

DRAWING BASICS

MDL[®] Draw
Version 1.2
Participant's Guide

Drawing Basics

MDL[®] Draw Version 1.2 Participant's Guide

Elsevier MDL
14600 Catalina Street
San Leandro, CA 94577

© Copyright (2004-2005) MDL Information Systems, Inc. All rights reserved.

No part of this document may be reproduced by any means except as permitted in writing by MDL Information Systems, Inc.

U.S. GOVERNMENT RESTRICTED RIGHTS NOTICE

The materials are provided with RESTRICTED RIGHTS. Use, duplication or disclosure by: (i) the Department of Defense ("DOD") shall be subject to MDL Information System, Inc.'s standard commercial license and (ii) by any unit or agency of the U.S. Government other than the DOD, shall be governed by clause 52.227-19(c) of the FAR (or any successor regulations) and (iii) by NASA, shall be governed by clause 48 1827.405(a) (or any successor regulations) and, in any such case, the U.S. Government acquires only "restricted rights" in the materials. Contractor/Manufacturer is: MDL Information Systems, Inc. 14600 Catalina St., San Leandro, CA 94577.

MDL is a registered trademark and DiscoveryGate is a registered service mark in the United States, of MDL Information Systems, Inc. All other product and company names may be trademarks or registered trademarks of their respective holders in the United States and other countries.

TABLE OF CONTENTS

DRAWING BASICS

Drawing Basics.....	1-1
Module objectives.....	1-2
MDL Draw interface.....	1-3
All-Purpose Drawing tool.....	1-4
Draw omeprazole.....	1-5
Right-click menu options	1-6
Other drawing tools	1-7
Erasing atoms and bonds	1-8
Using templates	1-9
Using the Template Selector.....	1-10
Building reactions.....	1-11
Duplicating structures.....	1-12
Adding stereo bonds	1-13
Saving a molecule or reaction.....	1-14
Summary.....	1-15
Exercises	
Draw oxaziridine	1-17
Draw a reaction.....	1-19

REFERENCE

To use the All-Purpose Drawing tool	2-1
To draw a bond at any angle.....	2-1
To delete an object.....	2-1
To delete all the objects in the drawing area	2-1
To undo a drawing operation.....	2-1
To redo a drawing operation.....	2-2
To move an object	2-2
To place a template.....	2-2
To fuse a template.....	2-2
To sprout a template	2-2
To use the Template Directory	2-2
To build a reaction	2-2
To select a molecule	2-2

To duplicate a molecule.....	2-3
To move a molecule.....	2-3
To add stereo bonds	2-3
To save a molecule or reaction	2-3

POWERING *the process of* INVENTION

Drawing Basics

Key points

- This module presents the basic skills required to draw molecules and reactions in MDL Draw.
- If you are drawing structures to be used as search queries, there are search-related properties that you will need to add to your structures. Learning how to apply search properties will be covered in the appropriate searching courses.

Notes

Module objectives

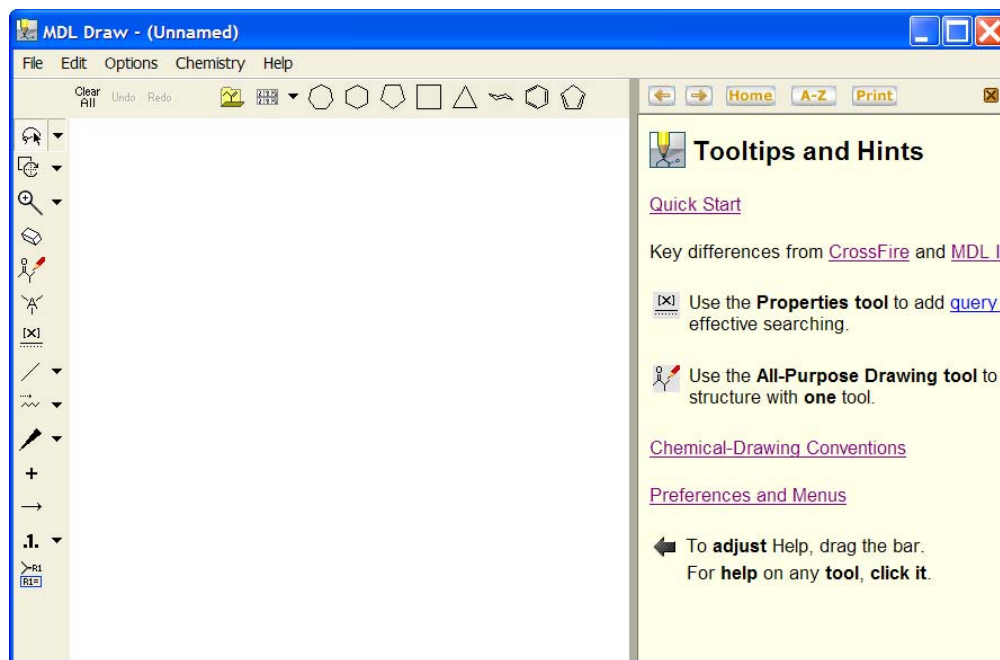
- ❑ Draw molecule structures efficiently
- ❑ Build reactions from component molecules
- ❑ Know where to find more information as needed

Key points

- MDL Draw has many flexible drawing tools, so there are several ways to accomplish any given task. The method you use will be one of personal style.
- Our goal is to show some of the most efficient drawing pathways so that you can draw molecules and reactions quickly.
- Where applicable, we will briefly touch on some of the other tools, to promote awareness of other options. However, the online help offers instructions on all tools and methods, so that you can explore these topics on your own.

Notes

MDL Draw interface

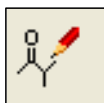


Key points

- As you rest the cursor over any tool, a tool tip displays the name of the tool or brief instructions.
- The online help will display information about the currently selected tool. To find help on other topics, click A-Z in the help pane.
- You can resize the help pane by dragging the bar on the left side of the pane.
- To close the help pane, click the Close button (x), choose Help > Show/Hide Help, or press F1.

Notes

All-Purpose Drawing tool



Use the All-Purpose Drawing tool to:

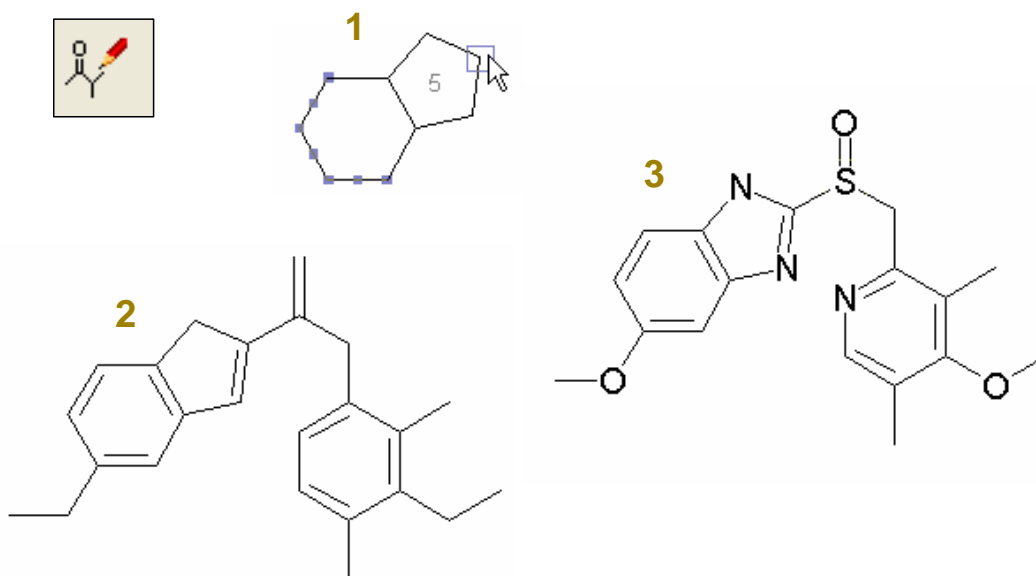
- ☐ Draw atoms, bonds, and chains
- ☐ Pull out a ring
- ☐ Change atom or bond type
- ☐ Change atom or bond properties

Key points

- You can use this single tool to perform almost all of your drawing needs.
- You can use the All-Purpose Drawing tool to draw atoms, bonds, chains, and rings.
- You can click to select an atom, or shift-click to select multiple atoms, and then perform a drawing operation on the selected atoms.
- You can click a bond to change its bond order.

Notes

Draw omeprazole



Key points

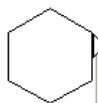
- To draw omeprazole using the All-Purpose Drawing tool, begin by drawing a six-membered ring. To obtain the same orientation as shown on the slide, start the first bond by dragging horizontally. When the ring is complete, pull the 5-membered ring from the ring bond.
- Draw the additional bonds by dragging the All-Purpose Drawing tool. Create double bonds by clicking single bonds.
- Shift-click to select the nitrogen atom positions. Then right-click, choose Atom Symbol, and click N. (Or, select the atoms, and then type N from the keyboard). Repeat for the oxygen atoms and sulfur atom.

Notes

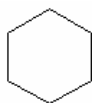
Right-click menu options



All-Purpose Drawing tool



Atom Property	
Atom symbol...	
Charge...	
Isotope	▸
Valence...	
Radical	▸
Number of nonhydrogen substituents...	
Prevent hydrogen substituents	▸
Unsaturated bond to atom	▸
Ring bonds to atom	▸
Repeat atom 1 to N...	
Allow these atoms	▸
Prohibit these atoms	▸
Stereoconfiguration	▸
Remove Properties	



Bond Property	
Bond order	▸
Stereobond	▸
Query bond type	
Chain or ring bond	▸
Remove properties	

Right-click bond menu

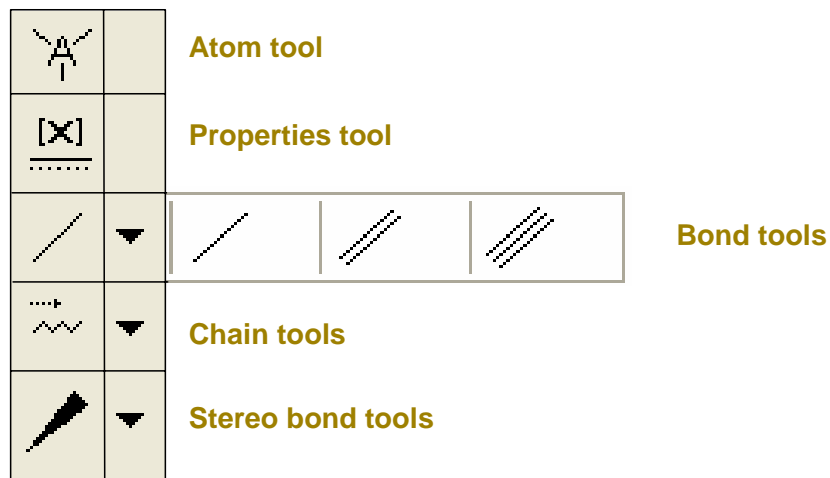
Right-click atom menu

Key points

- Several options for changing atom and bond properties are available from the right-click menu.
- When you right-click an atom with the All-Purpose Drawing tool, a menu for applying atom properties appears.
- When you right-click a bond with the All-Purpose Drawing tool, a menu for applying bond properties appears.

Notes

Other drawing tools

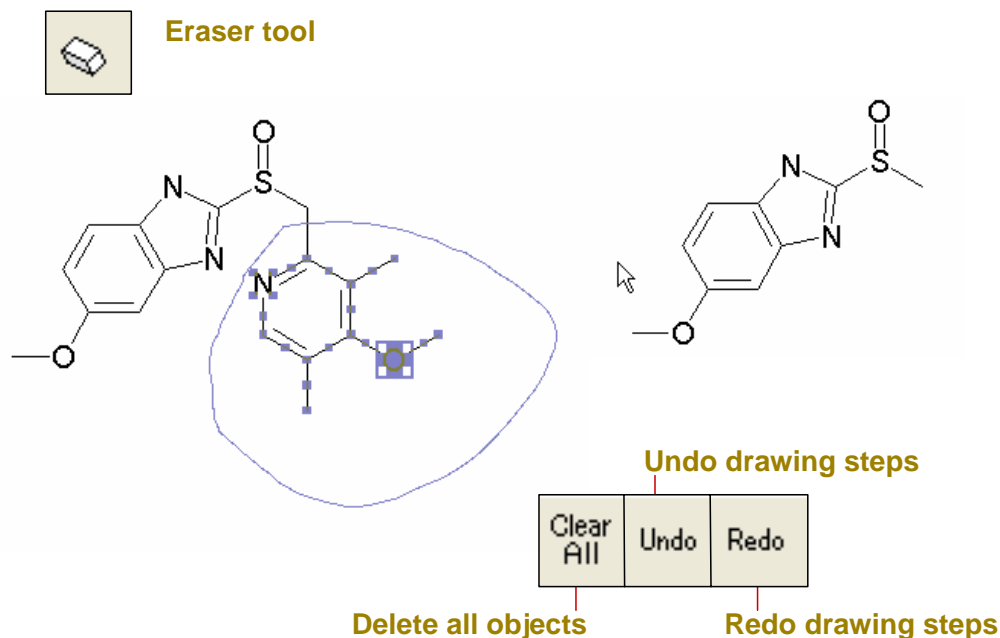


Key points

- All of these tools have right-click menus that allow you to change additional atom, bond, or molecule properties.
- A down arrow next to a tool indicates a tool palette. Click the arrow to display the palette, and then choose the tool you wish to use.
- With any of the Bond tools, you can drag to draw a bond at any angle.

Notes

Erasing atoms and bonds



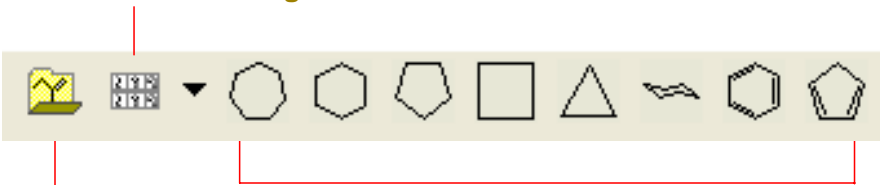
Key points

- To delete a bond or atom, click it using the Eraser tool. When you delete an atom, the Eraser tool automatically deletes any attached bonds.
- To delete a fragment or entire structure, drag the tool to encircle the object.
- You can also delete any selected object by pressing the Delete key.
- To delete all of the objects in the drawing area, click the Clear All button.
- Use the Undo button to successively undo the last drawing steps.
- Use the Redo button to successively redo steps that were undone.

Notes

Using templates

Toolbar Manager



Template Directory **Default template tools**

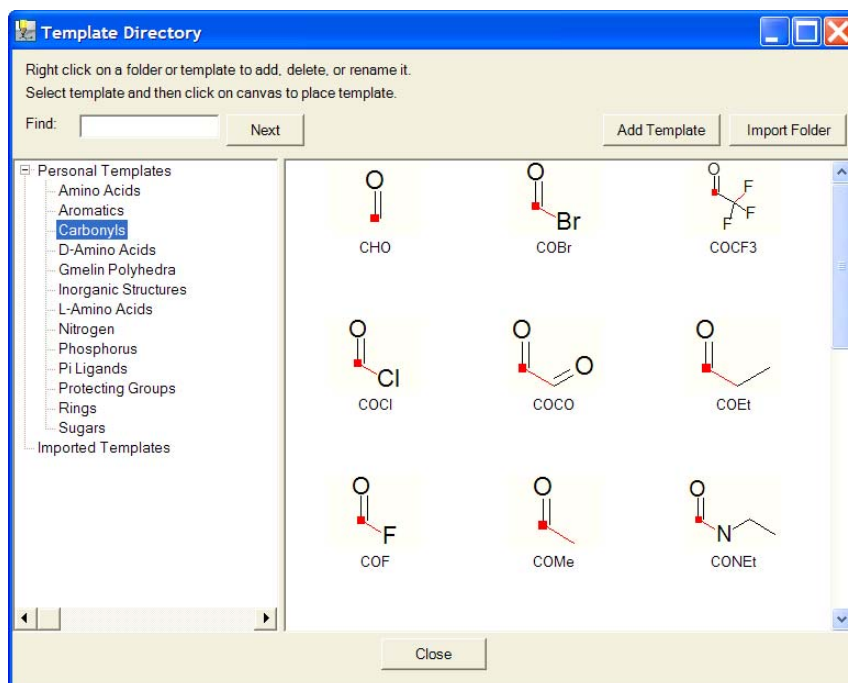
Click to place the template Click a bond to fuse the template Click an atom to sprout the template

Key points

- Templates are predrawn fragments that you can add to your structure.
- The default templates are displayed as tools along the top menu bar. The Toolbar Manager lets you change to a different tool bar. The Template Directory provides access to a library of templates.
- After you select a template tool, click the drawing area to place an isolated template.
- Click a bond to fuse a template.
- Click an atom to sprout a template.

Notes

Using the Template Directory

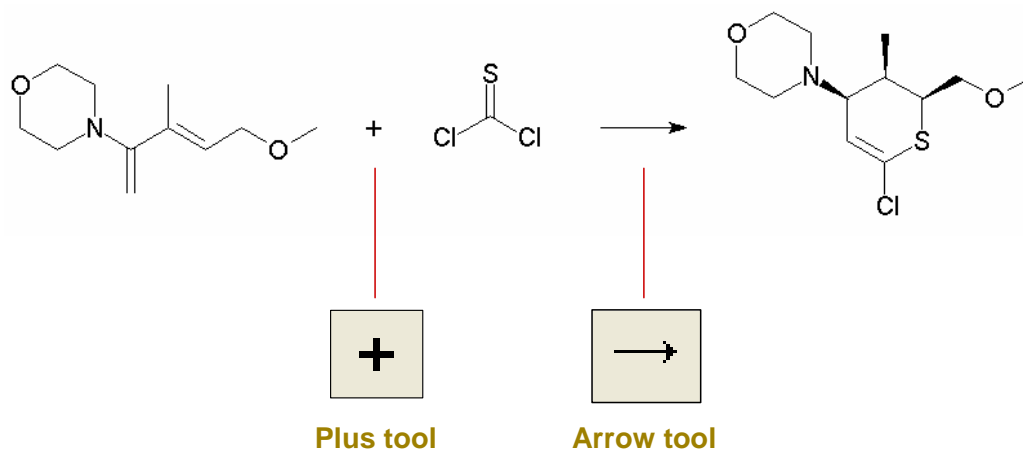


Key points

- The Template Directory contains several folders of templates.
- Click a folder to display the templates contained in the folder.
- Click a template to select it for use. Then click the drawing area to place the template.
- Click the Close button to close the Template Directory window.

Notes

Building reactions



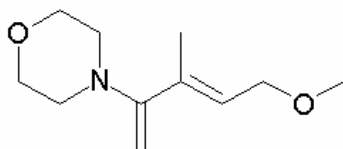
Key points

- To build a reaction, draw the reactants and products.
- Use the Plus tool to place a plus sign between multiple reactants or multiple products.
- Use the Arrow tool to place an arrow between the reactants and products.
- This is the reaction that you will build. In the process of building the reaction, we will be introducing some additional molecule drawing techniques.

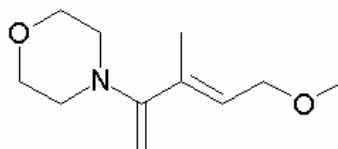
Notes

Duplicating structures

1. Draw molecule.

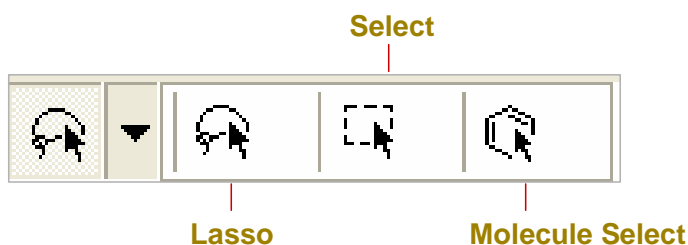


3. Choose Edit > Duplicate.



2. Select molecule.

4. Drag duplicate to new location.

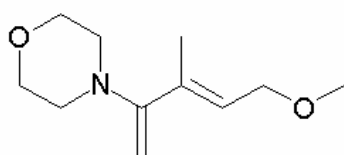


Key points

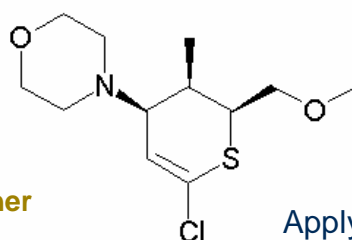
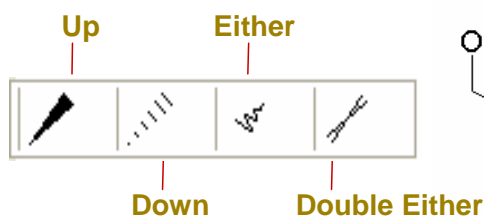
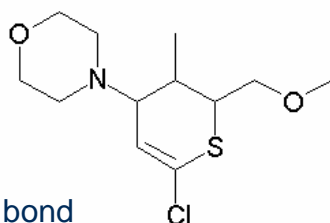
- To begin, you will draw the first reactant structure, and then duplicate it to use for the product structure.
- To duplicate a molecule, you need to select it. There are three different select tools available on the tool palette.
- After you select the reactant, choose Edit > Duplicate to duplicate the structure. Drag the duplicate to the right side of the drawing area.

Notes

Adding stereo bonds



Draw new bonds, change bond order, add atom symbols.



Apply stereo bonds.

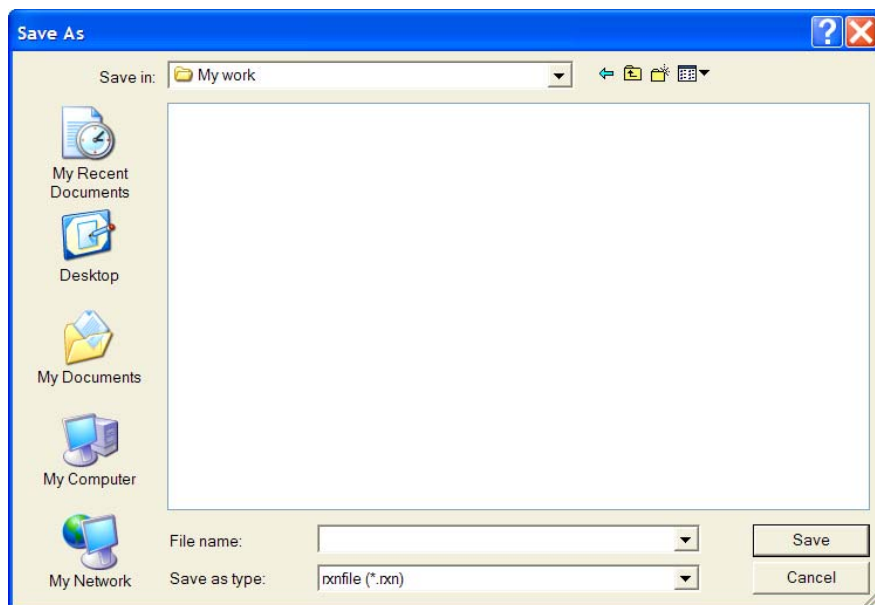
Key points

- To create the product structure, we need to modify the duplicate structure by drawing new bonds, changing bond order, and adding atom symbols. You can use the All-Purpose Drawing tool to perform these operations.
- There are four stereo bond tools on the tool palette.
- You can use the All-Purpose Drawing tool to add the stereo bonds by using the right-click menu, but you will have more control of the stereo bond direction by using the Up Wedge tool.
- With the Up Wedge tool, you can click an up bond to change its direction.

Notes

Saving a molecule or reaction

File > Save As



Key points

- You can save molecules and reactions in external files called molfiles and rxnfiles.
- The files can then be read by other structure-based applications.

Notes

Summary

In this module, you learned how to:

- ☐ Draw bonds and atoms using different tools
- ☐ Erase atoms and bonds
- ☐ Undo and redo drawing actions
- ☐ Use templates
- ☐ Select, duplicate, and move structures
- ☐ Build reactions
- ☐ Save molecules and reactions

Key points

- You learned how to use the All-Purpose Drawing tool with its right-click menus to draw complete structures and change atom and bond properties.
- You also worked with some of the other drawing tools and used predrawn templates.
- You learned how to erase objects, and how to undo and redo drawing actions.
- In building the sample reaction, you learned how to select, duplicate, and move structures.
- And you learned how to save molecules and reactions in external files for future use.

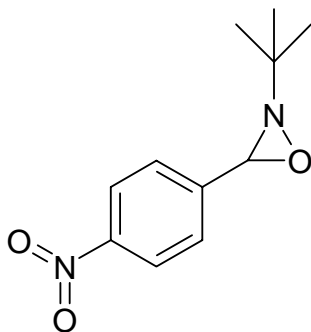
Notes

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

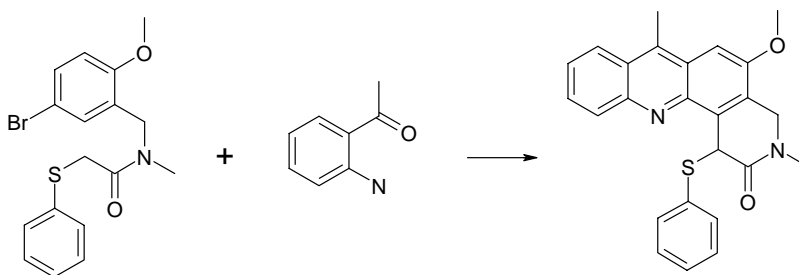
Draw the following molecule and save it as a molfile.



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

Exercise 2

Draw the following reaction and save it as a rxnfile.



For a step-by-step solution, see page 1-19.

Exercise 1

Draw the rings

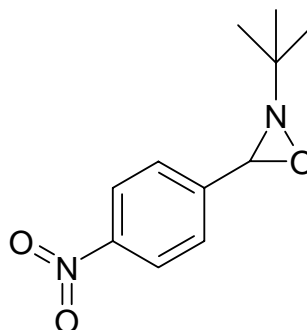


Draw the additional bonds

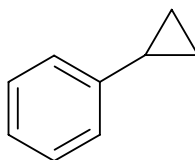


Draw oxaziridine

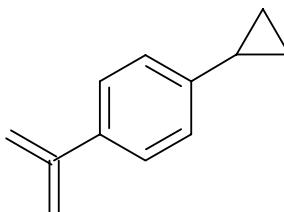
Draw the following molecule and save it as a molfile.



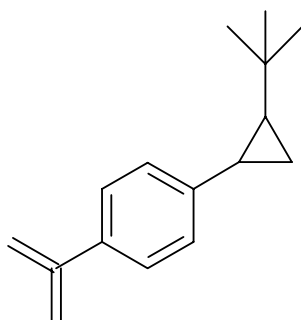
1. Click the **benzene** tool, and then click the drawing area to place the ring.
2. Click the **cyclopropane** tool, and then click an atom on the benzene ring to sprout the three-membered ring.



3. Click the **All-Purpose Drawing** tool. Drag to draw the bonds for the nitro group. Click the single bonds to change them to double bonds.

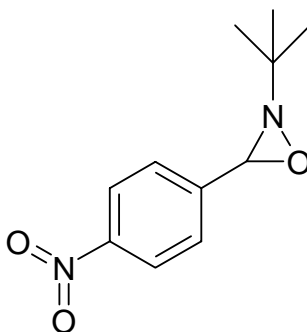


4. Click the **Single Bond** tool. Drag to draw the bonds for the tri-methyl group. Using the Single Bond tool lets you draw bonds at any angle.



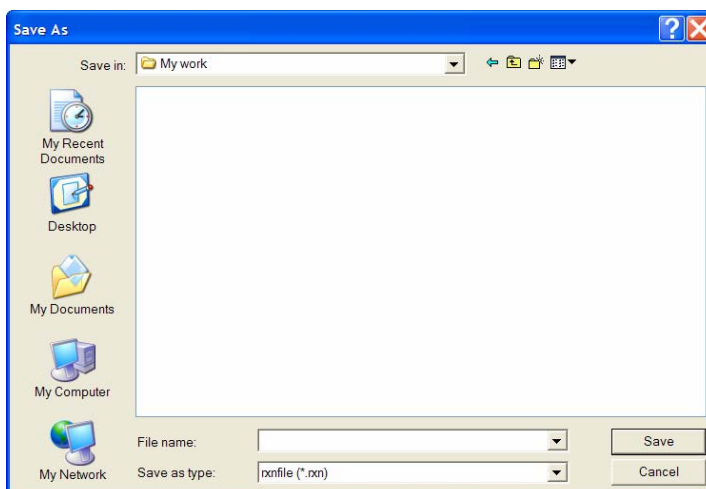
Add the atoms

- Click the **All-Purpose Drawing** tool. Shift-click to select the oxygen atom positions. Then type **O**.
- Shift click to select the nitrogen atom positions. Then type **N**. Press **Enter**.



Save the molecule

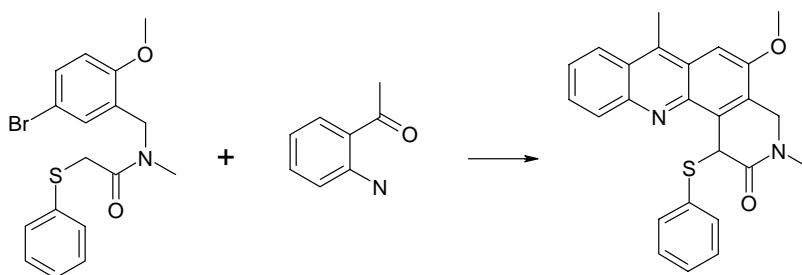
- Choose **File > Save As**. Enter **oxaziridine** as the file name. Click **Save**.



Exercise 2

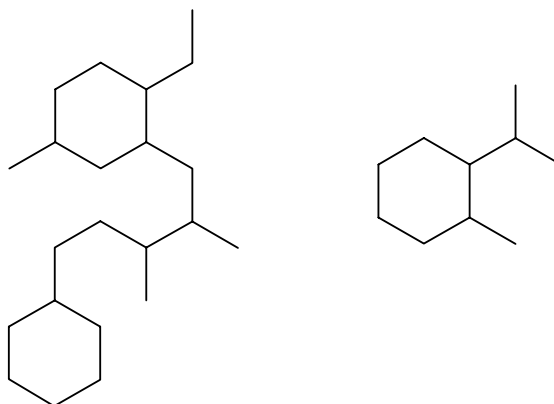
Draw a reaction

Draw the following reaction and save it as a rxnfile.

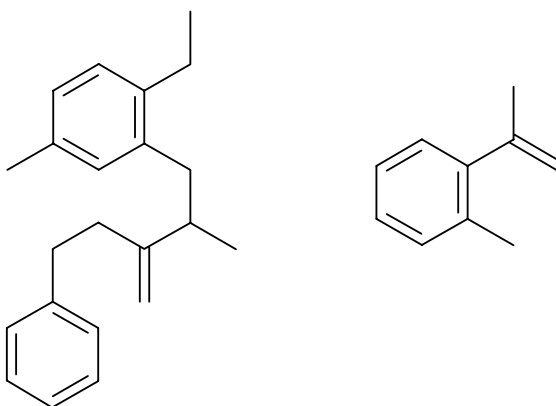


Draw the reactions

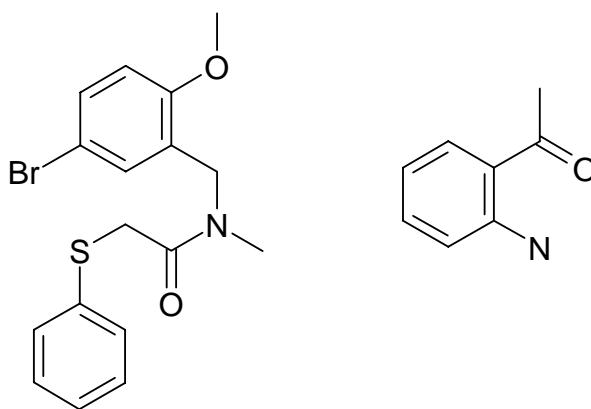
1. Delete the previous query.
2. Use the **All-Purpose Drawing** tool to draw the bonds for the two reactants.



3. Click the appropriate bonds to change them to double bonds.



4. Shift-click to select the atom positions for the oxygens. Right-click one of the selected atoms, and choose **Atom Symbol**. Click **O**.
5. Repeat to place the nitrogen atoms and the sulfur and bromine atoms.

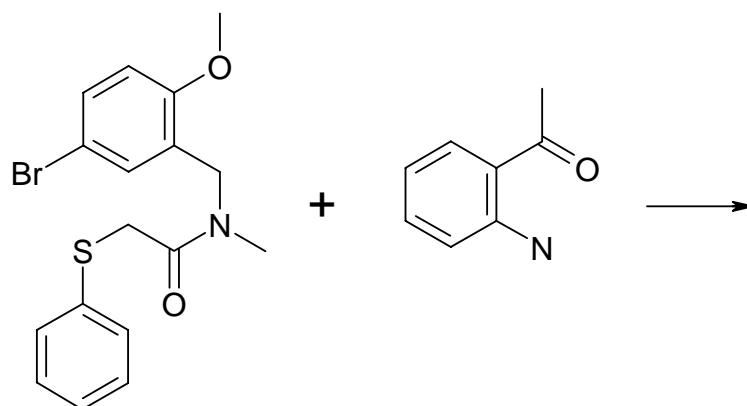


Place the reaction symbols

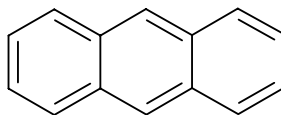


6. Click the **Plus** tool. Click the drawing area between the two reactants to place the plus sign.
7. Click the **Arrow** tool. Click the drawing area to the right of the second reactant.

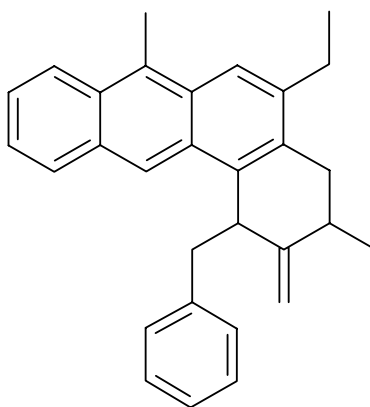
Draw the product



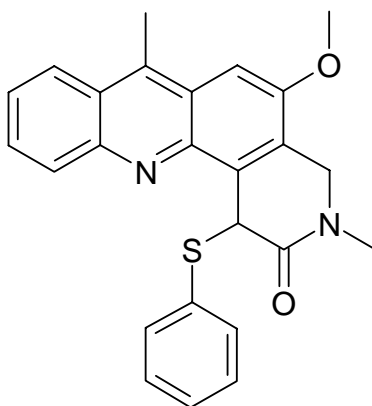
8. Click the **benzene** template, and then click the drawing area to the right of the arrow. Click the shared bond to fuse two more benzene rings.



9. Click the **All-Purpose Drawing** tool and draw the rest of the bonds.



10. Add the nitrogen, oxygen, and sulfur atoms.



Save the reaction

11. Choose **File > Save As**. Enter **reaction1** as the file name. Click **Save**.

To use the All-Purpose Drawing tool



1. Click the **All-Purpose Drawing** tool.
2. Choose a task from the table, and follow the instructions given.

To	Instructions
draw a bond	Drag at the desired angle
draw an atom	Click the screen and type a symbol
draw a chain or ring	Drag the cursor away from an atom
pull out a ring	Press the bond, and drag outward
change bond order	Click the bond
change atom type	Right-click the atom, and click Atom symbol
change multiple atom properties	Shift-click to select multiple atoms, and right-click to change a property
change multiple bond properties	Shift-click to select multiple bonds, and right-click to change a property

To draw a bond at any angle



1. Select a bond tool from the tool palette. (Click the arrow next to the bond tool to display the tool palette.)
2. Drag the mouse to draw the bond at the desired angle.

To delete an object



1. Click the **Eraser** tool.
2. Click an atom or bond to delete it, or drag the cursor to enclose the objects you want to delete.

To delete all the objects in the drawing area





1. Click **Clear All**.

To undo a drawing operation

1. Click **Undo**.
2. Repeat as needed to successively undo previous drawing operations.

To redo a drawing operation

1. Click **Redo**.
2. Repeat as needed to successively redo previously undone drawing operations.

To move an object	<ol style="list-style-type: none">1. Select the object(s).2. Drag to move the object in the desired direction.
To place a template	<ol style="list-style-type: none">1. Click the template tool.2. Click to place the template in the drawing area.
To fuse a template	<ol style="list-style-type: none">1. Click the template tool.2. Click the shared bond to fuse the template.
To sprout a template	<ol style="list-style-type: none">1. Click the template tool.2. Click an atom to sprout the template.
To use the Template Directory 	<ol style="list-style-type: none">1. Click the Template Directory.2. Click a folder to display the templates contained in the folder.3. Click to select the desired template.4. Click the drawing area to place the template; click a bond to fuse the template; click an atom to sprout the template.
To build a reaction  	<ol style="list-style-type: none">1. Draw the reactants and products.2. If there are multiple reactants or products, click the Plus tool and then click the drawing area to place a plus sign between the reactants or products.3. Click the Arrow tool. Then click the drawing area to place the reaction arrow between the reactants and products.
To select a molecule 	<ol style="list-style-type: none">1. Click the Molecule Select tool.2. Click the molecule.

To duplicate a molecule

1. Select the molecule.
2. Choose **Edit > Duplicate**.

To move a molecule

1. Select the molecule.
2. Drag the molecule to its new location.

To add stereo bonds

1. Click the **All-Purpose Drawing** tool.
 2. Right-click the bond and choose the **Stereobond** option.
- Or –
1. Choose a stereo bond tool from the tool palette.
 2. Click an existing bond to change it, or drag to draw a new stereo bond.
 3. If needed, click the stereo bond to change its direction.

To save a molecule or reaction

1. Choose **File > Save As**.
2. Type the name of the file.
3. Click **Save**.