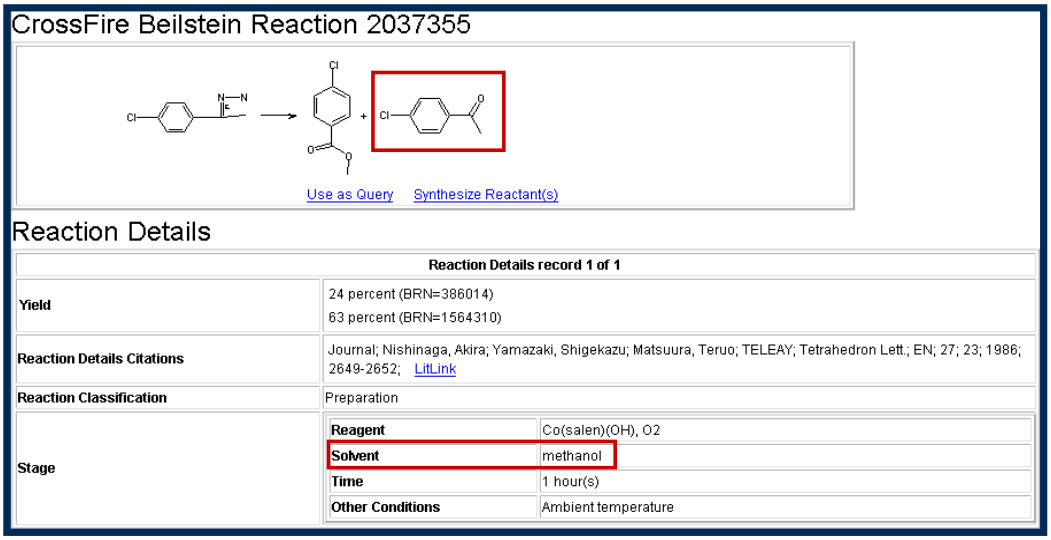


Key points

- When searching for reaction conditions, it is best to use the “Find Reaction by Conditions” form.

Notes

Structure/data search results



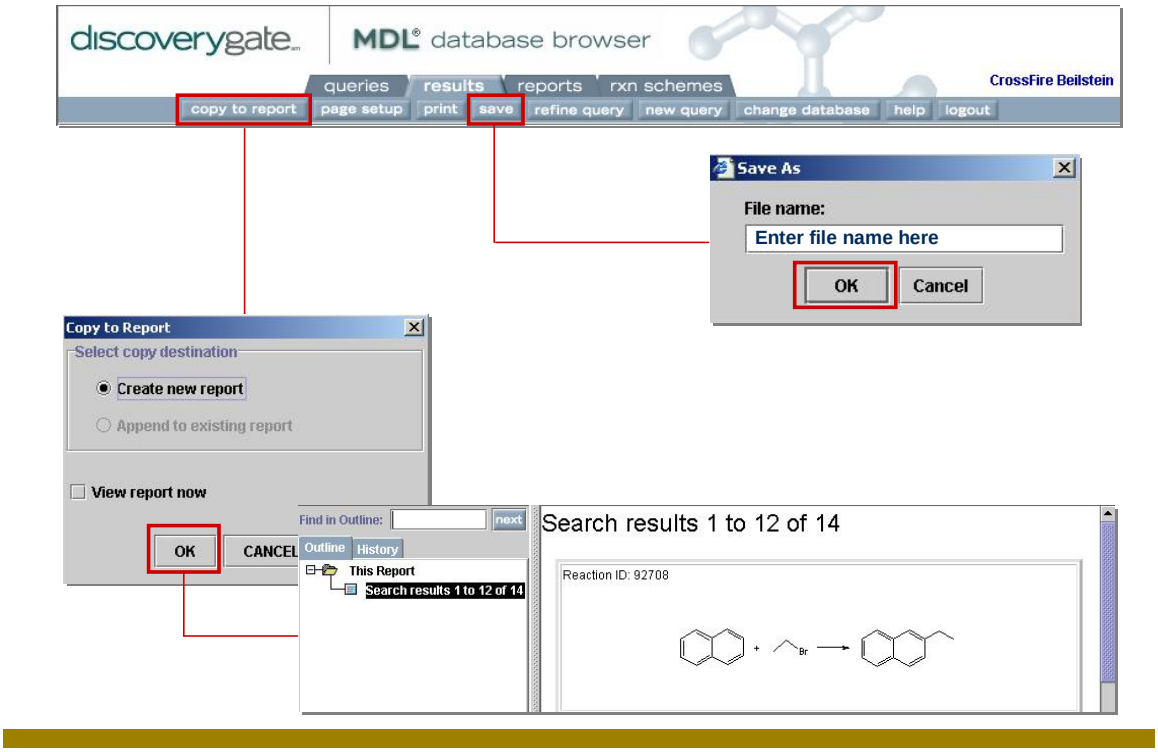
Conducting the structural search retrieves greater than 300 records.
Conducting the structure/data search retrieves approximately 20 records.

Key points

- Using a partial reaction query does not limit use to a specific type of reaction.
- Doing this portion of the search alone could retrieve too many results. The inclusion of the data parameter keeps the list focused.

Notes

Create a report and save a list



Key points

- You can copy your search results to a report that can be printed or exported.
- To create a report, click "copy to report" on the menu bar.
- You have the option of creating a new report or appending the data to an existing report. If you want to view the report immediately, check the box.
- To save a search, click the save button on the top menu bar.
- Saved searches are placed in the Saved Searches folder and stored permanently.

Notes

Exercise descriptions

The following descriptions explain the goal of each exercise. If you like to figure things out on your own, use the descriptions to conduct the exercises. If you prefer step-by-step instructions, go to the page listed below the description.

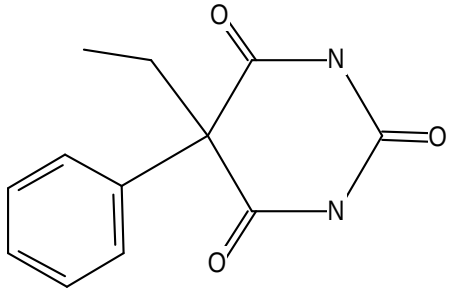
Exercise 1

Conduct a Chemical Name search to retrieve ibuprofen. Review the results. Conduct a second search for only those ibuprofen compounds that display pharmacological data. Review the results and link to the pharmacological data.

For a step-by-step solution, see page 1-26.

Exercise 2

Conduct a combination factual/structure search to retrieve all compounds that have a phenobarbital core structure and a melting point restriction greater than or equal to 150°C.



For a step-by-step solution, see page 1-28.

Exercise 3

Conduct a factual search to retrieve reactions where the product was derived from a demethylation of various groups.

For a step-by-step solution, see page 1-30.

Conduct a Chemical Name search to retrieve ibuprofen

Exercise 1

Conduct a Chemical Name search to retrieve ibuprofen. Review the results. Conduct a second search for only those ibuprofen compounds that display pharmacological data. Review the results and link to the pharmacological data.

Start DiscoveryGate

1. If you have already started the application, go to Step 3. Launch your internet browser and enter the DiscoveryGate URL (www.discoverygate.com).

2. Enter your user name and password. If necessary, enter your company id. Click **go discover**.

3. Under Applications, click **Search individual databases**.

Open the CrossFire Beilstein database

4. Under Chemistry Information, click **CrossFire Beilstein**.

5. Click the **Find Compounds by Property** link.

Open the Easy Data Search form

6. In the Field Index pane, open the **Easy Data Search** folder. Double-click the **Substance Identification Data** folder.

7. For the Chemical Name field, select the **Contains** operator.

8. Click the **Data Lookup** link below the text entry box.

Use the Data Lookup table

9. In the Data Look up – Chemical Name dialog box, type **ibuprofen** in Find text box and click **Find**.

10. In the Frequency: Values: box, double-click the **ibuprofen** entry.

11. When the entry appears in the Query box, click **OK**.

12. Click **start search**.

13. Click the **Details** link. Note that a number of records have the BIO label in the structure result box.

Isolate the list of compounds

14. Click the **refine query** button.

15. In the Field Index pane, click to expand the **Easy Data Search** category.

16. Double-click the **Pharmacological Data** form.

17. Check the **Pharmacological data exists** box.

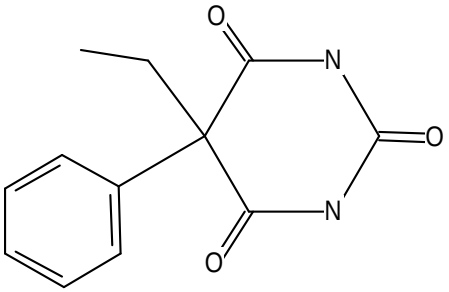
18. Click **start search**.

19. Click the **Details** link for any record.

Combination factual/structure search

Exercise 2

Conduct a combination factual/structure search to retrieve all compounds that have a phenobarbital core structure and a melting point restriction greater than or equal to 150°C.



Prepare for a new search

new query

1. Click the **new query** button.

2. Click the **Custom Search** link.

3. In the Field Index pane, double-click the **Structure** field.

4. In the Find Field Index text box, type **melting point**.

5. Open the **Melting Point (MP)** folder and double-click the **Melting Point (MP)** data field.

6. Double-click the structure box and draw phenobarbital using MDL Draw. Click **Done**.

7. In the MDL Database Browser select:

   - **Find this compound and its properties**
   - **Substitution as drawn, exclude tautomers**
   - Under Allow, check **Multi-component substances**, **Ring closure through substitution**, **Isotopes**, **Charges**, and **Radicals**.
   - Search Stereoinformation, select **Off**

8. If necessary, choose the **AND** operator between the fields.

9. For the melting point field, select the **greater than or equal to (>=)** operator and enter **150** in the text box.

10. Click **start search** and view the results.

11. Click the **Details** link for BRN 551715.

12. Under Available Data, click the **Melting Point** link.

Retrieve reactions using a factual query

Exercise 3

Conduct a factual search to retrieve reactions where the product was derived from a demethylation of various groups.

Prepare for a new search

1. Click the **new query** button.

2. Click the **Custom Search** link.

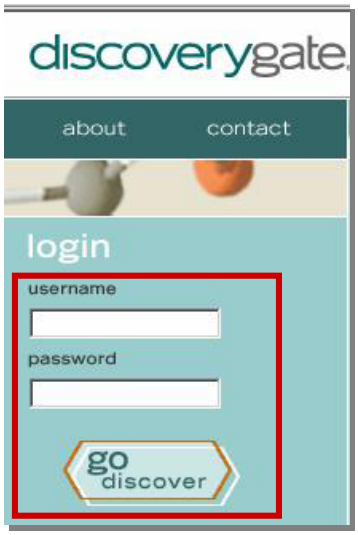
3. In the Field Index pane, type **conditions** in the Find Field Index text box, if necessary. Click the **Next** button until you obtain the **Other Conditions (RX.COND)** data field.

4. In the Field Index pane, double-click the **Other Conditions (RX.COND)** data field. If necessary, select the **Contains** operator and type **demethylation** in the text box on the form.

5. Click **start search** and view the results.

To launch the DiscoveryGate application

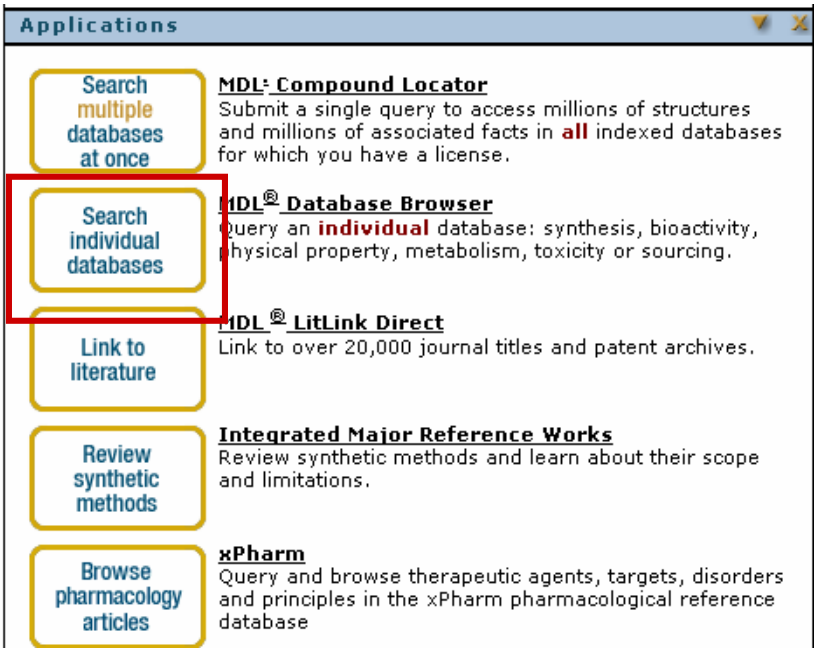
1. Launch your internet browser and enter the DiscoveryGate URL (www.discoverygate.com).
2. Enter your username and password.
3. If necessary, enter your company ID.



4. Click **go discover**.

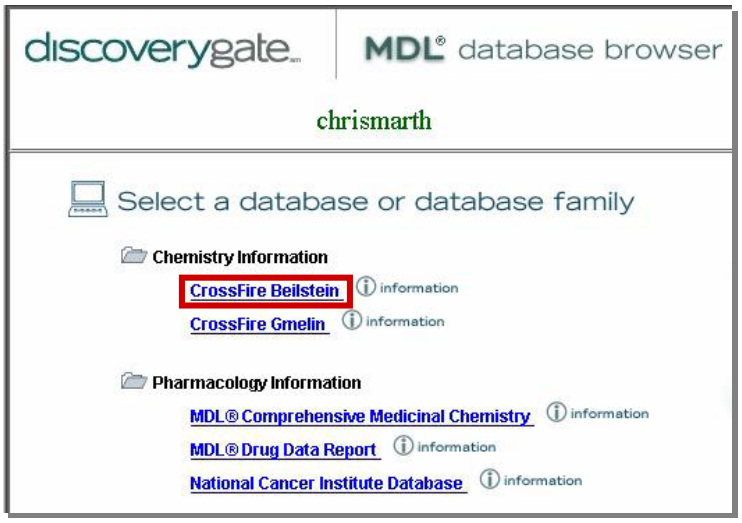
To select an individual database

1. Under Applications, click **Search individual databases**.



To select CrossFire Beilstein

1. Under Chemistry Information, click **CrossFire Beilstein**.



To configure CrossFire

1. Click the personal **Settings** tab.
2. In the My CrossFire Login Information box, enter your **User Name**, **Password**, **Confirm Password**, **Group**, and **Confirm Group** information.

3. Click **Update**.

To create a factual query

1. In the Select the Search of Interest window, click **Find Compounds by Property**, **Find Reaction by Conditions**, or **Custom Search**.

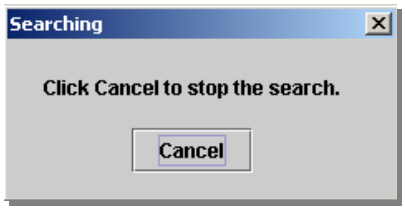
2. In the Field Index pane, open a predefined EDS form, or open a folder and double-click to select individual data fields.
3. Select a data operator and enter a text or numeric data entry into the associated text box.

To start a search

1. Enter a query into one or more data fields.
2. Click **start search**.

To stop a search

1. After a query is launched, click **Cancel**.



To modify a search query

1. At the top of the window, click the **refine query** button.

To clear the query

1. On the query tab, click **clear query**.

To open an Easy Data Search form

1. (Optional) Click **clear query**.
2. In the Field Index pane, expand the **Easy Data Search** folder.
3. Double-click the appropriate form.

To add a data field to the query

1. In the Field Index pane, expand the folders to locate the field.

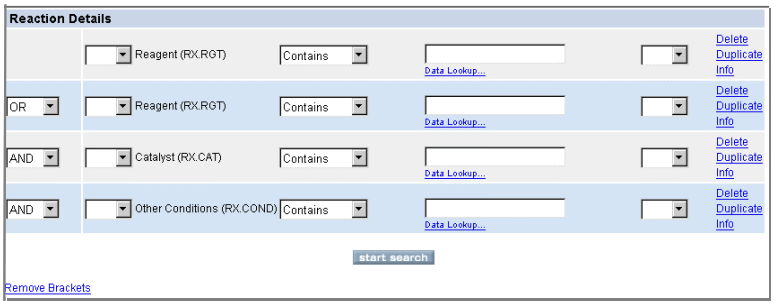
   – Or –

   Type the name of the field and click **Find**.
2. Double-click the field name to add it to the query.

To add the same data field to the query form twice

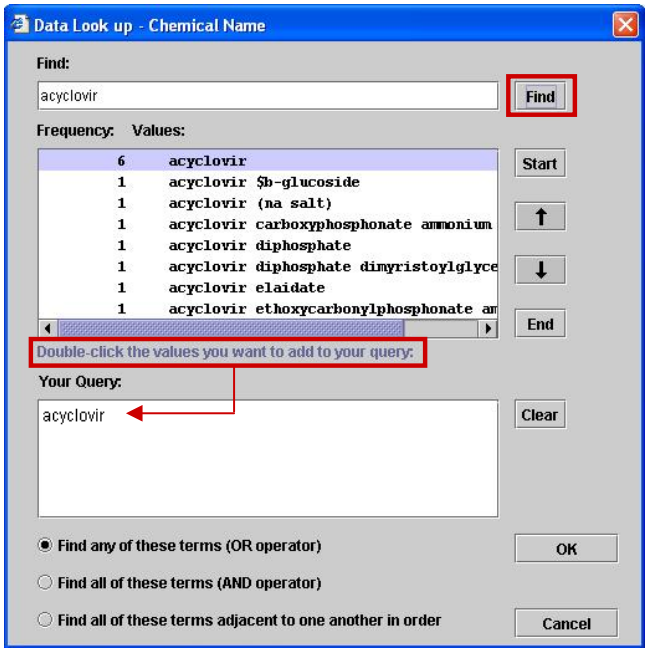
1. In the Field Index pane, expand the folders to locate the field and double-click the field name.

   – Or –
2. If the data field is currently on the form, click the **Duplicate** command to the right of the data field.



To use a Data Lookup table

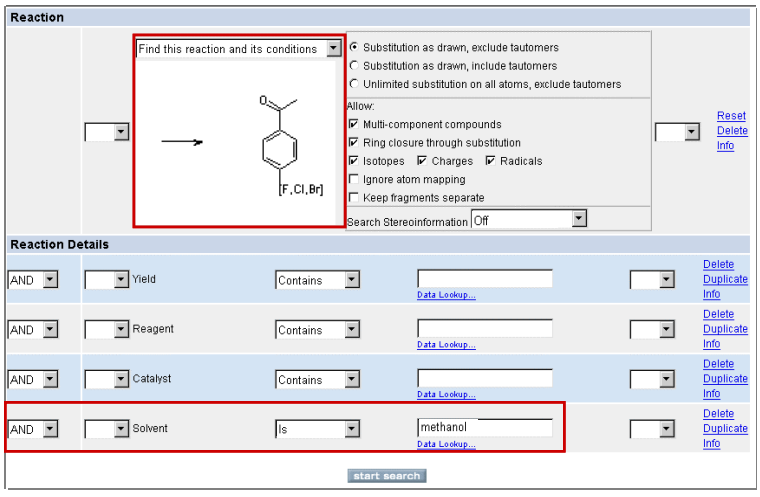
1. Click **Data Lookup**.
2. Type the value of interest.
3. Click **Find**.
4. Double-click to add a value to your query.



5. Repeat Steps 2 – 4 until all of the desired values have been added.
6. Click **OK**.

To conduct a combination factual/structure search

1. Place a structure in the Structure box using MDL Draw.
2. Set the Structure and Global search options.
3. Under Allow, set the search limits.

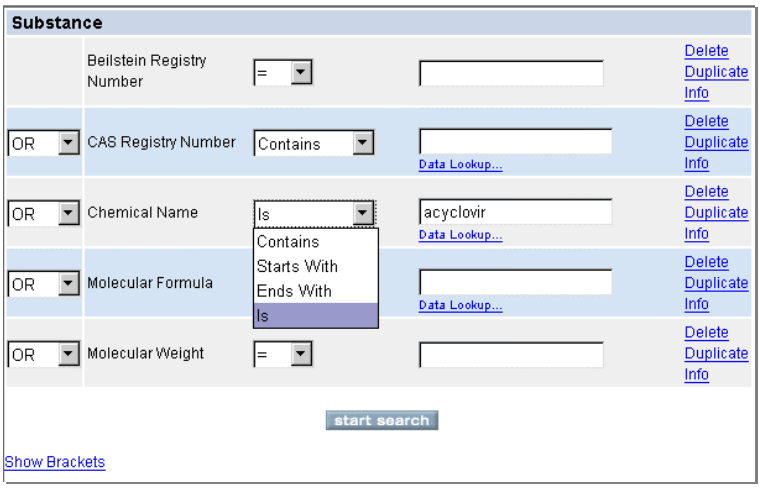


4. In the Field Index pane, navigate to the data field and double-click to add it to the form.

5. Select a data operator and type your search entry into the available text box.
6. Click **start search**.

To conduct a Chemical Name search

1. Under Easy Data Search, double-click **Identification Data**.
2. For the Chemical Name field, select a data operator and type your data entry in the available text box.



3. Click **start search**.

To conduct a CAS Number search

1. Under Easy Data Search, double-click **Identification Data**.
2. For the CAS Number field, select a data operator and type your data entry in the available text box.
3. Click **start search**.

To view search results

1. When the search is complete, the system automatically displays the results tab.
2. If necessary, click the **results** tab at the top of the window.
3. On the History tab, double-click to open the **Today's Searches** folder.
4. Double-click to open a **Search**.

To view details of a search

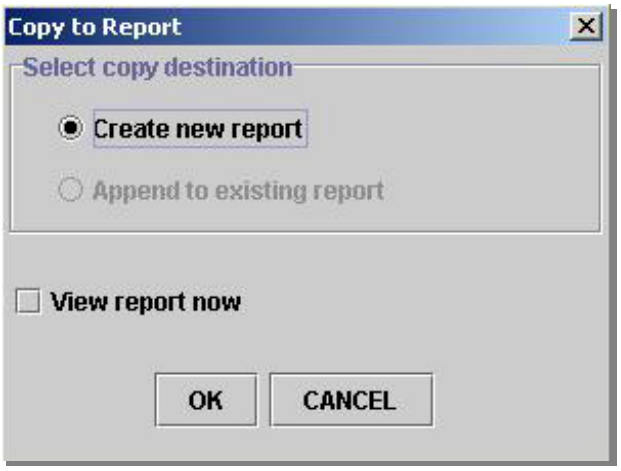
1. On the results tab, click the **Details** link found under the structure.
2. In the **Available Data** box, click a link to view the specific data.
3. Click the **Top of Page** link and repeat Step 2 to view more data.

To save search results

1. At the top of the results tab, click the **save** button.
2. Type a name into the Save As box and click **OK**.

To create a report

1. At the top of the results tab, click the **copy to report** button.
2. Select **Create new report** or **Append to existing report**.
3. Check the **View report now** box and click **OK**.



To use MDL LitLink to retrieve a publication

1. On the results tab or in the Details window, click **LitLink**.
2. In the MDL LitLink window, click the data source from which you would like to retrieve the article.