Introduction to DiscoveryGate

***using* DiscoveryGate v2.5**

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Course Objectives

- In this workshop, you will learn how to:
  - Log into DiscoveryGate
  - Change Personal Settings for DiscoveryGate
  - Conduct structure and data searches using the Database Browser and individual databases
  - View the search results using the Grid, Database, and Properties views
  - Save search results as Temporary and Permanent lists, and Combine lists
  - Create Reports
  - Modify Query Forms and Save as Default Forms
  - Introduce Synthetic Methods

What is DiscoveryGate?

- **An online content platform (www.discoverygate.com)**
- **For accessing a collection of reference databases**
  - Symyx scientific content
  - 3rd Party databases
- **Which are integrated and cross-indexed**
  - **Symyx Compound Index** – 27 million unique chemical structures
  - Compiled from compounds covered in the underlying databases
  - Every search retrieves relevant records from all databases
- **Augmented by direct retrieval of the original publications**
  - Abstracts, papers and patents
  - Delivered directly to the user's desktop
  - Using out-of-box citation service or commercial OpenURL services

DiscoveryGate – Delivers Lots of Individual Databases

Chemistry Reference

- CrossFire Beilstein (Elsevier)
- CrossFire Gmelin (Elsevier)
- OHS Pure Substance MSDS
- Index Chemicus (Thomson)

Bioactivity

- MDDR (Drug Data Report)
- Symyx Metabolite Database
- Symyx Toxicity Database
- National Cancer Institute Database
- Symyx Comp. Medicinal Chemistry
- PubChem (NIH)
- PharmaPendium (Elsevier)

Synthetic Methodology

- ChemInform Reaction Library (FIZ Chemie)
- Current Synth Methodology (FIZ Chemie)
- Derwent J. of Synth. Methods (Thomson)
- OrgSyn Database (OrgSyn)
- Symyx Solid Phase Org Rxns (FIZ Chemie)
- ISI Current Chemical Reactions (Thomson)
- Integrated Major Ref Works (Elsevier; Springer; InfoChem)

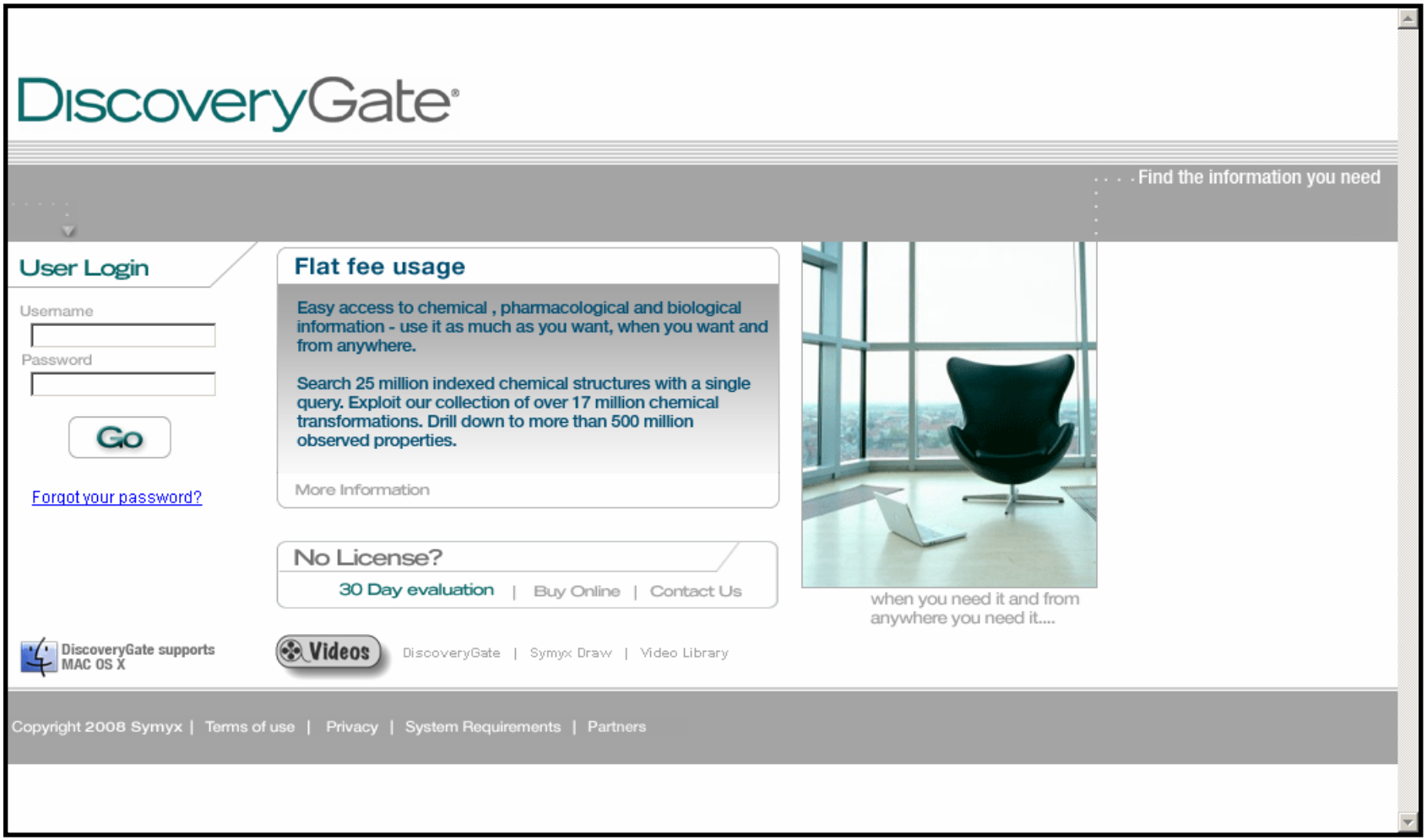
Patent Sources

- Patent Chemistry Database (Elsevier)
- Derwent World Patent Index (Thomson)

Sourcing Databases

- Symyx Available Chemicals Directory
- Symyx Screening Compounds Directory

Login to DiscoveryGate



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DiscoveryGate Home Page

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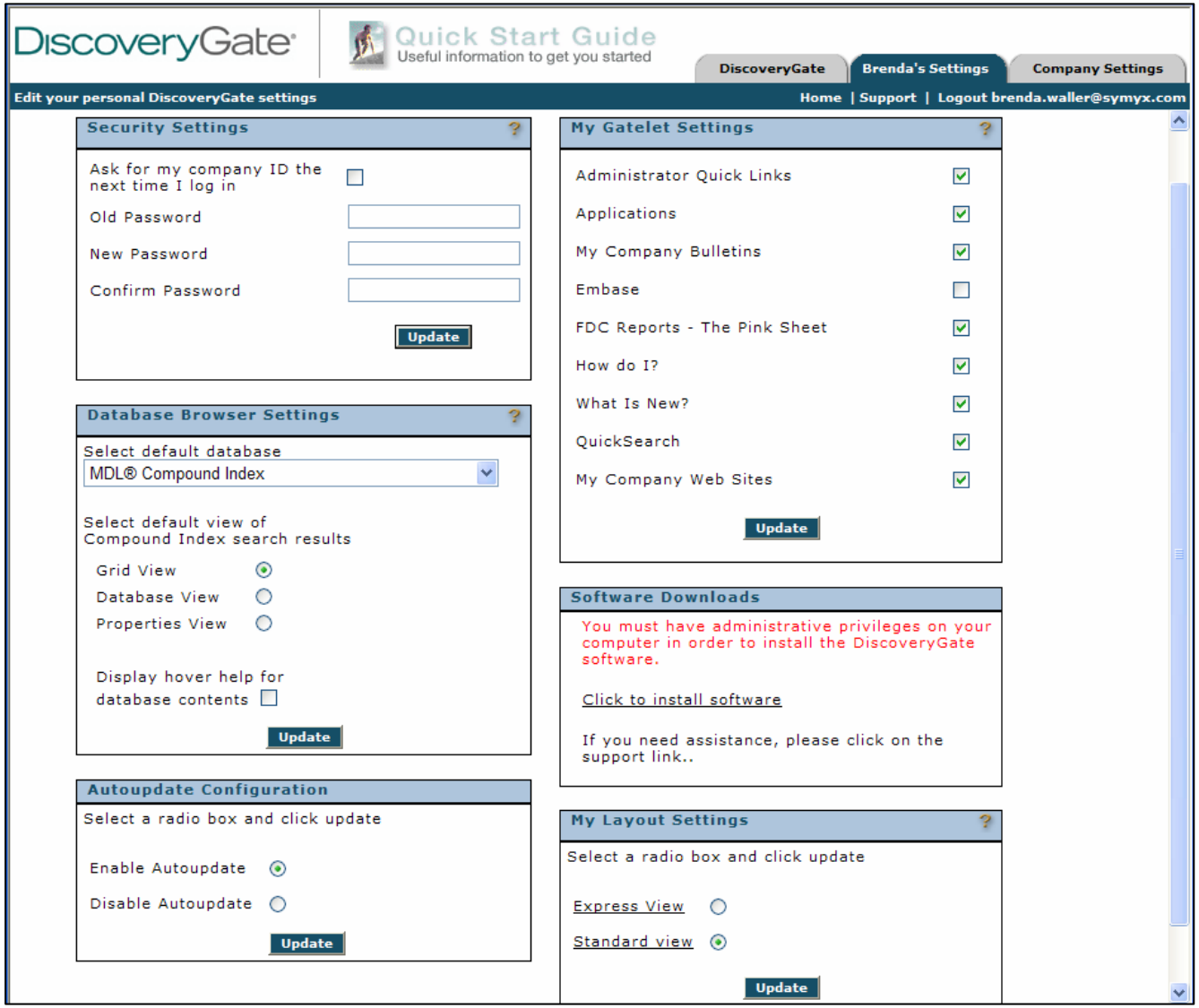
Personal Settings Tab



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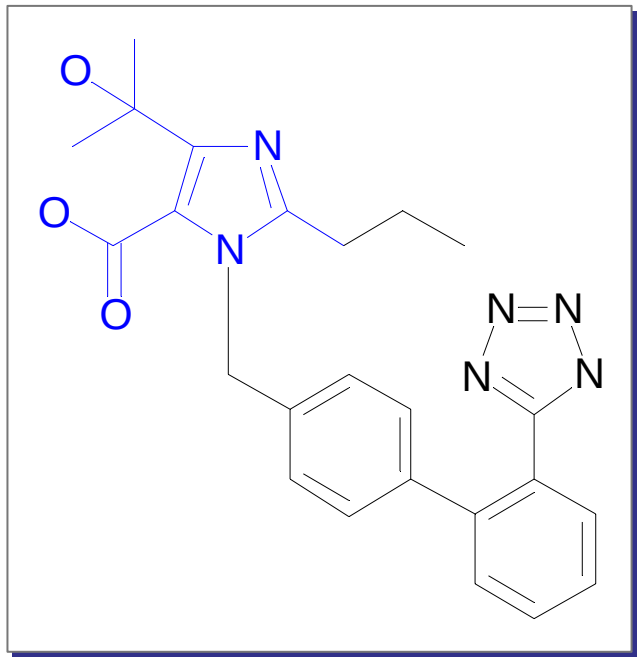
Structure Searching

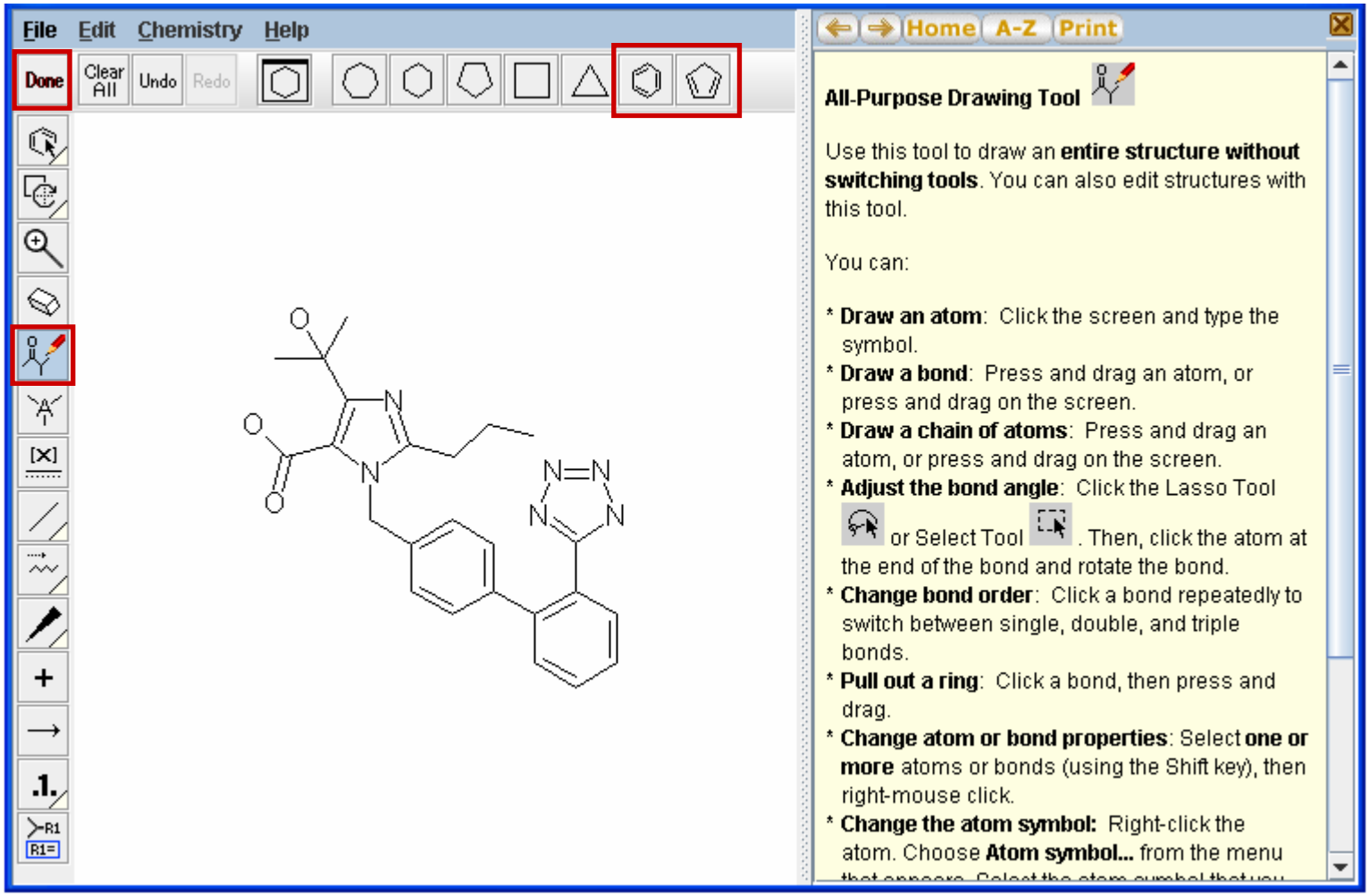
- In this module, you will learn how to:
  - Conduct an Exact Match and Substructure Search using the Database Browser
  - View Search Results using the Grid, Database, and Properties Views
  - Conduct a Combination Structure and Data Search

Search Scenario

Olemesartan is an antihypertensive agent, acting as an angiotensin II receptor agonist. You want to retrieve available information for the compound, as well as determine other known 2-alkyl-, 4-carboxy-, 5-alkylhydroxy-imidazole derivatives.



Draw the Structure Query



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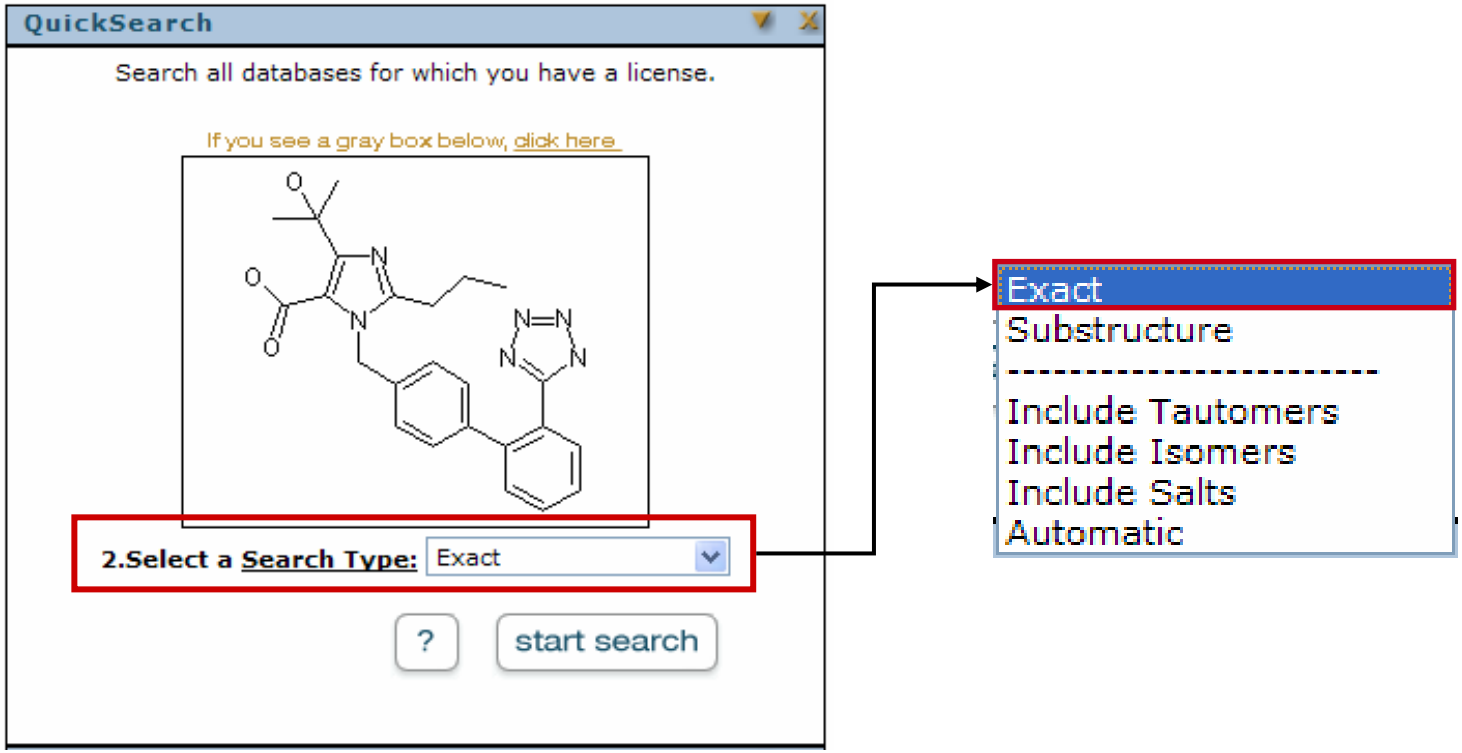
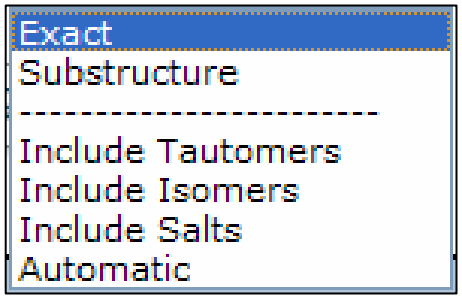
Conduct an Exact Match Search

QuickSearch is a shortcut to the molecule searching functionality.



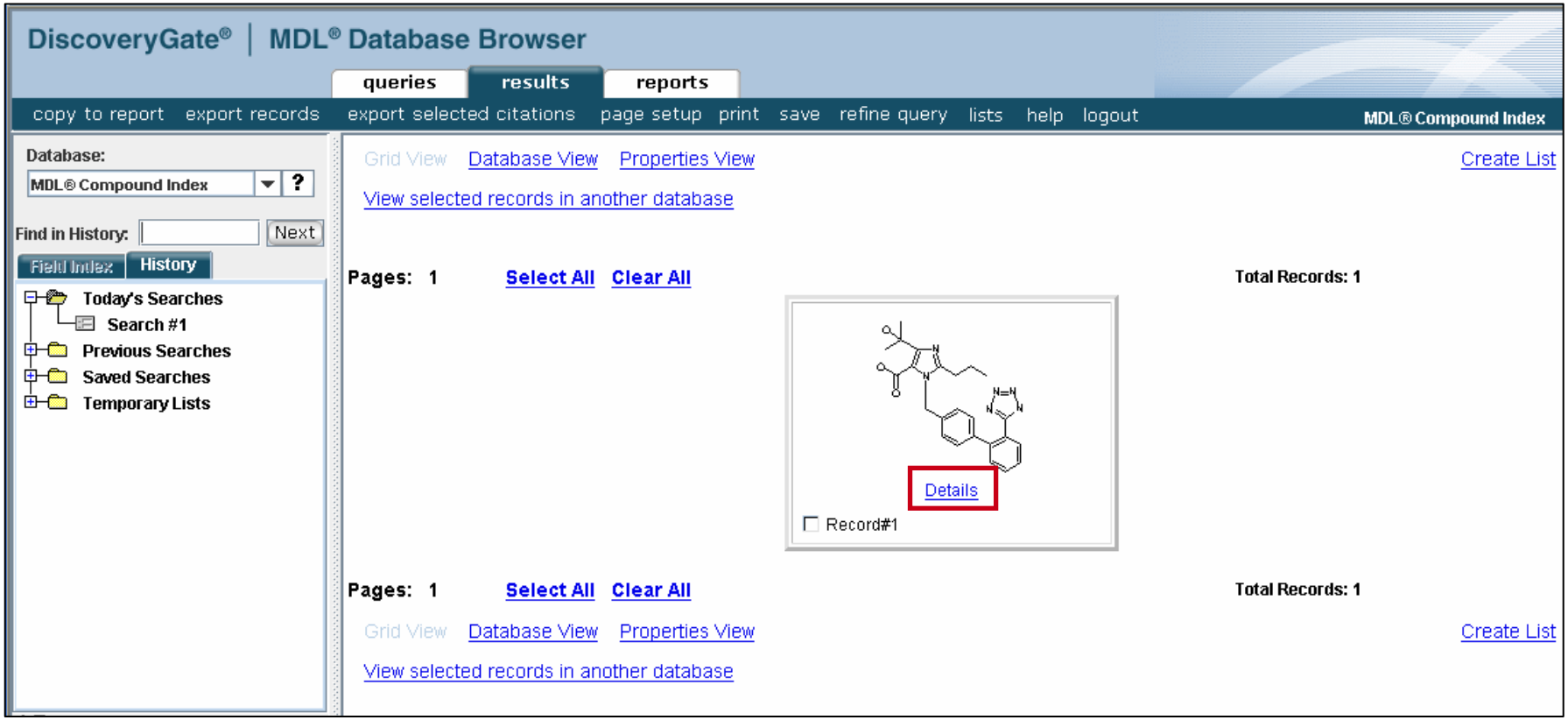
Structure Search Types



DiscoveryGate conducts a series of searches until it retrieves at least one compound that matches your query. Each subsequent search is more general than the preceding search. The order is listed below.

- **Exact Match:** Search for substances that match your structural query exactly.
- **Include Isomers:** Search for all stereoisomers (all R and S configurations, all E and Z configurations, and so on).
- **Include Tautomers:** Search for all tautomers, and also for structures with different charges and different isotopes.
- **Include Salts:** Search for substances that include different salts.
- **Substructure:** Search for substances that contain your query wholly embedded within them.
- **Similarity:** Search for substances that are structurally similar to your query.

View the Retrieved Compound



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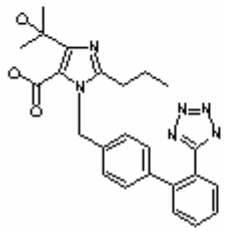
View the Detailed Information

Return to Search Results View selected records in another database Record # 1 **Total Records:** 1

Also found in: ACD Beilstein CMC DWPI Index Chemicus MDDR MetaCore MetaDrug Metabolite Patent Chemistry

Select / deselect all citations from this page.



Use as Query

☐ Select current record

Torsional degree of freedom	5
clogP (Syracuse Res. Center)	3.63
Molecular Formula	C24 H26 N6 O3
Mol. Weight/Largest Fragment	446.508
Proton Acceptors (O+N)	9
Molecular Weight	446.508
Total Polar Surface Area	129.81
Rule of Five	0
Proton Donors	3

Return to Search Results View selected records in another database Record # 1 **Total Records:** 1

Also found in: ACD Beilstein CMC DWPI Index Chemicus MDDR MetaCore MetaDrug Metabolite Patent Chemistry

Information for this compound can also be found in these databases

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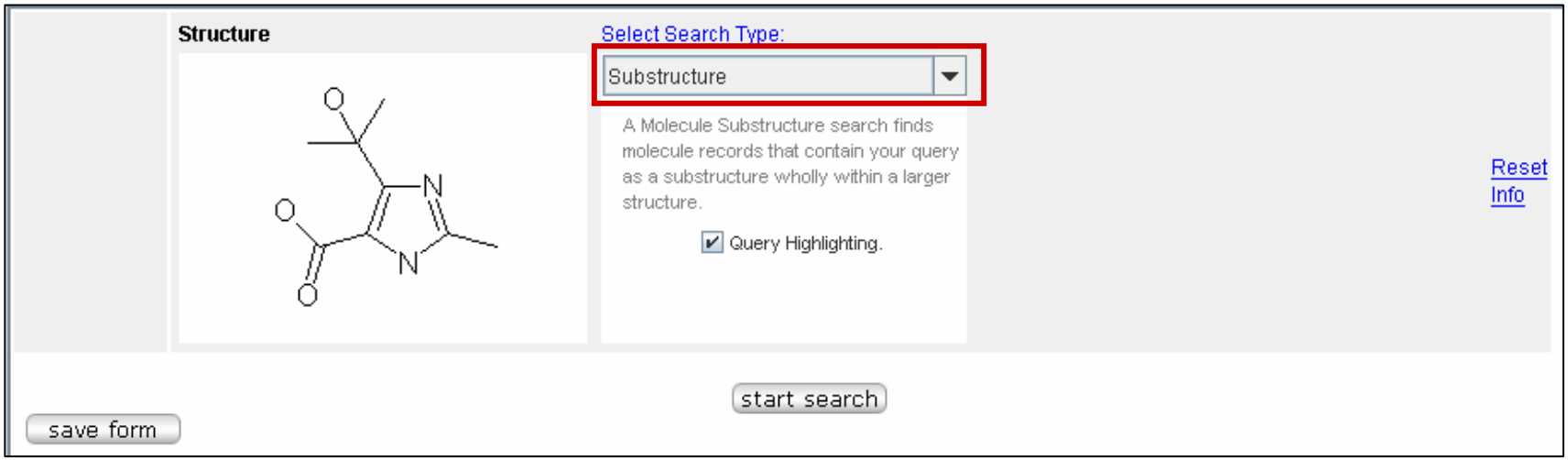
Conduct a Substructure Search

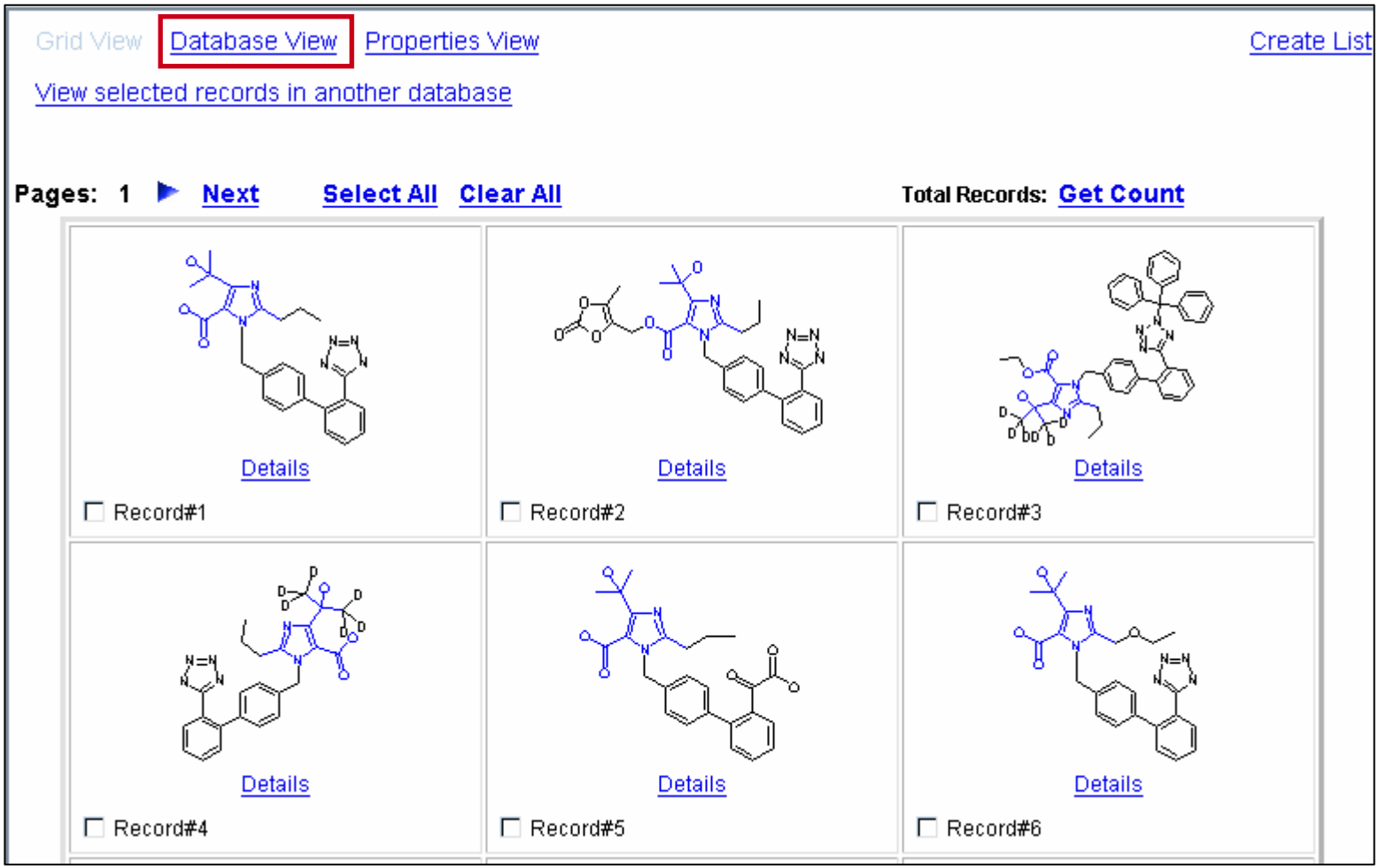
Determine other known 2-alkyl-, 4-carboxy-, 5-alkylhydroxy-imidazole derivatives.



Substructure search rules:

- The core structure must be embedded in all compounds retrieve
- Substitution can occur at any open valence

Substructure Results – Grid View



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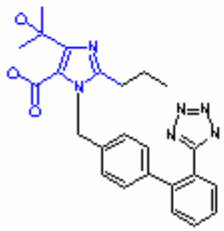
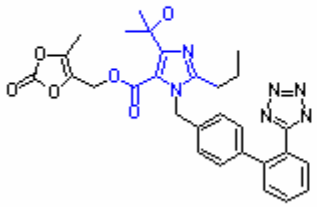
Database View

Grid View | Database View | Properties View | Create List

View selected records in another database

Pages: 1 2 3 4 5 6 7 8 9 10 ▶ **Next** **Next 10** **Select All** **Clear All** **Total Records: 248**

1	 Record#1	ACD	Beilstein
		CMC	DWPI
		Index Chemicus	MDDR
		MetaCore	MetaDrug
		Metabolite	Patent Chemistry
2	 Record#2	ACD	Beilstein
		DWPI	Index Chemicus
		MDDR	Metabolite
		Patent Chemistry	PharmaPendium
		Toxicity	

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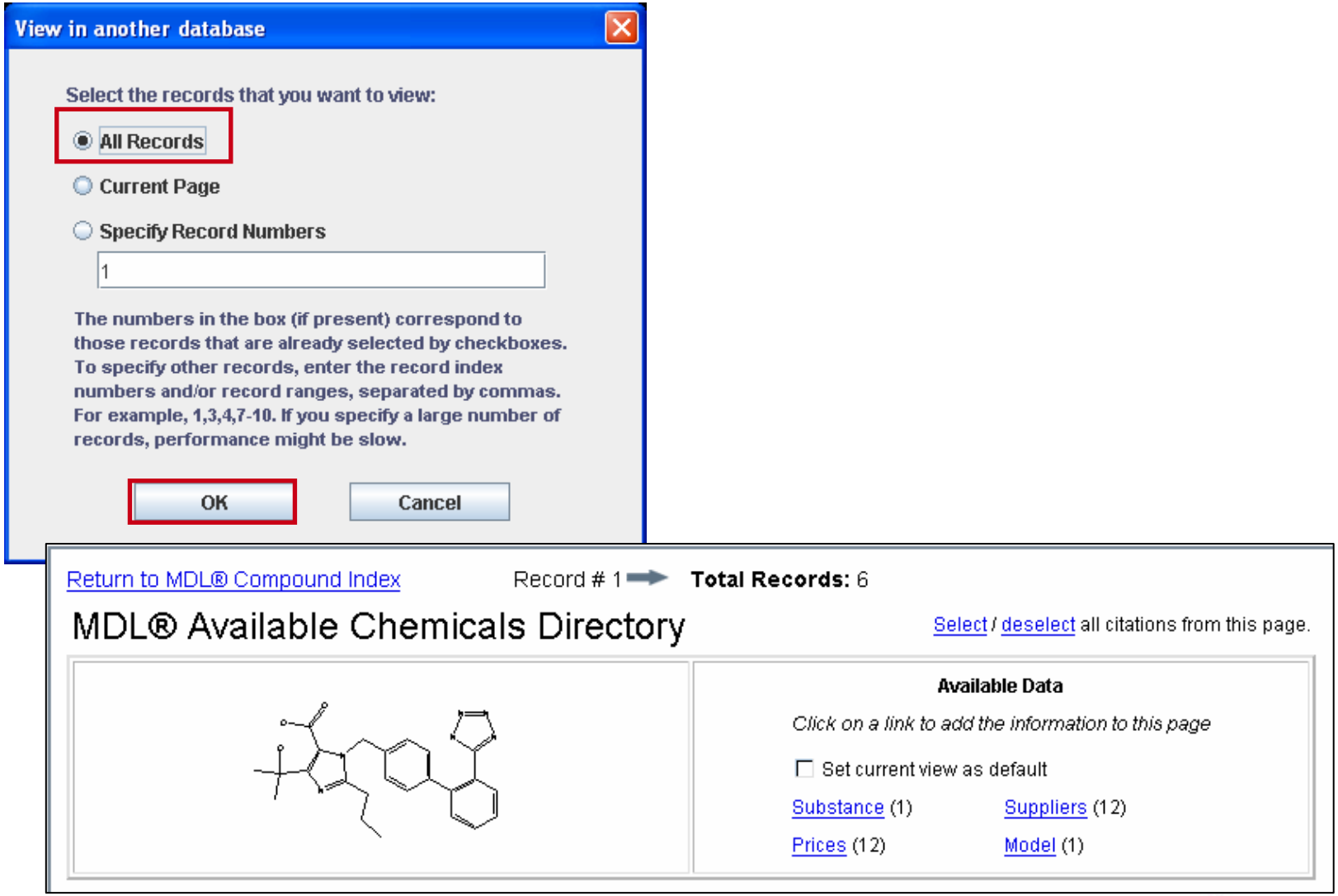
Viewing Compounds by Database



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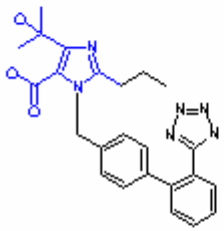
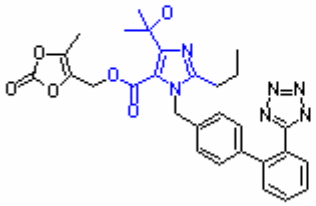
Properties View

Grid View | Database View | Properties View | Create List

View selected records in another database

Pages: 1 2 3 4 5 6 7 8 9 10 ▶ **Next** **Next 10** **Select All** **Clear All** **Total Records: 248**

1	 Record#1	3d Configuration, ADME, Agrochemical, Analytical, Chemical, Commercially Available, Information Source, Metabolism, Name, **Pharmacological**, Physical Chemical, Preparation
2	 Record#2	3d Configuration, ADME, Adverse Effects, Agrochemical, Analytical, Chemical, Commercially Available, Information Source, Metabolism, Name, Pharmacological, Physical Chemical, Preparation, Toxicity

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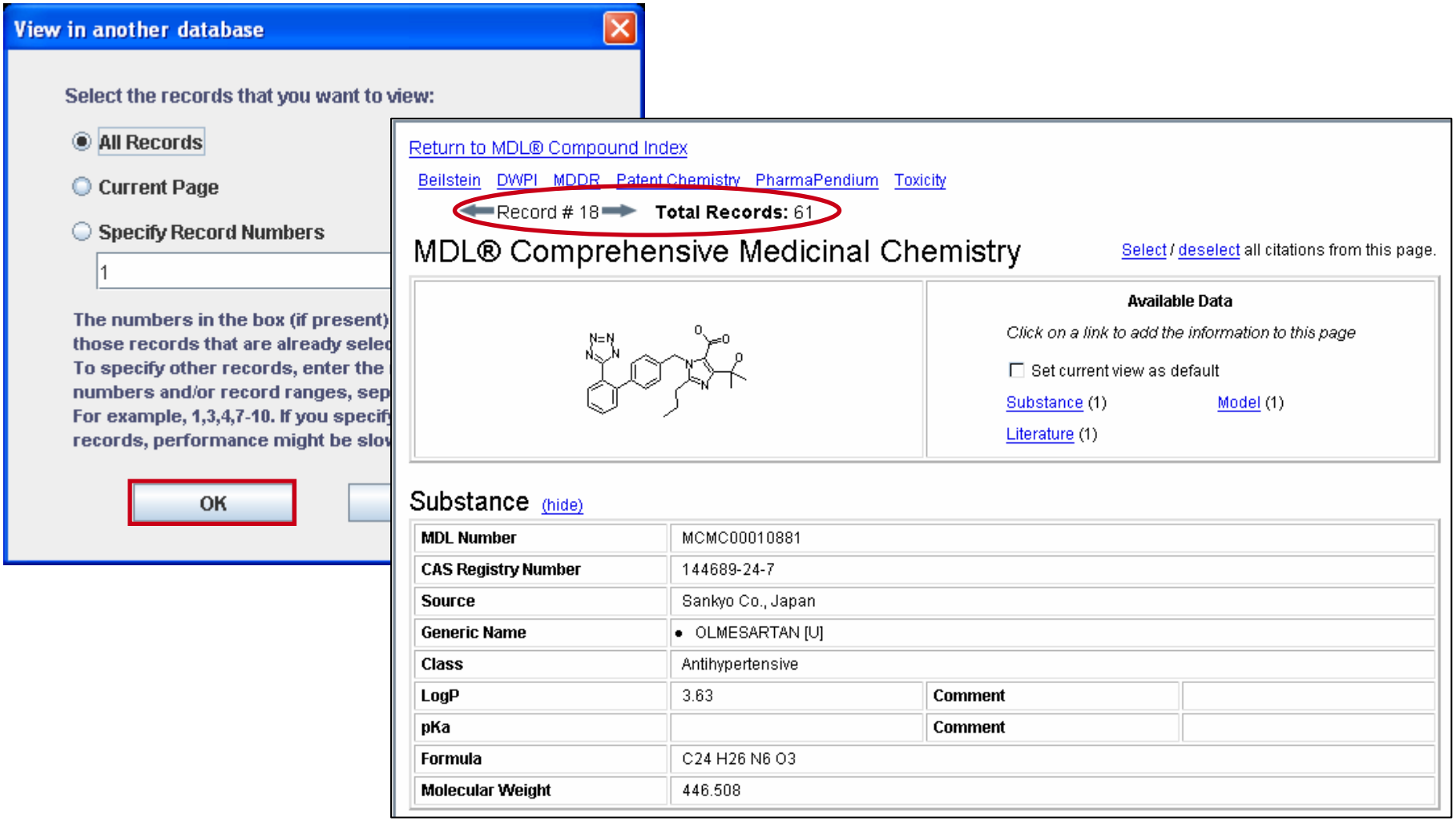
Viewing Compounds by Property



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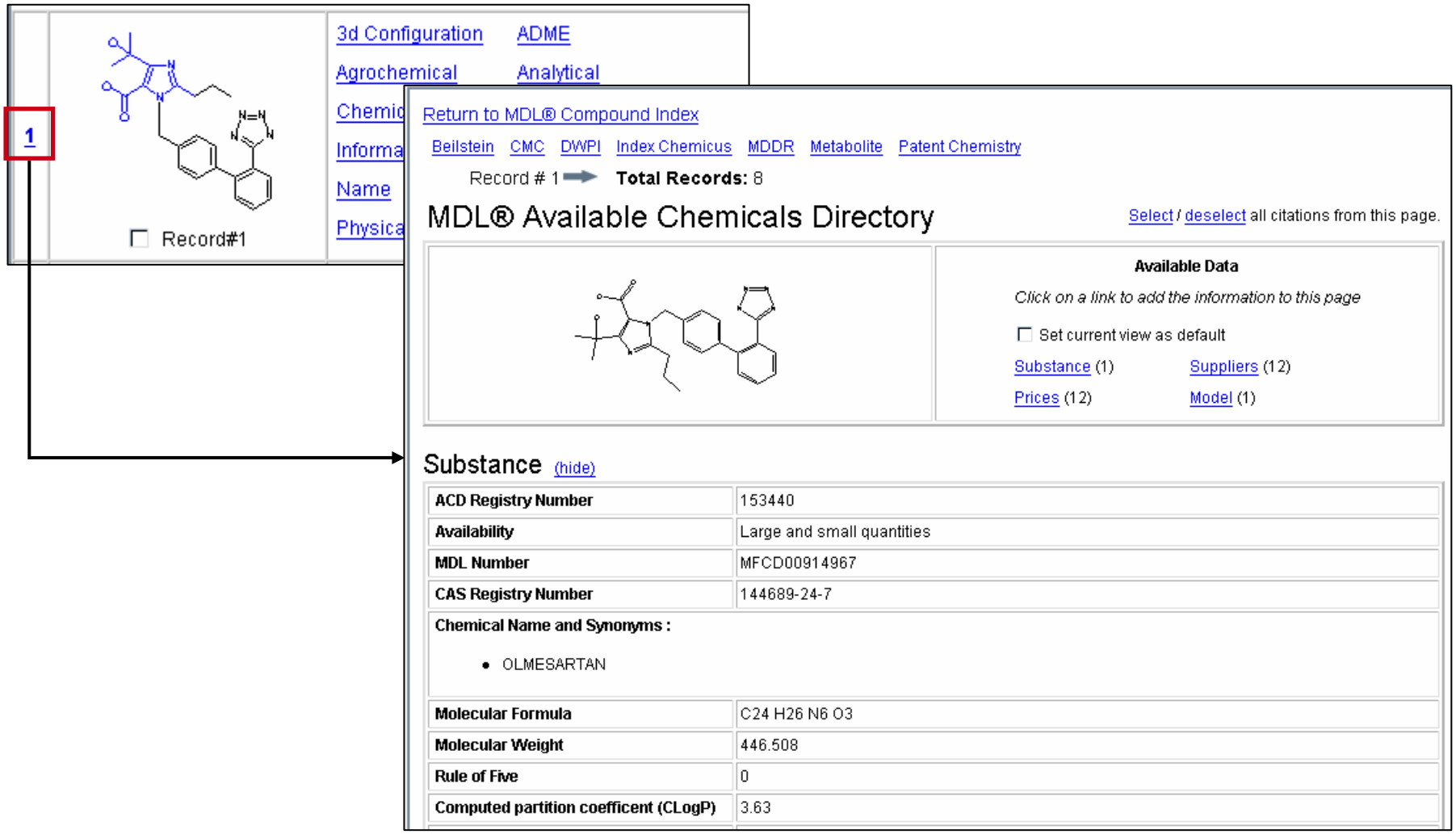
Viewing Data for a Single Record



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CMC

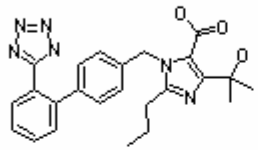
Return to MDL® Compound Index

ACD Beilstein DWPI Index Chemicus MDDR Metabolite Patent Chemistry

Record # 3 **Total Records:** 8

MDL® Comprehensive Medicinal Chemistry

Select / deselect all citations from this page.



Available Data

Click on a link to add the information to this page

☐ Set current view as default

Substance (1) Model (1)

Literature (1)

Substance (hide)

MDL Number	MCMC00010881		
CAS Registry Number	144689-24-7		
Source	Sankyo Co., Japan		
Generic Name	• OLMESARTAN [U]		
Class	Antihypertensive		
LogP	3.63	**Comment**	
pKa		**Comment**	
Formula	C24 H26 N6 O3		
Molecular Weight	446.508		

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MDDR

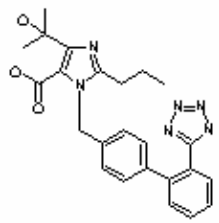
Return to MDL® Compound Index

ACD Beilstein CMC DWPI Index Chemicus Metabolite Patent Chemistry

Record # 6 **Total Records:** 8

MDL® Drug Data Report

Select / deselect all citations from this page.



Available Data

Click on a link to add the information to this page

Set current view as default

Substance (1) Model (1)

Biology (1) Identification (1)

Literature and Patent (1)

Substance (hide)

External Registration Number	188868
Prous Entry Number	188868
Preview Number	
CAS Registry Number	144689-24-7
Derivative	

Chemical Name :

- 4-(1-HYDROXY-1-METHYLETHYL)-2-PROPYL-1-[2'-(1H-TETRAZOL-5-YL)BIPHENYL-4-YLMETHYL]IMIDAZOLE-5-CARBOXYLIC ACID

Symyx

Metabolite

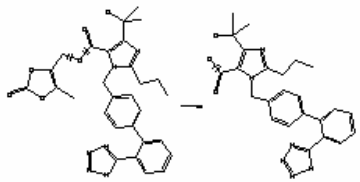
Return to MDL® Compound Index

ACD Beilstein CMC DWPI Index Chemicus MDDR Patent Chemistry

← Record # 7 → **Total Records:** 8

MDL® Metabolite Database

Select / deselect all citations from this page.



Available Data

Click on a link to add the information to this page

☐ Set current view as default

View results as **transformations:**

Transformation (1)
Reference (3)
Species (3)
Enzyme (3)

View results as **molecules:**

Parent (1)
Species (3)
Substrate (1)
Metabolite (1)

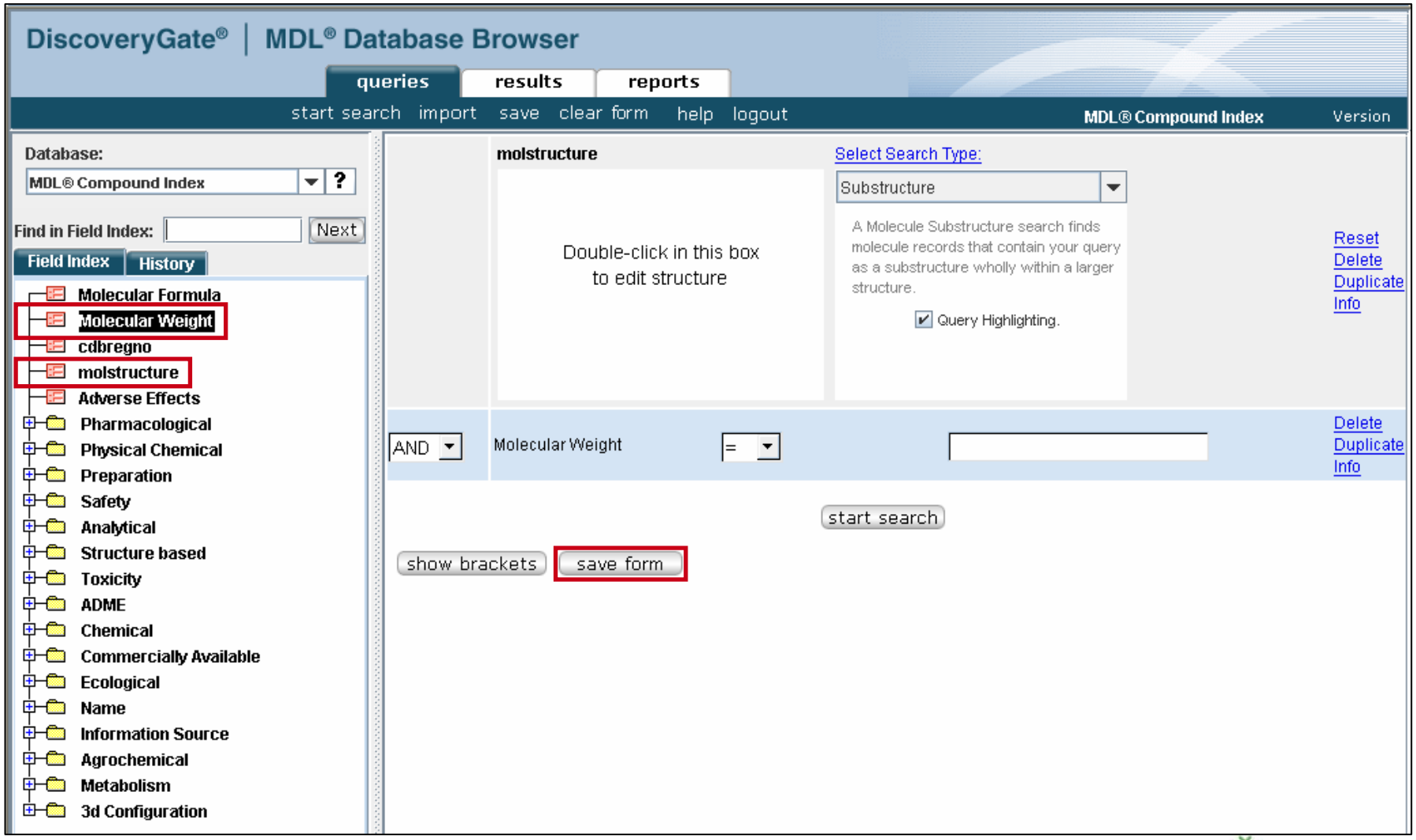
Transformation Results -- Transformation (hide)

MDL number	RMTB00058294
Path	MTB9122-A
Step	1 Step
Scheme	MTB9122

Chemical Name and Synonyms :

- CS-866
- (5-Methyl-2-oxo-1,3-dioxol-4-yl)methyl 4-(1-hydroxy-1-methylethyl)-2-propyl-1-((2'-(1H-tetrazol-5-yl)-1,1'-biphenyl-4-yl)methyl)-1H-imidazole-5-carboxylate
- Olmesartan medoxomil
- CS 866
- 5-Methyl-2-oxo-1,3-dioxol-4-ylmethyl 4-(1-hydroxy-1-methylethyl)-2-propyl-1-((2'-(1H-tetrazol-5-yl)biphenyl-4-yl)methyl)imidazole-5-carboxylate

Adding a Data Criterion to Your Structure Search



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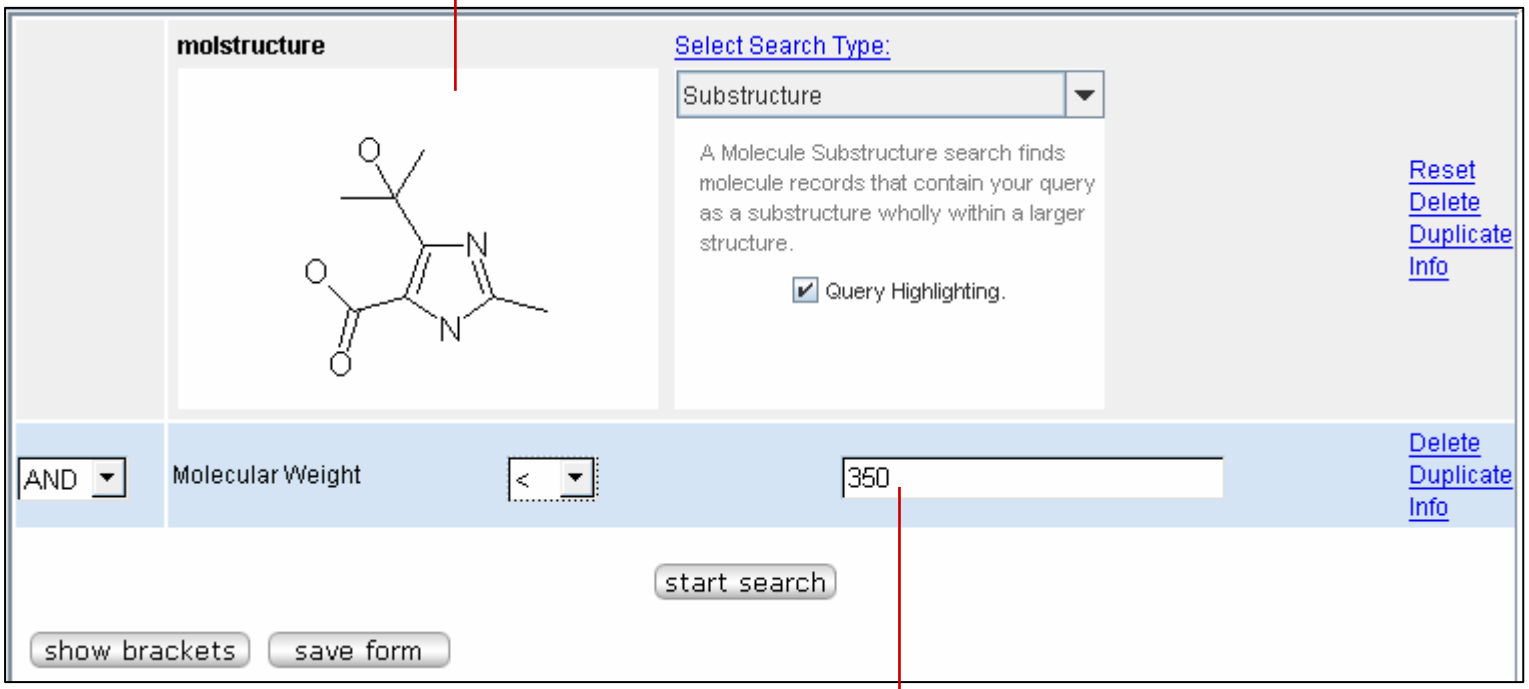
Completed Search Form

Enter the core structural fragment



Enter data and specify an operator

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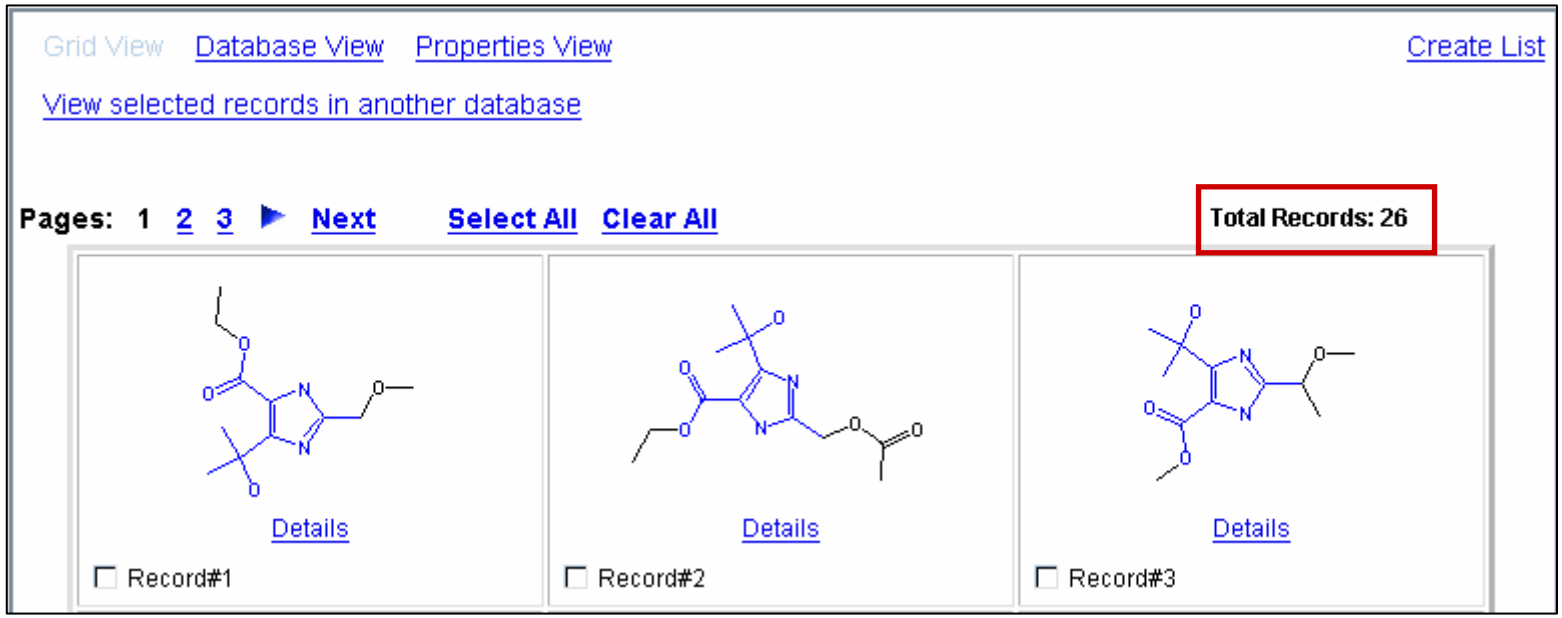
Results of the Structure and Data Search



Substructure search results – 248 compounds

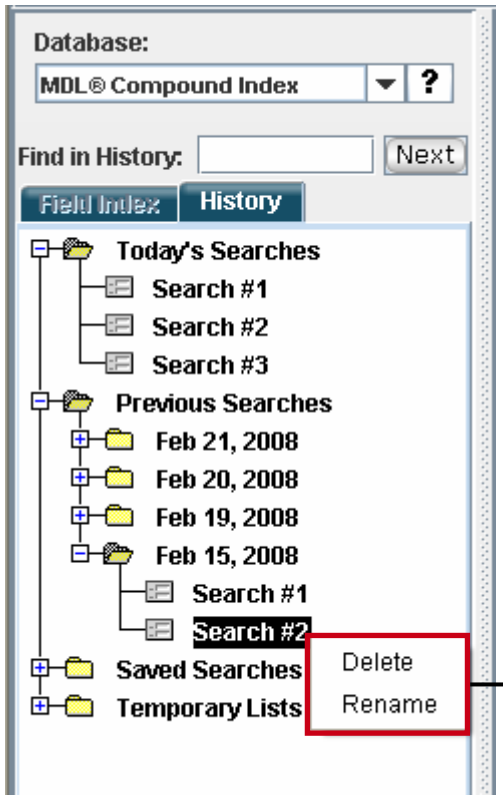
Substructure search with data constraint results – 26 compounds

Manipulating Search Results

- In this module, you will learn how to:
  - Work with the History Tab
  - Create a Temporary List
  - Save a Permanent List
  - Combine Temporary Lists
  - Export Results

Working with the History Tab

The History tab is unique to the database you are using.



Using the “results” tab, double click to open

Right-click a list to Delete or Rename

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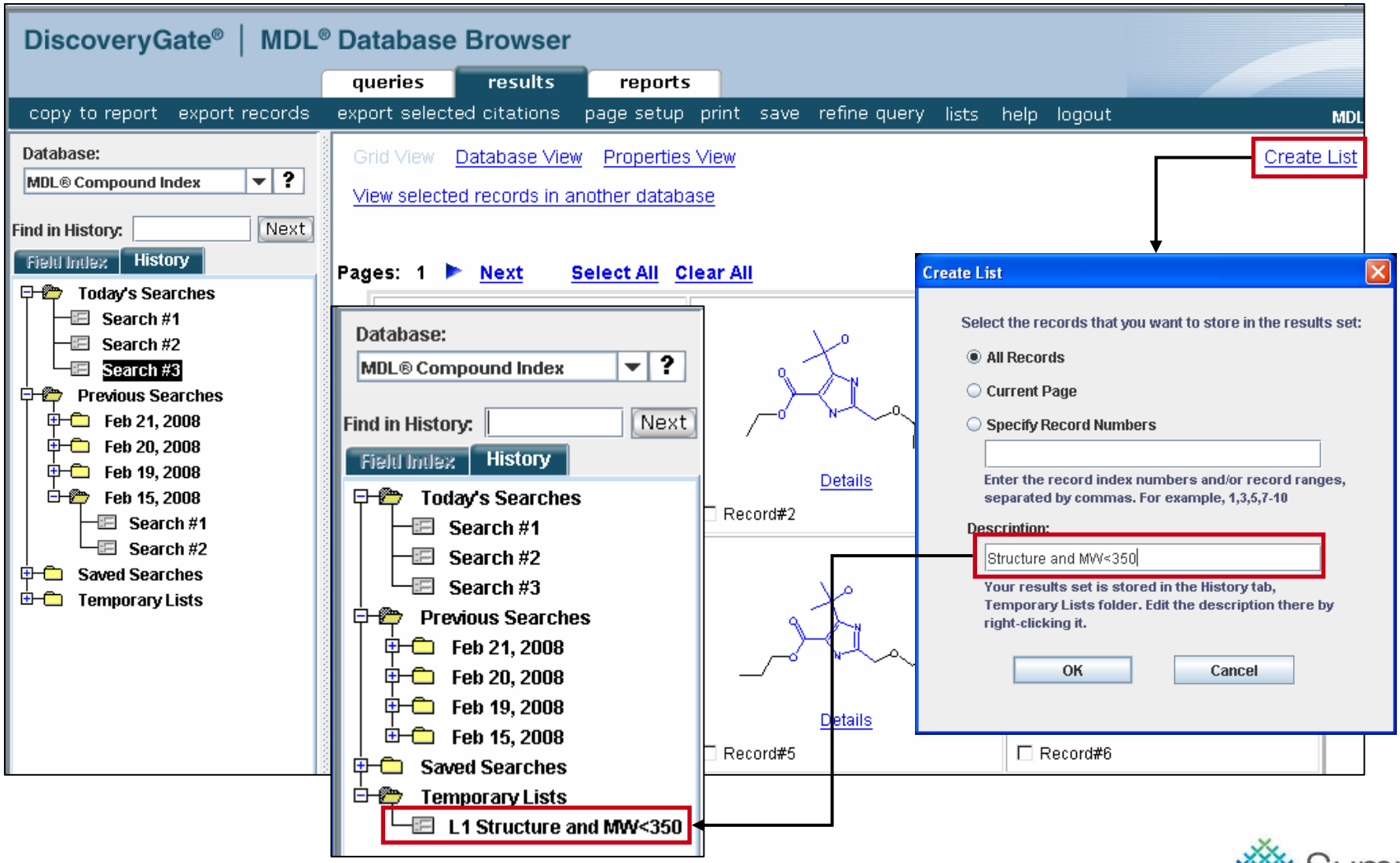
Create a Temporary List



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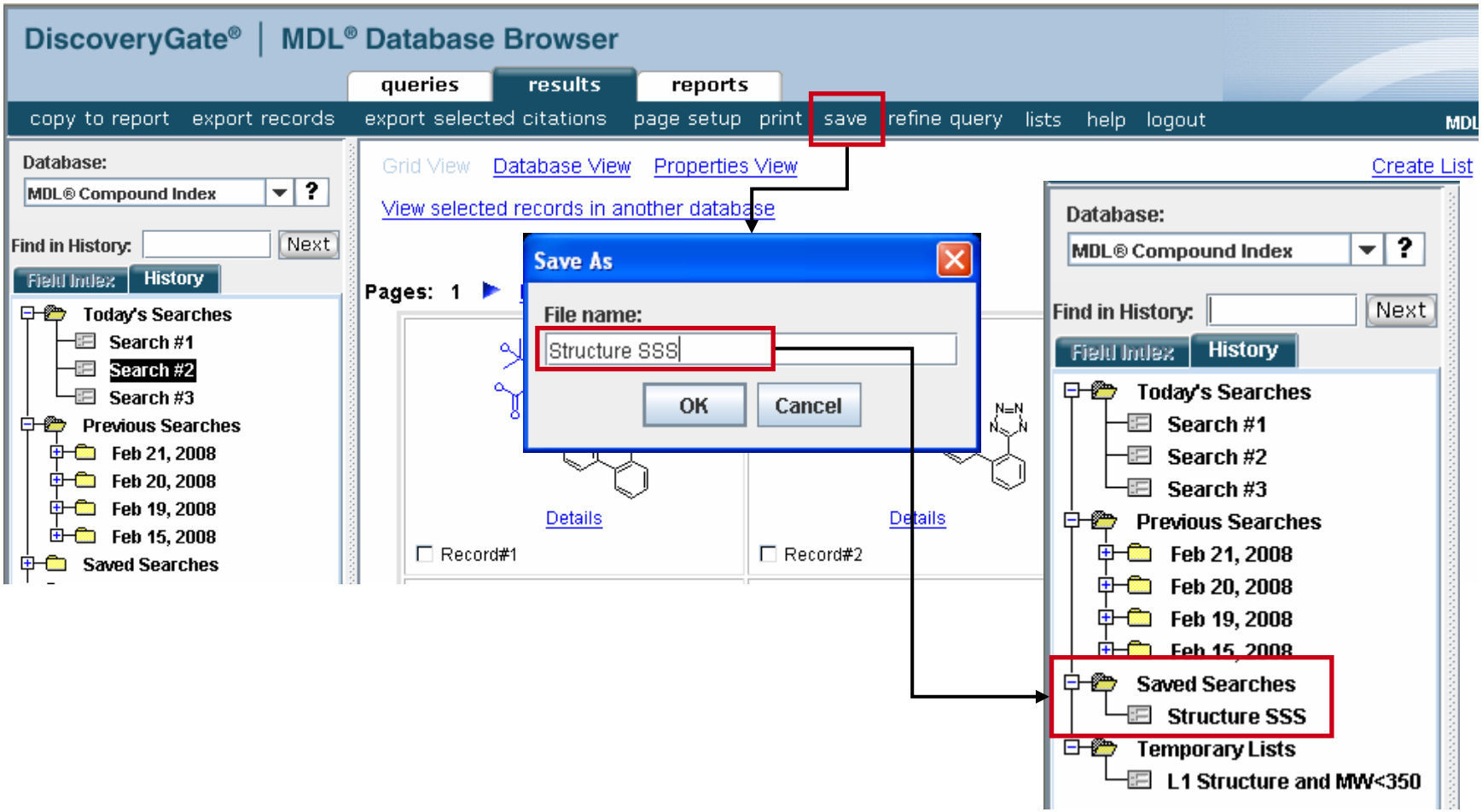
Create a Permanent List



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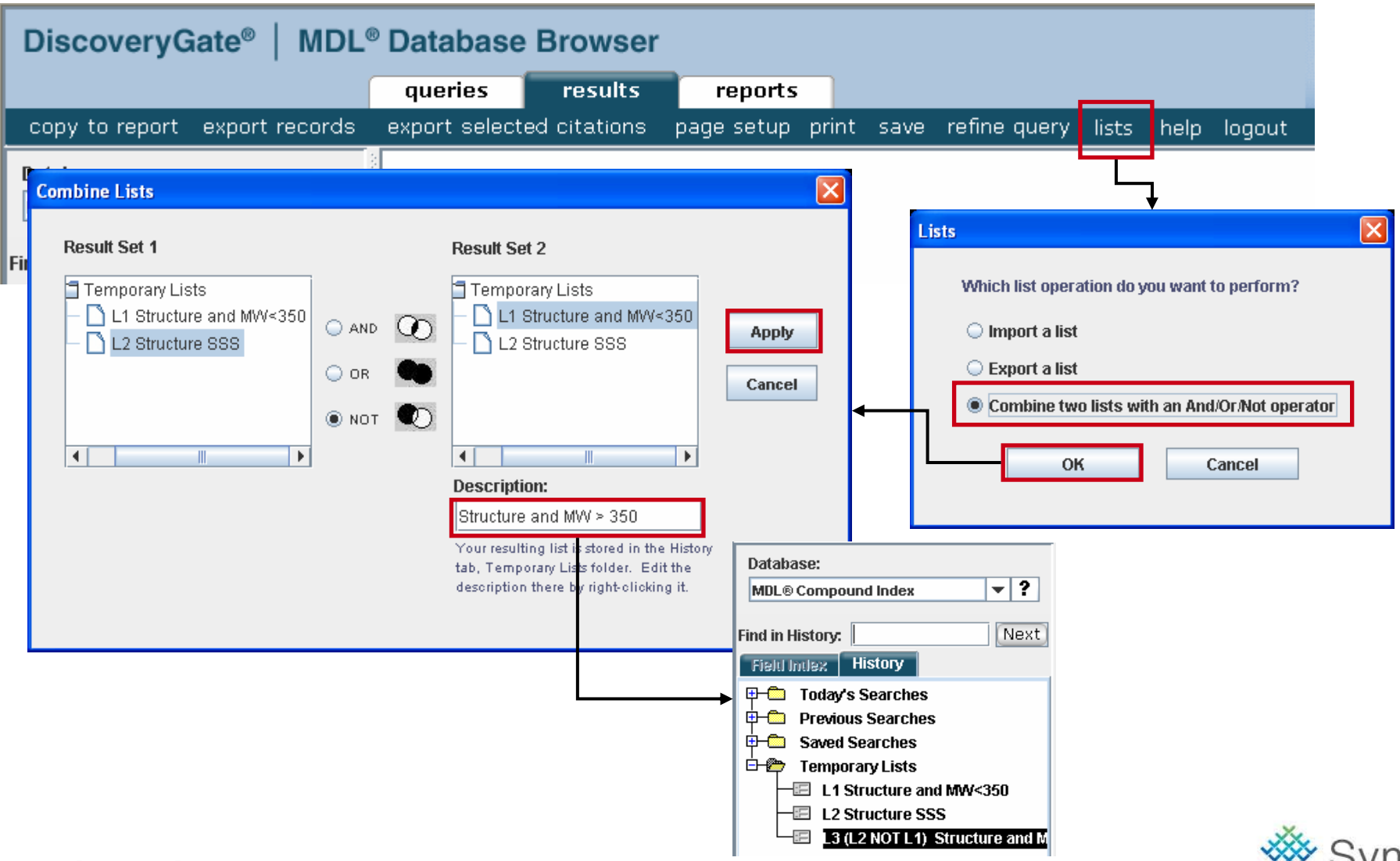
Combining Lists



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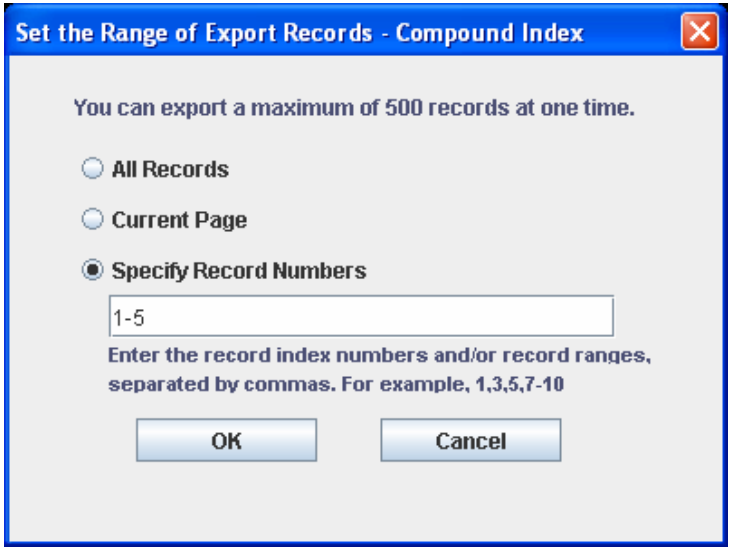
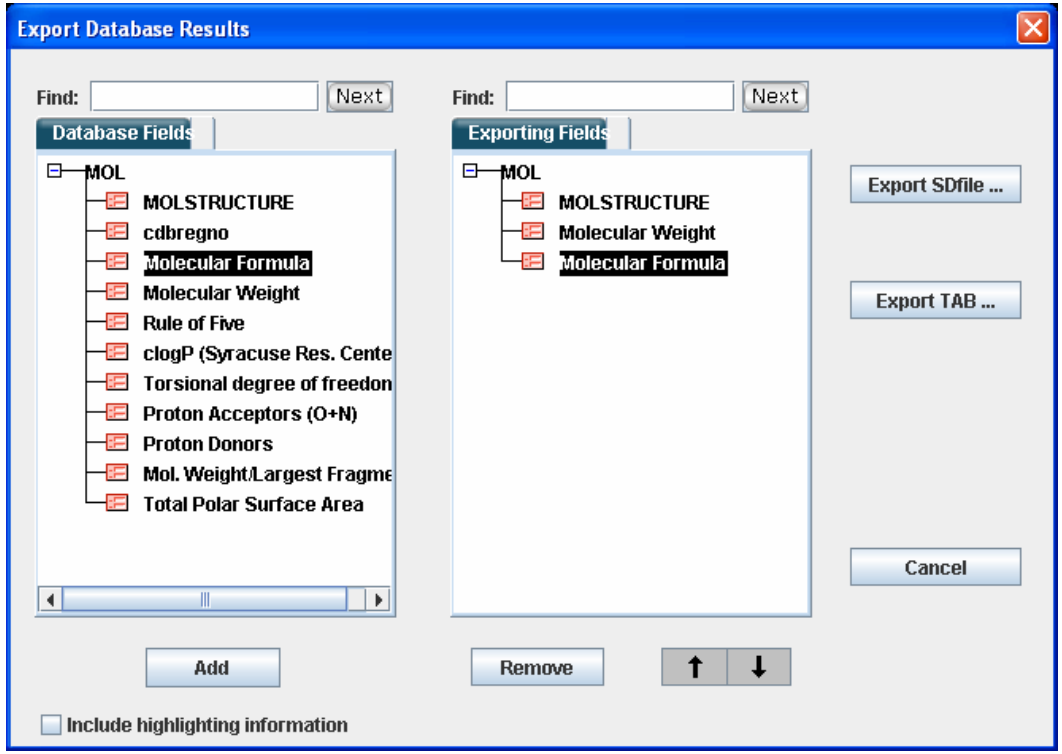
Export a List





Export format selection and the exported lists are supported by the database.

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Export Formats

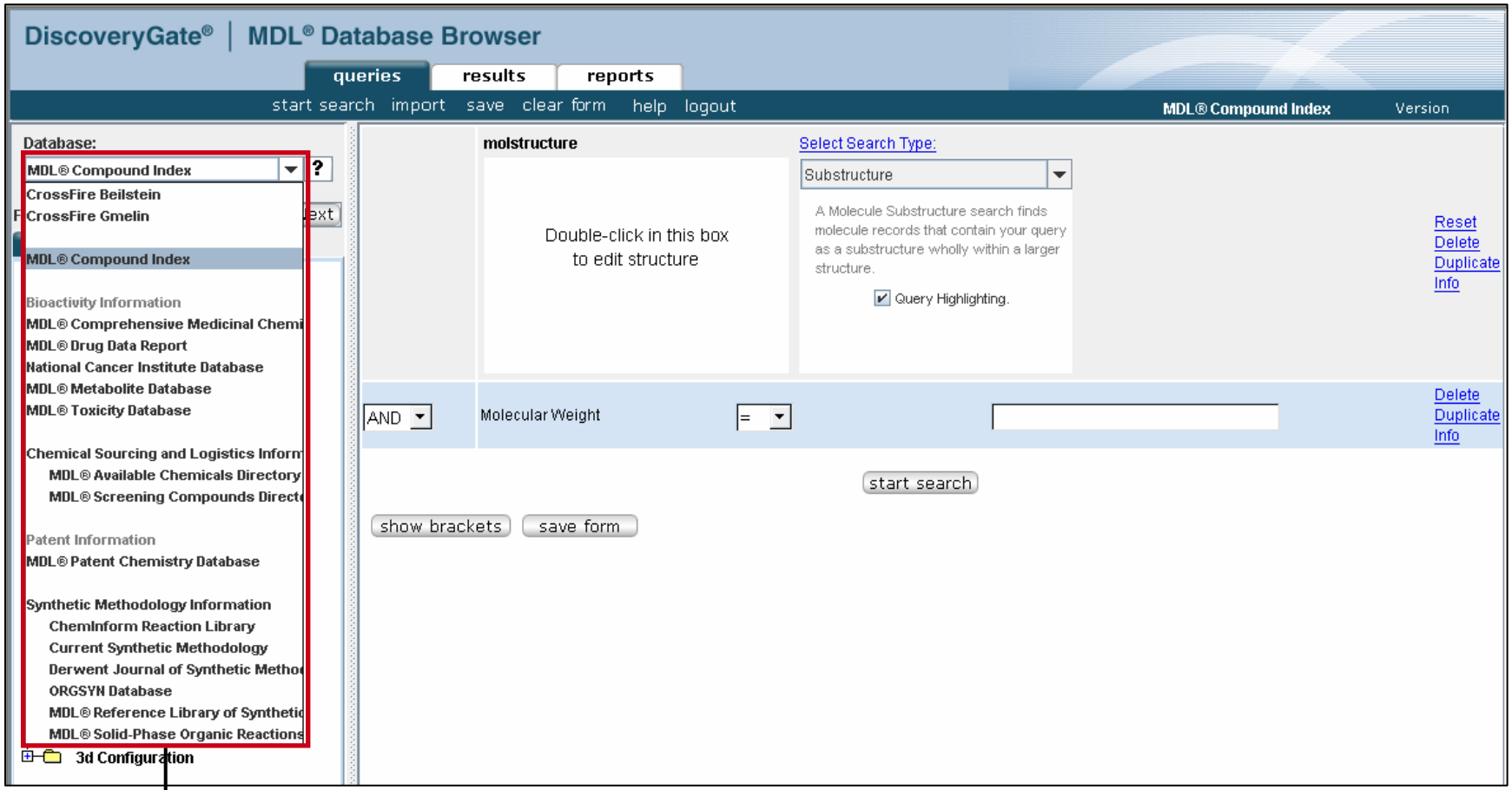
You can export results, both structures and data, in the following formats:

.sdf	▪ **This is a flat file format and can store structures, but not reactions.** ▪ **This format is suitable for files to be exported to ISIS for Excel and to ISIS/Base databases.** ▪ **The "results" tab needs to be active.**
.rdf	▪ **This is a hierarchical file format and can store reactions.** ▪ **This format is suitable for files to be exported to ISIS/Base databases.** ▪ **The "results" tab needs to be active.**
.tab	▪ **This format is suitable for files to be exported to ISIS for Excel.** ▪ **The "results" tab needs to be active.** ▪ **You require Chime software to view the structures.**

Data Searching

- In this module, you will learn how to:
  - Search Individual Databases
  - Select your Preferred Data Fields
  - Save the Modified Query Form as Your Default Form for the Current Database
  - Display Hidden Data in Details View
  - Create a Report

Selecting an Individual Database



Select an individual database from the drop-down list

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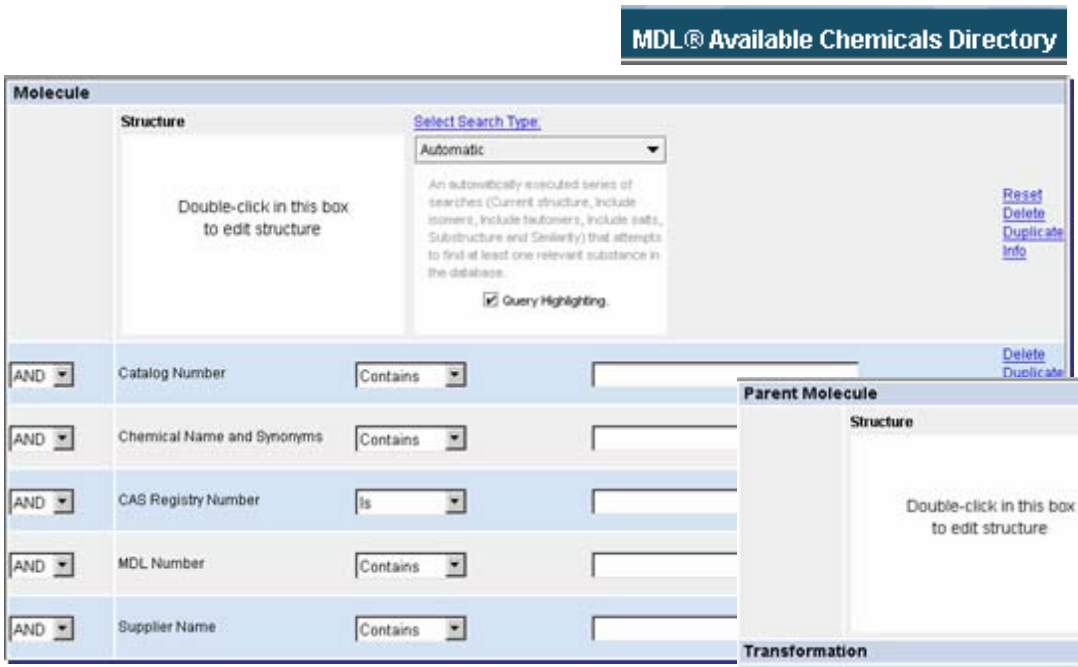
Using Default Forms



Each database has a defined default form

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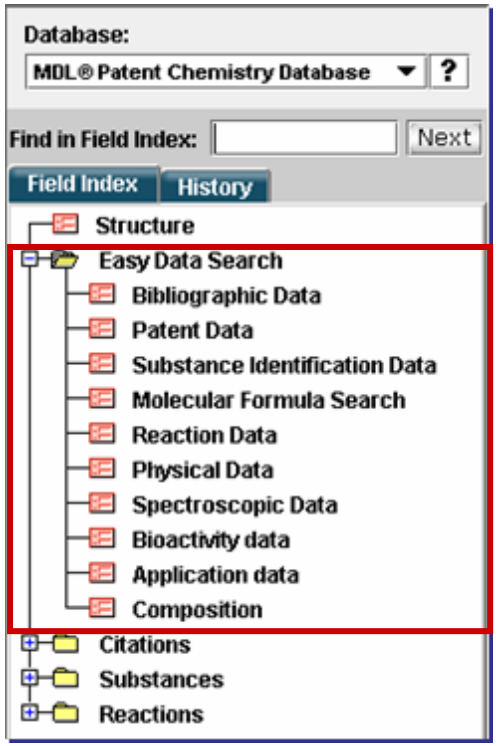
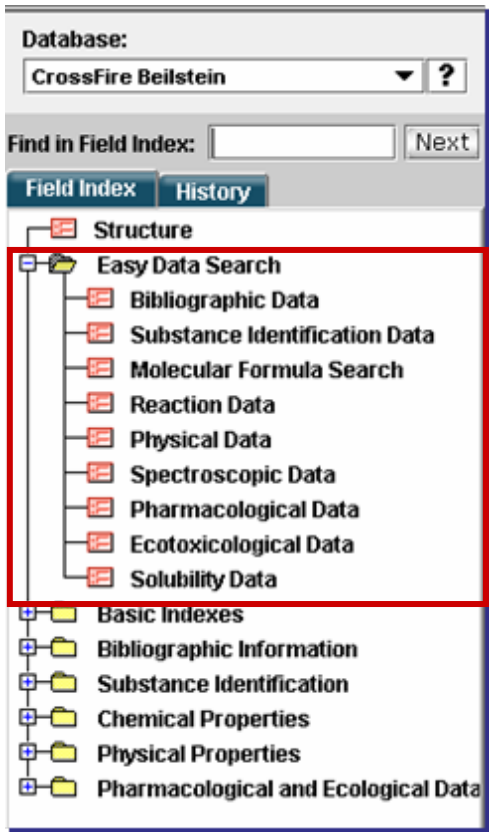
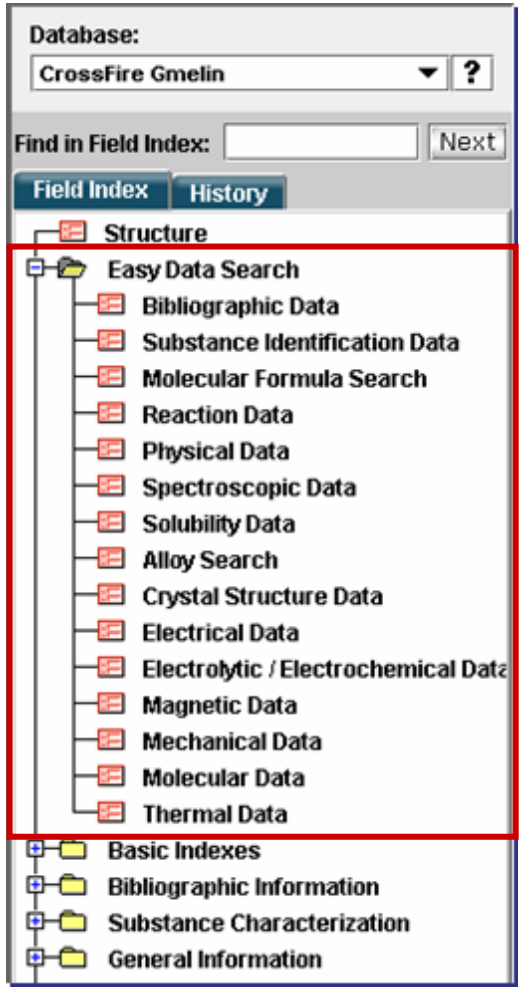
Predefined Search Forms

In addition to the default forms, the CrossFire Beilstein, CrossFire Gmelin, and the Patent Chemistry databases have a series of predefined forms.

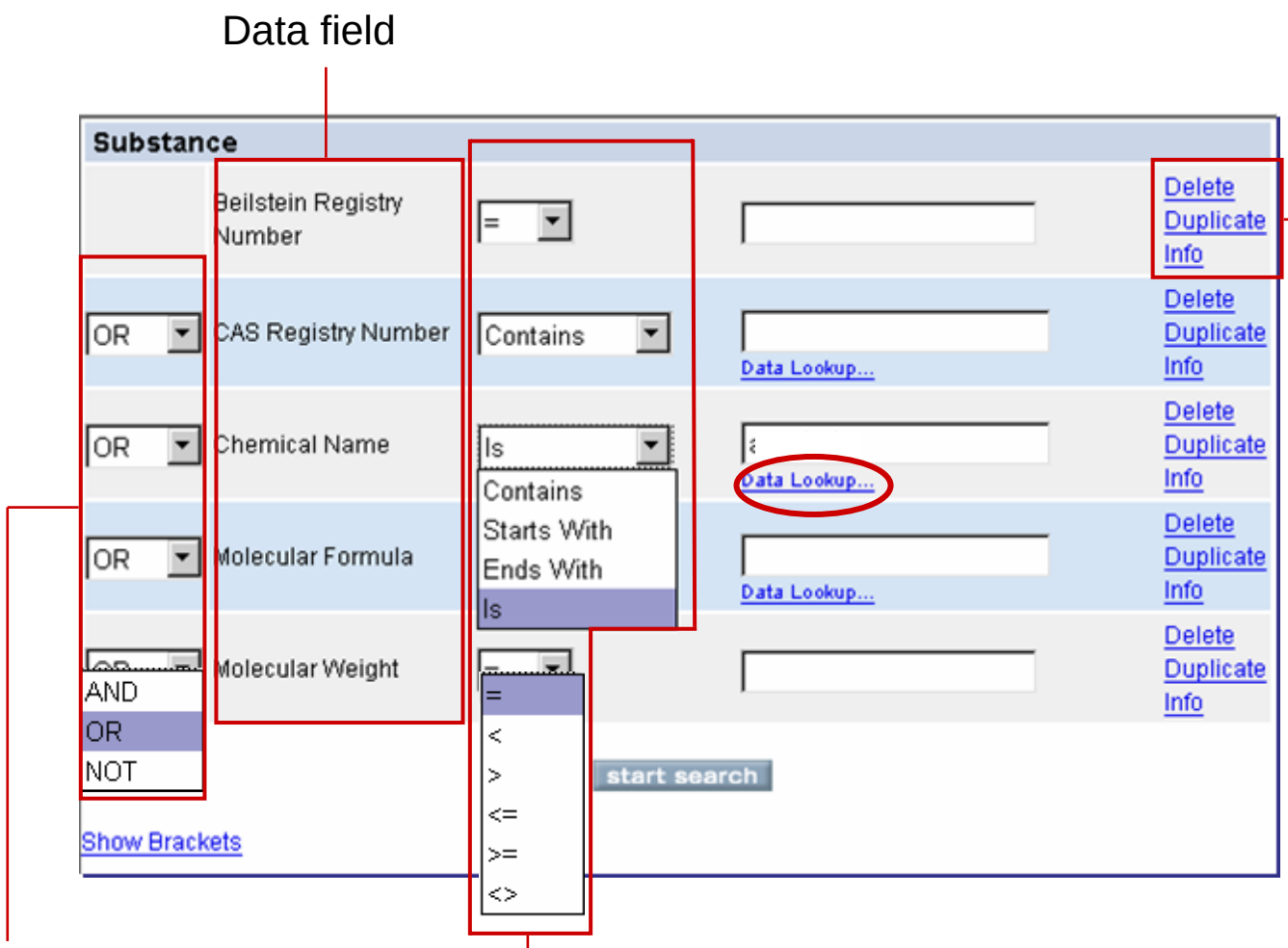






Symyx

Data Search Features



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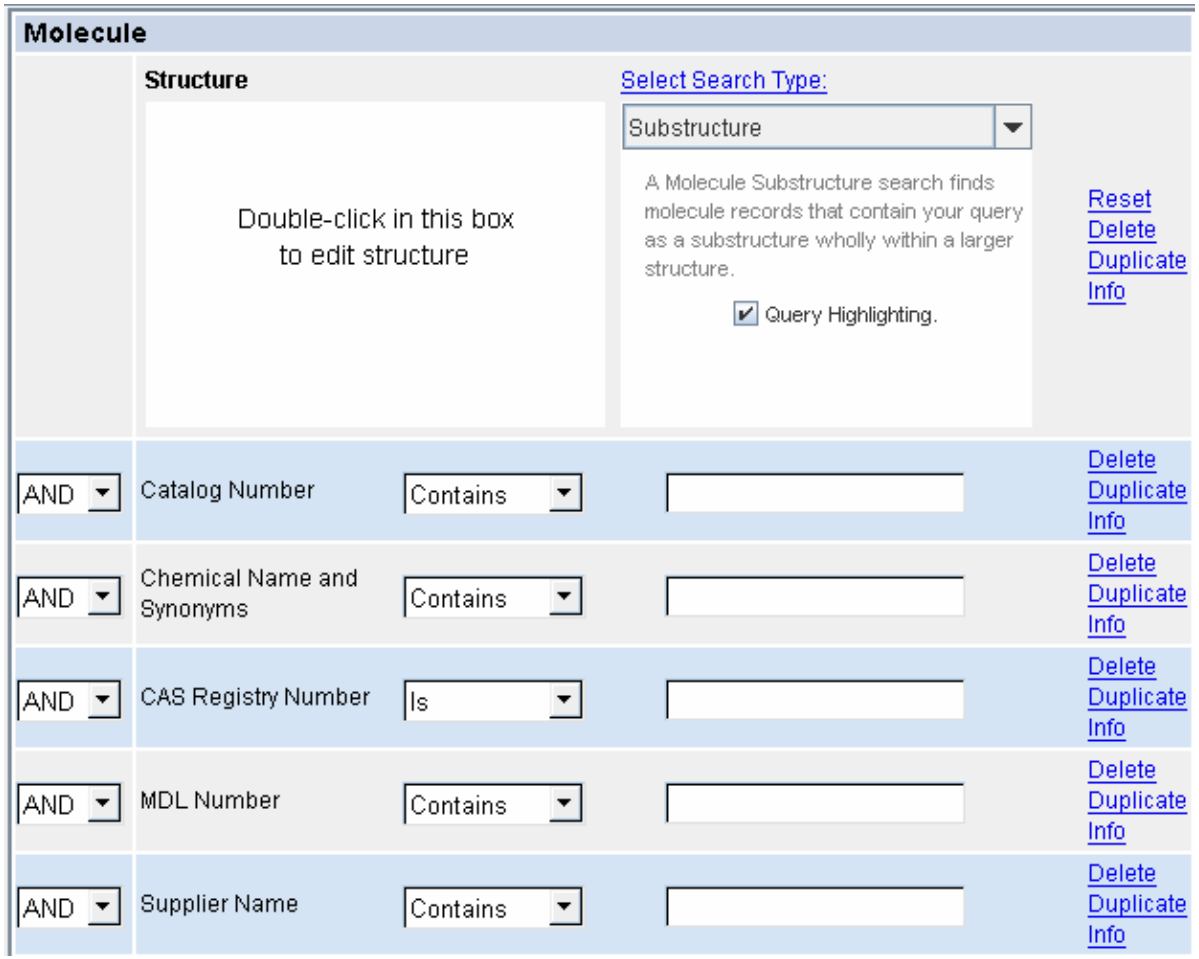
Data Operators and Wildcards

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

Search for a Specific Compound

Conduct two different data searches to retrieve the compound acyclovir (CAS number 59277-89-3) from the ACD database.



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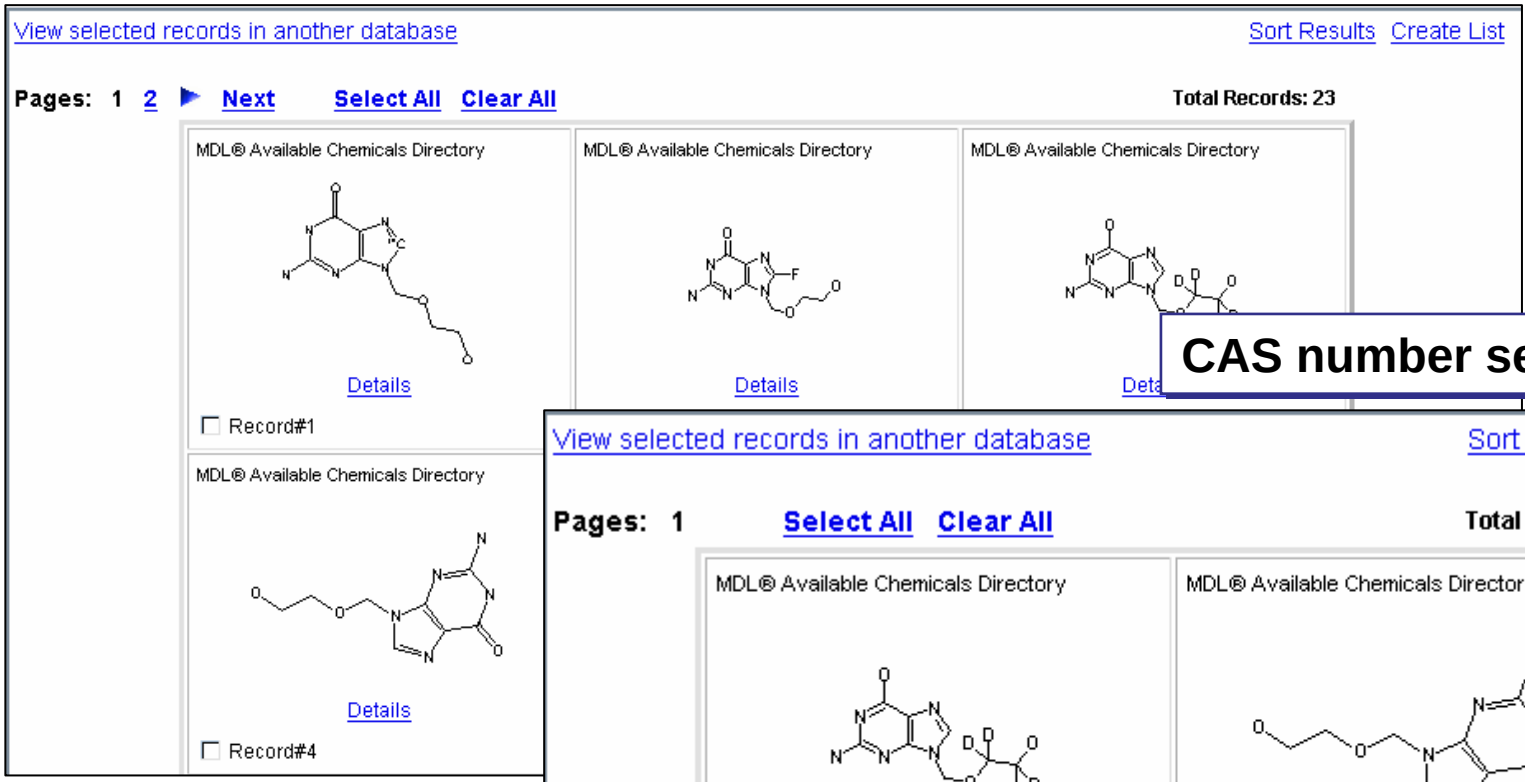
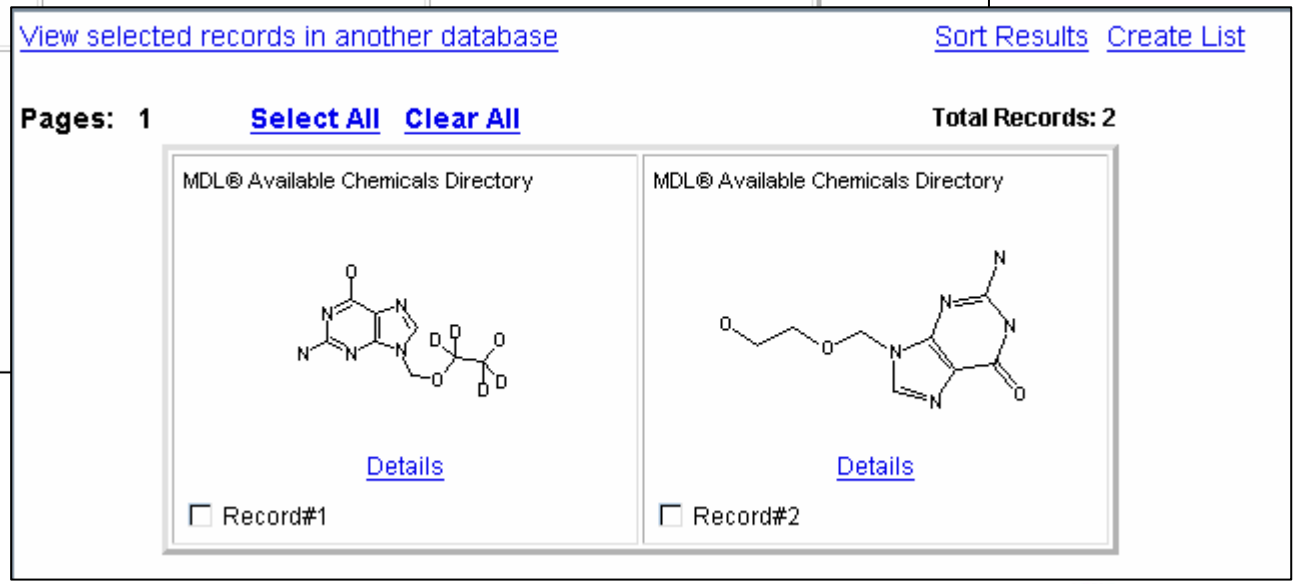
Search Results

Chemical Name search results

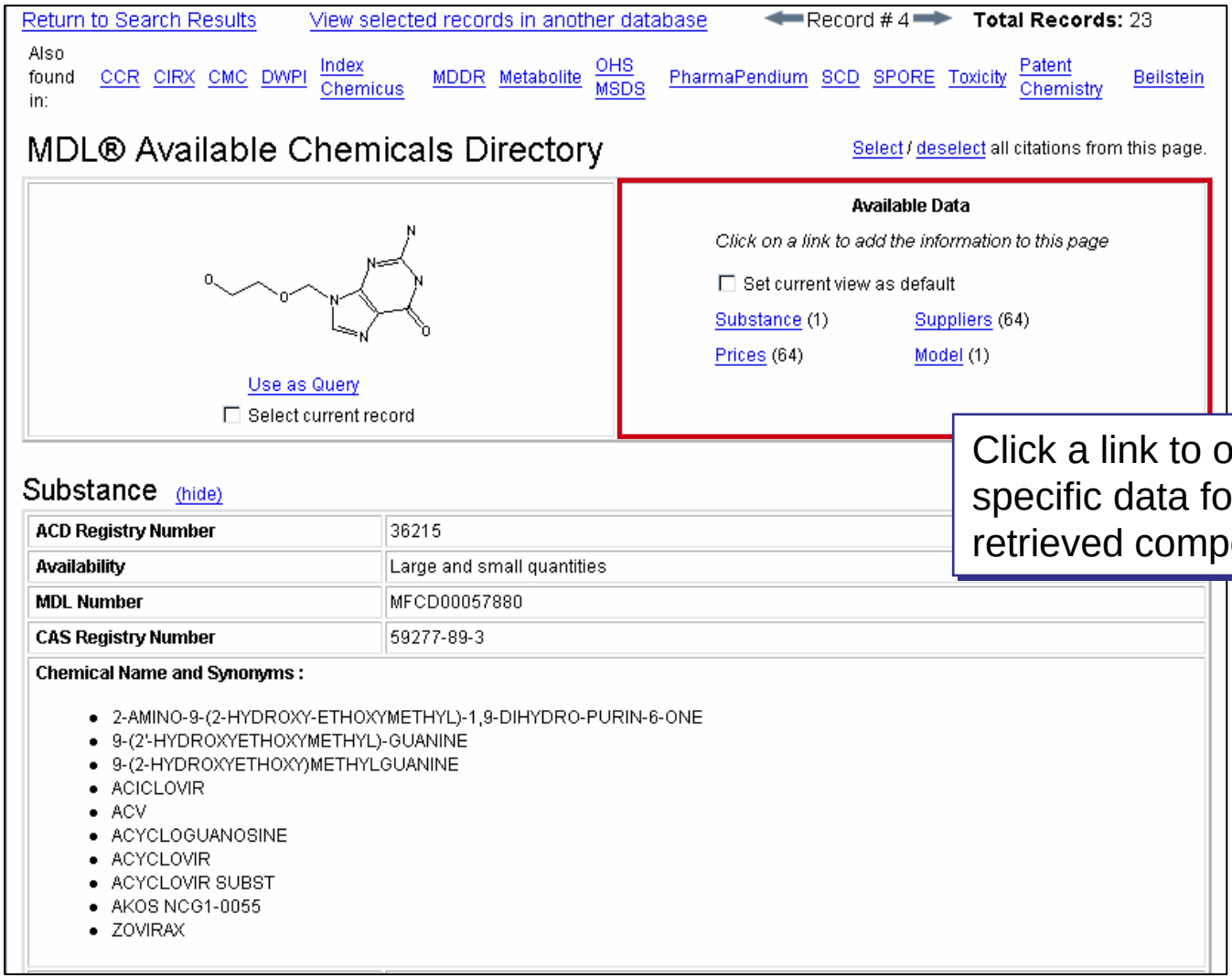


CAS number search results



Symyx

Link to Additional Data

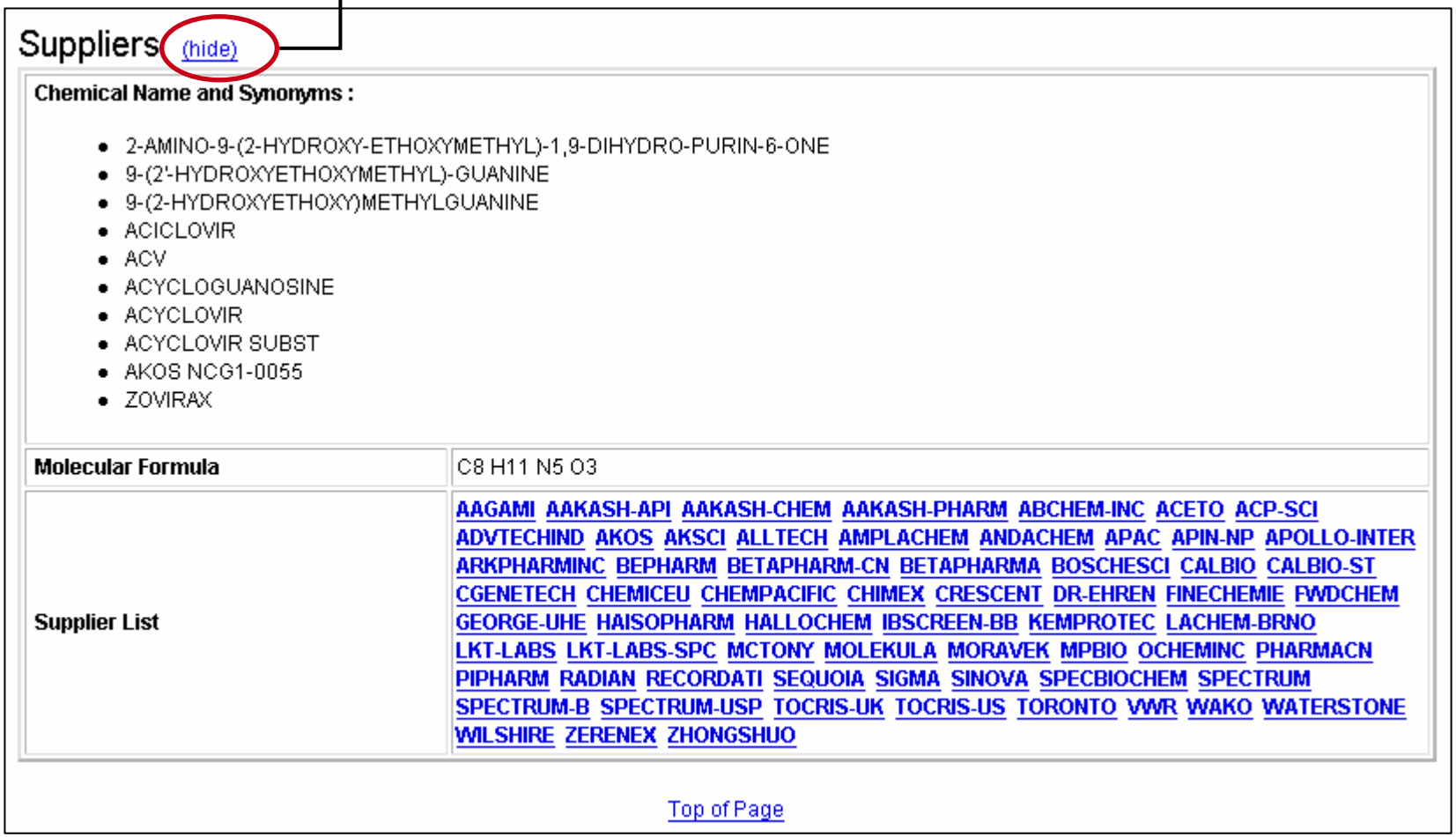


Click a link to obtain specific data for the retrieved compound.

Symyx

View Supplier Information

Displays or hides the data



Suppliers (hide)

Chemical Name and Synonyms :

- 2-AMINO-9-(2-HYDROXY-ETHOXYMETHYL)-1,9-DIHYDRO-PURIN-6-ONE
- 9-(2'-HYDROXYETHOXYMETHYL)-GUANINE
- 9-(2-HYDROXYETHOXY)METHYLGUANINE
- ACICLOVIR
- ACV
- ACYCLOGUANOSINE
- ACYCLOVIR
- ACYCLOVIR SUBST
- AKOS NCG1-0055
- ZOVIRAX

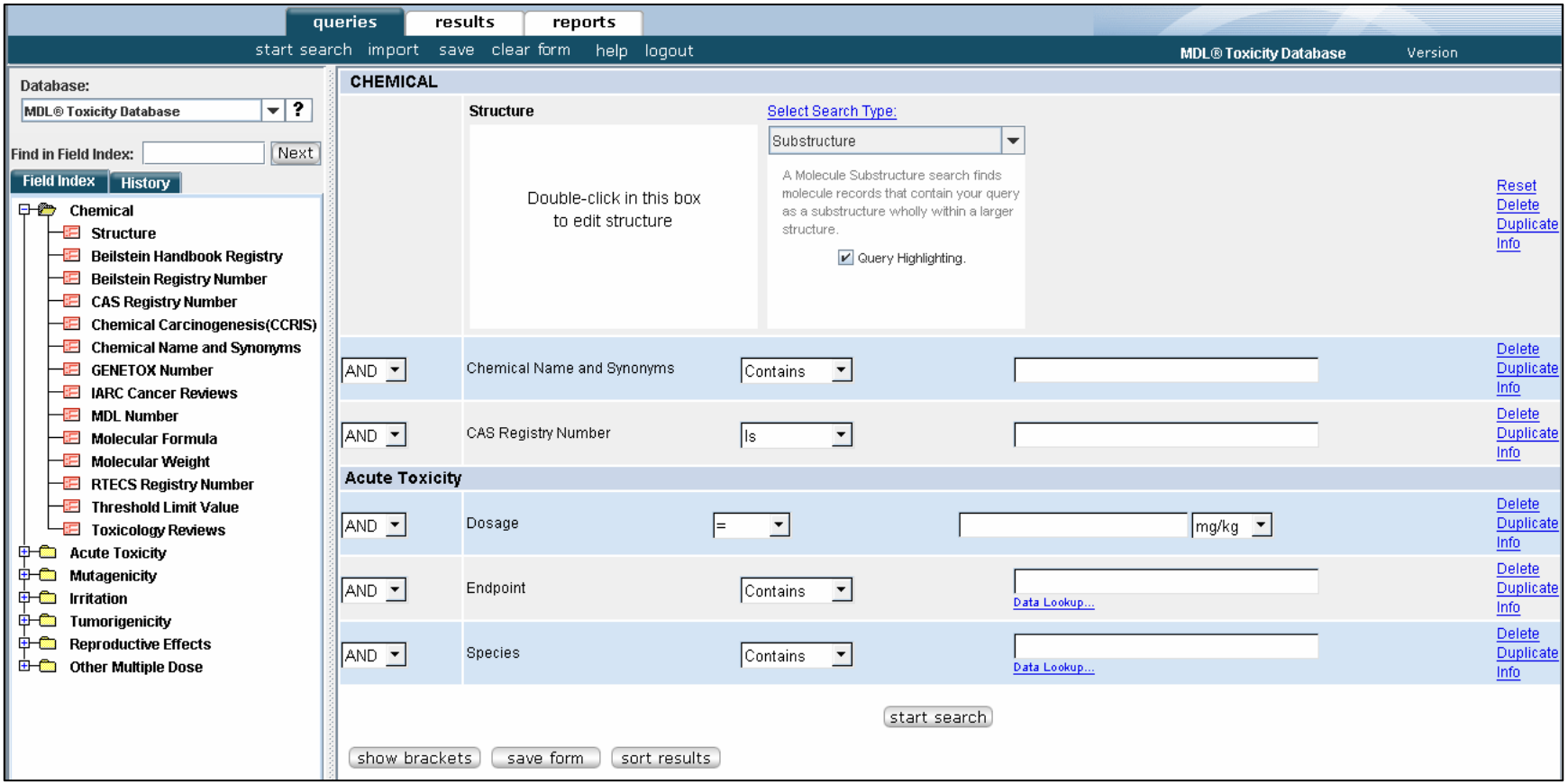
Molecular Formula	C8 H11 N5 O3
Supplier List	AAGAMI AAKASH-API AAKASH-CHEM AAKASH-PHARM ABCHEM-INC ACETO ACP-SCI ADVTECHIND AKOS AKSCI ALLTECH AMPLACHEM ANDACHEM APAC APIN-NP APOLLO-INTER ARKPHARMINC BEPHARM BETAPHARM-CN BETAPHARMA BOSCHESCI CALBIO CALBIO-ST CGENETECH CHEMICEU CHEMPACIFIC CHIMEX CRESCENT DR-EHREN FINECHEMIE FWDCHEM GEORGE-UHE HAISOPHARM HALLOCHEM IBSCREEN-BB KEMPROTEC LACHEM-BRNO LKT-LABS LKT-LABS-SPC MCTONY MOLEKULA MORAVEK MPBIO OCHEMINC PHARMACN PIPHARM RADIAN RECORDATI SEQUOIA SIGMA SINOVA SPECBIOCHEM SPECTRUM SPECTRUM-B SPECTRUM-USP TOCRIS-UK TOCRIS-US TORONTO VWR WAKO WATERSTONE WILSHIRE ZERENEX ZHONGSHUO

Top of Page

Symyx

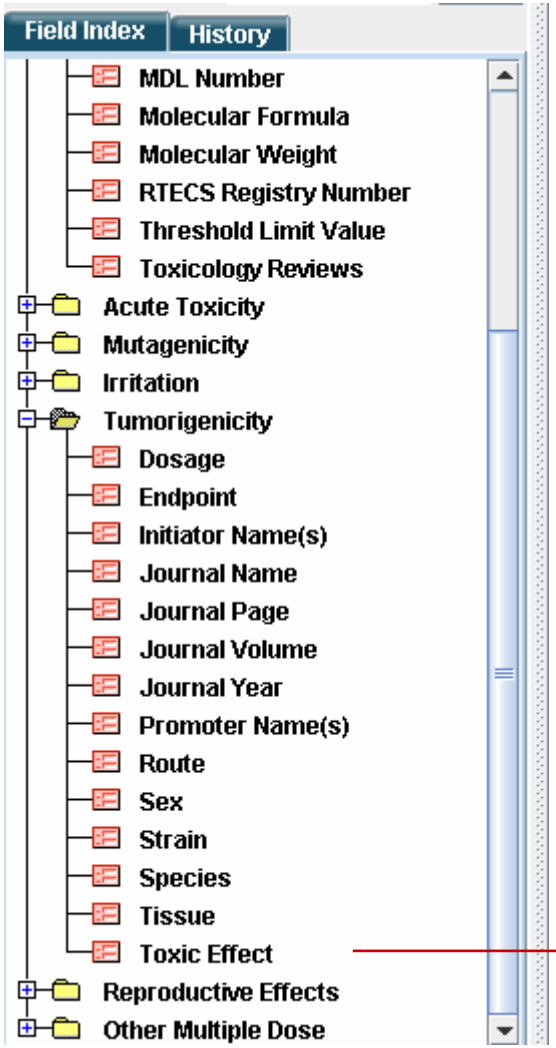
Search the Toxicity Database

Conduct a search, using the Toxicity database to retrieve compounds that have tumorigenicity data associated with fatty liver degeneration.



Symyx

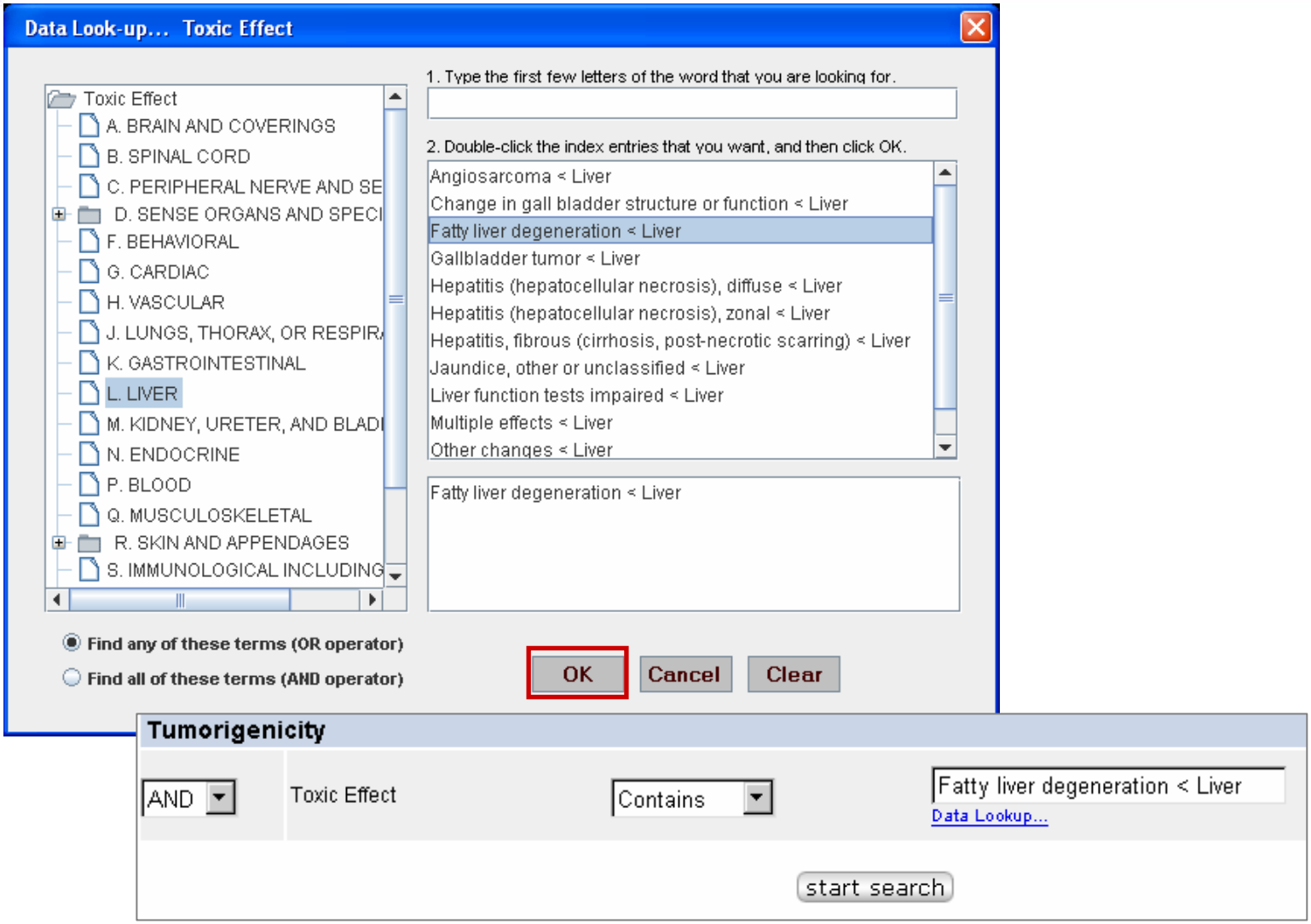
Create a Custom Form



Double-click to add field to query form

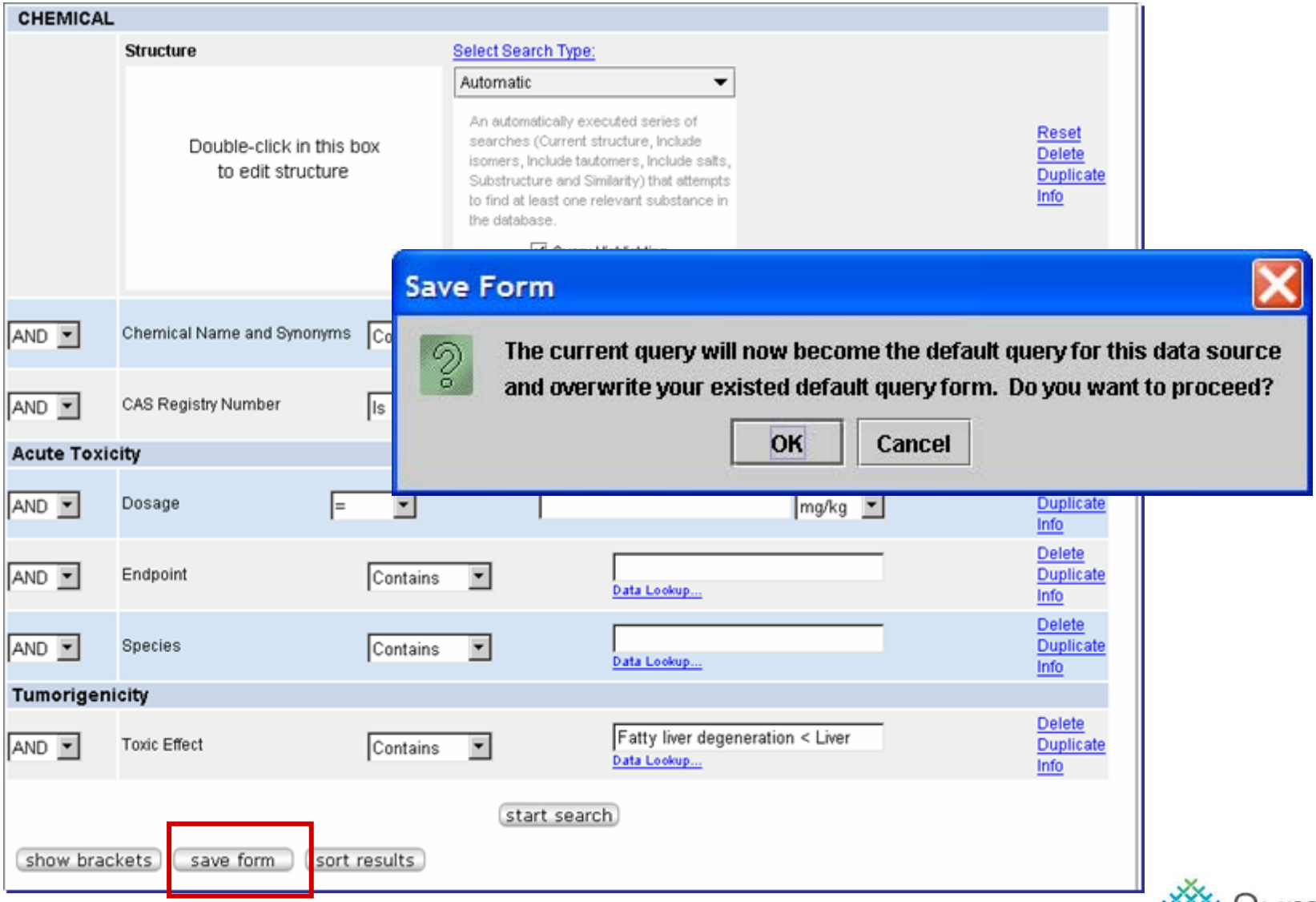
Symyx

Enter the “Toxic Effect” Data Constraint



Symyx

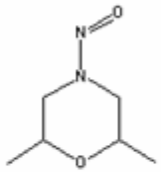
Saving a Form



Symyx

Tumorigenicity Data

MDL® Toxicity Database



Use as Query

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

Chemical (1) Acute Toxicity (4)

Mutagenicity (35) Tumorigenicity (35)

Review (1) Model (1)

Tumorigenicity (hide)

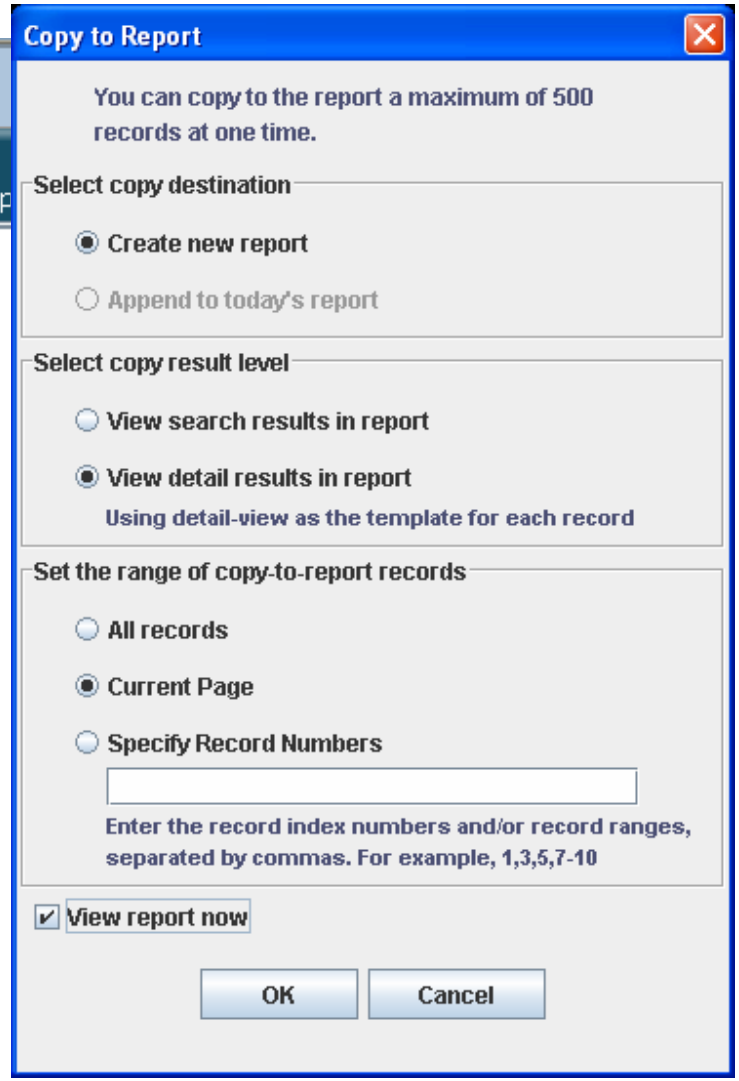
Full Citation 1 of 35	
Journal of the National Cancer Institute 64,529,1980	
Source ID : QE2150000	**Source :** RTECS
Chemical Name	MORPHOLINE, 2,6-DIMETHYL-N-NITROSO-
Species	guinea pig
Route	ORAL
Dosage	400 MG/KG/23W-I
Endpoint :	TD
Endpoint (Incidence) :	(Carcinogen, Carcinogen+Inhibitor, %Diff., Significance)
Endpoint (Multiplicity) :	
Endpoint (Latency) :	(Carcinogen, Carcinogen+Inhibitor, Significance)

Toxic Effects :

- Carcinogenic by RTECS criteria < Tumorigenic
- Fatty liver degeneration < Liver
- Tumors < Liver

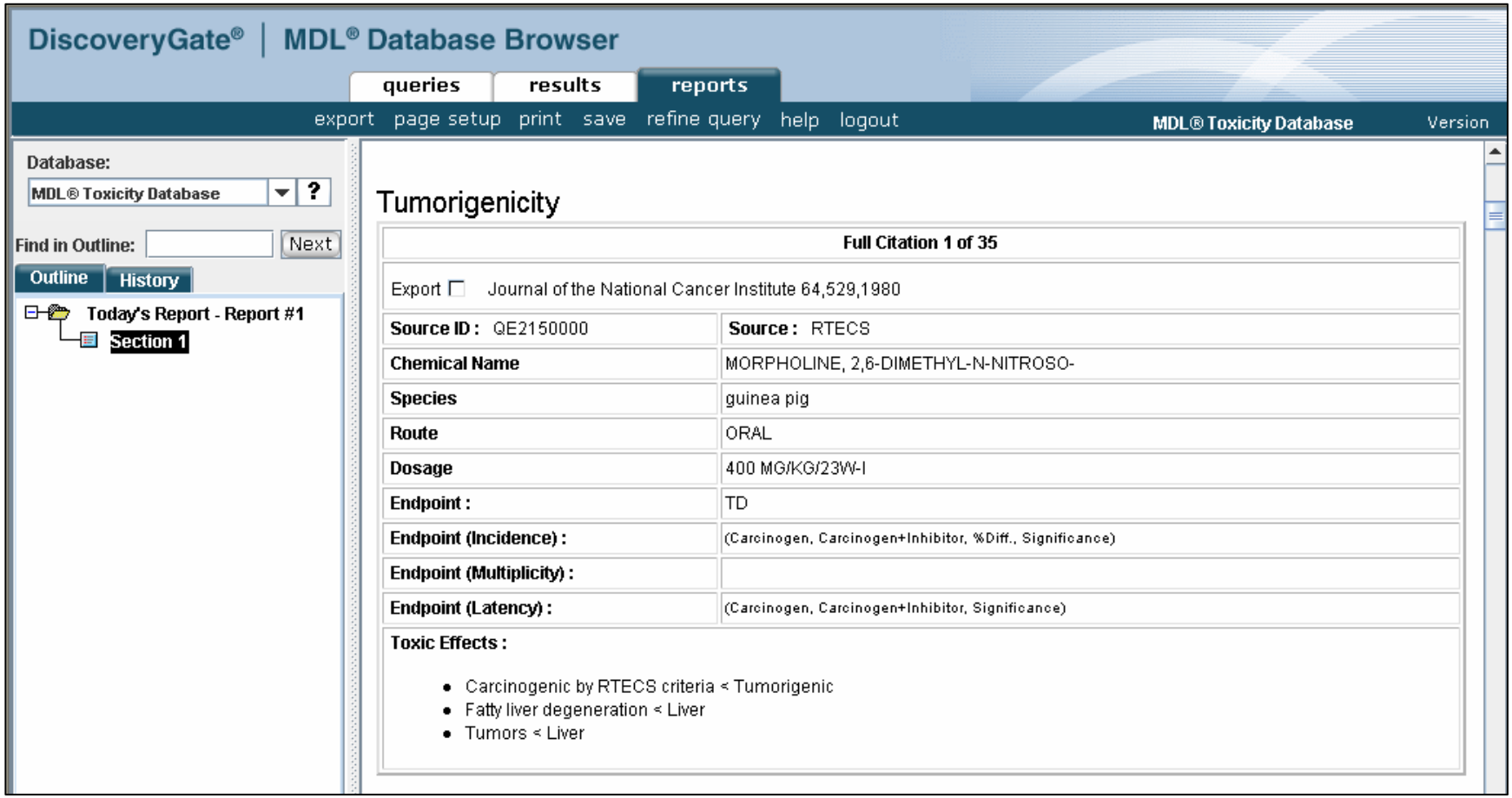
Symyx

Creating a Report



Symyx

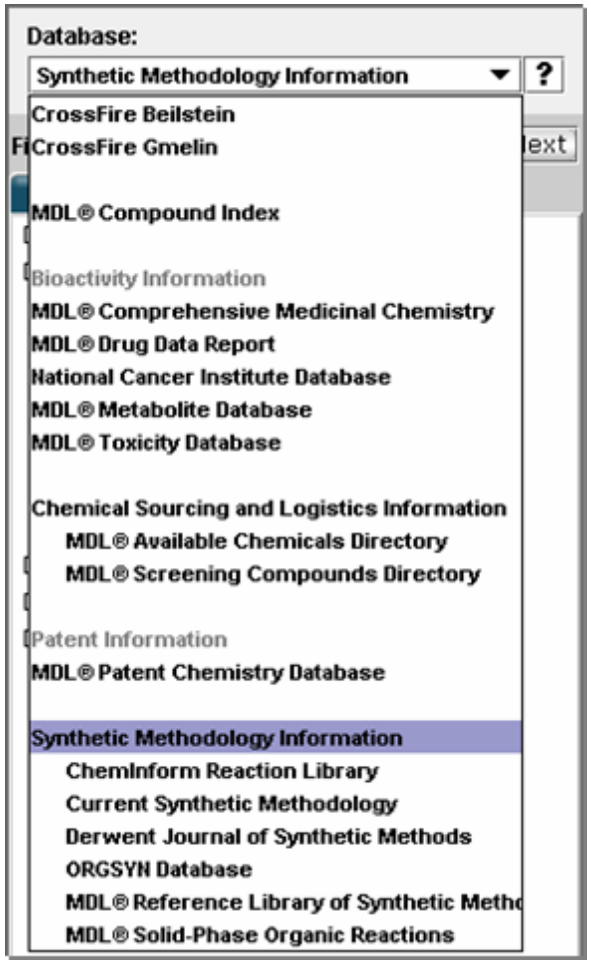
Reports tab



Symyx

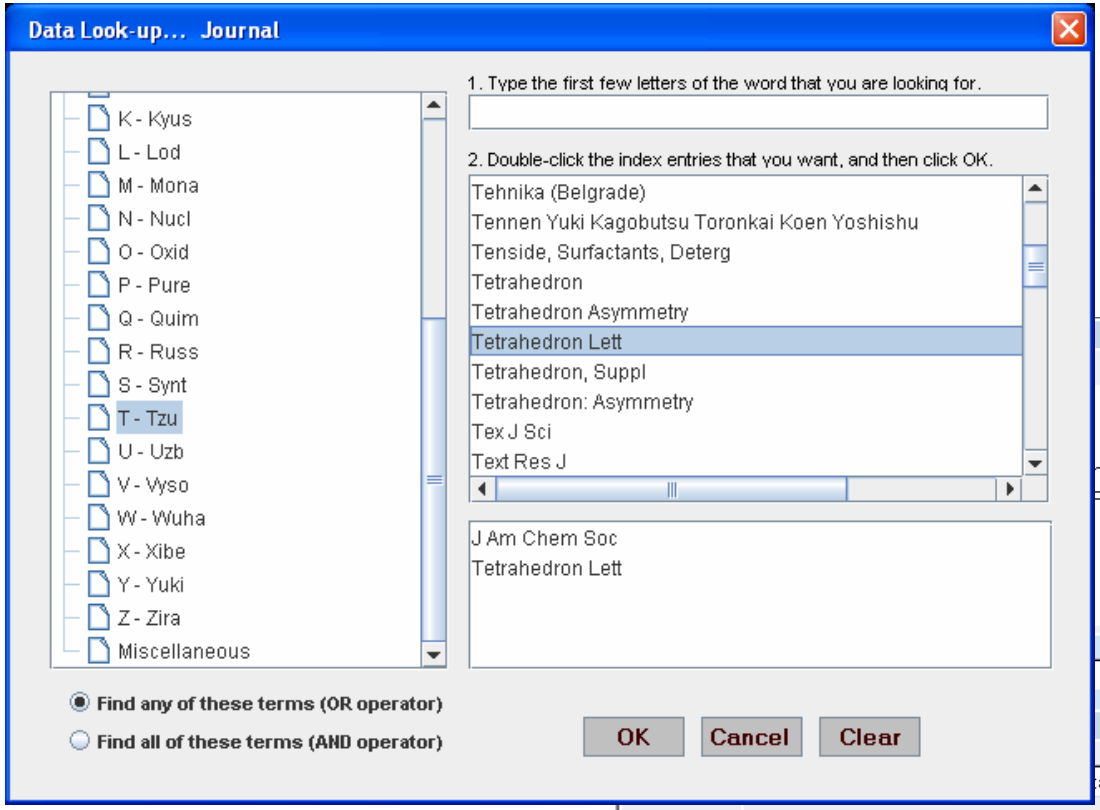
Retrieving Reactions using a Data Query

Conduct a search to retrieve hydrogenation reactions published in the Journal of the American Chemical Society or Tetrahedron Letters.

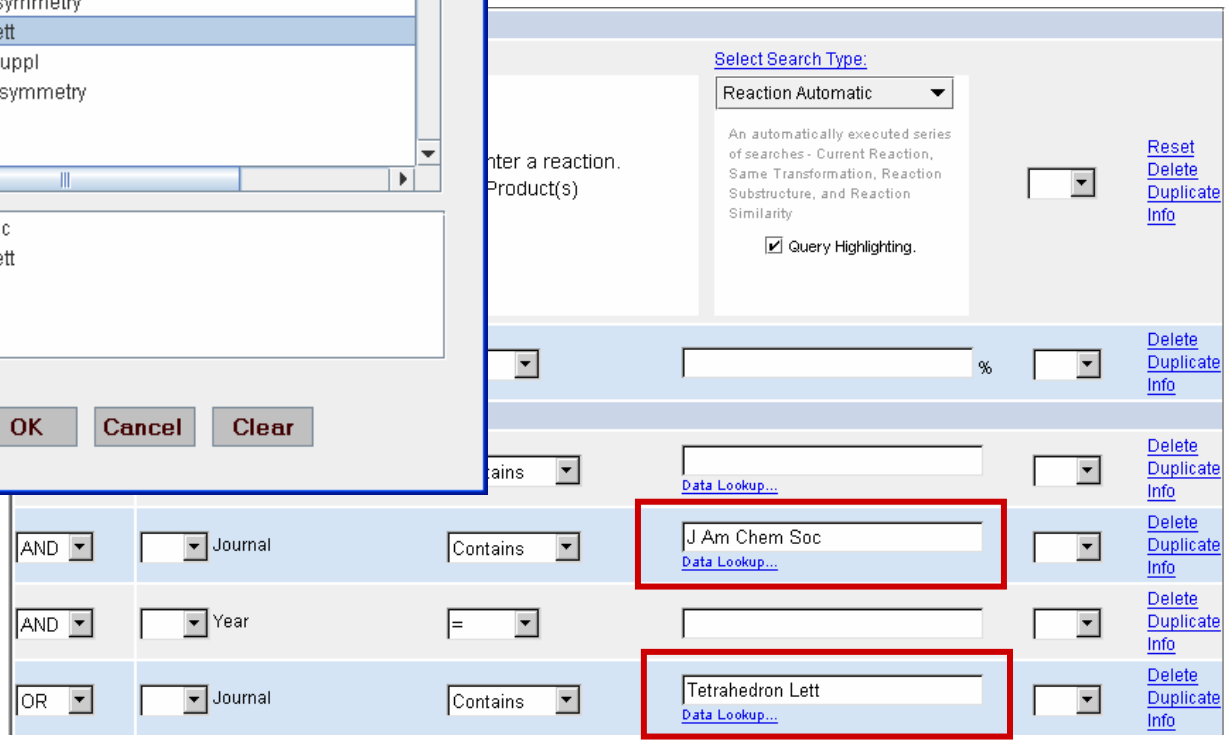


Symyx

Additional Data Fields

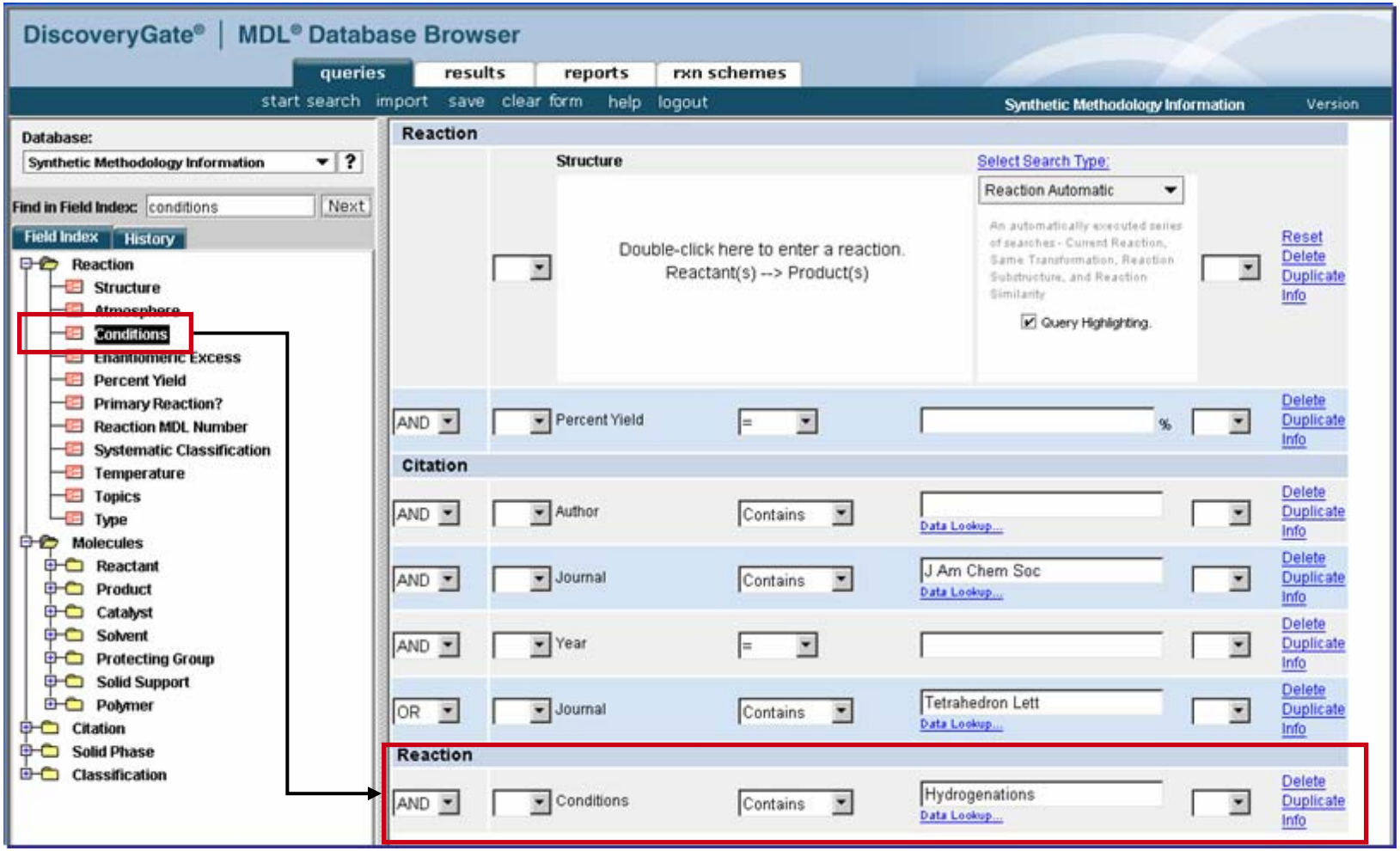


When multiple selections are made in the Data Lookup dialog box additional fields are added to the form



Symyx

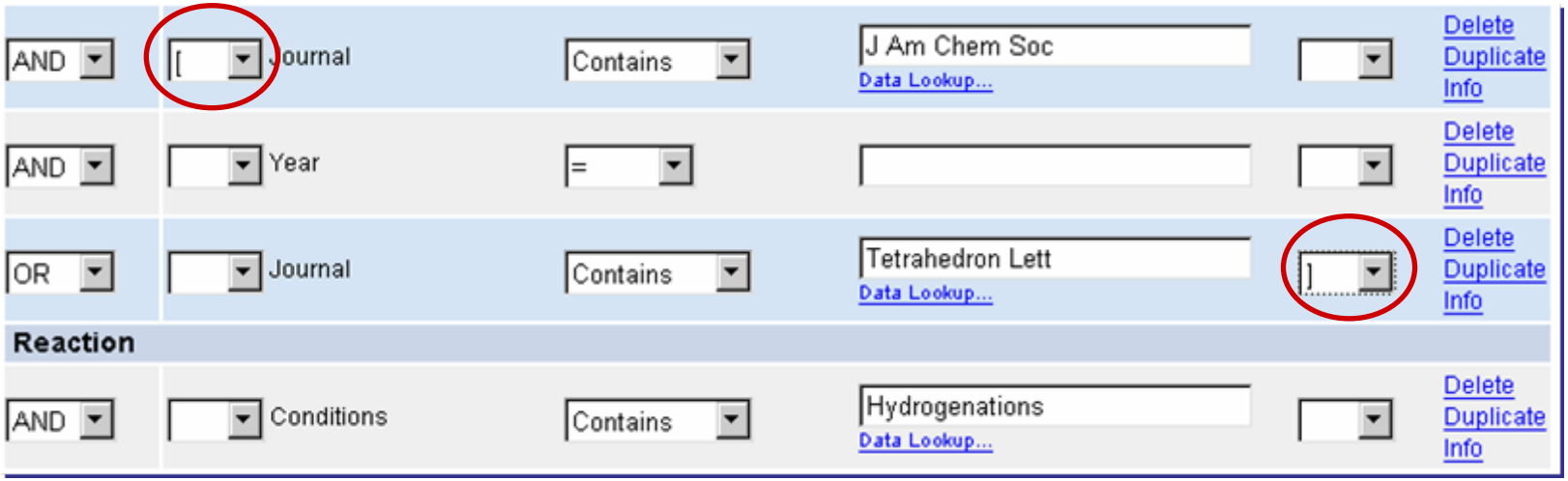
Manually Add a Data Field



Use the Field Index to find the data field. Double-click to add it to the form.

Symyx

Setting Search Logic

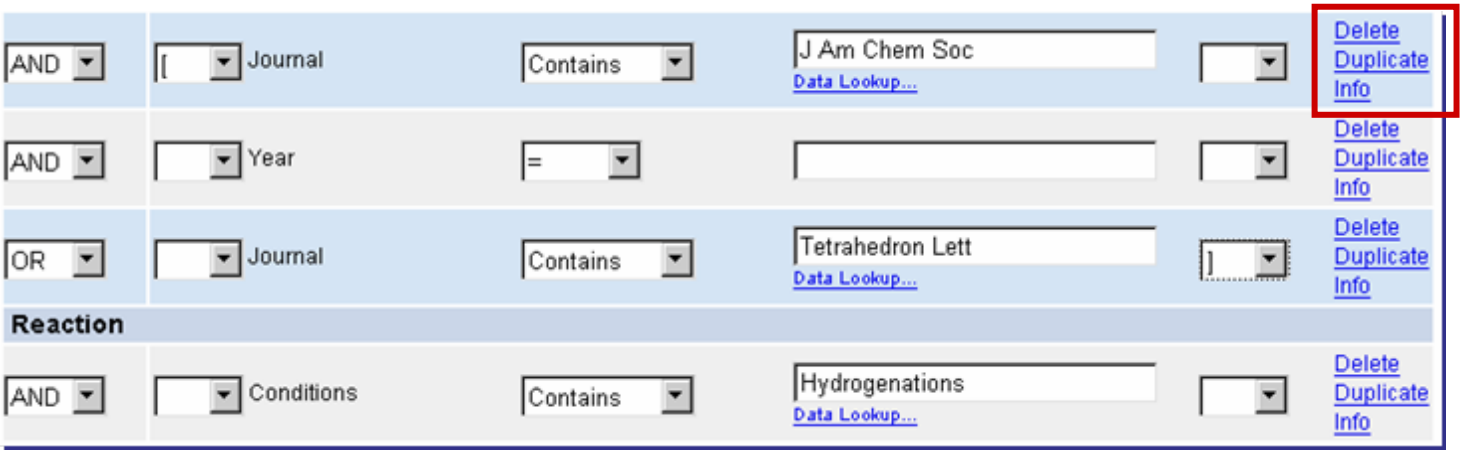


Setting the parenthetical statement forces the search.

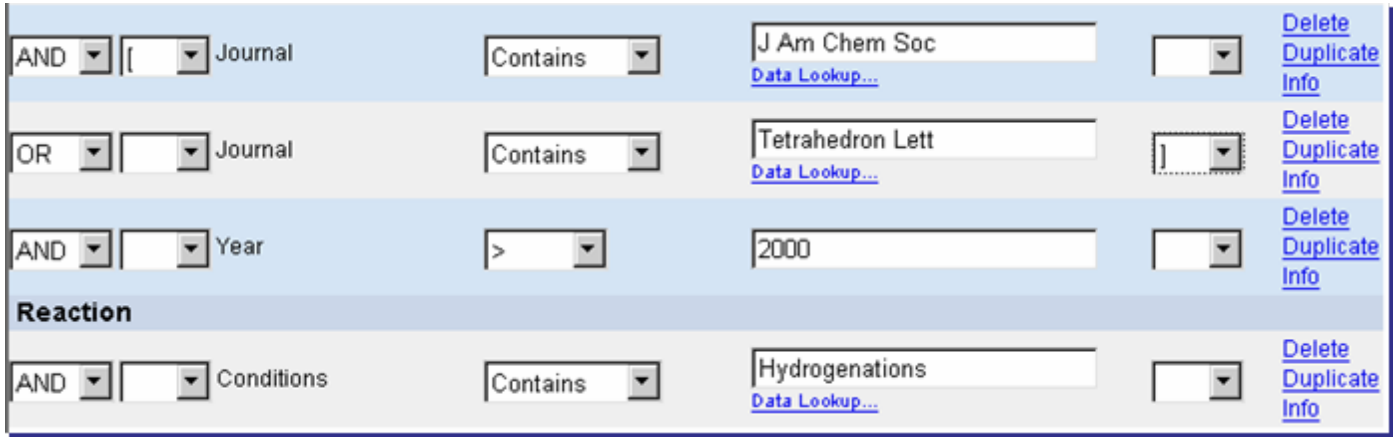
(Journal Contains J. Am.Chem.Soc. OR Journal Contains Tetrahedron Letters) AND Conditions Contains Hydrogenations

Setting Parenthetical Statements

Initial search



Modified search

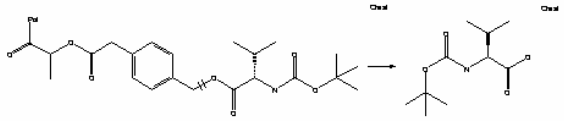


Manually adjust fields to create the correct parenthetical statements.

Symyx

Search Results

MDL® Solid-Phase Organic Reactions



Use as Query

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

Reaction Details (4) Reactant (1)

Product (1)

Reaction Details (hide)

RSPO69000650 **Reaction Variation 1 of 4**

Product no.	% Yield	Grade	%cs	%ds	%de	%ee	Reactant no.	Reactant Grade
1	50	(S)-isomer	100				1	(S)-isomer

Step no.	Catalysts and Solvents	Catalyst ID click ID for details	Solvent ID click ID for details
1	H2 Pd(O-Ac)2 (cat.) DMF	18137 48	9

Detailed Data	Conditions References	Solid Support Protecting Group	External Registry No.	Path	Step
			698000501	I	4 OF 4

TAM, J. P.; TJOENG, F. S.; MERRIFIELD, R. B.; J Am Chem Soc [JACSAT] 1980, 102 (19), 6117-6127.
TAM, J. P.; TJOENG, F. S.; MERRIFIELD, R. B.; Tetrahedron Lett [TELEAY] 1979, 51, 4935-4938.
WHITNEY, D. B.; TAM, J. P.; MERRIFIELD, R. B.; Tetrahedron [TETRAB] 1984, 40 (21), 4237-4244.

Conditions

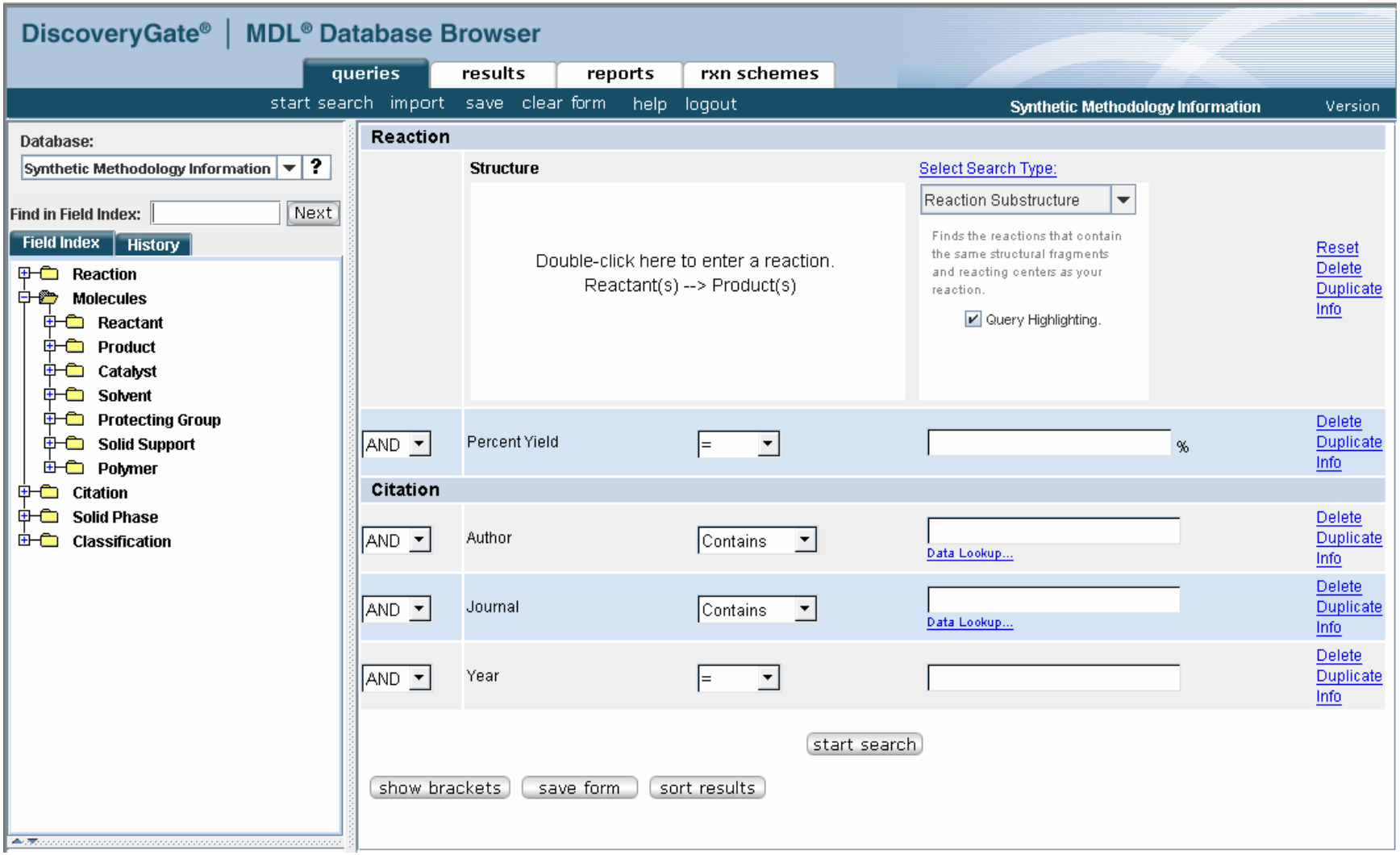
Step	1
Hours	17
Temp (C)	50
Conditions	Hydrogenations Transition Metal Salts Thermal

Symyx

Reaction Searching

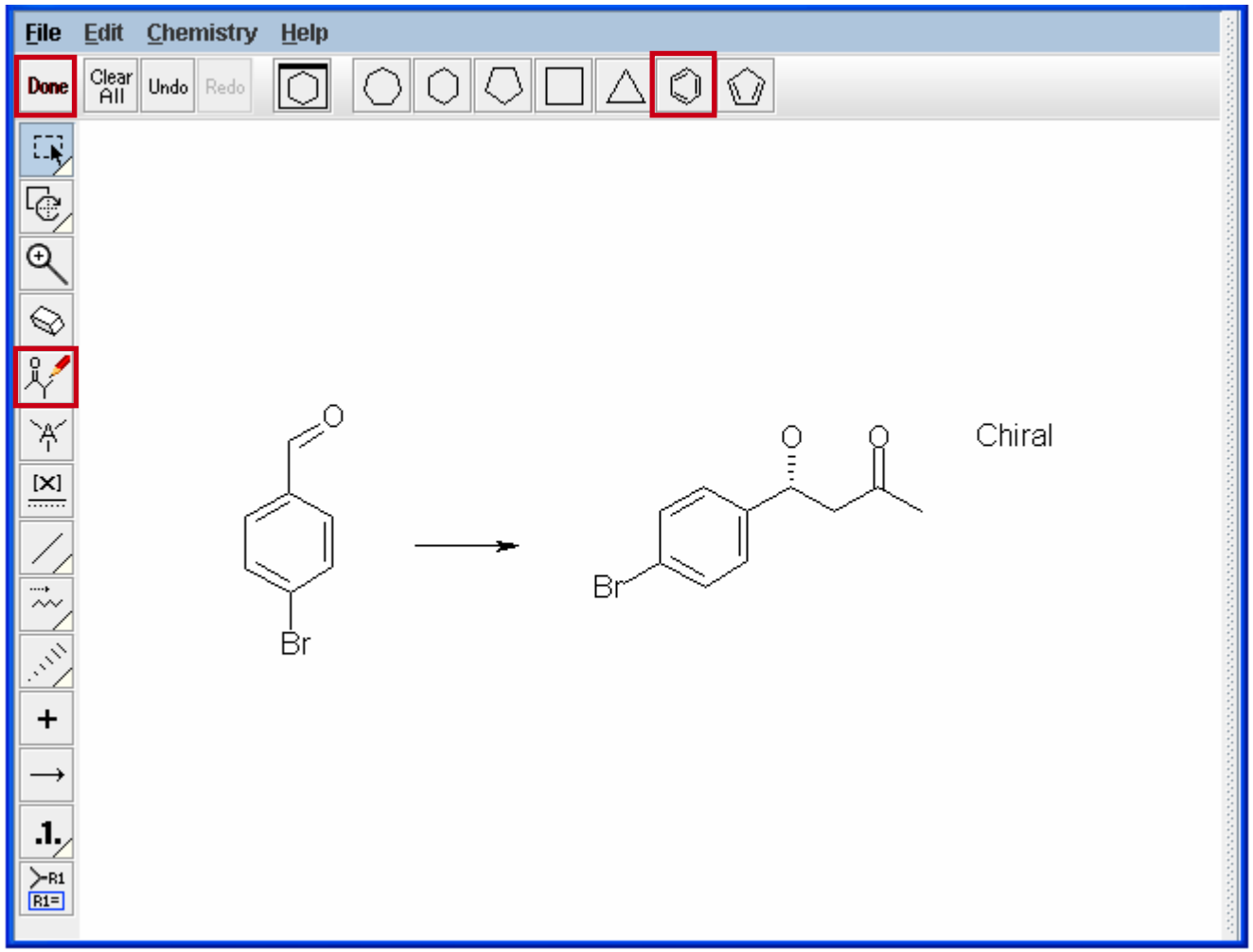
- In this module, you will learn how to:
  - Conduct a Reaction Substructure Search
  - View Reactant and Product Data from Another Database
  - Link to Literature References
  - Find Similar Reactions

Synthetic Methodology Information



Symyx

Draw the Reaction Query in Symyx Draw

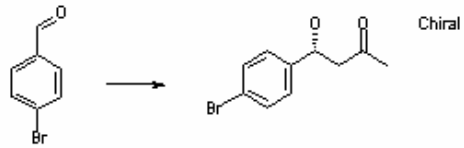


Symyx

Conduct a Reaction Substructure Search

Reaction

Structure



Select Search Type:

Reaction Substructure

Finds the reactions that contain the same structural fragments and reacting centers as your reaction.

☑ Query Highlighting.

Reset
Delete
Duplicate
Info

AND	Percent Yield	=	%	Delete Duplicate Info

Citation

AND	Author	Contains	Data Lookup...	Delete Duplicate Info
AND	Journal	Contains	Data Lookup...	Delete Duplicate Info
AND	Year	=		Delete Duplicate Info

start search

show brackets | save form | sort results

Symyx

Search Results

queries | results | reports | rxn schemes

export selected citations | page setup | print | save | refine query | lists | help | logout

Synthetic Methodology Information

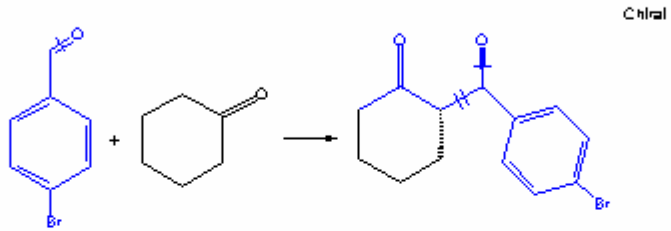
View selected records in another database

Sort Results | Create List

Pages: 1 2 ▶ Next Select All Clear All

Total Records: 18

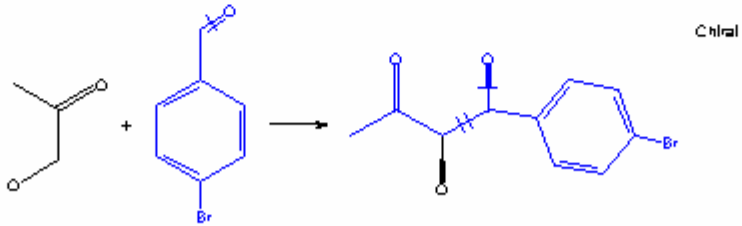
ChemInform Reaction Library



Details | Synthesize Reactants | Find Similar Reactions

☐ Record#1

ChemInform Reaction Library



Details | Synthesize Reactants | Find Similar Reactions

☐ Record#2

Symyx

Details View

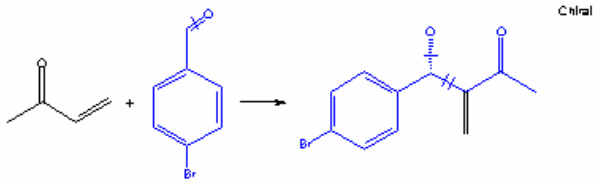
Return to Search Results | View selected records in another database | Find Similar Reactions | Record # 12 | Total

Records: 18

Also found in: ACD | DWPI | Index Chemicus | NCI | OHS MSDS | PubChem | SCD | Toxicity | Patent Chemistry | Beilstein

ChemInform Reaction Library

Select / deselect all citations from this page.



Use as Query

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

Reaction Details (1) Reactant (2)

Product (1)

Reaction Details (hide)

RXCI03010134 **Reaction Variation 1 of 1**

Product no.	% Yield	Grade	%cs	%ds	%de	%ee	Reactant no.	Reactant Grade
1	31	(S)-isomer	100			27		

Step no.	Catalysts and Solvents	Catalyst ID click ID for details	Solvent ID click ID for details
1	COMPOUND182 [oxygen-bridged quinidine deriv.] (cat.) D-proline (cat.) DMF	667533 2806	38

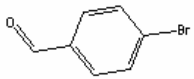
Symyx

ACD Data for Reactant 1

Return to Synthetic Methodology Information Record # 1 → **Total Records:** 3

MDL® Available Chemicals Directory

Select / deselect all citations from this page.



Available Data

Click on a link to add the information to this page

☐ Set current view as default

Substance (1) Suppliers (67)

Prices (67) Model (1)

Substance (hide)

ACD Registry Number	3253
Availability	Large and small quantities
MDL Number	MFCD00003377
CAS Registry Number	1122-91-4

Chemical Name and Synonyms :

- 4-BBA
- 4-BROMOBENZALDEHYDE
- 4-BROMOBENZYLALDEHYDE
- AKOS BBS-00003194
- LABOTEST-BB LT00929178
- LABOTEST-BB LT03333287
- P-BROMOBENZALDEHYDE

Molecular Formula	C7 H5 Br O
Molecular Weight	185.02
Rule of Five	0
Computed partition coefficent (CLogP)	2.6
Molecular weight of largest fragment	185.019
Number of proton acceptors	1
Number of proton donors	0
Number of rotatable bonds (TDF)	0

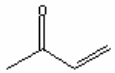
Symyx

ACD Data for Reactant 2

Return to Synthetic Methodology Information ← Record # 2 → **Total Records:** 3

MDL® Available Chemicals Directory

Select / deselect all citations from this page.



Available Data

Click on a link to add the information to this page

☐ Set current view as default

Substance (1) Suppliers (35)

Prices (35) Model (1)

Substance (hide)

ACD Registry Number	8372
Availability	Large and small quantities
MDL Number	MFCD00008777
CAS Registry Number	78-94-4
Chemical Name and Synonyms : • 1-BUTEN-3-ONE • 3-BUTEN-2-ONE • METHYL VINYL KETONE • MVK • VINYL METHYL KETONE	
Molecular Formula	C4 H6 O
Molecular Weight	70.0904
Rule of Five	0
Computed partition coefficent (CLogP)	0.41
Molecular weight of largest fragment	70.09
Number of proton acceptors	1
Number of proton donors	0
Number of rotatable bonds (TDF)	0

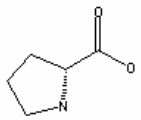
Symyx

ACD Data for Catalyst

Return to Synthetic Methodology Information ← Record # 3 **Total Records:** 3

MDL® Available Chemicals Directory

Select / deselect all citations from this page.



Available Data

Click on a link to add the information to this page

☐ Set current view as default

Substance (1) Suppliers (65)

Prices (65) Model (1)

Substance (hide)

ACD Registry Number	39629
Availability	Large and small quantities
MDL Number	MFCD00064317
CAS Registry Number	344-25-2

Chemical Name and Synonyms :

- (2R)-PYRROLIDINE-2-CARBOXYLIC ACID
- (R)-(+)-PROLINE
- (R)-PYRROLIDINE-2-CARBOXYLIC ACID
- D(+)-PROLINE
- D-2-PYRROLIDINECARBOXYLIC ACID
- D-PRO
- D-PROLINE
- D-PYRROLIDINE-2-CARBOXYLIC ACID
- H-D-PRO-OH
- H-D-PYRD(2)-OH
- PROLINE

Molecular Formula	C5 H9 N O2
Molecular Weight	115.131
Rule of Five	0
Computed partition coefficent (CLogP)	-2.15
Molecular weight of largest fragment	115.131
Number of proton acceptors	3
Number of proton donors	2

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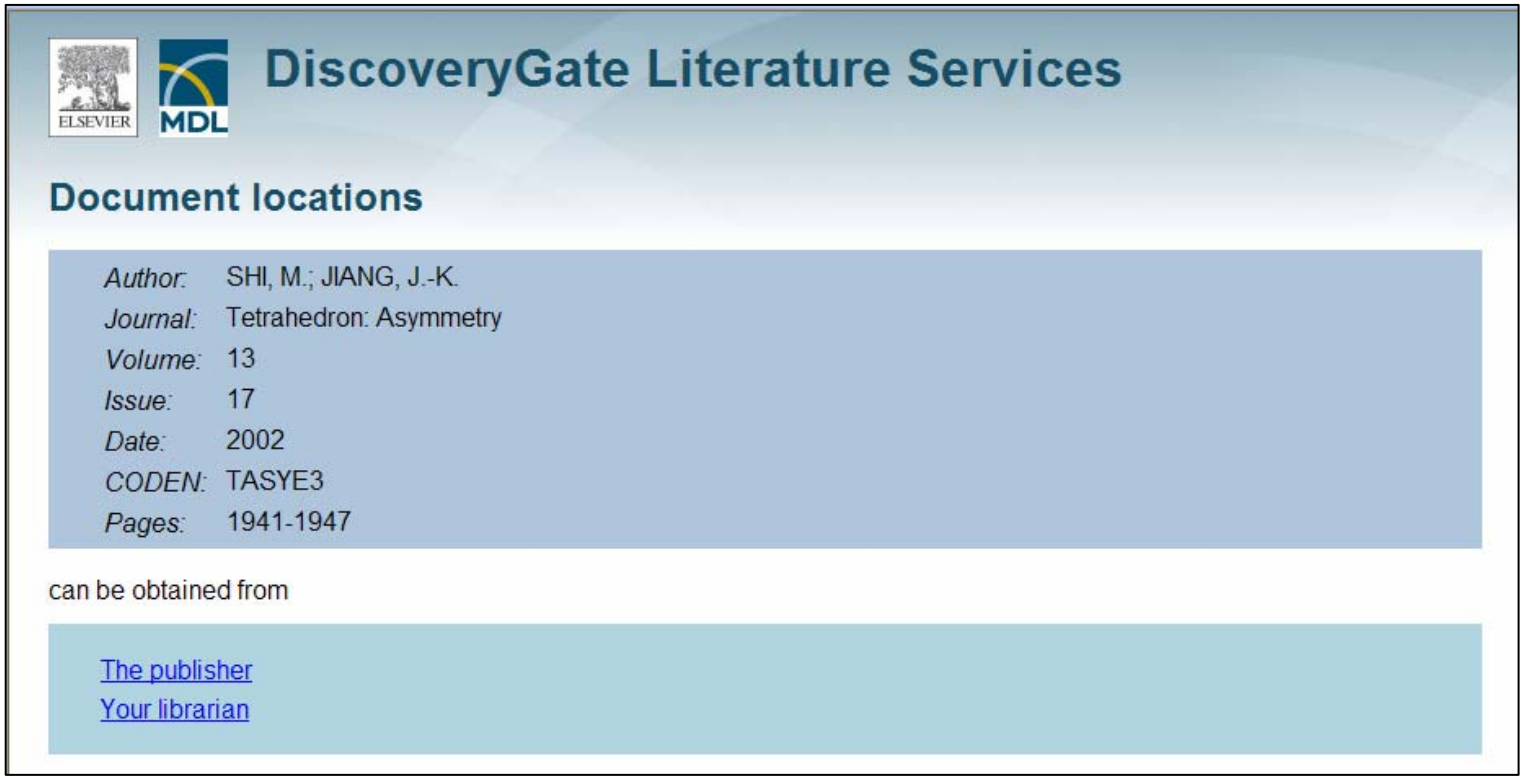
Link to Literature References

Detailed Data	Conditions References Scheme	External Registry No.	Path	Step
		1030803202	A	1 STEP

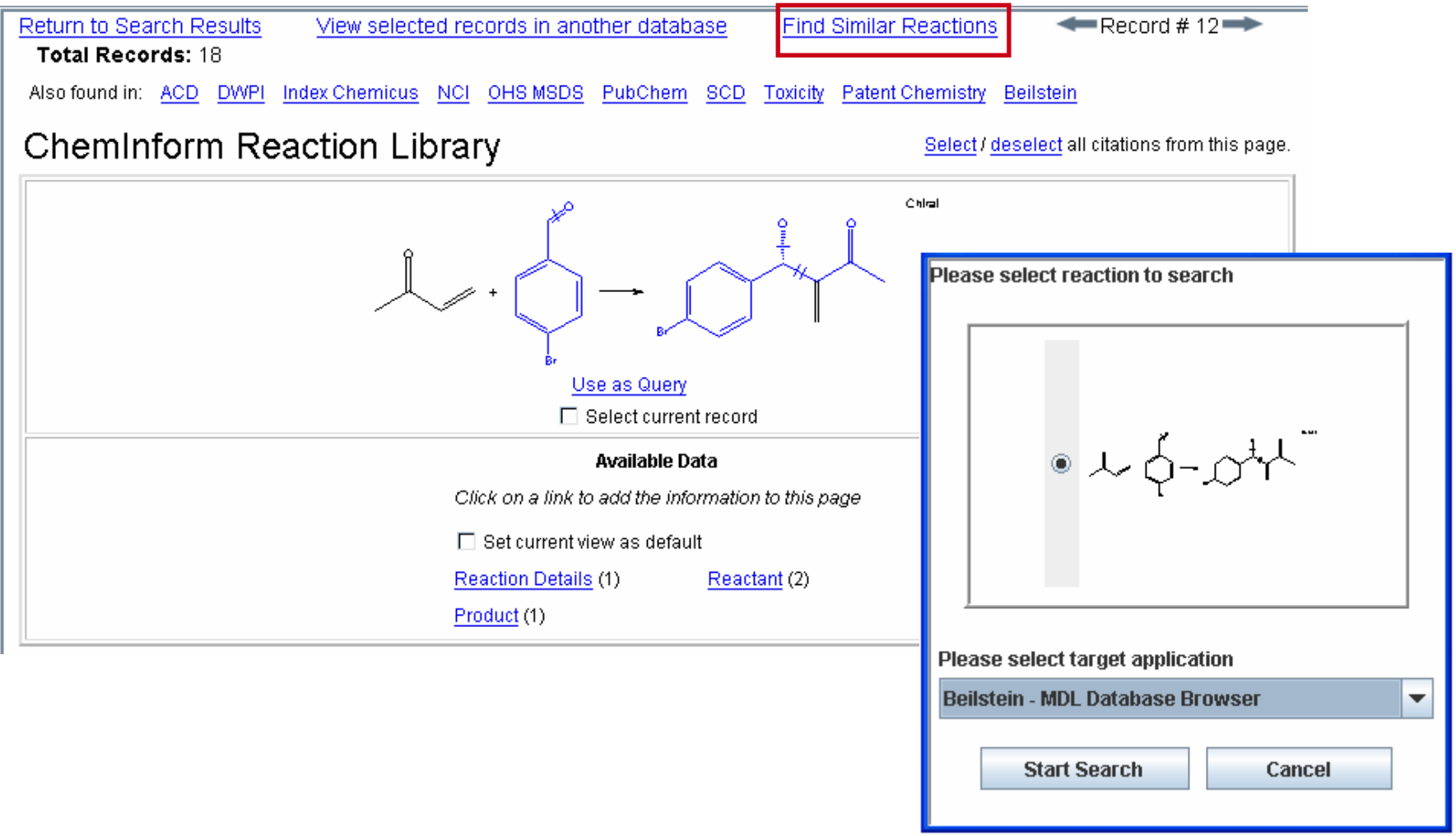
Export

☐ SHI, M.; JIANG, J.-K.; Tetrahedron: Asymmetry [TASYE3] 2002, 13 (17), 1941-1947.



Symyx

Find Similar Reactions



Symyx

Narrow Search Results

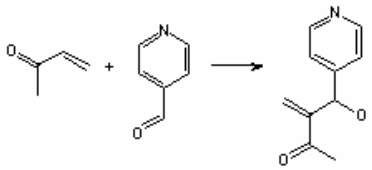
Reaction Classification Search Results

Reaction Parent.Reaction code (broad) Parent.Reaction code (broad): 3488 Hits
Reaction Parent.Reaction code (broad) Parent.Reaction code (medium): 626 Hits
Reaction Parent.Reaction code (broad) Parent.Reaction code (narrow): 143 Hits

Return to Reaction Classification Results

Pages: 1 2 3 4 5 6 7 8 9 10 Next Next 10 Select All Clear All Total Records: 143

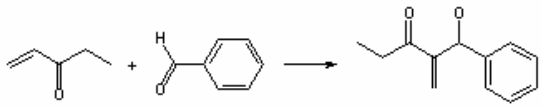
Reaction ID: 1524228



Details Synthesize Reactant(s) Find Similar Reactions

Record#1

Reaction ID: 2678985

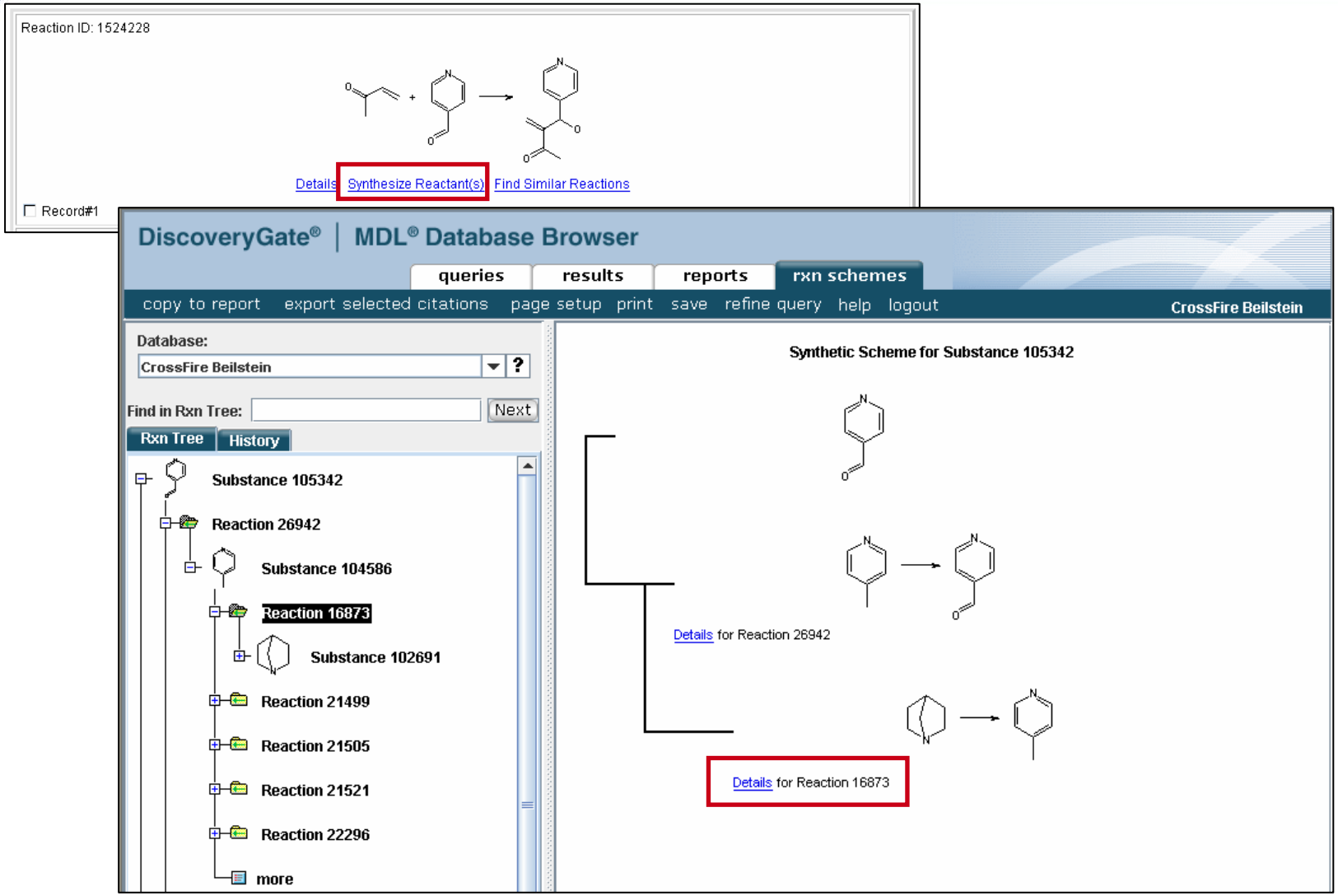


Details Synthesize Reactant(s) Find Similar Reactions

Record#2

Symyx

Synthesize Reactant(s)



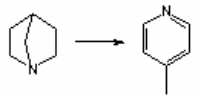
Symyx

Reaction Details

Return to Reaction Scheme Find Similar Reactions

CrossFire Beilstein Reaction 16873

Select / deselect all citations from this page.



Use as Query

Reaction

Reaction record 1 of 1		
Reaction ID	16873	
Reactant	**Reactant BRN**	102691
	Reactant	1-aza-bicyclo[2.2.1]heptane
Product	**Product BRN**	104586
	Product	4-methyl-pyridine
No of Reaction Details	2	
Reaction Entry Date	1988/06/27	
Reaction Update Date	1988/06/27	

Top of Page

Reaction Details

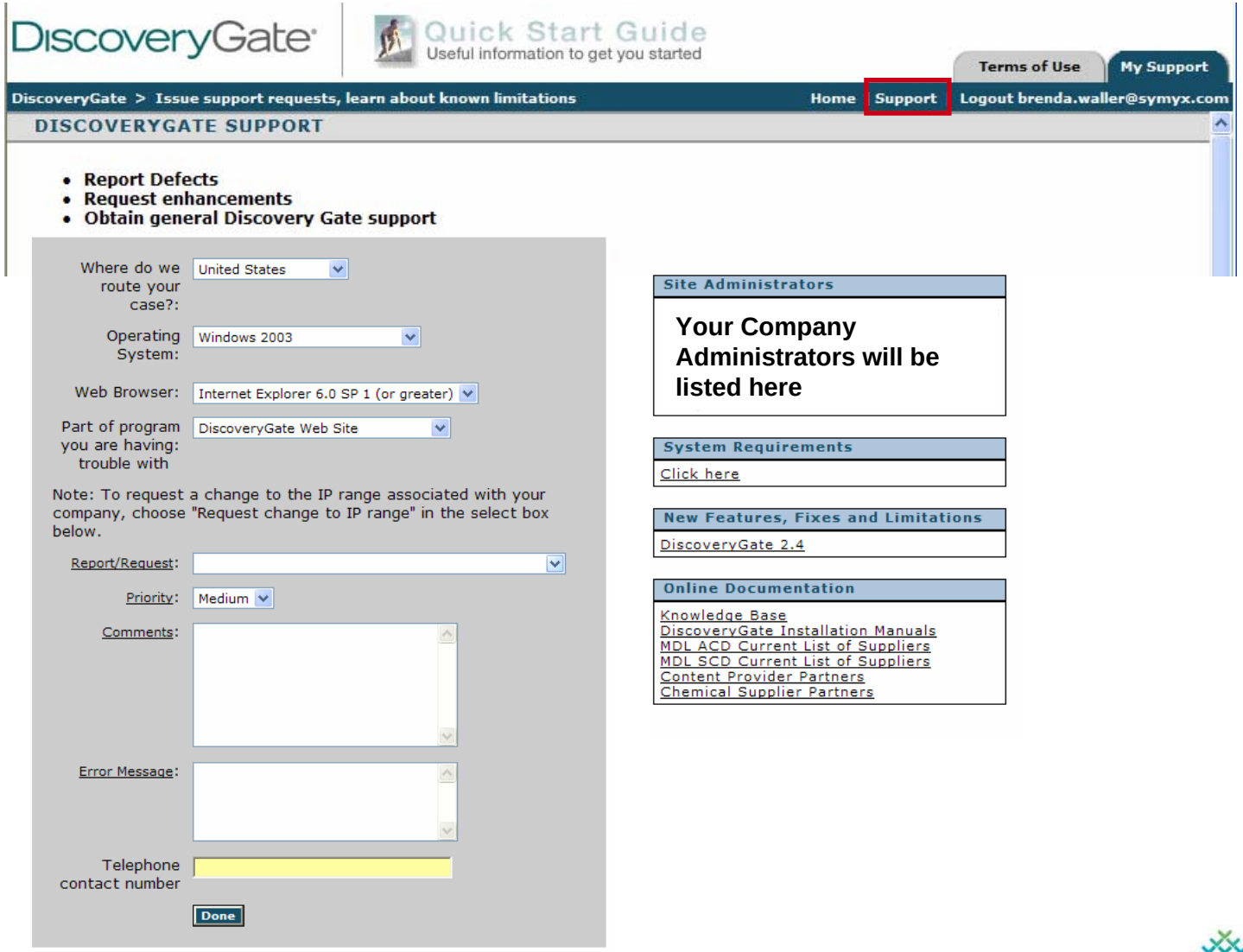
Reaction Details record 1 of 2		
Citation Pointer	• 983616	
Reaction Detail ID	16873.2	
Reaction Classification	• Preparation	
Stage	**Reagent**	palladium/charcoal
	Temperature	330 C

Symyx

Course Summary

- In this Workshop, we have covered how to:
  - Log into DiscoveryGate
  - Change Personal Settings for DiscoveryGate
  - Conduct structure and data searches using the Database Browser and individual databases
  - View the search results using the Grid, Database, and Properties views
  - Save search results as Temporary and Permanent lists, and Combine lists
  - Create Reports
  - Modify Query Forms and Save as Default Forms
  - Introduce Synthetic Methods

Support for DiscoveryGate



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