Citation Searching in CrossFire Beilstein

DiscoveryGate℠
Version 1.4
Participant's Guide

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Participant's Guide

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San Leandro, CA 94577

TRDG-05V1.4PG

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CITATION SEARCHING IN CROSSFRIE BEILSTEIN

Exercises

REFERENCE

POWERING *the process of* INVENTION

Citation Searching in CrossFire Beilstein

Key points

- Welcome to the *Citation Searching in CrossFire Beilstein* module.
- In this module, we will present the basics required to retrieve citations from` the Beilstein database through DiscoveryGate using the MDL Database Browser.

Notes

Module objectives

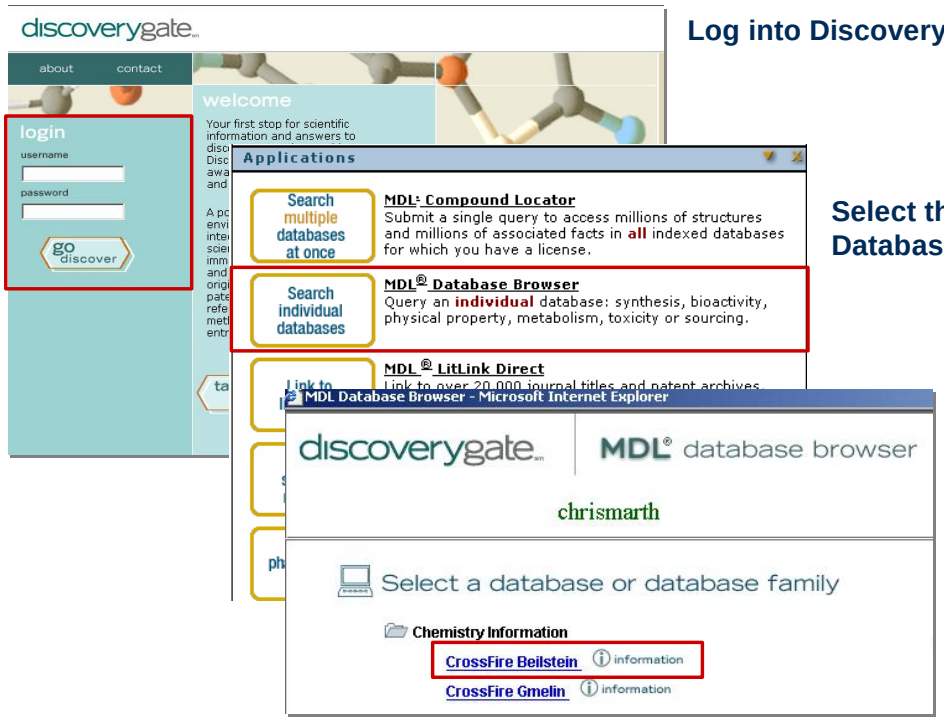
- Use various strategies to conduct a citation search
- Conduct a multiple data search to retrieve a list of citations
- Conduct a structure search to retrieve a list of citations
- Use Data Lookup tables
- Use hyperlinks to access data from integrated sources

Key points

- This module demonstrates various strategies for retrieving a list of citations and associated information.
- You will learn how to conduct a data search over multiple fields.
- You will learn how to use a structure query to retrieve a list of citations.
- You will learn how and when to use a Data Lookup table.
- You will learn to how to use hyperlinks to access data from integrated sources.

Notes

Launch the application and database



Log into DiscoveryGate

Select the MDL Database Browser

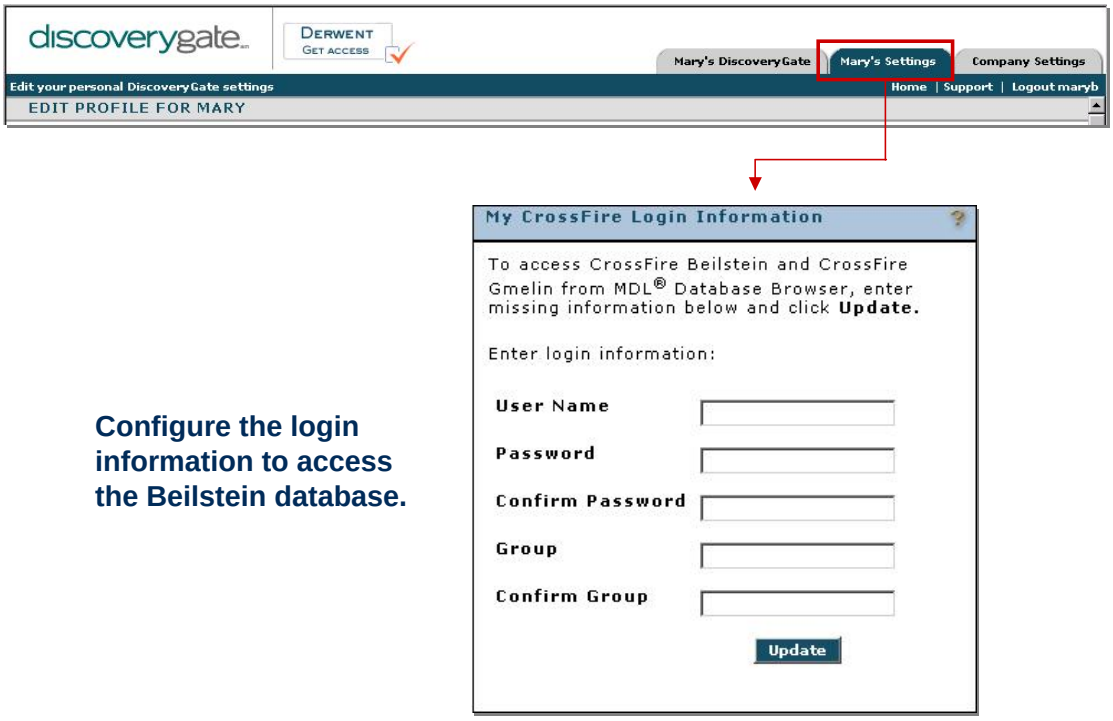
Select the CrossFire Beilstein database

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, such as CrossFire Beilstein.
- CrossFire Beilstein is one of the individual database selections. It is an essential source of information for generating leads, planning syntheses, and determining bioactivity and physical properties.

Notes

Configure CrossFire access information



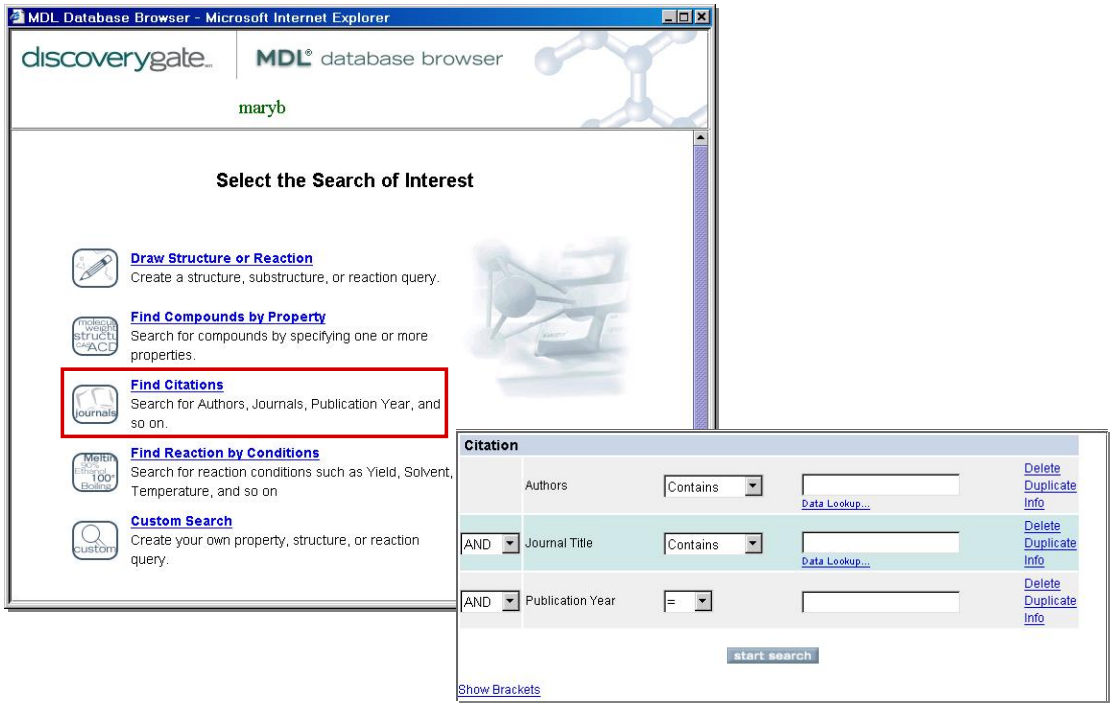
Configure the login information to access the Beilstein database.

Key points

- Prior to searching the CrossFire Beilstein database, you will need to enter the CrossFire login information.
- If your login information 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

- To retrieve citations, you must search on citation fields such as Authors, Journals, Publication Year, Title, Abstract, or Keywords.
- The "Find Citations" link directs you to a predefined form that allows you to input search criteria for one or more of these fields.

Notes

Search scenario

Search the Beilstein database, using the MDL Database Browser, to retrieve articles which:

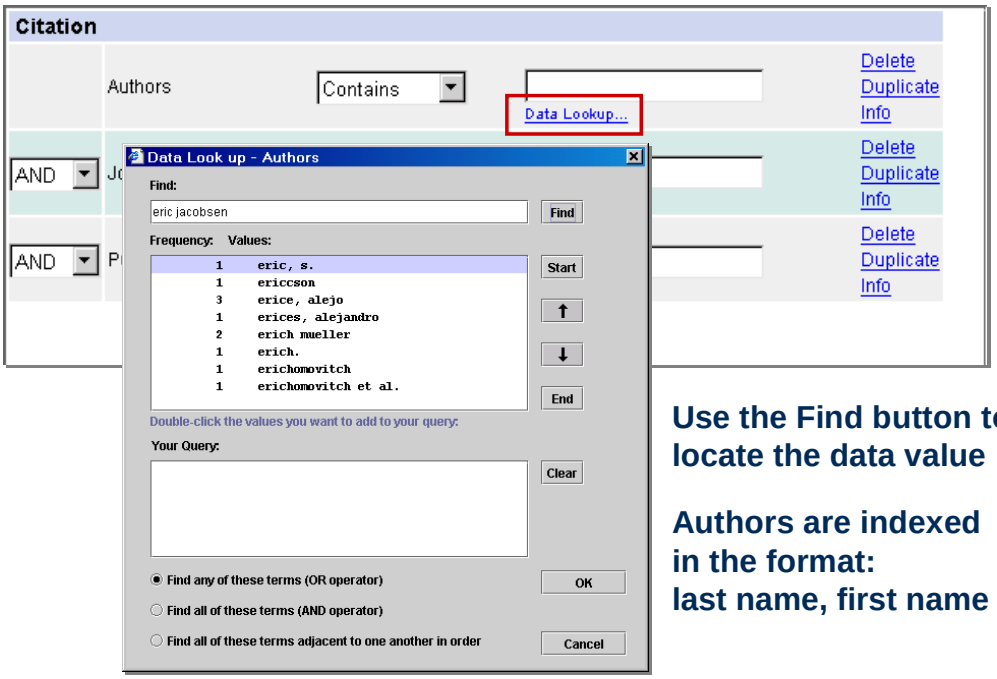
- are published by Eric Jacobsen.
- discuss epoxidation reactions.

Key points

- In this example, you will conduct a data search to find publications authored by Eric Jacobsen. You are not sure of the exact spelling of the author's first and last name.
- After the publications are retrieved, you will narrow the list to those references that discuss epoxidation reactions.

Notes

Use a Data Lookup



Use the Find button to locate the data value

Authors are indexed in the format: last name, first name

Key points

- The Data Lookup feature allows you to view the contents of the database.
- When you attempt to find eric jacobsen, you learn that authors are indexed using the format last name, first name.
- Your query must contain the appropriate format for the author's name.

Notes

Search by author

Author can be Erik Jacobsen, Erik Jacobson, Eric Jacobsen, or Erik Jacobson

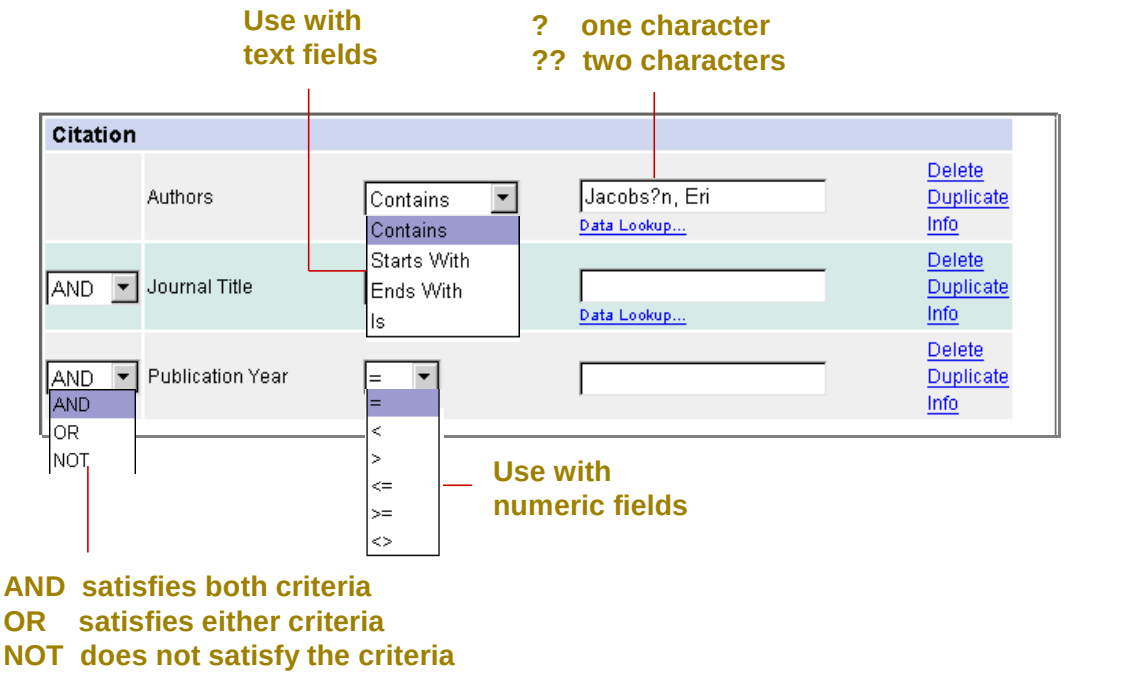
Fields that do not specify a criteria are ignored by the search

Key points

- You learned that the author field is indexed in the format "last name, first name". You must type the data value in the correct format that it appears in the database, otherwise it will not be found.
- You can use a wildcard (?) to take the place of one character in the last name.
- Citations that have an author with the last name "Jacobsen" and a first name that starts with the letters "Eri" will be retrieved.

Notes

Data operators and wildcards

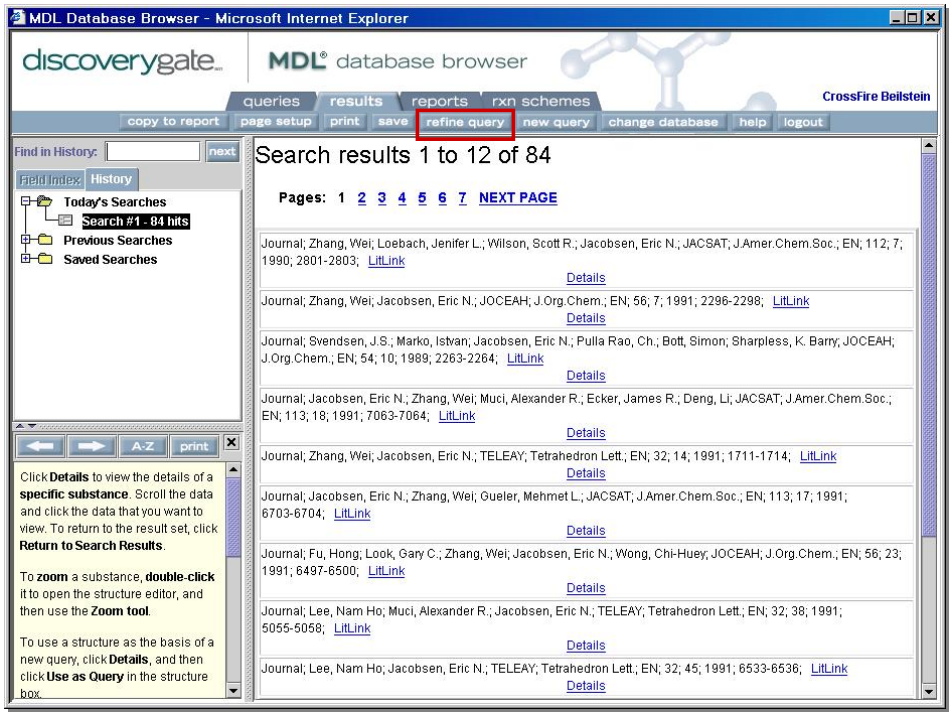


Key points

- For text fields, you can use the following operators: Contains, Starts With, Ends With, and Is.
- Wildcards take the place of one or more characters in a text string.
- When using multiple fields, you must use an operator.

Notes

Search results



Key points

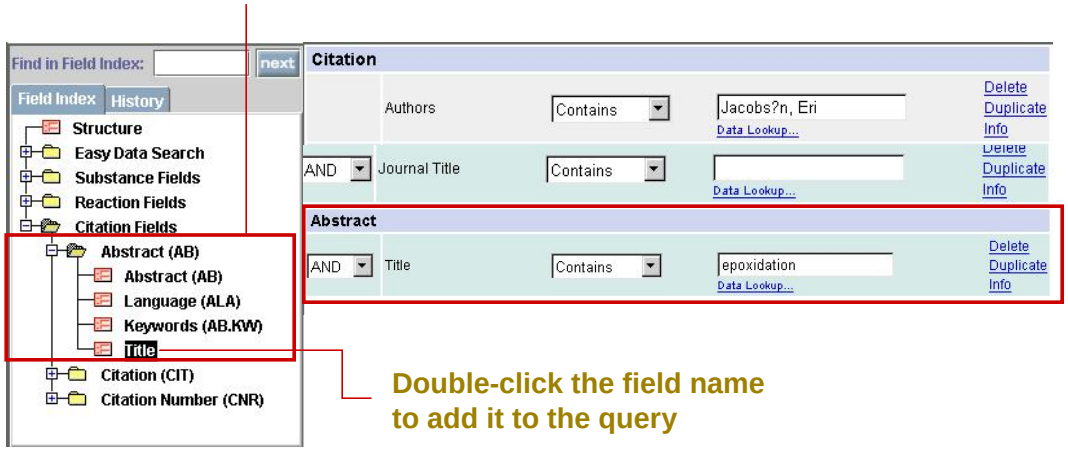
- The hit list consists of citations published by Eric Jacobsen.
- You are interested in finding publications by Jacobsen that discuss epoxidation chemistry.
- You will refine the search to retrieve only those publications that meet this criteria.

Notes

Add data to the query

Refine the search to retrieve articles which cite epoxidation reactions.

To locate a field, expand the Field Index or use the Find box



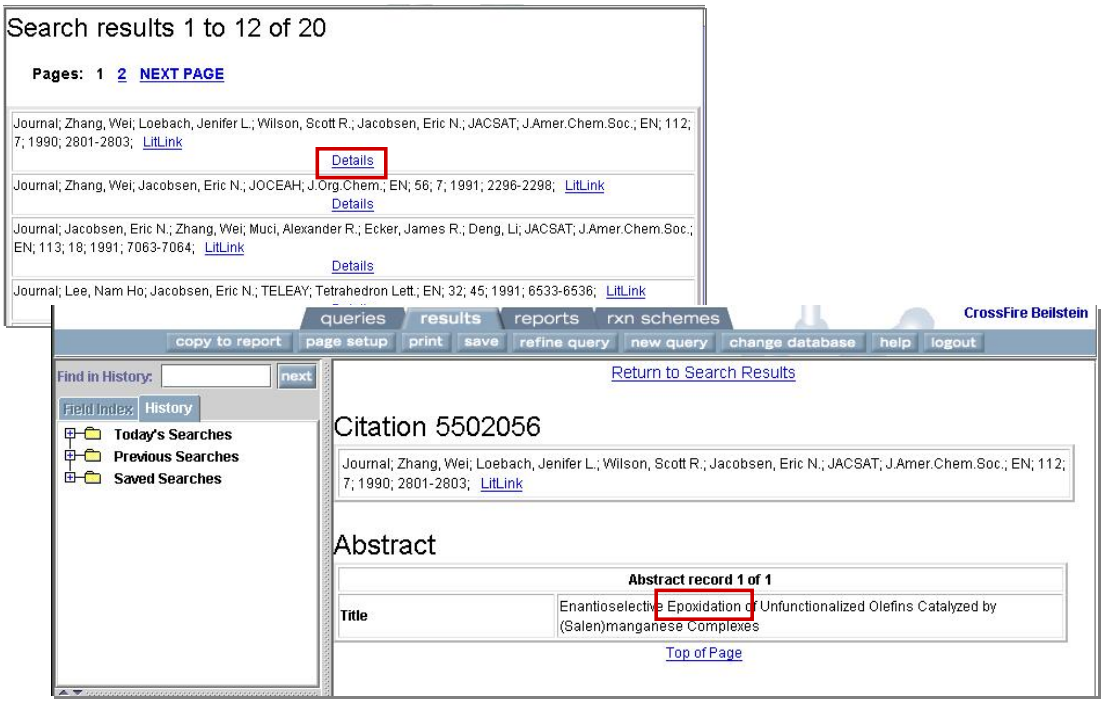
Double-click the field name to add it to the query

Key points

- You can refine the search by adding a data criteria to the original query.
- In order to retrieve a list of citations, you must choose the additional data fields from the Citation Fields area.
- To add a data field, double-click the field name in the Field Index.
- By default, the AND operator is inserted before the data field.

Notes

Display the citation details



Key points

- The search results show that the citations retrieved are authored by Eric Jacobsen.
- To view more details about a specific citation, click the "Details" link. You are shown the Title of the citation.
- The title contains the term "epoxidation". This citation discusses the enantioselective epoxidation of olefins by a particular catalyst.

Notes

Multiple data search

Search the CrossFire Beilstein database, using the MDL Database Browser, to retrieve articles which:

- cite the topic of hydroxylation reactions.
- are published in Synthesis or the Journal of Organic Chemistry.
- are published in or after 2002.

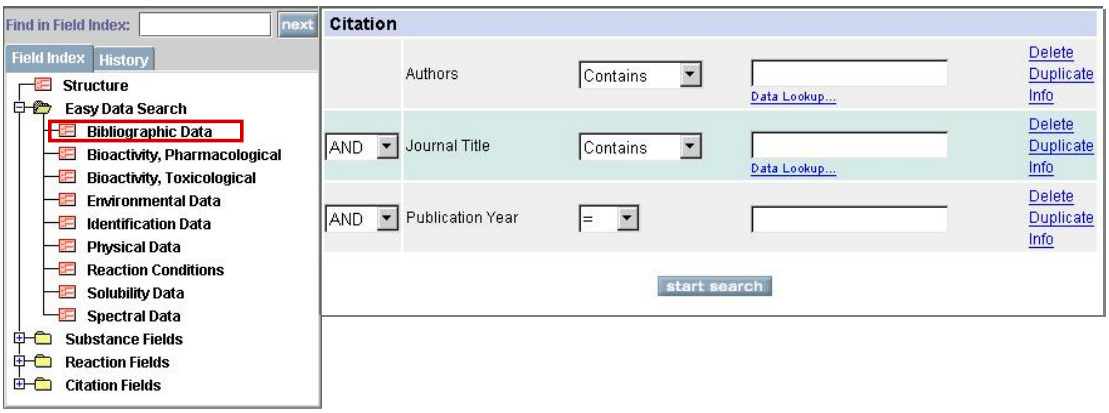
Key points

- In this example, you will conduct a search to find publications that meet multiple criteria.
- You are interested in retrieving information on the topic of hydroxylation reactions found in Synthesis or the Journal of Organic Chemistry, published in or after 2002.

Notes

Easy Data Search

Easy Data Search query forms contain common search criteria.

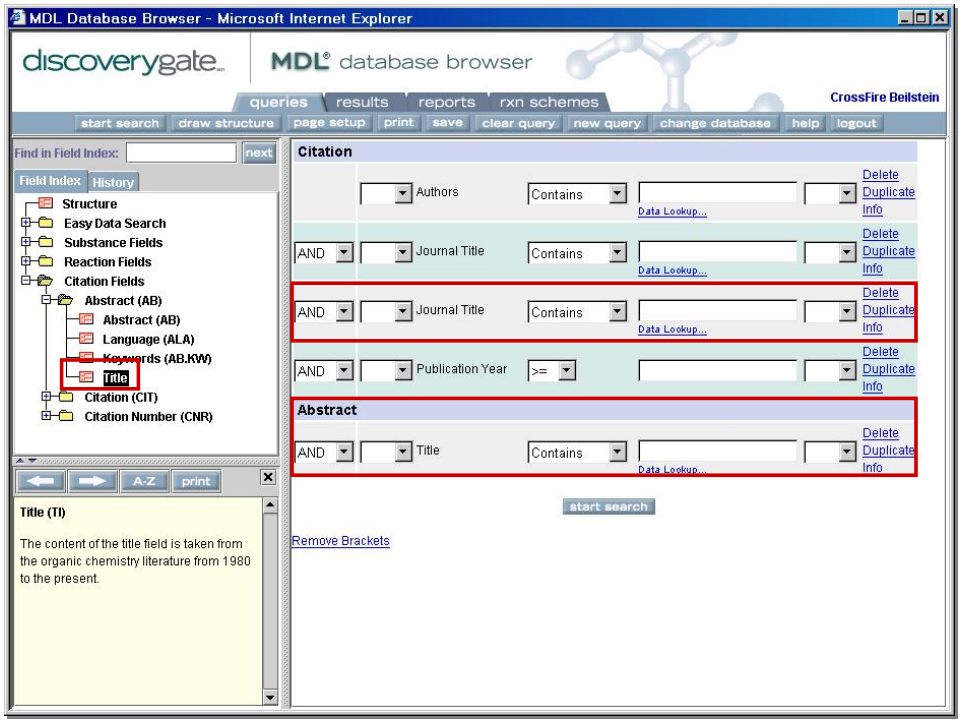


Key points

- 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.
- The Bibliographic form contains common search criteria for bibliographic fields.

Notes

Select the fields

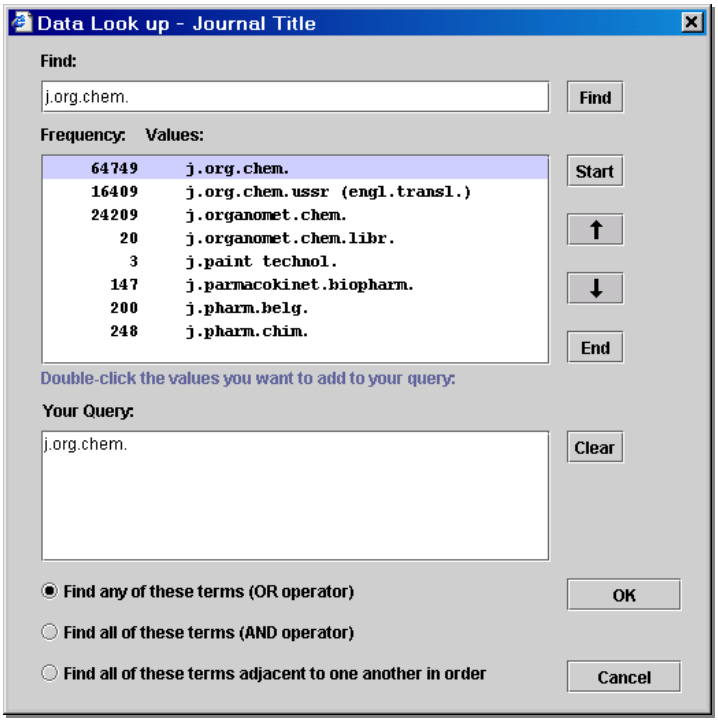


Key points

- In order to construct the query, you must add data fields to the Bibliographic form.
- If the field is already selected, you can click Duplicate to add another copy to the query form.
- In this scenario, you have a specific citation in mind that contains the word "hydroxylation" in its title.
- To locate the Title field, expand Citation Fields > Abstract on the Field Index tab.

Notes

Use Data Lookup for an abbreviation

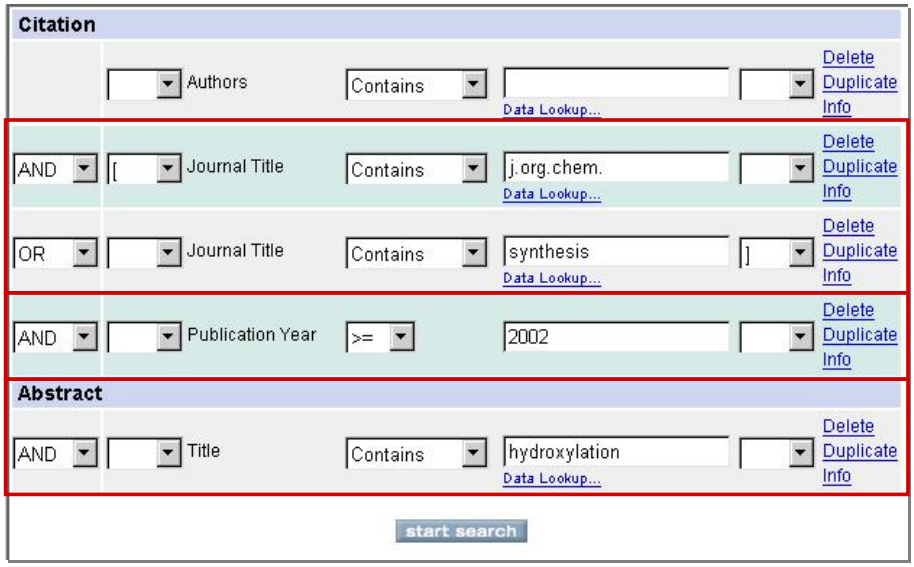


Key points

- Journal titles are abbreviated in the database. The abbreviations are in a standard format, so you may already be aware of many of them.
- To be sure that the abbreviation is spelled correctly, use the Data Lookup feature.

Notes

Construct the query



Journal Title contains j.org.chem. OR synthesis

AND Publication Year is greater than or equal to 2002

AND Title contains hydroxylation

Key points

- Now that the fields are selected, you will construct the query by adding values, data operators, and brackets, where appropriate.
- You can use brackets to show the order of precedence in the query.
- First, the query will locate citations from the Journal of Organic Chemistry, then it will proceed to the second journal listed, Synthesis.

Notes

Sample citation result

Abstract

Abstract record 1 of 1	
Title	Regioselective Hydroxylation of 2,4-Lutidine: A Practical Synthesis of 4-Hydroxymethyl-2-methylpyridine
Abstract	A practical synthesis of 4-hydroxymethyl-2-methylpyridine has been developed which makes use of Evans' regioselective lithiation of readily available 2,4-lutidine and trapping with dimethylformamide.
Language	EN
Keywords	lithiation; hydroxylation; regioselectivity; pyridines

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Citation

Citation record 1 of 1	
Document Type	Journal
Authors	Ragan, John A.; Jones, Brian P.; Meltz, Clifford N.; Teixeira, John J.
CODEN	CODEN: SYNTBF Journal Title: Synthesis Language Code: EN Number: 4 Publication Year: 2002 Page: 483 - 486

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Citation Number

Citation Number record 1 of 1	
Citation Entry Date	2002/09/30

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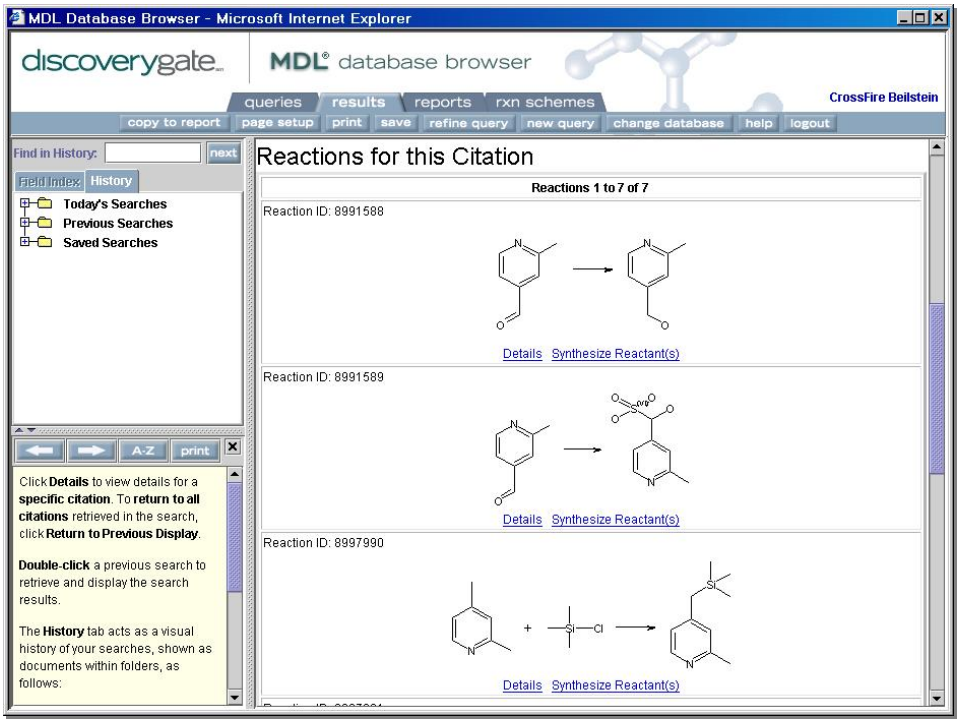
Show Substances for this Citation Show Reactions for this Citation

Key points

- The results tab shows the citaions that matched the multiple data criteria.
- The sample search result was published in Synthesis in 2002 and contained the word “hydroxylation” in its title.
- You have the option of viewing the substances for this citation or the reactions for this citation.

Notes

Show Reactions for this Citation

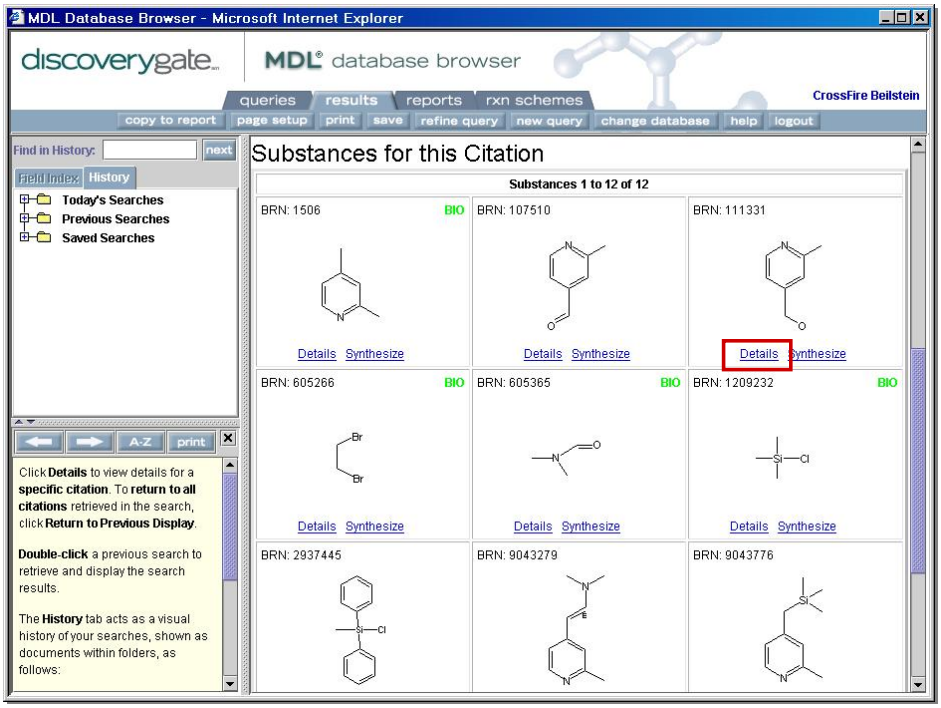


Key points

- Seven reactions are reported in this citation.
- To view additional data about a reaction, click Details.
- To learn how to synthesize the reactants in a reaction, click Synthesize Reactant(s).

Notes

Show Substances for this Citation

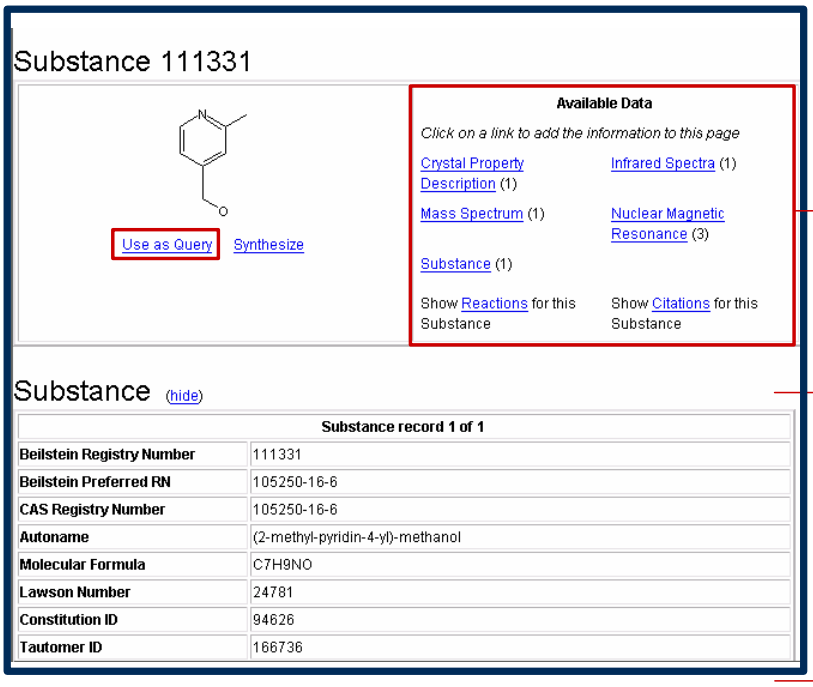


Key points

- There are 12 substances reported in this citation.
- To view additional data about a substance, click Details.
- To view synthetic routes to the substance, click Synthesize.

Notes

Substance details



Click a link to obtain specific data for the retrieved compound

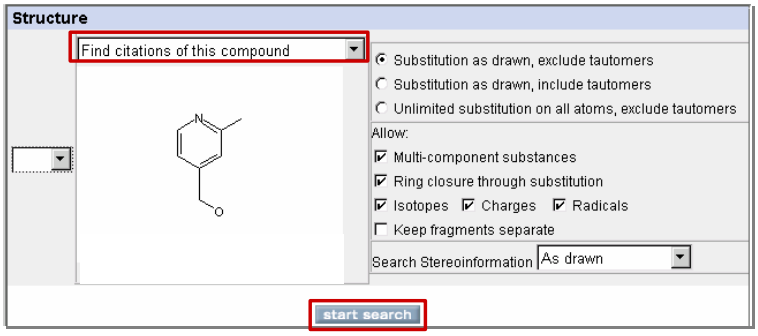
Substance data

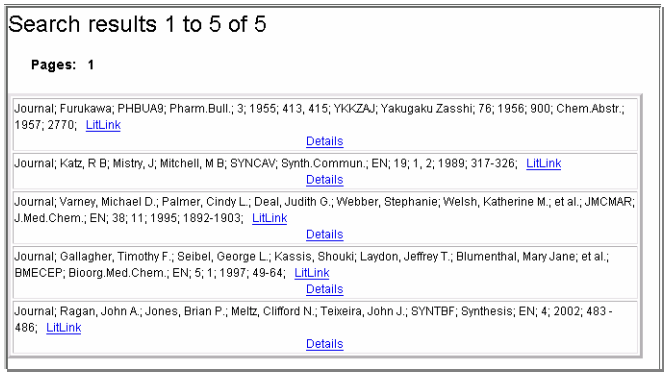
Key points

- The Substance data is shown, which includes identification information, such as registry numbers and the molecular formula.
- To obtain specific data for the compound, click a link in the Available data box.
- To use the structure in a new query, click “Use as Query”.

Notes

Use as Query





Key points

- You can search for substances, reactions, or citations that involve this compound.
- In this case, you are interested in retrieving citations that report this compound.
- There are five citations that report this compound.

Notes

Search scenario

Use the MDL Database Browser and MDL LitLink to retrieve an abstract from the Beilstein database that:

- is authored by K. Barry Sharpless.
- is published after 1995.

Key points

- In this example, you will conduct a search to find publications authored by K. Barry Sharpless after 1995.

Notes

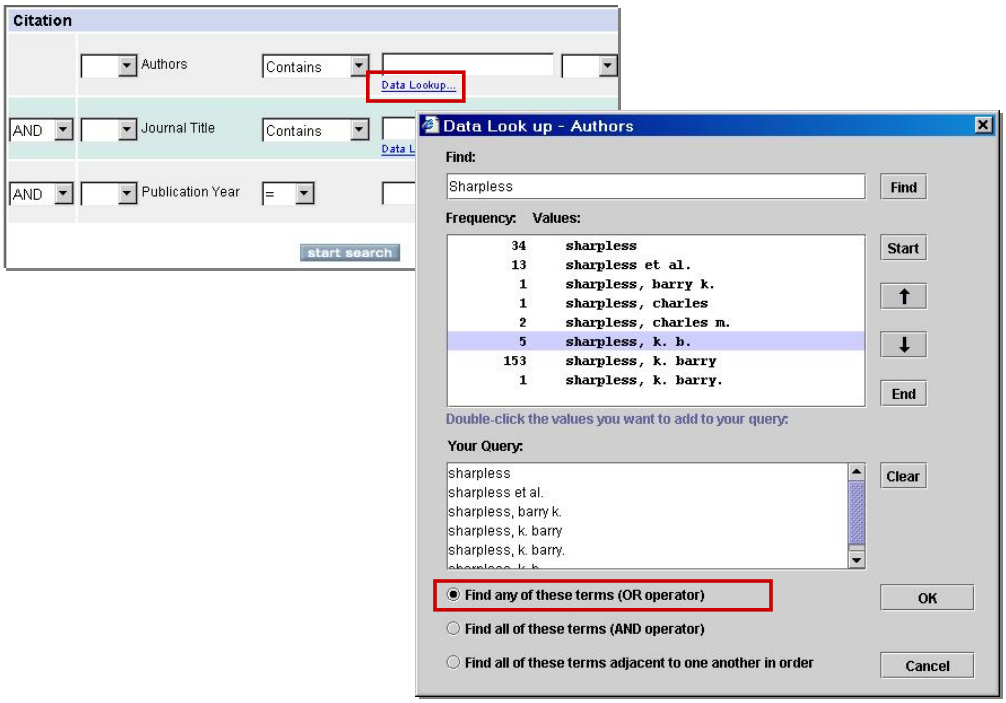
Create a new query

Key points

- Click the new query button to clear the previous query and start a new one.

Notes

Multiple occurrences of a value



Key points

- The Data Lookup dialog box shows that there are multiple occurrences of the value “Sharpless”.
- In your query, you must include every occurrence that can match “K. Barry Sharpless”.
- By default, “Find any of these terms (OR operator)” is selected. That means that an OR operator will be used to connect each value you have selected.

Notes

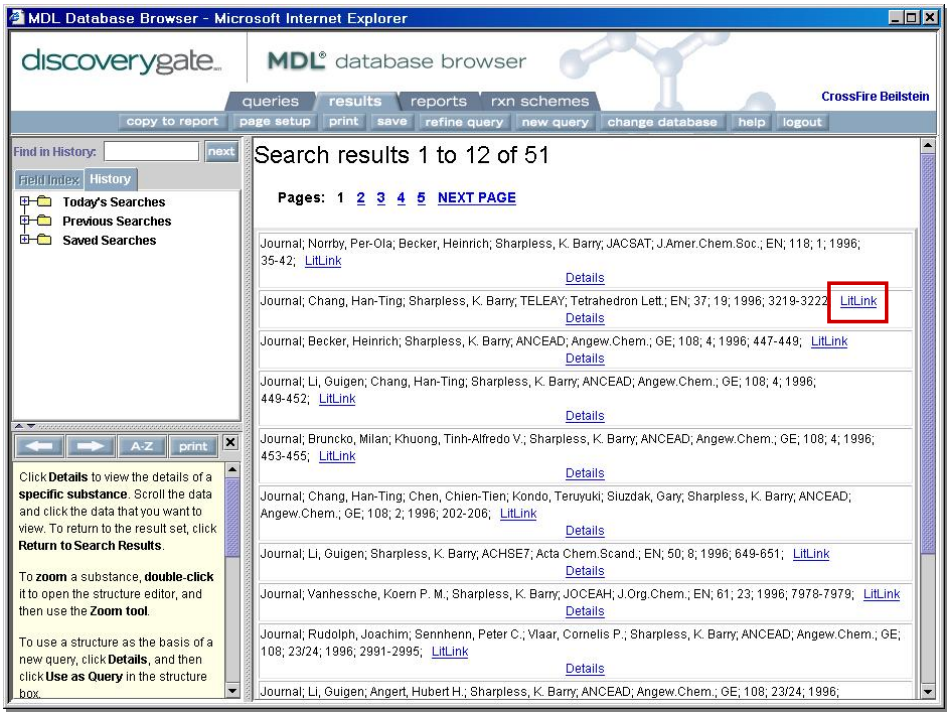
Query interpretation

Key points

- If a citation contains one of the six possible values for the author and is published after 1995, then it will be retrieved as a hit.

Notes

Search results

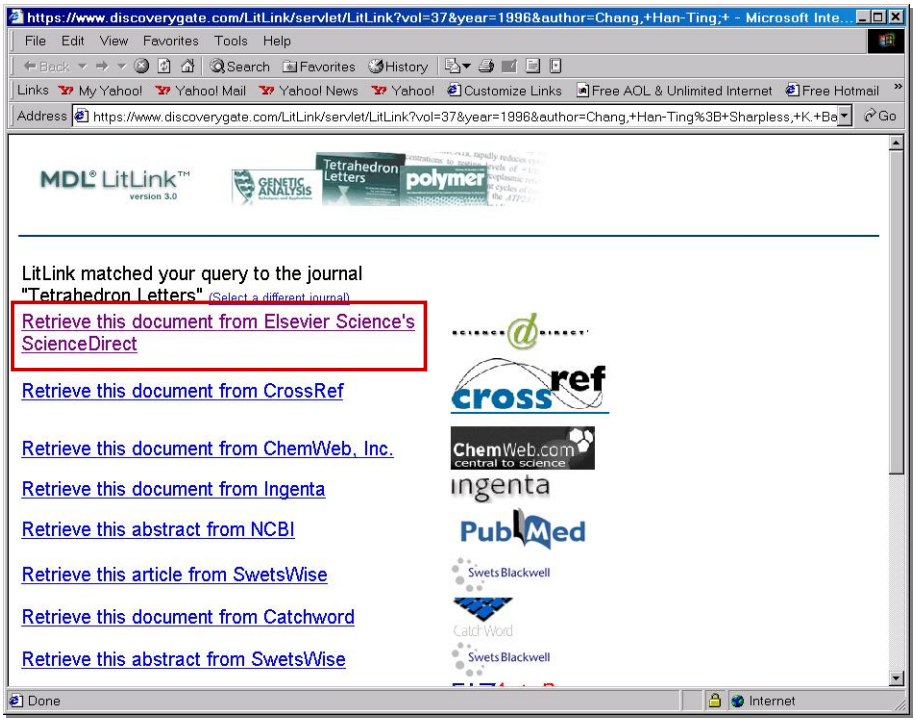


Key points

- The results tab show the publications retrieved that were published by K. Barry Sharpless after 1995.
- You can use MDL LitLink to link to an original literature reference.

Notes

Use MDL LitLink

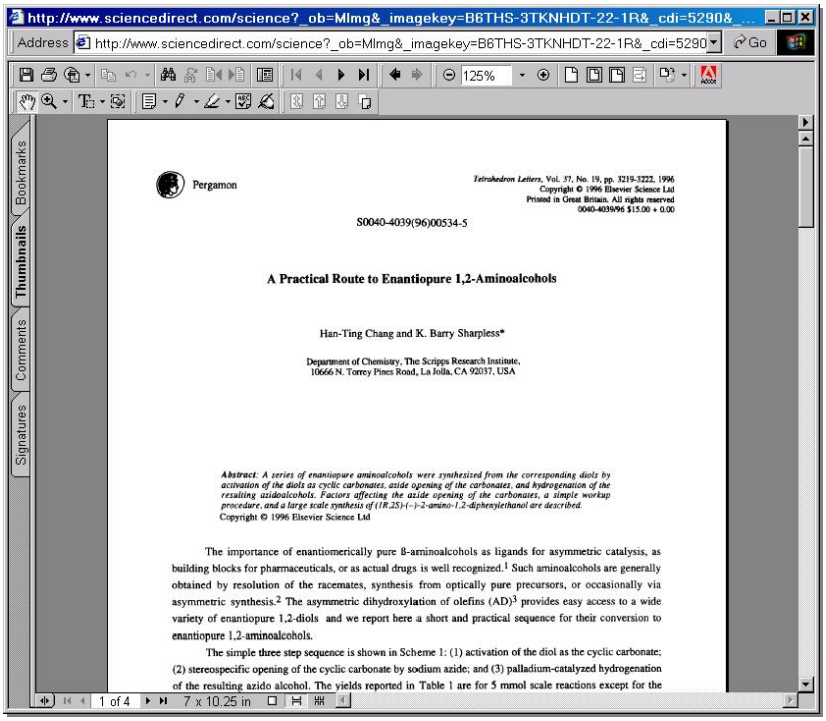


Key points

- Click the publication link to view the abstract.
- MDL LitLink provides a direct link from the citation to the source of the primary literature. You must have the appropriate access rights in order to view the primary literature.

Notes

Document retrieved



Pergamon

Tetrahedron Letters, Vol. 37, No. 19, pp. 3219-3222, 1996

0040-4039/96 $15.00 + 0.00

S0040-4039(96)00534-5

A Practical Route to Enantiopure 1,2-Aminoalcohols

Han-Ting Chang and K. Barry Sharpless*

Department of Chemistry, The Scripps Research Institute,
10666 N. Torrey Pines Road, La Jolla, CA 92037, USA

Abstract: *A series of enantiopure aminoalcohols were synthesized from the corresponding diols by activation of the diols as cyclic carbonates, azide opening of the carbonates, and hydrogenation of the resulting azidoalcohols. Factors affecting the azide opening of the carbonates, a simple workup procedure, and a large scale synthesis of (1R,2S)-(−)-2-amino-1,2-diphenylethanol are described.*

The importance of enantiomerically pure β-aminoalcohols as ligands for asymmetric catalysis, as building blocks for pharmaceuticals, or as actual drugs is well recognized.[1] Such aminoalcohols are generally obtained by resolution of the racemates, synthesis from optically pure precursors, or occasionally via asymmetric synthesis.[2] The asymmetric dihydroxylation of olefins (AD)[3] provides easy access to a wide variety of enantiopure 1,2-diols and we report here a short and practical sequence for their conversion to enantiopure 1,2-aminoalcohols.

The simple three step sequence is shown in Scheme 1: (1) activation of the diol as the cyclic carbonate; (2) stereospecific opening of the cyclic carbonate by sodium azide; and (3) palladium-catalyzed hydrogenation of the resulting azido alcohol. The yields reported in Table 1 are for 5 mmol scale reactions except for the

Key points

- The publication was retrieved from Tetrahedron Letters via ScienceDirect.
- K. Barry Sharpless authored the publication in 1996. This reference meets all of the criteria specified in the query.
- The document discusses the synthesis of enantiopure aminoalcohols from their corresponding diols.

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 search to retrieve articles published by Larry Overman. Refine the search to locate those articles that contain the term “heck reaction” in the abstract.

For a step-by-step solution, see page 1-31.

Exercise 2

Use the results from Exercise 1 to do the following:

- View the reactions reported in a citation.
- View the substances reported in a citation.
- Use a substance reported in the citation as a new query.

For a step-by-step solution, see page 1-34.

Retrieve citations by an author on a particular topic

Exercise 1

Conduct a search to retrieve articles published by Larry Overman. Refine the search to locate those articles that contain the term "heck reaction" in the abstract.

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

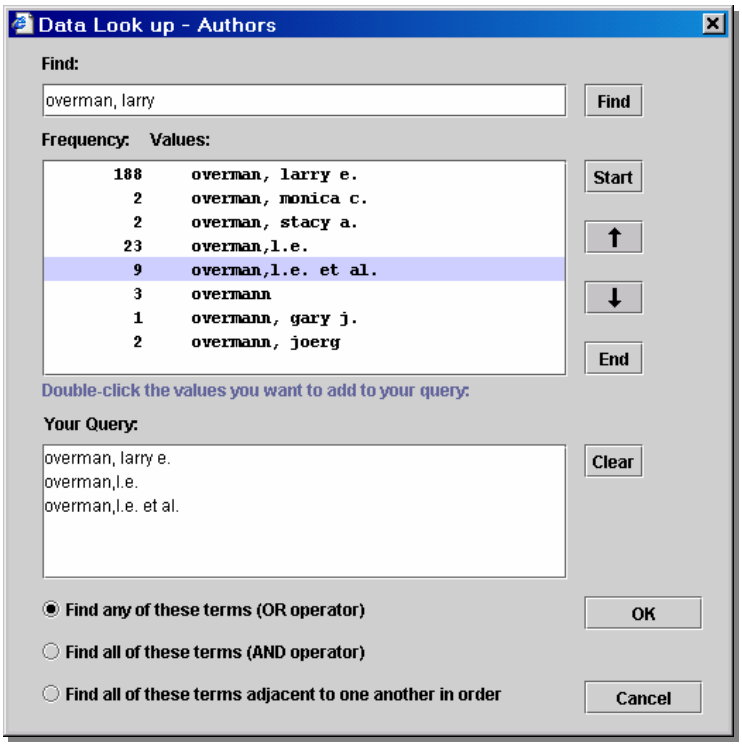
4. Under Chemistry Information, click **CrossFire Beilstein**.

5. Click the **Find Citations** link.

6. Under the Authors data field, click **Data Lookup**. Type **overman, larry** and click **Find**.

Use Data Lookup

7. Double-click to add the terms **overman, larry e.**, **overman,l.e.**, and **overman,l.e. et al.** to the Your Query box. Click **OK**.



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

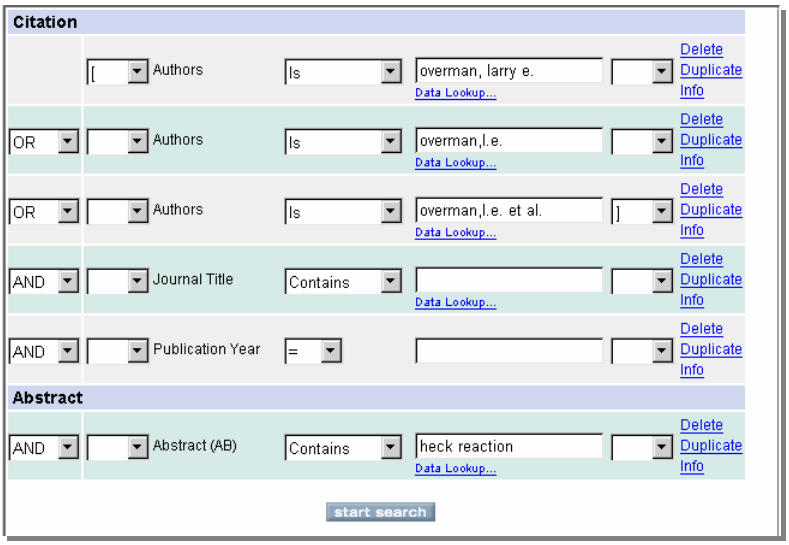
9. Click **refine query**.

Add a data field to the query form

10. On the Field Index tab, click the plus (+) to expand **Citation Fields**. Then, click the plus (+) to expand **Abstract (AB)**.

11. Double-click **Abstract (AB)**.

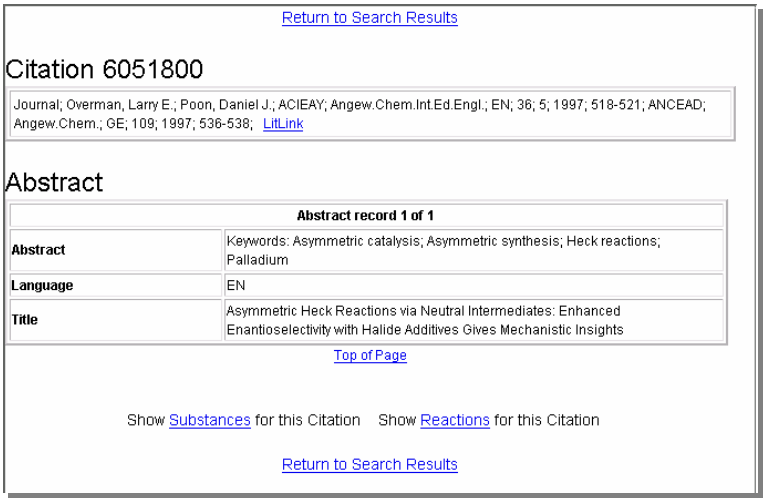
12. Type **heck reaction** in the Abstract (AB) field. Your final query should look like this:



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

Inspect the citation details

14. Click the **Details** link under the first citation.



Note: Do not close this window. You will use this result in Exercise 2.

Display detailed information about a citation

Exercise 2

Use the results from Exercise 1 to do the following:

- View the reactions reported in a citation.
- View the substances reported in a citation.
- Use a substance reported in the citation as a new query.

Show Reactions for this Citation

1. For the citation selected in Exercise 1, click **Show Reactions for this Citation**.

Return to Search Results

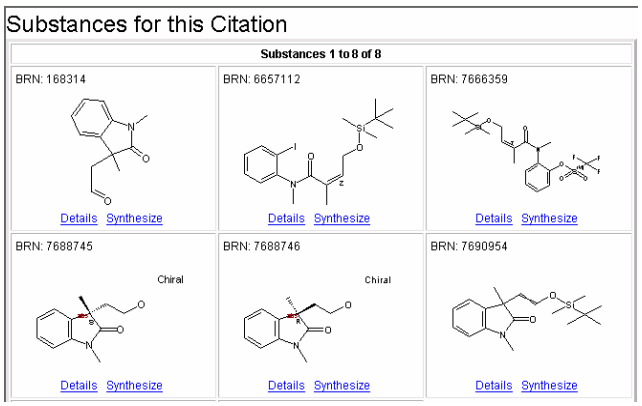
2. View the results. Scroll to the bottom of the page, and click the **Return to Search Results** link.

3. Click the **Details** link for the first citation.

Show Substances for this Citation

4. Click the **Show Substances for this Citation** link.

5. View the results.



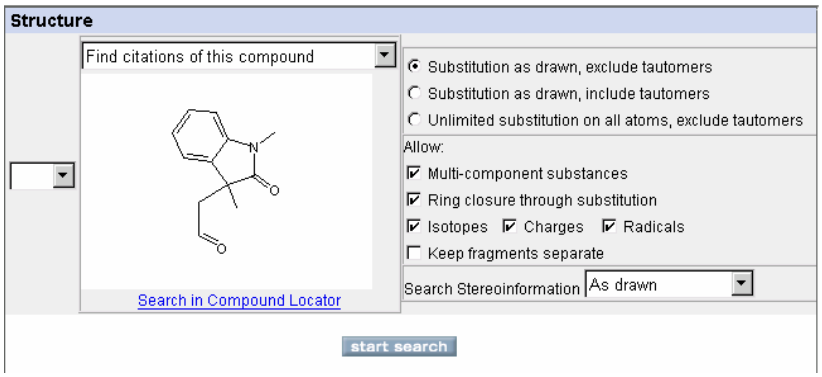
6. Click the **Details** link for substance BRN: 168314.

Use as Query

7. Click the **Use as Query** link.

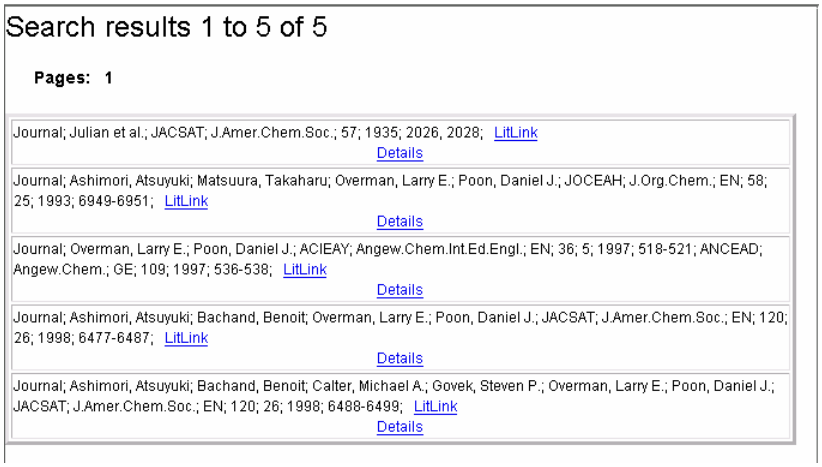
Find citations of this compound

8. Choose **Find citations of this compound**.



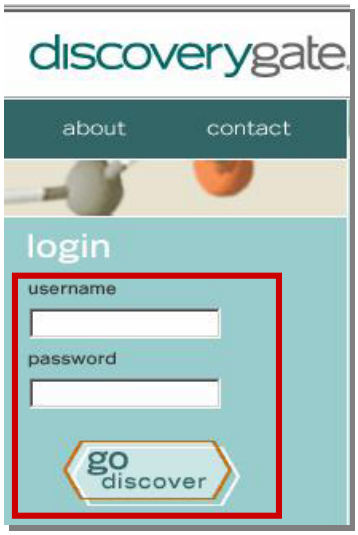
9. Click **start search**.

10. View the results.



To launch the DiscoveryGate application

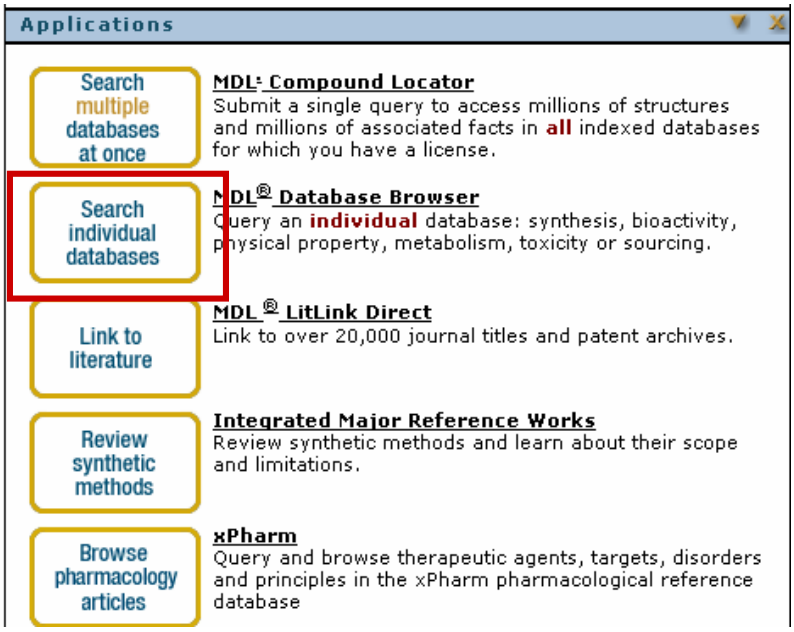
1. Launch your internet browser and enter the DiscoveryGate URL (www.discoverygate.com).
2. Enter your user name and password.
3. If necessary, enter your company ID.



4. Click **go discover**.

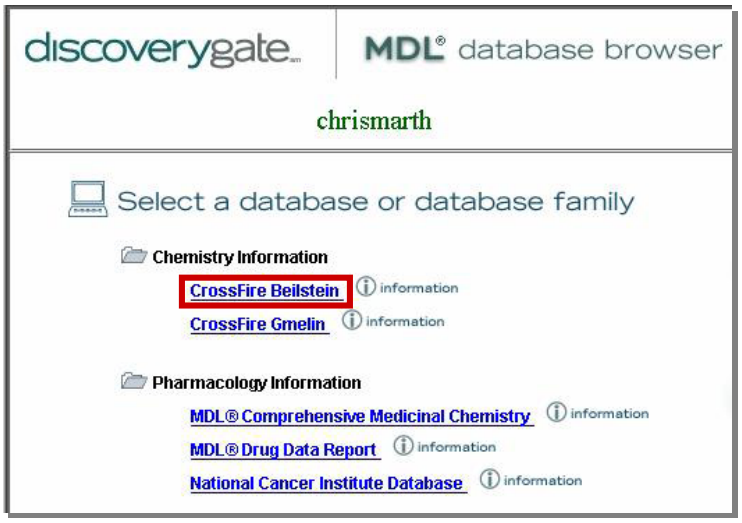
To select an individual database

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



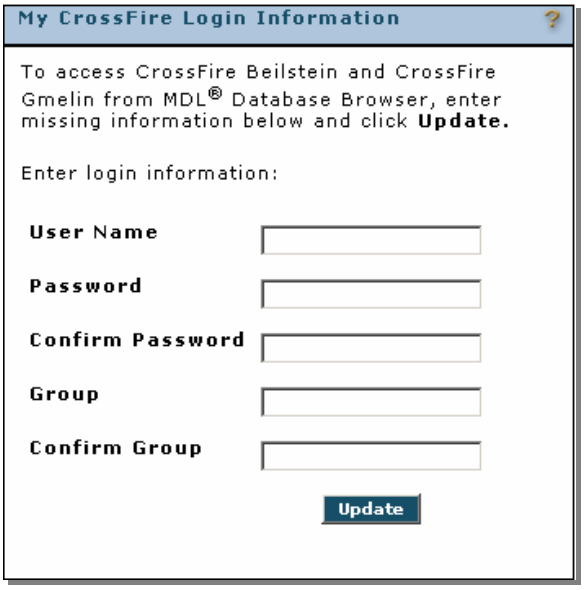
To select CrossFire Beilstein

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 new query

1. (Optional) If you are already logged into MDL Database Browser, click **new query**.

2. In the Select the Search of Interest window, click **Find Citations**.
3. Type the field values and select the data operators, as needed.

4. Click **start search**.

To clear the query

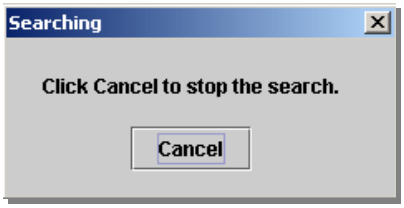
1. On the query tab, click **clear query**.

To start a search

1. Enter a query using the Bibliographic form.
2. Click **start search**.

To stop a search

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



To use a Data Lookup

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 add a data field to the query

1. In the Field Index, 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 modify a search query

1. Click the **refine query** button.

To open an Easy Data Search form

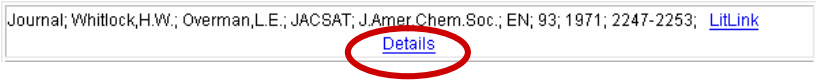
1. (Optional) If necessary, click **clear query**.
2. In the Field Index, expand the **Easy Data Search** folder.
3. Double-click the appropriate form.

To view search results

1. After a search is complete, the system automatically displays the results tab.
2. On the History tab, expand the **Today's Searches** folder.
3. Double-click to open a **Search**.

To view details of a retrieved citation

1. On the results tab, click the **Details** link for the citation.



To show reactions for a citation

1. On the results tab or in the Details window, click the **Show Reactions for this Citation** link.

To show substances for a citation

1. On the results tab or in the Details window, click the **Show Substances for this Citation** link.

To return to the search results

1. On the results tab or in the Details window, scroll to the bottom of the page.
2. Click the **Return to Search Results** link.

To use a structure or reaction in a new query

1. When you are viewing a list of substances or reactions from a citation, click **Use as Query** for the substance or reaction of interest.
2. Choose **Find citations for this substance**.

   – Or –

Choose **Find citations for this reaction**.

3. Click **start search**.

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.

To view search results

1. After a search is complete, the system automatically displays the results tab.
2. On the History tab, double-click to open the **Today's Searches** folder.
3. Double-click to open a **Search**.

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**.