

CITATION SEARCHING IN CROSSFIRE BEILSTEIN

DiscoveryGateSM
Version 1.4
Participant's Guide

Citation Searching in CrossFire Beilstein

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Version 1.4
Participant's Guide

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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.

My CrossFire Login Information

To access CrossFire Beilstein and CrossFire Gmelin from MDL® Database Browser, enter missing information below and click **Update**.

Enter login information:

User Name

Password

Confirm Password

Group

Confirm Group

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

The screenshot shows the MDL Database Browser interface in Microsoft Internet Explorer. The main heading is "Select the Search of Interest". Below this, there are five search options, each with an icon and a description:

- Draw Structure or Reaction**: Create a structure, substructure, or reaction query.
- Find Compounds by Property**: Search for compounds by specifying one or more properties.
- Find Citations**: Search for Authors, Journals, Publication Year, and so on. (This option is highlighted with a red box.)
- Find Reaction by Conditions**: Search for reaction conditions such as Yield, Solvent, Temperature, and so on.
- Custom Search**: Create your own property, structure, or reaction query.

To the right of these options is a small image of a laboratory flask. Below the search options is a "Citation" search form with the following fields:

Citation			
	Authors	Contains	<input type="text"/>
			Data Lookup...
			Delete Duplicate Info
AND	Journal Title	Contains	<input type="text"/>
			Data Lookup...
			Delete Duplicate Info
AND	Publication Year	=	<input type="text"/>
			Delete Duplicate Info

At the bottom of the form is a "start search" button and a "Show Brackets" link.

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:

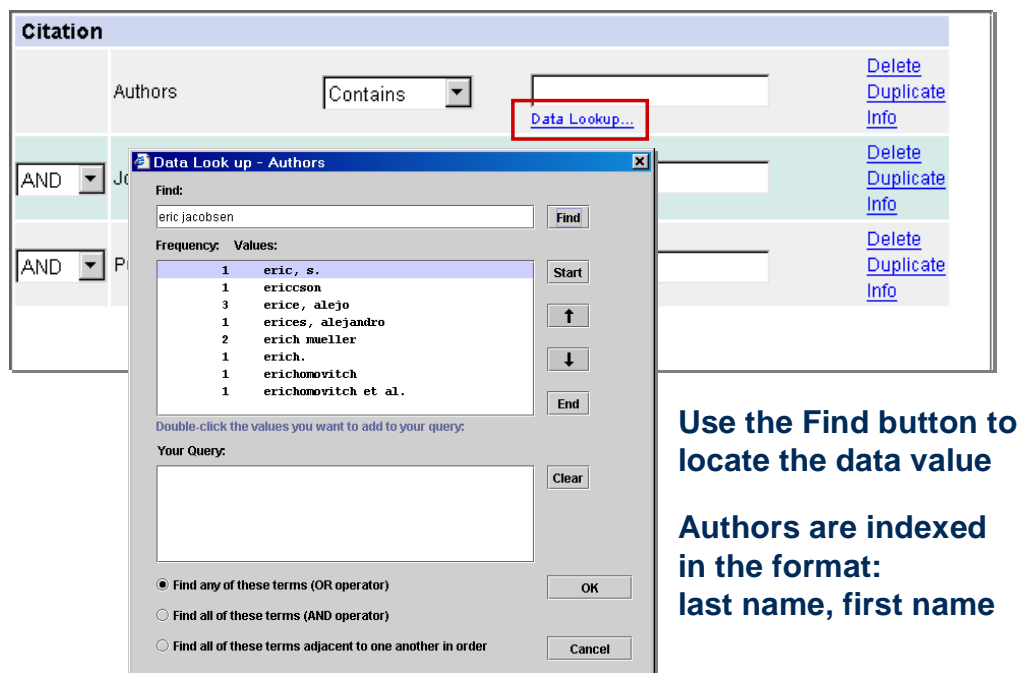
- are published by Eric Jacobsen.
- discuss epoxidation reactions.

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



Key points

- The Data Lookup feature allows you to view the contents of the database.
- When you attempt to find eric jacobson, 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

Citation				
	Authors	Contains	Jacobs?n, Eri	Delete Duplicate Info
AND	Journal Title	Contains		Delete Duplicate Info
AND	Publication Year	=		Delete Duplicate Info
<input type="button" value="start search"/>				
Show Brackets				

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

Use with text fields

? one character
?? two characters

Citation			
	Authors	Contains	Jacobs?n, Eri Data Lookup...
		Contains	Delete Duplicate Info
AND	Journal Title	Starts With	Delete Duplicate Info
		Ends With	Data Lookup...
		Is	Delete Duplicate Info
AND	Publication Year	=	Delete Duplicate Info
AND		=	
OR		<	
NOT		>	
		<=	
		>=	
		<>	

Use with numeric fields

AND satisfies both criteria
OR satisfies either criteria
NOT does not satisfy the criteria

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

The screenshot shows the CrossFire Beilstein search interface. On the left, the 'Field Index' is expanded, showing a tree structure with categories: Structure, Easy Data Search, Substance Fields, Reaction Fields, and Citation Fields. Under 'Citation Fields', the following fields are listed: Abstract (AB), Abstract (AB), Language (ALA), Keywords (AB.KW), and Title. A red box highlights the 'Abstract (AB)' field. On the right, the 'Citation' search results are displayed. The first result is for 'Authors' with the search term 'Jacobs?n, Eri'. The second result is for 'Journal Title' with the search term 'epoxidation'. The third result is for 'Abstract' with the search term 'epoxidation'. A red box highlights the 'Abstract' result. A red arrow points from the 'Abstract (AB)' field in the Field Index to the 'Abstract' result in the search results.

Find in Field Index: next

Field Index History

- Structure
- Easy Data Search
- Substance Fields
- Reaction Fields
- Citation Fields
 - Abstract (AB)
 - Abstract (AB)
 - Language (ALA)
 - Keywords (AB.KW)
 - Title
- Citation (CIT)
- Citation Number (CNR)

Citation

Field	Operator	Search Term	Actions
Authors	Contains	Jacobs?n, Eri	Delete Duplicate Info
AND			
Journal Title	Contains		Delete Duplicate Info
AND			
Abstract	Contains	epoxidation	Delete Duplicate Info

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

The screenshot displays the MDL Database Browser interface. At the top, a blue banner reads "Display the citation details". Below this, a search results page shows "Search results 1 to 12 of 20". A list of search results is shown, with the first result highlighted: "Journal; Zhang, Wei; Loebach, Jenifer L.; Wilson, Scott R.; Jacobsen, Eric N.; JACSAT; J.Amer.Chem.Soc.; EN; 112; 7; 1990; 2801-2803; [LitLink](#)". A red box highlights the "Details" link next to this result. Below the search results, a navigation bar includes tabs for "queries", "results", "reports", and "rxn schemes", along with buttons for "copy to report", "page setup", "print", "save", "refine query", "new query", "change database", "help", and "logout". On the left, a sidebar shows "Find in History:" with a "next" button and a "Field Index" section containing "Today's Searches", "Previous Searches", and "Saved Searches". The main content area shows the "Citation 5502056" details for the selected result. It includes the citation text: "Journal; Zhang, Wei; Loebach, Jenifer L.; Wilson, Scott R.; Jacobsen, Eric N.; JACSAT; J.Amer.Chem.Soc.; EN; 112; 7; 1990; 2801-2803; [LitLink](#)". Below this, the "Abstract" section shows "Abstract record 1 of 1" with the title "Enantioselective Epoxidation of Unfunctionalized Olefins Catalyzed by (Salen)manganese Complexes". A red box highlights the word "Epoxidation" in the title. A "Top of Page" link is also present.

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.

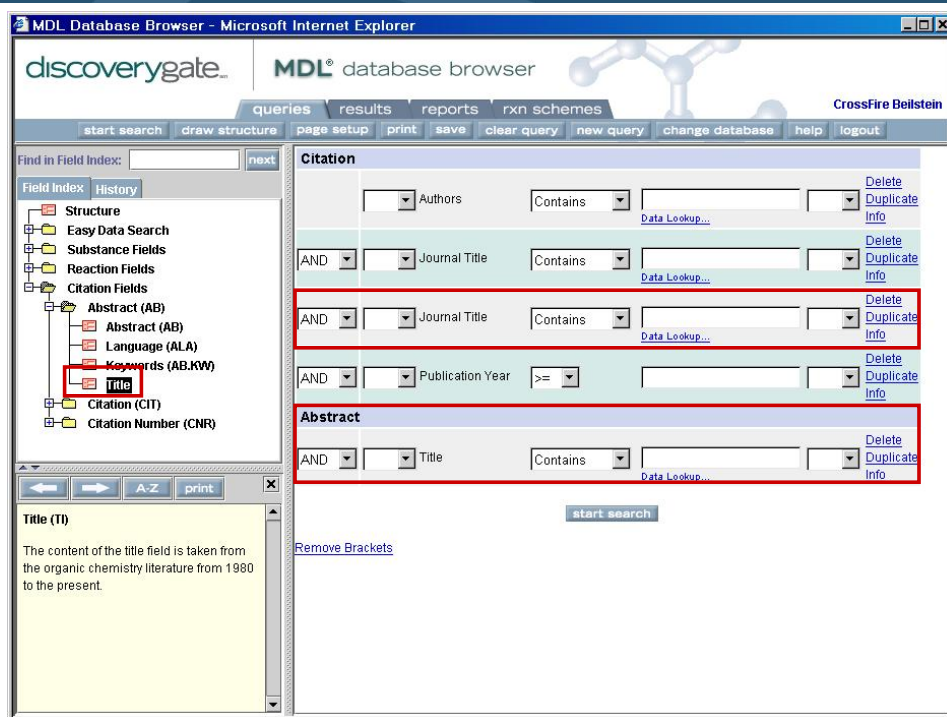
The screenshot shows the 'Easy Data Search' interface. On the left, a 'Field Index' tab is active, displaying a tree view of search categories. The 'Bibliographic Data' category is highlighted. The main area shows the 'Citation' search form. It includes three search criteria: 'Authors' (Contains), 'Journal Title' (Contains), and 'Publication Year' (=). Each criterion has a text input field and a 'Data Lookup...' button. The form also includes 'Delete', 'Duplicate', and 'Info' links for each criterion. A 'start search' button is located at the bottom of the form.

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

Data Look up - Journal Title

Find:
j.org.chem. Find

Frequency: Values:

64749	j.org.chem.
16409	j.org.chem.ussr (engl.transl.)
24209	j.organomet.chem.
20	j.organomet.chem.lib.
3	j.paint technol.
147	j.parmacokinet.biopharm.
200	j.pharm.belg.
248	j.pharm.chin.

Start ↑ ↓ End

Double-click the values you want to add to your query:

Your Query:
j.org.chem. Clear

☒ Find any of these terms (OR operator)
☐ Find all of these terms (AND operator)
☐ Find all of these terms adjacent to one another in order

OK Cancel

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

Citation					
	<input type="text"/>	Authors	Contains	<input type="text"/>	Delete Duplicate Info
				Data Lookup...	
AND	[<input type="text"/>	Journal Title	Contains	j.org.chem.
					Delete Duplicate Info
				Data Lookup...	
OR		<input type="text"/>	Journal Title	Contains	synthesis
					Delete Duplicate Info
				Data Lookup...	
AND		<input type="text"/>	Publication Year	>=	2002
					Delete Duplicate Info
				Data Lookup...	
Abstract					
AND		<input type="text"/>	Title	Contains	hydroxylation
					Delete Duplicate Info
				Data Lookup...	
start search					

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

[Top of Page](#)

Citation

Citation record 1 of 1													
Document Type	Journal												
Authors	Ragan, John A.; Jones, Brian P.; Meltz, Clifford N.; Teixeira, John J.												
CODEN	<table><tbody><tr><td>CODEN</td><td>SYNTRF</td></tr><tr><td>Journal Title</td><td>Synthesis</td></tr><tr><td>Language Code</td><td>EN</td></tr><tr><td>Number</td><td>4</td></tr><tr><td>Publication Year</td><td>2002</td></tr><tr><td>Page</td><td>483 - 486</td></tr></tbody></table> <div>Top of Page</div>	CODEN	SYNTRF	Journal Title	Synthesis	Language Code	EN	Number	4	Publication Year	2002	Page	483 - 486
CODEN	SYNTRF												
Journal Title	Synthesis												
Language Code	EN												
Number	4												
Publication Year	2002												
Page	483 - 486												

Citation Number

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

[Top of Page](#)

Show [Substances](#) for this Citation

Show [Reactions](#) for this Citation

Key points

- The results tab shows the citations 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

The screenshot displays the MDL Database Browser interface within a Microsoft Internet Explorer window. The browser shows the 'CrossFire Beilstein' database. The main content area is titled 'Reactions for this Citation' and lists 'Reactions 1 to 7 of 7'. Three reactions are visible:

- Reaction ID: 8991588**: A chemical reaction showing the conversion of a pyridine derivative to another pyridine derivative.
- Reaction ID: 8991589**: A chemical reaction showing the conversion of a pyridine derivative to a pyridine derivative with a sulfonate group.
- Reaction ID: 8997990**: A chemical reaction showing the conversion of a pyridine derivative and a silane reagent to a pyridine derivative with a silyl ether group.

Each reaction entry includes a 'Details' link and a 'Synthesize Reactant(s)' link. On the left side, there is a 'Find in History' section with a search bar and a 'next' button. Below this, there is a 'Field Index' section with a tree view showing 'Today's Searches', 'Previous Searches', and 'Saved Searches'. At the bottom left, there is a 'History' tab with instructions on how to use it.

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

The screenshot displays the MDL Database Browser interface in a Microsoft Internet Explorer window. The main content area is titled "Substances for this Citation" and shows a grid of 12 chemical structures, each with its BRN (Beilstein Reference Number) and a "Details" link. The "Details" link for the substance with BRN 111331 is highlighted with a red box. The sidebar on the left contains a "Find in History" search bar and a "History" tab with a tree view showing "Today's Searches", "Previous Searches", and "Saved Searches".

Substances 1 to 12 of 12		
BRN: 1506 Details Synthesize	BRN: 107510 Details Synthesize	BRN: 111331 Details Synthesize
BRN: 605266 Details Synthesize	BRN: 605365 Details Synthesize	BRN: 1209232 Details Synthesize
BRN: 2937445 Details Synthesize	BRN: 9043279 Details Synthesize	BRN: 9043776 Details Synthesize

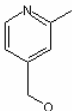
Key points

- 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

Substance 111331



[Use as Query](#)
[Synthesize](#)

Available Data

Click on a link to add the information to this page

[Crystal Property Description \(1\)](#)
[Infrared Spectra \(1\)](#)

[Mass Spectrum \(1\)](#)
[Nuclear Magnetic Resonance \(3\)](#)

[Substance \(1\)](#)

[Show Reactions for this Substance](#)
[Show Citations for this Substance](#)

Substance [\(hide\)](#)

Substance record 1 of 1	
Beilstein Registry Number	111331
Beilstein Preferred RN	105250-16-6
CAS Registry Number	105250-16-6
Autoname	(2-methylpyridin-4-yl)-methanol
Molecular Formula	C7H9NO
Lawson Number	24781
Constitution ID	94626
Tautomer ID	166736

Click a link to obtain specific data for the retrieved compound

Substance data

Key points

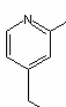
- The Substance data is shown, which includes identification information, such as registry numbers and the molecular formula.
- To obtain specific data for the compound, click a link in the Available data box.
- To use the structure in a new query, click “Use as Query”.

Notes

Use as Query

Structure

Find citations of this compound



Substitution as drawn, exclude tautomers
Substitution as drawn, include tautomers
Unlimited substitution on all atoms, exclude tautomers

Allow:

☒ Multi-component substances
☒ Ring closure through substitution
☒ Isotopes ☒ Charges ☒ Radicals
☐ Keep fragments separate

Search Stereoinformation As drawn

start search

Search results 1 to 5 of 5

Pages: 1

Journal; Furukawa, PHBUA9; Pharm.Bull.; 3; 1955; 413, 415; YKJZAJ; Yakugaku Zasshi; 76; 1956; 900; Chem.Abstr.; 1957; 2770; LitLink	Details
Journal; Katz, R B; Mistry, J; Mitchell, M B; SYNCAV; Synth.Communi.; EN; 19; 1, 2; 1989; 317-326; LitLink	Details
Journal; Varney, Michael D.; Palmer, Cindy L.; Deal, Judith G.; Webber, Stephanie; Welsh, Katherine M.; et al.; JMCMAJ; J.Med.Chem.; EN; 38; 11; 1995; 1892-1903; LitLink	Details
Journal; Gallagher, Timothy F.; Seibel, George L.; Kassiss, Shouki; Laydon, Jeffrey T.; Blumenthal, Mary Jane; et al.; BMECEP; Bioorg.Med.Chem.; EN; 5; 1; 1997; 49-64; LitLink	Details
Journal; Ragan, John A.; Jones, Brian P.; Meltz, Clifford N.; Teixeira, John J.; SYNTBF; Synthesis; EN; 4; 2002; 483 - 486; LitLink	Details

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:

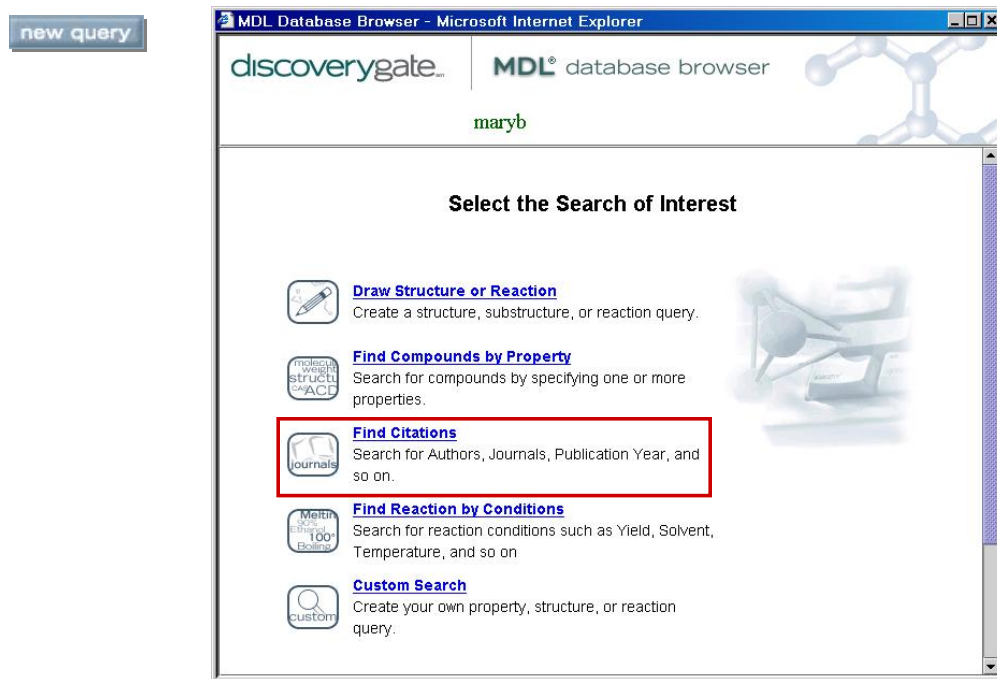
- is authored by K. Barry Sharpless.
- is published after 1995.

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

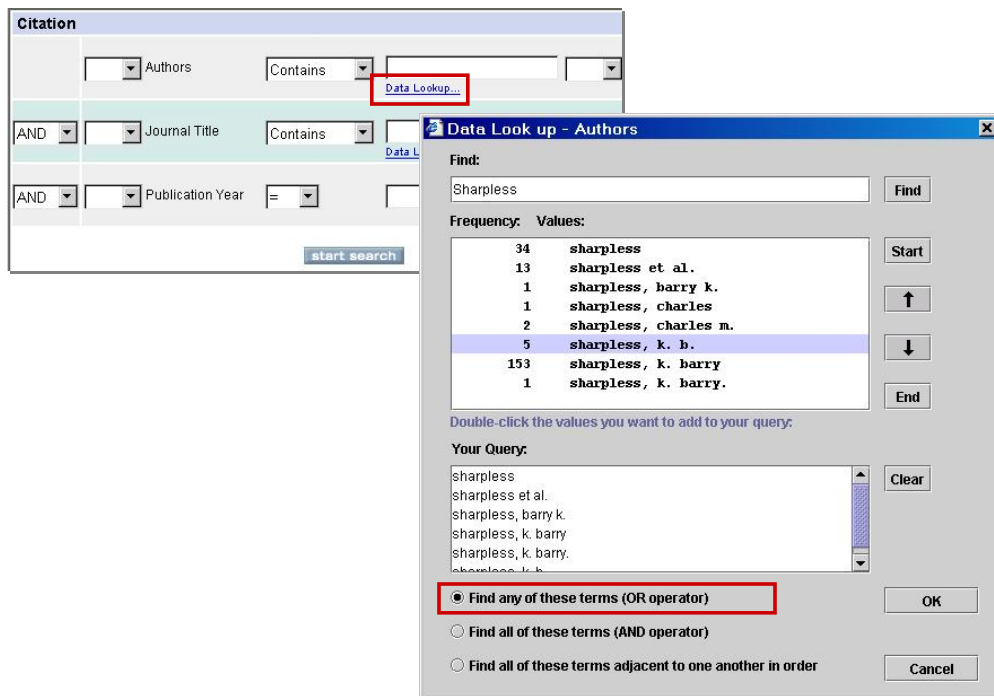


Key points

- 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

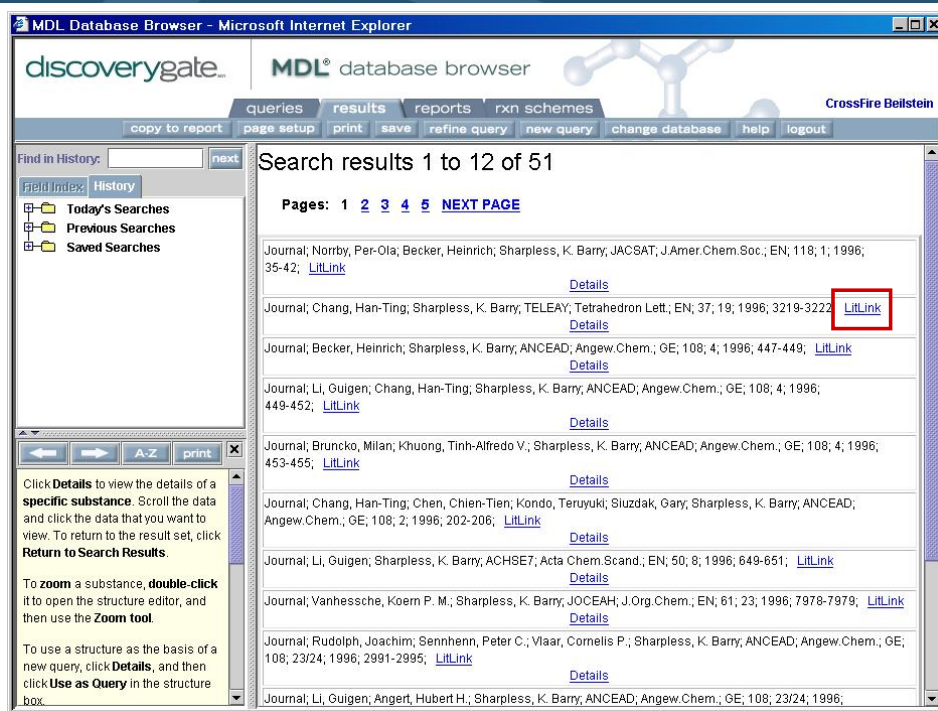
Citation					
	[Authors	Is	sharpless	Delete Duplicate Info
				Data Lookup...	
OR		Authors	Is	sharpless et al.	Delete Duplicate Info
				Data Lookup...	
OR		Authors	Is	sharpless, barry k.	Delete Duplicate Info
				Data Lookup...	
OR		Authors	Is	sharpless, k. b.	Delete Duplicate Info
				Data Lookup...	
OR		Authors	Is	sharpless, k. barry	Delete Duplicate Info
				Data Lookup...	
OR		Authors	Is	sharpless, k. barry.	Delete Duplicate Info
				Data Lookup...	
AND		Journal Title	Contains		Delete Duplicate Info
				Data Lookup...	
AND		Publication Year	>	1995	Delete Duplicate Info
start search					

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

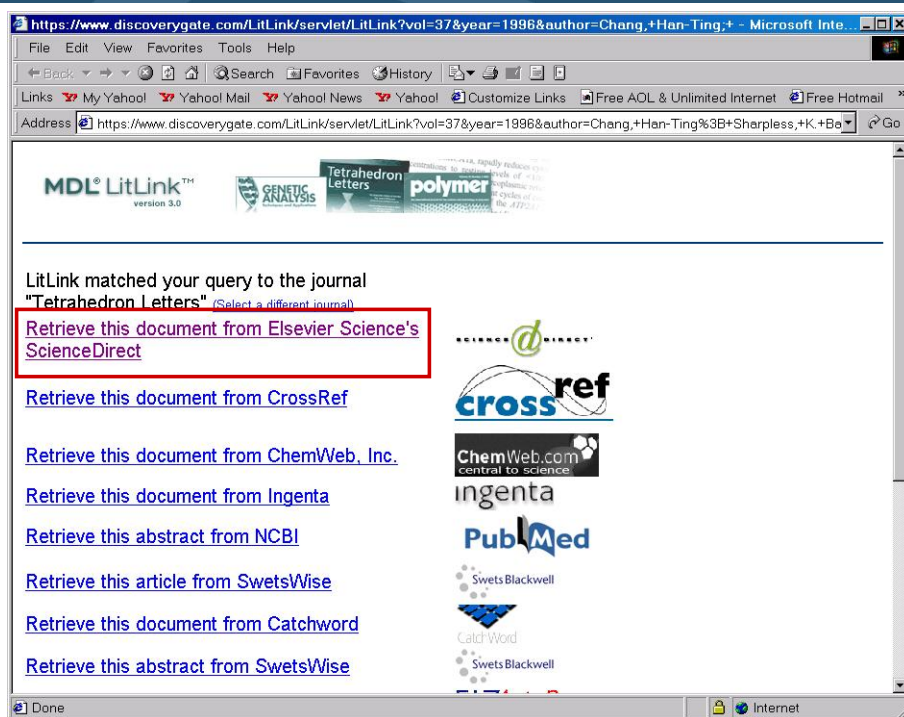


Key points

- 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

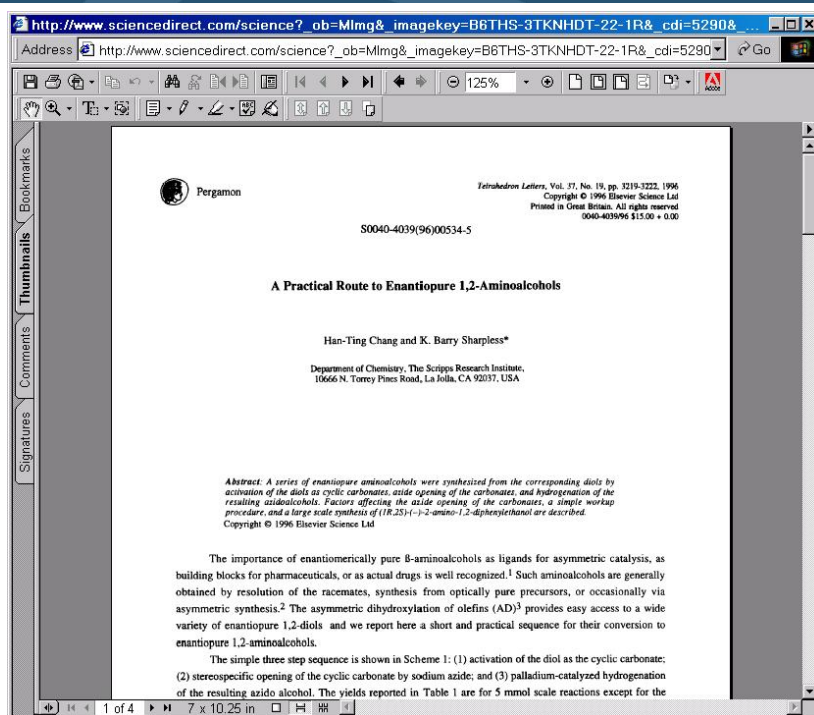


Key points

- 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



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**.

Data Look up - Authors

Find:
overman, larry Find

Frequency: Values:

188	overman, larry e.
2	overman, monica c.
2	overman, stacy a.
23	overman, l.e.
9	overman, l.e. et al.
3	overmann
1	overmann, gary j.
2	overmann, joerg

Start ↑ ↓ End

Double-click the values you want to add to your query:

Your Query:
overman, larry e.
overman, l.e.
overman, l.e. et al.

Clear

☒ Find any of these terms (OR operator)
☐ Find all of these terms (AND operator)
☐ Find all of these terms adjacent to one another in order

OK Cancel

start search

refine query

Add a data field to the
query form

8. Click **start search** and view the results.
9. Click **refine query**.
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:

start search

Inspect the citation details

Citation					
	[]	Authors	Is	Overman, Larry E.	Delete Duplicate Info Data Lookup...
OR		Authors	Is	Overman, L. E.	Delete Duplicate Info Data Lookup...
OR		Authors	Is	Overman, L. E. et al.	Delete Duplicate Info Data Lookup...
AND		Journal Title	Contains		Delete Duplicate Info Data Lookup...
AND		Publication Year	=		Delete Duplicate Info
Abstract					
AND		Abstract (AB)	Contains	Heck reaction	Delete Duplicate Info Data Lookup...
start search					

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

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

[Return to Search Results](#)

Citation 6051800

Journal: Overman, Larry E.; Poon, Daniel J.; ACIEAY; Angew.Chem.Int.Ed.Engl.; EN; 36; 5; 1997; 518-521; ANCEAD; Angew.Chem.; GE; 109; 1997; 536-538; [LitLink](#)

Abstract

Abstract record 1 of 1	
Abstract	Keywords: Asymmetric catalysis; Asymmetric synthesis; Heck reactions; Palladium
Language	EN
Title	Asymmetric Heck Reactions via Neutral Intermediates: Enhanced Enantioselectivity with Halide Additives Gives Mechanistic Insights

[Top of Page](#)

Show [Substances](#) for this Citation Show [Reactions](#) for this Citation

[Return to Search Results](#)

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

Exercise 2

Show Reactions for
this Citation

Return to Search Results

Show Substances for this
Citation

Use as Query

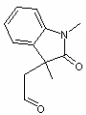
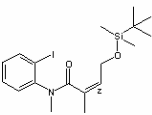
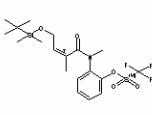
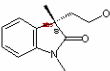
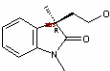
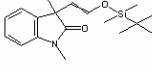
Display detailed information about a citation

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.

1. For the citation selected in Exercise 1, click **Show Reactions for this Citation**.
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.
4. Click the **Show Substances for this Citation** link.
5. View the results.

Substances for this Citation

Substances 1 to 8 of 8		
BRN: 168314  Details Synthesize	BRN: 6657112  Details Synthesize	BRN: 7666359  Details Synthesize
BRN: 7688745  Details Synthesize	BRN: 7688746  Details Synthesize	BRN: 7690954  Details Synthesize

6. Click the **Details** link for substance BRN: 168314.
7. Click the **Use as Query** link.

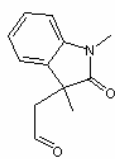
Find citations of this compound

start search

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

Structure

Find citations of this compound



[Search in Compound Locator](#)

start search

☒ Substitution as drawn, exclude tautomers
☐ Substitution as drawn, include tautomers
☐ Unlimited substitution on all atoms, exclude tautomers

Allow:

☒ Multi-component substances
☒ Ring closure through substitution
☒ Isotopes ☒ Charges ☒ Radicals
☐ Keep fragments separate

Search Stereoinformation As drawn

9. Click **start search**.

10. View the results.

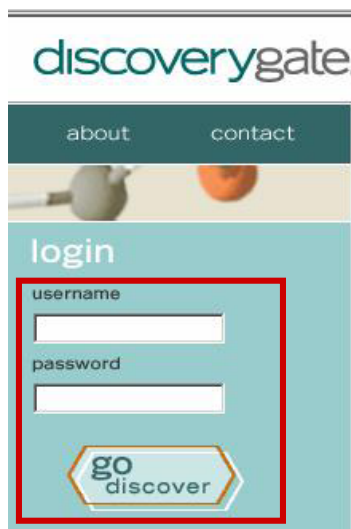
Search results 1 to 5 of 5

Pages: 1

Journal; Julian et al.; JACSAT; J.Amer.Chem.Soc.; 57; 1935; 2026, 2028; LitLink Details
Journal; Ashimori, Atsuyuki; Matsuura, Takaharu; Overman, Larry E.; Poon, Daniel J.; JOCEAH; J.Org.Chem.; EN; 58; 25; 1993; 6949-6951; LitLink Details
Journal; Overman, Larry E.; Poon, Daniel J.; ACIEAY; Angew.Chem.Int.Ed.Engl.; EN; 36; 5; 1997; 518-521; ANCEAD; Angew.Chem.; GE; 109; 1997; 536-538; LitLink Details
Journal; Ashimori, Atsuyuki; Bachand, Benoit; Overman, Larry E.; Poon, Daniel J.; JACSAT; J.Amer.Chem.Soc.; EN; 120; 26; 1998; 6477-6487; LitLink Details
Journal; Ashimori, Atsuyuki; Bachand, Benoit; Caller, Michael A.; Govek, Steven P.; Overman, Larry E.; Poon, Daniel J.; JACSAT; J.Amer.Chem.Soc.; EN; 120; 26; 1998; 6488-6499; LitLink Details

**To launch the
DiscoveryGate application**

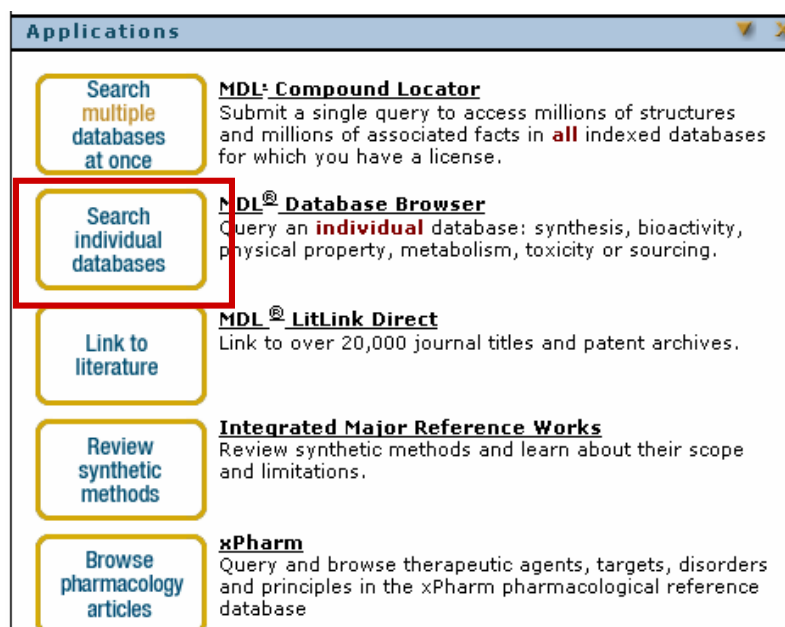
1. Launch your internet browser and enter the DiscoveryGate URL (www.discoverygate.com).
2. Enter your user name and password.
3. If necessary, enter your company ID.



4. Click **go discover**.

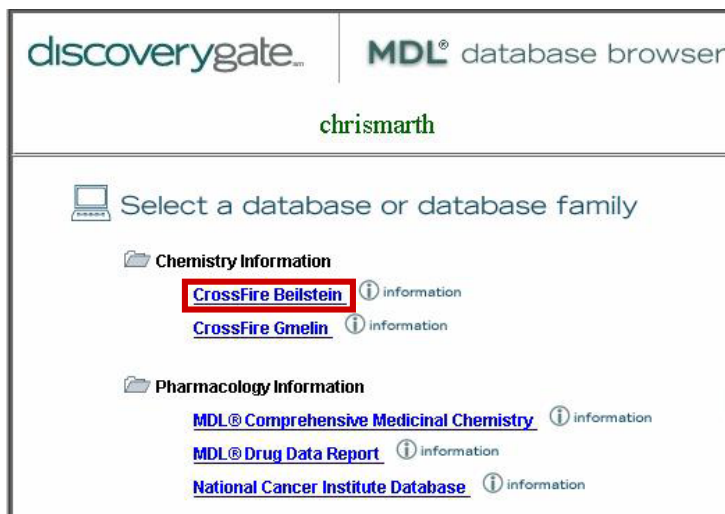
**To select an individual
database**

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.

The screenshot shows a form titled 'My CrossFire Login Information' with a help icon. The text inside says: 'To access CrossFire Beilstein and CrossFire Gmelin from MDL® Database Browser, enter missing information below and click **Update**.' Below this is the instruction 'Enter login information:'. There are five input fields labeled 'User Name', 'Password', 'Confirm Password', 'Group', and 'Confirm Group'. At the bottom right is a blue 'Update' button.

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**.

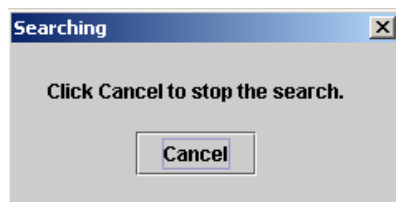
To start a search



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.



Journal; Whitlock,H.W.; Overman,L.E.; JACSAT; J.Amer.Chem.Soc.; EN; 93; 1971; 2247-2253; [LitLink](#)
[Details](#)

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 –

To use MDL LitLink to retrieve a publication

Choose **Find citations for this reaction**.

3. Click **start search**.

To view search results

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.

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**.