



# **Reaction Searching using DiscoveryGate**

DiscoveryGate®  
Exercise Guide

# Reaction Searching using DiscoveryGate

## DiscoveryGate<sup>®</sup> Exercise Guide

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Developed: May 2008, Symyx Educational Services

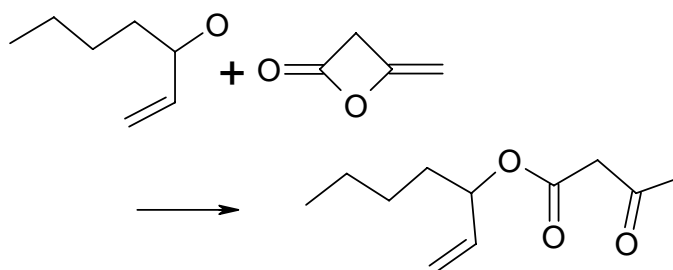
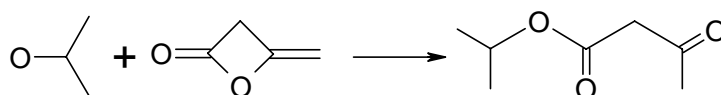
TRDG-22V2.5EG

## 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 reaction substructure search for synthesis of keto esters. Examples of the desired transformations are shown below. Do not draw each of the reactions shown. Draw a single reaction that is representative of the desired transformation.

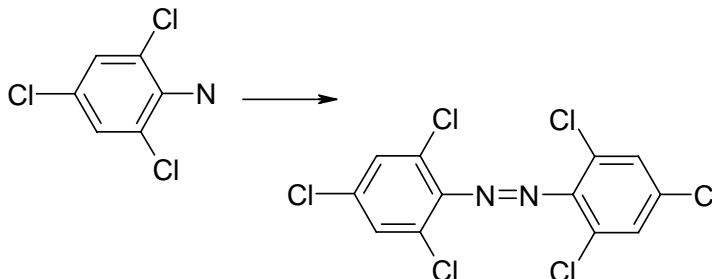
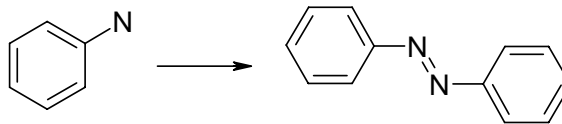


- View the details for one of the reactions retrieved.

For a step-by-step solution, see page 1-4.

### Exercise 2

- Conduct a search to retrieve methods for preparing azo compounds from aniline. Examples of the desired transformations are shown below. Do not draw each of the reactions shown. Draw a single reaction that is representative of the desired transformation. Use substitution count to specify the unsubstituted nitrogen on the reactant and prevent amine oxides in the product.

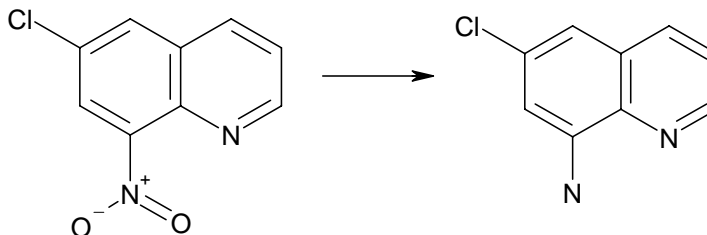


- Use one of the reactions retrieved to find similar reactions in IMRW.

For a step-by-step solution, see page 1-7.

### Exercise 3

- Search for the reduction of a halogenated aromatic nitro group to a primary amine. An example of this type of reaction is shown below.

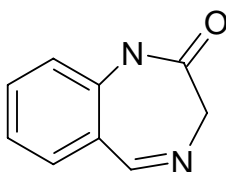


- Use one of the reactions retrieved to find similar reactions in MDL Patent Chemistry.

For a step-by-step solution, see page 1-11.

### Exercise 4

- Retrieve synthetic methods for 1,4 benzodiazepine that use THF or ethanol as a solvent. Conduct a substructure search with benzodiazepine as product not reactant. Conduct a formula search for the solvent.



THF  
C<sub>4</sub>H<sub>8</sub>O

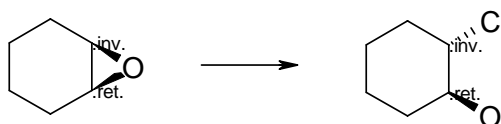
Ethanol  
C<sub>2</sub>H<sub>6</sub>O

## Exercise 5

- Use one of the reactions retrieved to find similar reactions in CrossFire Beilstein.

For a step-by-step solution, see page 1-17.

- Retrieve reactions that open epoxide rings with stereo inversion and halogenation. Allow five- and six-membered rings.



For a step-by-step solution, see page 1-24.

### Exercise 1

Launch the MDL Database Browser

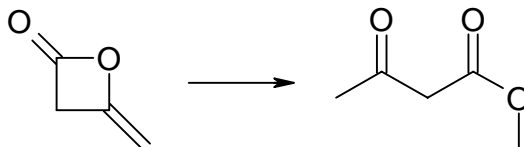
Choose the Synthetic Methodology Information database

Draw the reactant

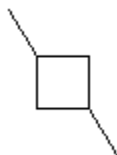


### Synthesis of esters

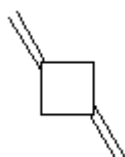
Conduct a reaction substructure search to retrieve methods for the synthesis of keto esters.



1. From the DiscoveryGate home page, click **Search Databases**.
2. Choose **Synthetic Methodology Information** from the Database list.
3. Double-click the **Reaction** box to launch MDL Draw.
4. Click the **cyclobutane** template. Click the drawing area.
5. Click the **All-Purpose Drawing** tool. Drag the mouse to draw the two single bonds.



6. Click the single bonds to change them to double.

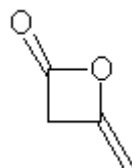


Draw the reaction arrow

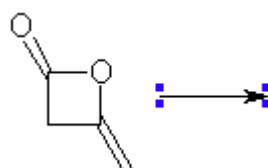


Draw the product

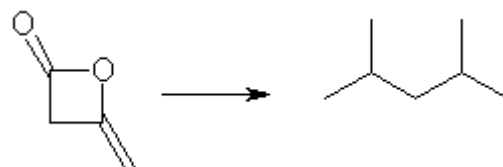
7. Shift-click to select the atoms that you want to change to oxygen. Type **o**.



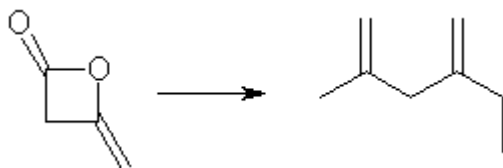
8. Click the **Arrow** tool. Then click the drawing area to the right of the reactant structure.



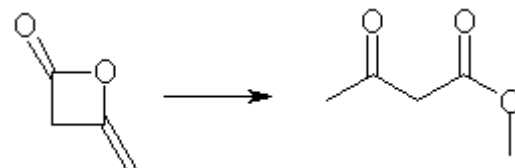
9. Click the **All-Purpose Drawing** tool. Drag to draw the carbon framework.



10. Click the bonds to change them to double.



11. Shift-click to select the atoms that you want to change to oxygen. Type **o**.



Conduct the search

12. Click **Done**.

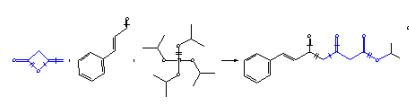
13. Choose **Reaction Substructure** as the search type.

14. Click **start search**. The results are displayed.

[View selected records in another database](#) [Sort Results](#) [Create List](#)

Pages: 1 2 3 4 5 6 7 8 9 10 [Next](#) [Next 10](#) [Select All](#) [Clear All](#) Total Records: 152

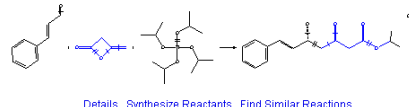
ChemInform Reaction Library



[Details](#) [Synthesize Reactants](#) [Find Similar Reactions](#)

Record#1

ChemInform Reaction Library



[Details](#) [Synthesize Reactants](#) [Find Similar Reactions](#)

Record#2

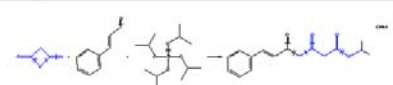
View the search results

15. Click **Details** for one of the reactions. Scroll to view the data.

[Return to Search Results](#) [View selected records in another database](#) [Find Similar Reactions](#) Record # 1 [Total Records: 152](#)

Also found in: [ACD](#) [DWPI](#) [Index Chemicus](#) [NCI](#) [OHS MSDS](#) [Patent Chemistry](#) [SCD](#) [Toxicity](#)

ChemInform Reaction Library



[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 \(5\)](#) [Reactant \(2\)](#)

[Product \(1\)](#)

**Reaction Details** [\(hide\)](#)

RXC00540653 **Reaction Variation 1 of 5**

Product no.	% Yield	Grade	%CS	%DS	%SE	Reactant no.	Reactant Grade
1	68		100		82	1	
						2	
						3	1 equiv.

Step no.	Catalysts and Solvents	Catalyst ID	Solvent ID
1	(S)-(2,5-Sbu2-2-OH-C6H2)-CPhuN-CH(OiPr)-CH2OH (cat) CH2Cl2	<a href="#">378952</a> click ID for details	<a href="#">32</a> click ID for details

Detailed Data	Conditions	External Registry No.	Path	Step
	<a href="#">References</a>	983902502	A	1 STEP

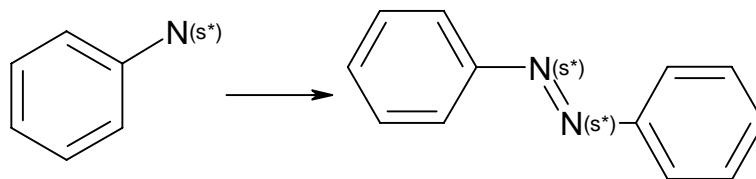
[OGUNI, N., TANAKA, K., ISHIDA, H., Synlett \[SYNLETS\] 1998, \(6\), 601-602](#)



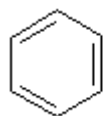
## Exercise 2

## Preparation of azo compounds from aniline

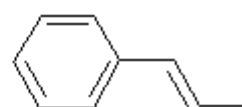
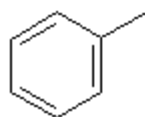
Conduct a reaction substructure search using the following query:



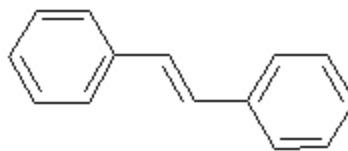
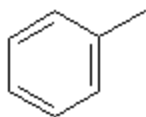
Draw the query



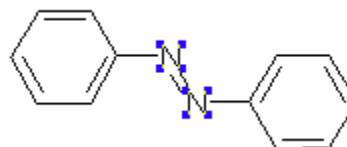
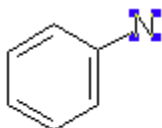
- Click the **All-Purpose Drawing** tool. Drag the mouse to draw the bonds shown. Click the single bond to change it to double.



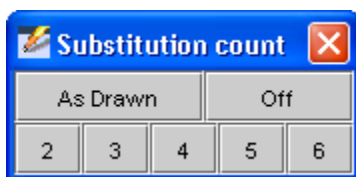
- Click the **benzene** template, and then click the end of the single bond to attach the ring.



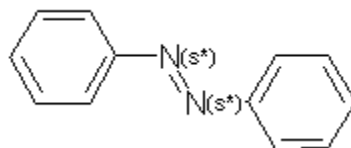
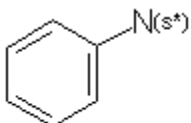
7. Click the **Lasso Select** tool. Shift-click to select the atoms that you want to change to nitrogen. Type **n**.



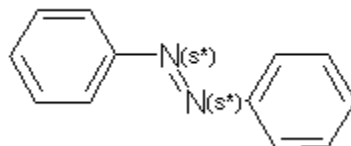
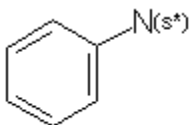
8. Right-click one of the selected nitrogen atoms, and choose **Number of nonhydrogen substituents**.



9. Click **As Drawn**.



10. Click the **Arrow** tool. Click the drawing area between the two structures.



11. Click **Done**.

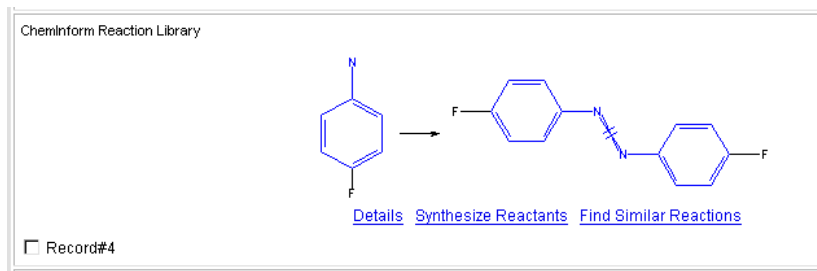
Conduct the search

From the results, find similar reactions in the Integrated Major Reference Works

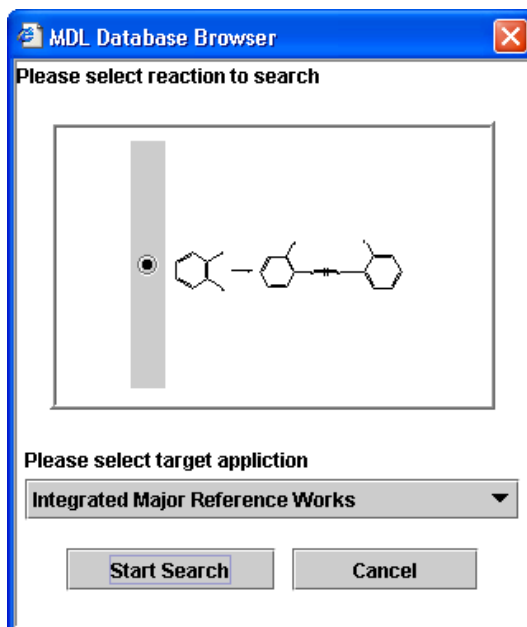
12. Choose **Reaction Substructure** as the search type.

13. Click **start search**.

14. For one of the reactions retrieved, click **Find Similar Reactions**. For example:



15. Choose **Integrated Major Reference Works** as the target application. Click **Start Search**.



16. If necessary, enter your Username and Password to login to the IMRW database.

17. Click a link for Broad, Medium, or Narrow search results from one of the licensed IMRW publications. In this

example, you would click the **Narrow: 3Hits** link for COFGT.

### Results from All Licensed IMRW Publications

■ CAC	<a href="#">Broad: 0 Hits</a>	<a href="#">Medium: 0 Hits</a>	<a href="#">Narrow: 0 Hits</a>
■ COFGT	<a href="#">Broad: 5 Hits</a>	<a href="#">Medium: 3 Hits</a>	<a href="#">Narrow: 3 Hits</a>
■ EROS	<a href="#">Broad: 22 Hits</a>	<a href="#">Medium: 18 Hits</a>	<a href="#">Narrow: 18 Hits</a>
■ Science of Synthesis	<a href="#">Broad: 0 Hits</a>	<a href="#">Medium: 0 Hits</a>	<a href="#">Narrow: 0 Hits</a>

### COFGT Results

#### Query Data

Your Query:  
[CLS=broad:225702704381200,medium:265989766633421,narrow:320813278212335,]

3 hits. 5 hits per page:

[Return to Results](#)  
[Return to Query](#)  
[New Query](#)



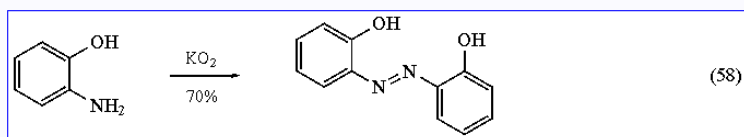
#### Search Results

- [2.15 Vinyl- and Arylnitrogen Compounds](#)  
1 [2.15.8 HYDRAZINES AND RELATED FUNCTIONS](#)  
[2.15.8.2 Azo Compounds](#)

Related reactions in

18. Click the reference link to view the article text. For example:

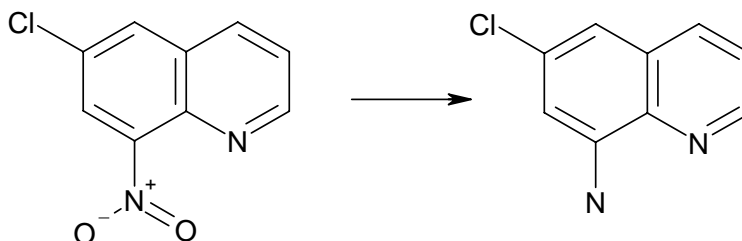
Other reagents which bring about the oxidation of aromatic amines to the corresponding azo derivatives and more details on the subject may be found in an excellent review by Gilchrist [561]. These include silver oxide on celite, lead tetraacetate, barium manganate, bispyridinesilver permanganate, sodium perborate, and sodium hypochlorite. Potassium superoxide has been found to be capable of selectively oxidizing *ortho*- and *para*-substituted diamines and aminophenols to the corresponding azo compounds in good yield (Equation (58)) [562].



19. Close the IMRW publication windows.

**Exercise 3****Reduce halogenated aromatic nitro to an amine**

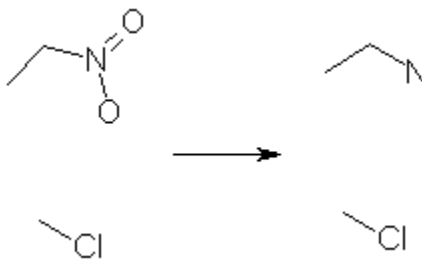
Conduct a reaction substructure search to retrieve reactions of the following type:



Return to the Query page

Draw the query

1. Click the **queries** tab.
2. Click the **Reset** link located to the right of the reaction box.
3. Double-click the **Reaction** box.
4. Click the **All-Purpose Drawing** tool. Draw the fragments shown below. Use the **Arrow** tool to draw the arrow.

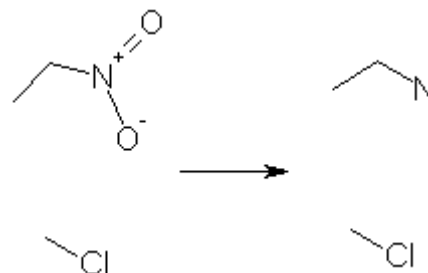


Apply charges

5. To apply the charges, right-click the nitrogen atom in the nitro group. Choose **Charge**, and then click **+1**.

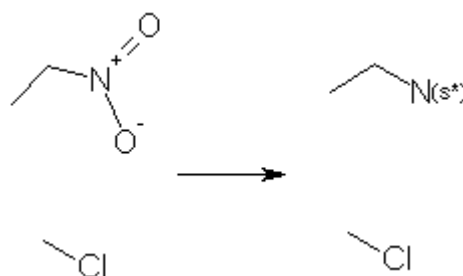


6. Use the same technique to add the **-1** charge to the oxygen.



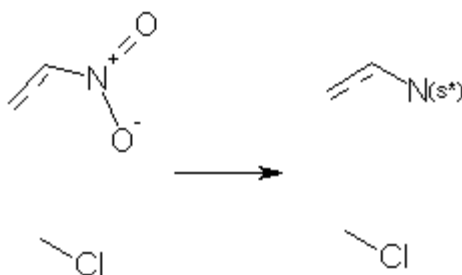
Specify substitution count

7. Right-click the uncharged nitrogen and choose **Number of nonhydrogen substituents**. Click **As Drawn**.



Apply Aromatic query bond

8. Shift-click to select the carbon-carbon bonds in the reactant and product fragments. Right-click one of the selected bonds, and choose **Query bond type > Aromatic**.



Conduct the search

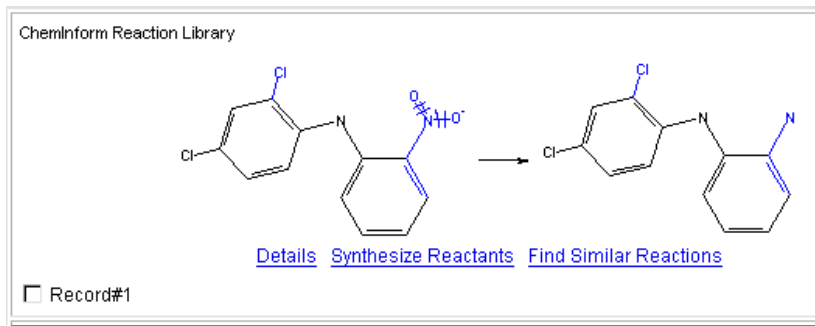
9. Click **Done**.

10. Choose **Reaction Substructure** as the search type.

11. Click **start search**.

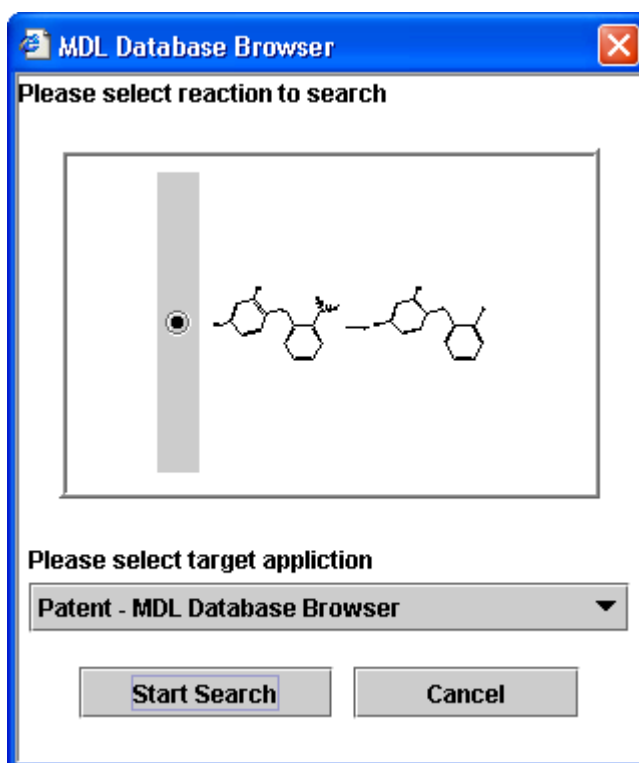
Find similar reactions in  
CrossFire Beilstein

12. For one of the reactions retrieved, click **Find Similar Reactions**. For example:



13. Choose **Patent – MDL Database Browser** as the target application. Click **Start Search**.



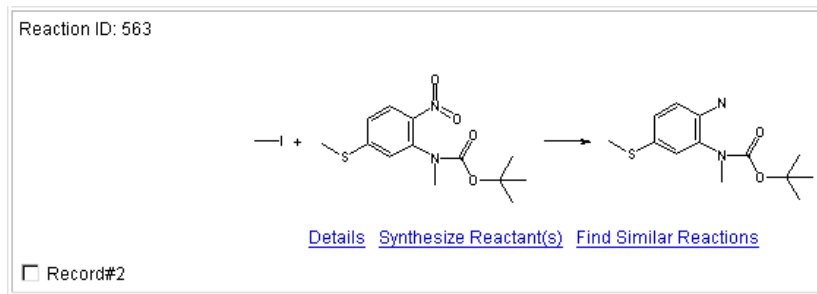


14. Click the link for the **Narrow Class Code** search results.

#### Reaction Classification Search Results

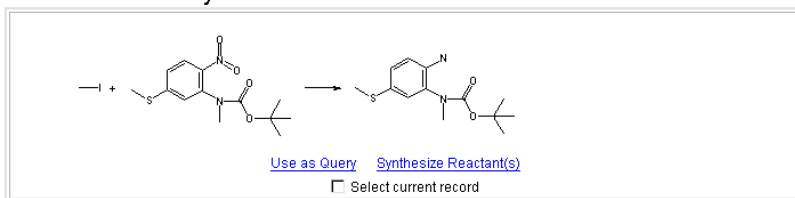
[Reaction Identification Parent.Broad Class Code Parent.Broad Class Code: 13283 Hits](#)  
[Reaction Identification Parent.Medium Class Code Parent.Medium Class Code: 12847 Hits](#)  
[Reaction Identification Parent.Narrow Class Code Parent.Narrow Class Code: 12441 Hits](#)

15. For one of the similar reactions, click **Details**. For example:



The reaction details are displayed.

### Patent Chemistry Reaction 563



### Reaction Identification

Reaction Identification record 1 of 1	
<b>Reaction ID</b>	563
<b>Reactant</b>	<b>Reactant PRN</b> 122294 <b>Reactant</b> iodo-methane
	<b>Reactant PRN</b> 134307 <b>Reactant</b> N-(2-nitro-5-methylthiophenyl)-N-methylcarbamic acid t-butyl ester
<b>Product</b>	<b>Product PRN</b> 134306 <b>Product</b> 2-(N-t-butoxycarbonyl-N-methylamino)-4-methylthioaniline
<b>Reaction Specification</b>	full reaction
<b>Reaction Entry Date</b>	2003/12/24
<b>Reaction Update Date</b>	2003/12/24

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### Reaction Details

Reaction Details record 1 of 1	
<b>Citation</b>	1073
<b>Topic of Interest</b>	Preparation
<b>Example Name</b>	Example 41
<b>Location in Patent</b>	Page 126
<b>Product</b>	<b>Product PRN</b> 134306 <b>Product</b> 2-(N-t-butoxycarbonyl-N-methylamino)-4-methylthioaniline
<b>Stage Number</b>	1
<b>Reactant</b>	<b>Reactant PRN</b> 122294 <b>Reactant</b> iodo-methane
	<b>Reactant PRN</b> 134307 <b>Reactant</b> N-(2-nitro-5-methylthiophenyl)-N-methylcarbamic acid t-butyl ester
<b>Reagent</b>	<b>Reagent PRN</b> 240067 <b>Reagent</b> 10 percent palladium on carbon
<b>Solvent</b>	<b>Solvent PRN</b> 7574 <b>Solvent</b> methanol <b>Quantity in Solvent Mixture</b> 300 ml
	<b>Solvent PRN</b> 126957 <b>Solvent</b> dioxane <b>Quantity in Solvent Mixture</b> 300 ml
<b>Reaction Details Citations</b>	<ul style="list-style-type: none"> <li>• <a href="#">Patent, Sankyo Company, Limited; Publ.: EP1167357 A1 (2002/01/02), Appl.: EP2000-915361 (2000/04/06)</a></li> </ul>

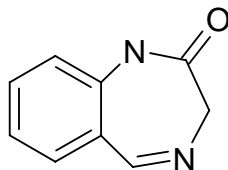
[Top of Page](#)

Show [Substances](#) for this Reaction   Show [Citations](#) for this Reaction

## Synthesis of benzodiazepine

### Exercise 4

Conduct a substructure search to retrieve synthetic methods for 1,4 benzodiazepines that use THF or ethanol as a solvent.



THF  
C<sub>4</sub>H<sub>8</sub>O

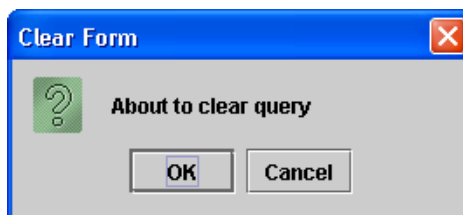
Ethanol  
C<sub>2</sub>H<sub>6</sub>O

Construct the query

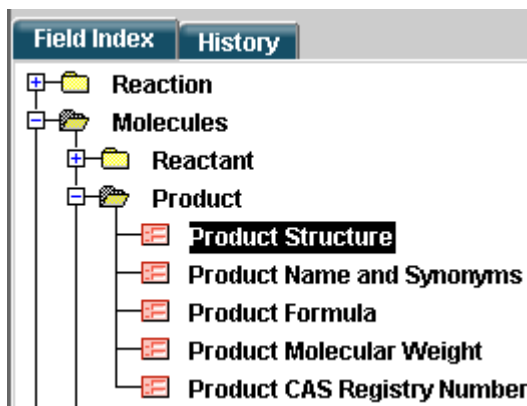
1. Click **queries**.
2. Choose **Synthetic Methodology Information** from the Database list.

Build a custom form

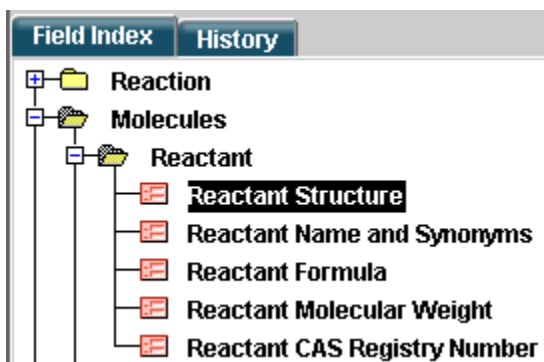
3. Click **clear form** on the top menu bar. Click **OK** at the confirmation prompt.



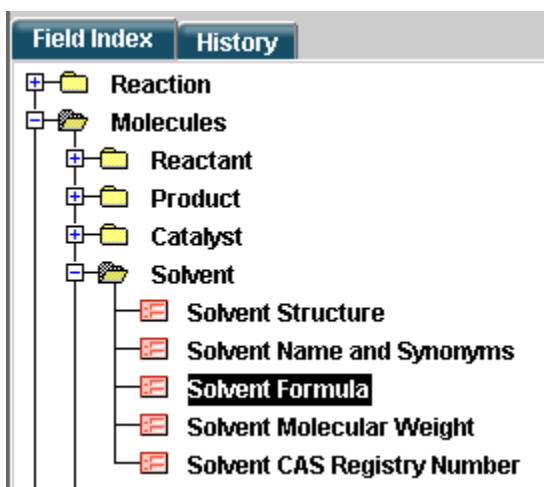
4. In the Field Index, open the **Molecules > Product** folder. Double-click **Product Structure**.



5. In the Field Index, open the **Molecules > Reactant** folder. Double-click **Reactant Structure**.



6. In the Field Index, open the **Molecules > Solvent** folder. Double-click **Solvent Formula**.

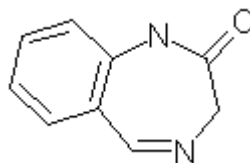


The query form looks like this:

Molecules			
	<b>Product Structure</b> Double-click in this box to edit structure	<b>Select Search Type:</b> Automatic An automatically executed series of searches (Current structure, include isomers, include tautomers, include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.	<a href="#">Reset</a> <a href="#">Delete</a> <a href="#">Duplicate</a> <a href="#">Info</a>
<input type="button" value="AND"/>	<b>Reactant Structure</b> Double-click in this box to edit structure	<b>Select Search Type:</b> Automatic An automatically executed series of searches (Current structure, include isomers, include tautomers, include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.	<a href="#">Reset</a> <a href="#">Delete</a> <a href="#">Duplicate</a> <a href="#">Info</a>
<input type="button" value="AND"/>	Solvent Formula	<input type="button" value="Contains"/>	<input type="text"/>
<input type="button" value="start search"/>			<a href="#">Delete</a> <a href="#">Duplicate</a> <a href="#">Info</a>

Draw the product structure

- Double-click the **Product Structure** box. Draw the structure for 1,4 benzodiazepine.



Copy and paste the product structure

- Click **Done**.
- Right-click the structure in the Product Structure box. Choose **Copy**.

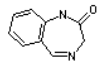
- Right-click the **Reactant Structure** box. Choose **Paste**.

Set the search type and logic

- Choose **Substructure** as the search type for both the Product and Reactant. Then change the logical operator for the Reactant Structure to **NOT**.

**Molecules**

**Product Structure** [Select Search Type:](#)



Substructure ▼

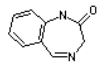
A Molecule Substructure search finds molecule records that contain your query as a substructure wholly within a larger structure.

[Reset](#)  
[Delete](#)  
[Duplicate](#)  
[Info](#)

---

**Reactant Structure** [Select Search Type:](#)

NOT ▼



Substructure ▼

A Molecule Substructure search finds molecule records that contain your query as a substructure wholly within a larger structure.

[Reset](#)  
[Delete](#)  
[Duplicate](#)  
[Info](#)

Enter the Solvent query

12. For the Solvent field, enter the formula query that will retrieve both THF (C<sub>4</sub>H<sub>8</sub>O) and Ethanol (C<sub>2</sub>H<sub>6</sub>O).

Solvent Formula Contains ▼ c(2-4) h(6-8) o

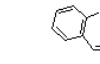
Use parentheses to clarify search logic

13. Click **show brackets**. Then apply parentheses around the two structure queries.

**Molecules**

**Product Structure** [Select Search Type:](#)

[ ] ▼



Substructure ▼

A Molecule Substructure search finds molecule records that contain your query as a substructure wholly within a larger structure.

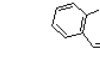
[Reset](#)  
[Delete](#)  
[Duplicate](#)  
[Info](#)

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**Reactant Structure** [Select Search Type:](#)

NOT ▼

[ ] ▼



Substructure ▼

A Molecule Substructure search finds molecule records that contain your query as a substructure wholly within a larger structure.

[Reset](#)  
[Delete](#)  
[Duplicate](#)  
[Info](#)

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[ AND ▼ ] Solvent Formula Contains ▼ c(2-4) h(6-8) o [Delete](#)  
[Duplicate](#)  
[Info](#)

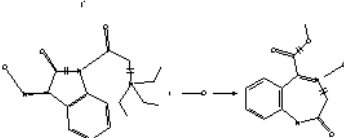
Execute the search

14. Click **start search**.

View details for a reaction

Pages: 1 2 3 4 ► Next Select All Clear All Total Records: 42

ChemInform Reaction Library



[Details](#) [Synthesize Reactants](#) [Find Similar Reactions](#)

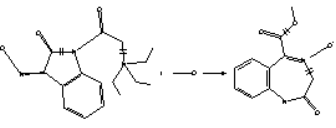
Record#1

15. For one of the reactions retrieved, click **Details**. For example:

[Return to Search Results](#) [View selected records in another database](#) [Find Similar Reactions](#) Record # 1 ► Total Records: 42

Also found in: [ACD](#) [CMC](#) [DWPI](#) [Index Chemicus](#) [NCI](#) [OHS MSDS](#) [Patent Chemistry](#) [SCD](#) [Toxicity](#)

## ChemInform Reaction Library



[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 [\(hide\)](#)

RXCI05004297 Reaction Variation 1 of 1

Product no.	% Yield	Grade	%cs	%ds	%de	%ee	Reactant no.	Reactant Grade
1	50		100					

Step no.	Catalysts and Solvents	Catalyst ID click ID for details	Solvent ID click ID for details
1	DMF		<a href="#">38</a>

Detailed Data	<a href="#">Conditions</a> <a href="#">References</a>	External Registry No.	Path	Step
		1050316101	A	4 OF 5
		1050316101	B	4 OF 5

[SIROHI, R.; SINGH, A.; SHASTRI, S.; KISHORE, D.; J Indian Chem Soc \[JICSAH\] 2004, 81 \(3\), 254-257.](#)

View Toxicity data for a reaction

16. Click the **Toxicity** link for “Also found in.” In this example, toxicity data for one of the reactants is retrieved.

[Return to Synthetic Methodology Information](#)

Record # 1 **Total Records:** 1

### MDL® Toxicity Database

0 —	<p><b>Available Data</b></p> <p><i>Click on a link to add the information to this page</i></p> <p><input type="checkbox"/> Set current view as default</p> <p> <a href="#">Chemical</a> (1)      <a href="#">Acute Toxicity</a> (46)  <a href="#">Mutagenicity</a> (27)      <a href="#">Skin/Eye Irritation</a> (12)  <a href="#">Reproductive Effects</a> (22)      <a href="#">Other Multiple Doses</a> (15)  <a href="#">Review</a> (10)      <a href="#">Model</a> (1)                 </p>
-----	--

#### Chemical [\(hide\)](#)

<b>Molecular Formula</b>	C H4 O
<b>Molecular Weight</b>	32.0416
<b>MDL Number</b>	MFCD00004595
<b>CAS Registry Number</b>	54841-71-3 , 67-56-1
<b>Beilstein Number</b>	
<b>Beilstein Handbook</b>	
<b>RTECS Number</b>	PC1400000
<b>CCRIS Number</b>	2301
<b>GENE-TOX Number</b>	286
<b>GENOTOXICITY Number</b>	
<b>CARCINO Number</b>	
<b>HEPATO Number</b>	
<b>NEPHRO Number</b>	
<b>Patch Test</b>	195
<b>Compound Descriptor</b>	Drug , Human Data , Primary Irritant , Reproductive Effector

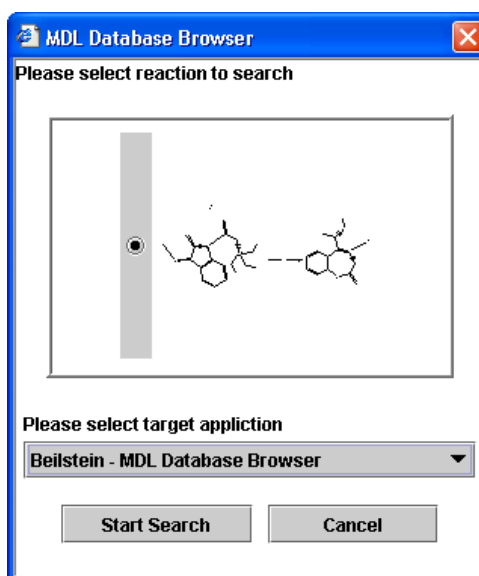
17. Click **Return to Synthetic Methodology Information**.

18. Click **Return to Search Results**.

Find similar reactions in  
CrossFire Beilstein

19. For one of the reactions, click **Find Similar Reactions**.  
Enter **Beilstein – MDL Browser** as the target application.  
Click **Start Search**.





20. Click the **narrow** results link.

#### Reaction Classification Search Results

[Reaction Parent.Reaction code \(broad\) Parent.Reaction code \(broad\): 4 Hits](#)  
[Reaction Parent.Reaction code \(broad\) Parent.Reaction code \(medium\): 4 Hits](#)  
[Reaction Parent.Reaction code \(broad\) Parent.Reaction code \(narrow\): 4 Hits](#)

21. View the similar reactions retrieved.

**Exercise 5**

Return to Synthetic  
Methodology Information

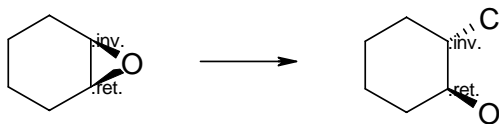
Draw the query



Draw stereo bonds

**Open epoxides with stereo inversion**

Conduct a reaction substructure search to retrieve reactions of the following type:



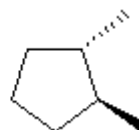
1. Click **queries**.
2. Choose **Synthetic Methodology Information** from the Database list.
3. Double-click the **Reaction** box.
4. Click the **cyclopentane** template. Click the drawing area twice to draw two separate rings.



5. Click the **Up Wedge** tool. Drag the mouse to draw the wedged bond. For the reactant, join the ends of the two wedge bonds.



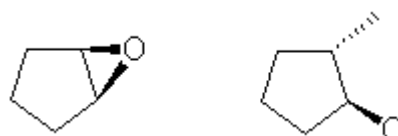
6. Click the **Down Wedge** tool. Drag the mouse to draw the bond on the product.



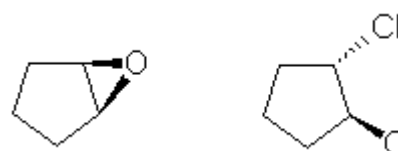
Add atom symbols



7. Click the **Lasso Select** tool. Shift-click to select the two atoms that you want to change to oxygen. Type **o**.



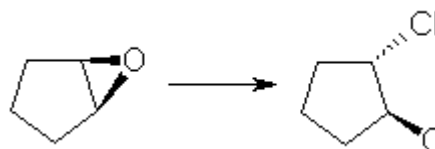
8. Select the atom that you want to change to chlorine. Type **cl**.



Draw the reaction arrow

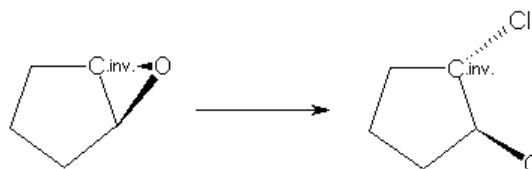


9. Click the **Arrow** tool. Click the drawing area between the two structures.



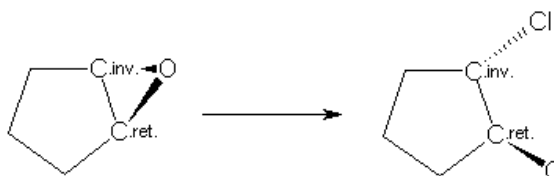
Add stereoconfiguration labels

10. Click the **Lasso Select** tool. Shift-click to select the stereocenters that will invert during the reaction. Right-click one of the selected atoms and choose **Stereoconfiguration at atom > Inverted in reaction**.

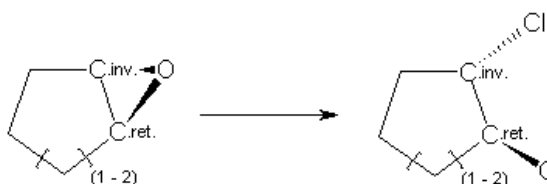


11. Shift-click to select the stereocenters that will be retained during the reaction. Right-click one of the selected atoms and choose **Stereoconfiguration at atom > Retained in reaction**.

Add repeat atoms to allow ring expansion



12. Shift-click to select the two atoms that can repeat to expand the rings from five-membered to six-membered rings. Right-click one of the selected atoms and choose **Repeat atom 1 to N**. Click **2**.



13. Click **Done**.

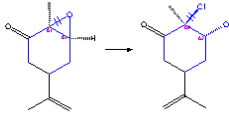
Conduct the search

14. Choose **Reaction Substructure** as the search type.

15. Click **start search**.

16. View the details for some of the reactions retrieved. Scroll to view the data. For example:

## ChemInform Reaction Library



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](#) (1)  
[Product](#) (1)

Reaction Details [\(hide\)](#)

RXCI05069381 Reaction Variation 1 of 1

Product no.	% Yield	Grade	%cs	%ds	%de	%ee	Reactant no.	Reactant Grade
1	90		100					

Step no.	Catalysts and Solvents	Catalyst ID click ID for details	Solvent ID click ID for details
1	1.5 equiv. 1-(carboxymethyl)-3-methylimidazolium chloride neat	<a href="#">1053340</a>	<a href="#">372397</a>

Detailed Data	<a href="#">Conditions</a> <a href="#">References</a>	External Registry No.	Path	Step
		1054406011	A	1 STEP

[RANU, B. C.; BANERJEE, S.; J Org Chem \[JOCEAH\] 2005, 70 \(11\), 4517-4519.](#)