MDL
Information Systems, Inc.

ISIS™/Draw Tutorial

Version 1.1

INTEGRATED SCIENTIFIC INFORMATION SYSTEM

August 1993

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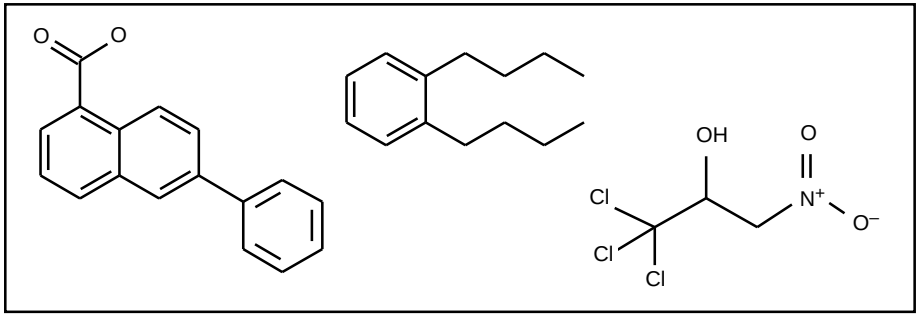
Drawing a Molecule

This chapter teaches you how to draw *chemically significant* molecules. This means that you can store the molecules in an ISIS/Base, MACCS-II, or REACCS database and search for them based on their structure.

Using a variety of drawing techniques, you will draw the following molecules:



When you complete this chapter you will know how to:

- Use templates
- Delete atoms and bonds
- Draw and edit bonds
- Add and edit atom symbols
- Move and resize molecules

✎ The exercises assume that ISIS/Draw on your workstation is using the factory-set defaults. If, *and only if*, the program operates differently than is described in this tutorial, check your workstation settings against those listed in “Defaults Affecting Molecule Drawing” on page 31.

ENHANCEMENTS FOR ISIS/DRAW VERSION 1.1

There are program changes in ISIS/Draw 1.1 which affect the tutorial. The cursors were changed, as was the visual feedback when moving the cursor over atoms, bonds, components, and sketches. Chapter 2 of the Tutorial has been updated to accurately describe these changes.

✎ Chapters 3 and 4 of the Tutorial were not updated, and contain some small inaccuracies.

Cursors

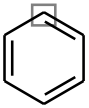
The ISIS/Draw cursors provide feedback on what tool is active. The following table displays the cursors used when you select a tool in ISIS/Draw 1.1:

Tools	Cursors	Tools	Cursors
Select		Eraser	
Sketch (Ellipse, Arc, Line, and so on)		Atom	
Rotate		Bond	
3D Rotate		Template	
3D Edit			

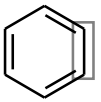
✎ You will see these cursors on your screen, but they are not displayed in the tutorial for reasons of clarity.

Object highlighting

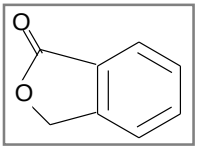
When you move the cursor over an object, the object highlights to indicate whether the cursor is over an atom, bond, component, or sketch:



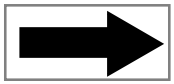
Square atom indicator shows that an atom is highlighted



Rectangular bond indicator shows that a bond is highlighted



A component is highlighted



A sketch is highlighted

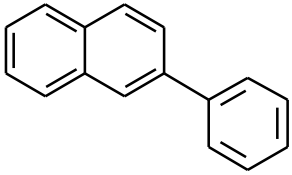
USING TEMPLATES

Templates are predrawn structures that you can use to quickly build molecules. ISIS/Draw has two types of templates:

- Template *pages*. A template page is a window that contains many structural fragments, such as rings or chains. You pick the template that you want to use from the window.
- Template *tools*. A template tool is a single structural fragment, such as a benzene ring, that you pick directly from the menu bar.

Exercise: Drawing with template tools

This exercise demonstrates three ways to use template tools. You will draw the following molecule:



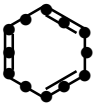
1. Template tools are only available when **Molecule** is highlighted on the menu bar. If the template tools are not displayed on the top menu bar, point to **Molecule** and press the mouse button.

✎ We usually use the word *click* to mean "point to an object and press the mouse button."

2. Click the **Benzene Ring** tool  . The tool highlights.

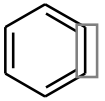
✎ If the error message “Unable to read drawing: tpl4.skc” appears, your workstation has not been properly configured to read the template files. See the *ISIS/Draw Installation & New Features* booklet for instructions.

3. Click the center of the drawing area. A benzene ring appears:



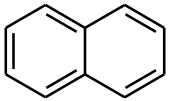
The black dots marking the ring are *selection handles*. When you draw an object, the object is automatically *selected*. When an object is selected, you can perform operations on it, such as deleting or moving it. You will learn more about selecting objects later. To simplify pictures, we usually do not show selection handles.

4. Point to the bond on the right side of the ring. The *entire* bond is surrounded by the *bond indicator*, which looks like a rectangle:



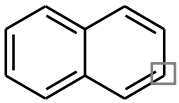
✎ Be precise when you point to an object. Before you go to the next step, make sure that you see the bond indicator, not the atom indicator. The bond indicator tells you that you are pointing to a bond.

5. Click the bond. A new ring is *fused* to that bond:



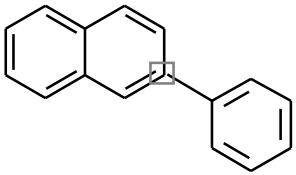
The double bonds in the structure change position to accommodate the aromaticity of the second ring.

6. Point to the atom shown below. The atom is surrounded by the *atom indicator*, which looks like a square:



✎ Again, be precise when you point to an object. Before you go to the next step, make sure that you see the atom indicator, not the bond indicator. The atom indicator tells you that you are pointing to an atom.

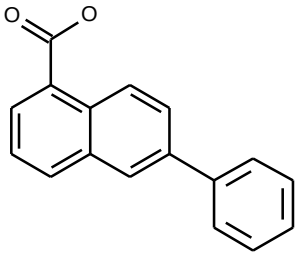
7. Click the atom. A benzene ring *sprouts* from that atom. Sprouting means that the ring is connected to the atom by a single bond:



Exercise: Drawing with template pages

Unlike a template tool, a template *page* displays several fragments for you to pick. When you pick a template from the page, you also define its attachment point. The *attachment point* is the atom or bond on the template that attaches it to the molecule you are building.

This exercise demonstrates one method of using template pages. In this exercise, you will add a carboxylic acid template to the existing molecule:

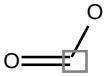


1. Point to **Templates** on the menu bar and press *and hold* the mouse button. The Templates menu appears.

2. Move the pointer down the menu. When the **Functional Groups** command highlights, release the mouse button. You see a window containing functional groups.

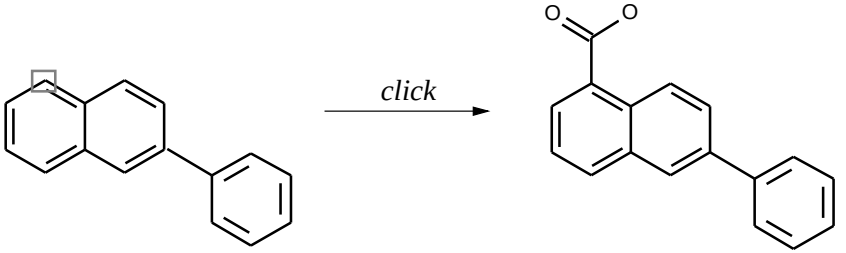
✎ We usually abbreviate Steps 1 & 2 to “Choose Functional Groups from the Templates menu.”

3. Click the carbon atom on the carboxylic acid template. Make sure that that you see the atom indicator before you click:



The atom that you click becomes the attachment point for the template. In this case, the template will attach to the molecule by the carbon atom. The template page disappears.

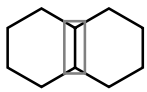
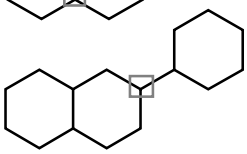
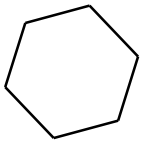
4. Click the atom shown below. The carboxylic acid group sprouts from that atom:



The next exercise shows you how to delete objects on your screen.

Summary: Four ways to use template tools and pages

For a template tool, click the tool. For a template page, choose the appropriate template page from the Templates menu and click an attachment point. Then:

Choose one method	
Click the work area to draw a template of standard bond length.	
Click a bond to fuse to it.	
Click an atom to sprout from it.	
Drag mouse for a variable-sized template.	

You can also attach templates by using the keyboard. See “Keyboard Drawing” in the *ISIS/Draw Reference*.

DELETING ATOMS AND BONDS

In this section, you learn how to:

- Delete a single atom or bond
- Delete an entire structure
- Delete all objects in the drawing area

You must have some molecule structures on the screen to practice deleting. Before you begin the exercises below, use the templates to draw a few simple molecules.

Exercise: Deleting a single object

In this exercise, you will use the Eraser tool to delete an atom and a bond. Use this method when you have only a few objects to delete. Later, you will learn a better method for deleting several objects at a time.

1. Click the **Eraser** tool  .
2. Click any bond. The bond disappears. (Any terminal atoms attached to the bond also disappear.)
3. Click any atom. The atom and any bonds attached to it disappear.

Exercise: Undoing the last command

If you make a mistake and want to immediately *undo* the last command, you can choose Undo from the Edit menu. However, not all commands can be reversed with Undo. If this is the case, the Undo command is dimmed on the menu and you cannot choose it.

In this exercise, you will use the Eraser tool to delete an atom, and then recover it by undoing the deletion.

1. Verify that the Eraser tool is highlighted, and then click an atom. The atom disappears.
2. Choose **Undo** from the **Edit** menu. The atom is restored.

Exercise: Selecting objects to delete

In this exercise, you learn how to *select* the objects to delete and then delete them. Use this method if you want to delete several objects at once.

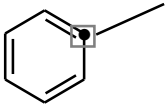
✎ It is very important to learn how to select objects. Many operations, such as moving and resizing objects, require that you select the objects first.

Select one object — click

1. Click the **Select** tool .

   ✎ The Select tool is the first tool on the menu bar. Do not confuse it with the Component tool which looks like this .

2. Click an atom to select it. A selection handle appears on the atom. For example:



Selection handle (inside the atom indicator)

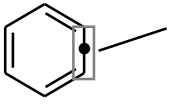
3. Choose **Cut** from the **Edit** menu, or press **Delete**. The selected atom and any attached bonds disappear.

   You can also use the *keyboard accelerator* to quickly delete the selected object. The keyboard accelerator for a command is shown on the menu next to the command name.

Select many objects — shift-click

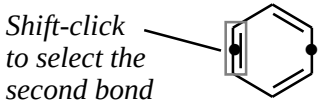
1. Verify that the **Select** tool is highlighted.

2. Click a bond to select it. A selection handle appears on the bond. For example:



Selection handle (inside the bond indicator)

3. To select another bond, press and hold the **Shift** key. Then click the bond:



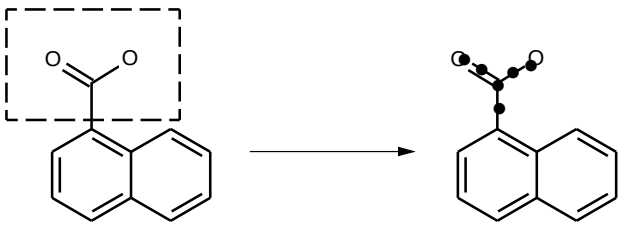
✎ We use the word *shift-click* to mean "press and hold the Shift key as you click an object." You must shift-click to select more than one object at a time. If you click a second object *without* pressing the Shift key, the second object is selected but the first object is then *deselected*.

4. Release the **Shift** key.

5. Choose **Cut** from the **Edit** menu, or press **Delete**. The selected bonds disappear.

Select many objects — use a frame

You can select objects by drawing a frame around them. For example, you can select a *portion* of a molecule by drawing a frame around it. All the atoms and bonds in the frame are selected:



1. Verify that the **Select** tool is highlighted.

2. Point to where you want to begin the frame.

3. Press *and hold* the mouse button as you move the mouse diagonally. The frame stretches from the starting point to the pointer. Stretch the frame until it encloses all of the atoms and bonds you want to delete.

✎ We usually use the word *drag* to mean "press and hold the mouse button as you move the mouse."

4. Release the mouse button. All of the atoms and bonds in the frame are selected.

5. Choose **Cut** from the **Edit** menu, or press **Delete**. The selected objects disappear.

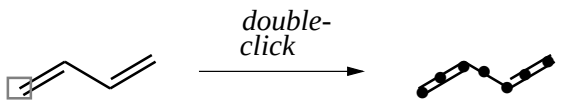
Select many objects — use the lasso tool

With ISIS/Draw 1.1, you can also select objects with a lasso. When you have finished this tutorial, you can change the selection method to the lasso. See page 5–3 in the *ISIS/Draw Installation & New Features* booklet for details on how to do this.

✎ All three chapters in this tutorial use the frame to select objects. Do not change the frame selection to the lasso until you have completed the tutorial.

Select a molecule — double-click

To select all of the atoms and bonds in a molecule, double-click any atom or bond in the molecule. For example:



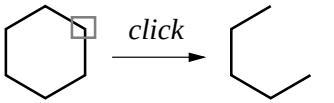
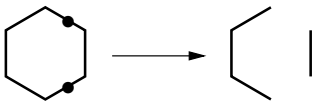
1. Verify that the **Select** tool is highlighted.
2. Point to an atom and then *quickly* press the mouse button twice. All of the atoms and bonds in the structure are selected. (If you do not press the mouse button quickly enough, only the one atom is selected. Try again.)

   ✎ We use the word *double-click* to mean "point to an object and quickly press the mouse button twice."
3. Choose **Cut** from the **Edit** menu, or press **Delete**. The molecule disappears.

Select all objects — choose Select All

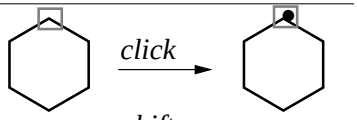
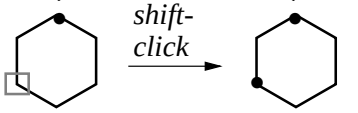
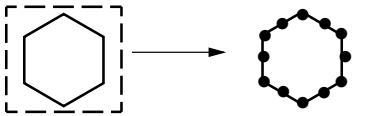
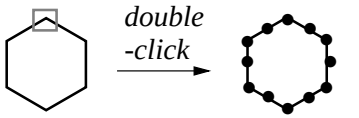
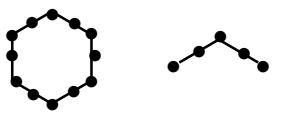
1. Choose **Select All** from the **Edit** menu. All of the objects in the window are selected.
2. Choose **Cut** from the **Edit** menu, or press **Delete**. All of the objects disappear.

Summary: Two ways to delete atoms and bonds

Choose one method	
Click the Eraser tool. Then click an atom or bond.	
Select multiple atoms or bonds. Then choose Cut from the Edit menu, or press Delete.	

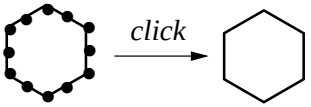
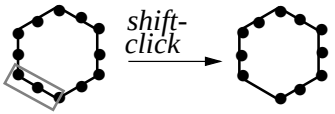
Summary: Five ways to select objects

Click the Select tool. Then:

Choose one method	
Click one object to select it.	
Shift-click to select multiple objects.	
Draw a frame to select multiple objects.	
Double-click an atom to select all atoms and bonds in the molecule.	
Choose Select All from the Edit menu to select all objects in the window.	

Summary: Two ways to deselect objects

Click the Select tool. Then:

Choose one method	
Click an empty space to deselect all objects.	
Shift-click one object to deselect it.	

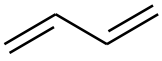
DRAWING AND EDITING BONDS

In this section you learn how to:

- Draw bonds using the *bond tools*
- Change bond types

Exercise: Drawing and editing bonds

This exercise demonstrates one method of drawing bonds. You will draw the following structure:

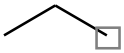


1. Click the **Single Bond** tool  .
2. Point to any empty space in the drawing area. This will be the starting point for your bond.
3. Drag the mouse away from the starting point. A new bond stretches from the starting point to the pointer:

4. Release the mouse button. The bond of standard length is fixed in place.

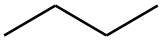
5. To draw the next bond, point to an atom at the end of the first bond:

6. Drag the mouse away from the starting point:



7. Release the mouse button to fix the bond in place.

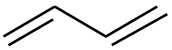
8. Repeat the procedure to draw the third bond:



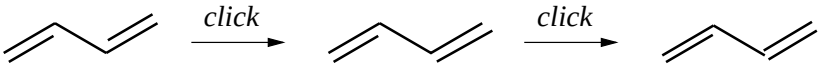
9. Click the **Double Bond** tool  .

10. Click the first bond. The bond changes to double:

11. Click the third bond. The bond changes to double:



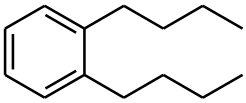
12. You can change the placement of a double bond by clicking it. To experiment, click the third bond twice more. The placement of the double bond rotates between these three positions:



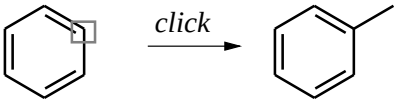
(centered)

Exercise: Sprouting bonds

Sprouting bonds is a fast way to draw bonds that are a standard length and angle. (The standard length is determined by a setting in Preferences on the Options menu.) In this exercise, you will sprout bonds to draw the following molecule:

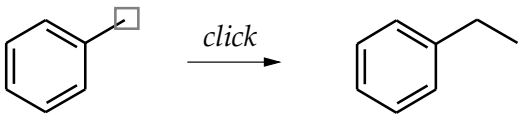


1. Click the **Benzene Ring** tool.
2. Click an empty space in the drawing area. A benzene ring appears.
3. Click the **Single Bond** tool.
4. Click the ring atom shown below. A single bond *sprouts* from that atom:

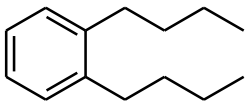


   The sprouted bond is the standard length and bisects the ring angle.

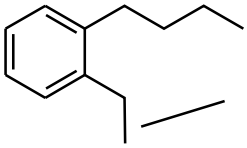
5. Click the end of the single bond. A new bond sprouts from that atom:



6. Continue sprouting bonds to complete the structure:



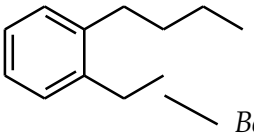
✎ Sometimes a bond sprouts in the wrong direction. For example, a bond may sprout like this:



Bond sprouts in wrong direction.

To delete the bond, choose Cut from the Edit menu, or press Delete. (This works because the bond is already selected.)

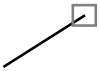
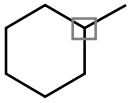
When you have deleted the bond, click the atom again. A new bond sprouts in the opposite direction:



Bond sprouts in opposite direction.

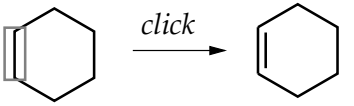
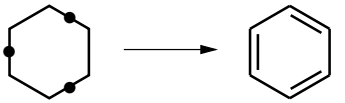
Summary: Two ways to draw bonds

Click a bond tool. Then:

Choose one method	
Drag and release the mouse to draw a bond of standard length.	
Click an atom (or empty space) to sprout a bond of standard length.	

You can use the compass or the keyboard to draw bonds with specific bond angles. See “Aids for precision drawing” and “Keyboard Drawing” in the *ISIS/Draw Reference* for more information.

Summary: Two ways to edit bonds

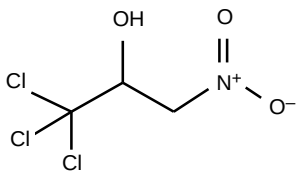
Choose one method	
Click a bond tool. Click the bond you want to change.	
Select multiple bonds. Choose Bond... from the Style menu. Change any bond properties. Click OK.	

ADDING AND EDITING ATOM SYMBOLS

When you draw a bond, there are implied carbon atoms at each end. To add heteroatoms to your molecule, you must edit the atom symbol. You can also edit an atom in other ways, such as adding charges, changing the isotope, or displaying attached hydrogens.

Exercise: Adding atom symbols

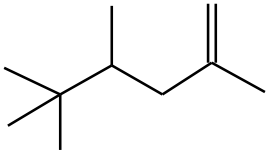
This exercise demonstrates two methods for adding atom symbols. You will draw the following molecule:



Before you begin, delete all objects from the window.

Draw the carbon skeleton

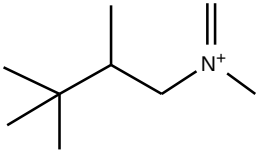
Use the appropriate bond tools to draw the structure below. Draw the bonds by dragging and releasing the mouse. The exact bond angles are not important:



If you wish, you can adjust the appearance of your molecule by moving the atoms. To move an atom, click the Select tool. Then drag the atom to its new position. The bonds attached to the atom stretch to accommodate the new atom position. Release the mouse button to fix the atom and bonds in place.

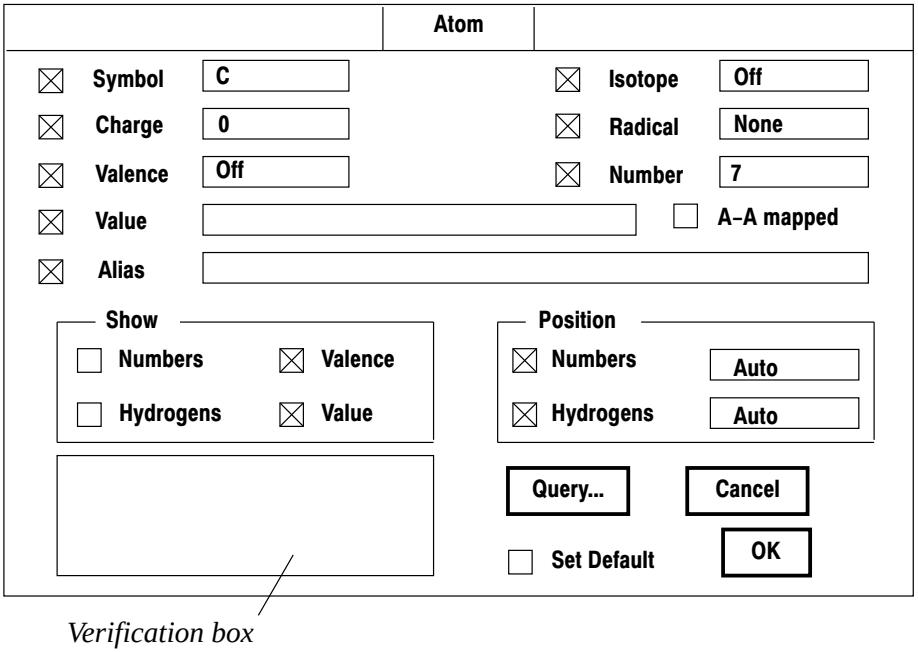
Add the nitrogen atom

Now you will add the nitrogen atom and the positive charge:

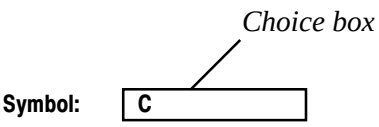


1. Click the **Atom** tool.

2. Double-click the atom that you want to change to nitrogen. The Atom dialog box appears:



3. Point to the Symbol choice box:



You want to change the symbol from C to N.

4. Press *and hold* the mouse button. A menu of atom symbols appears.

5. Move the pointer down the menu until N highlights.

6. Release the mouse button.

✎ We usually abbreviate Steps 3–6 as "Choose N from the Symbol choice box."

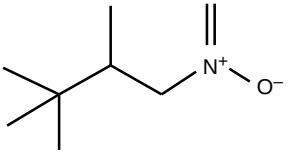
7. Choose **1+** from the **Charge** choice box.

8. Examine the atom displayed in the verification box. Make sure that you have defined a nitrogen atom with a single positive charge (N+).

9. Click **OK**. The dialog box disappears and the carbon atom changes to a positively charged nitrogen atom.

Add the oxygen atoms

You will now use the same method to add the negatively charged oxygen atom:



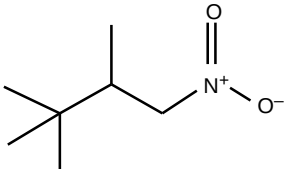
1. Double-click the atom you want to change to oxygen.

2. Choose **O** from the **Symbol** choice box.

3. Choose **1–** from the **Charge** choice box.

4. Click **OK**.

Now you will add the oxygen atom to the end of the double bond:

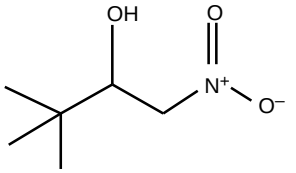


1. Double-click the atom at the end of the double bond.

2. Choose **O** from the **Symbol** choice box.

3. Click **OK**.

Now you will add the hydroxyl group:

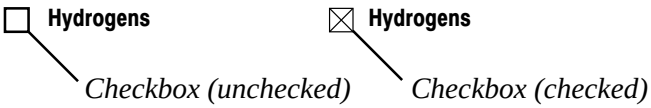


To draw the hydroxyl group, you will add an oxygen atom *and* display the hydrogen on it:

1. Double-click the atom that you want to change.

2. Choose **O** from the **Symbol** choice box.

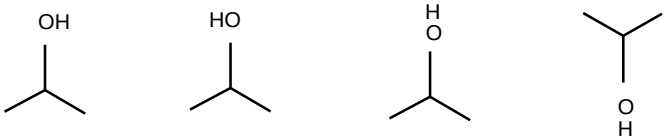
3. Click the **Show Hydrogens** checkbox to check it. This switches on the hydrogen display:



Checkbox (unchecked) *Checkbox (checked)*

4. Choose **Right** from the **Position Hydrogens** choice box. This positions the hydrogens to the right of the atom symbol. (The checkbox must be checked.)

You can position hydrogens to the right, left, above, or below the atom symbol. For example:



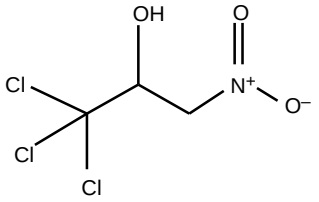
Right *Left* *Above* *Below*

You can also represent the hydrogen with a dot or circle.

5. Click **OK**.

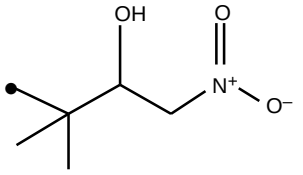
Add the chlorine atoms

Now you will add the chlorine atoms:

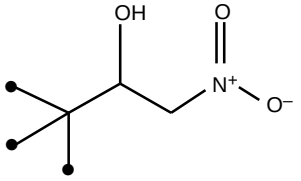


Because there are three atoms to change, it is faster to use the selection method to edit these atoms:

1. Click the **Select** tool.
2. Click one of the atoms that you want to change to chlorine. A selection handle appears on the atom:



3. Shift-click to select the second and third atoms:



✎ It is important that you select all three atoms at this point. If you made a mistake and the proper atoms are not selected, click an empty space in the drawing area. All of the selection handles disappear. Now try to select the atoms again.

4. Choose **Atom...** from the **Style** menu. The Atom dialog box appears.
5. Point to the Symbol choice box and press and hold the mouse button. A menu of atom symbols appears.

6. The symbol for chlorine is not on the menu. In this case, choose **Ptable...**. The Periodic Table appears.

7. Click the element **Cl**.

8. Click **OK**. The Periodic Table disappears.

9. Click **OK**. The selected atoms change to chlorine.

Save the molecule

You always save molecules in a *sketch file*. Sketch files save an image of the molecule, exactly as it is displayed on the screen, with all of the chemical information intact.

1. Choose **Save As...** from the **File** menu. A dialog box appears.

2. Change to the SAMPLE directory or folder if it is not already current. (If you did not follow the recommended installation procedure, your work directory or folder may have a different name.)

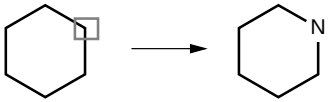
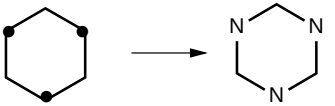
3. Type the filename **trichlor.skc** in the File Name text box. (Macintosh users type **trichlor** in the Save Document As? text box.) On IBM computers, the filename extension .SKC identifies the file as a sketch file.

4. If you make a typing mistake, use these editing keys:

To do this:	IBM	Mac
Move cursor left	←	←
Move cursor right	→	→
Delete left character	Backspace	Delete/Backspace
Delete right character	Delete	Del

5. Click **OK** (Mac=**Save**). The sketch file is saved on disk, and you see the name of the sketch in the title bar of the window.

Summary: Two ways to edit atom symbols

Choose one method	
Click the Atom tool. Double-click one atom. Choose the atom symbol from the Symbol choice box. Click OK.	
Select multiple atoms. Choose Atom... from the Style menu. Change any atom properties. Click OK.	

You can also edit atom symbols using the keyboard. See “Keyboard Drawing” in the *Drawing a Molecule*.

MOVING AND RESIZING MOLECULES

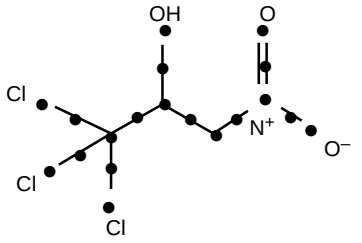
In this section, you learn how to move and resize molecules.

If the last molecule you drew (trichloro-nitropropanol) is displayed in the drawing area, go directly to the exercise below. If the molecule is not currently displayed, follow these steps to retrieve it:

1. Choose **Insert...** from the **File** menu. You see a dialog box,
2. Double-click the name **trichlor.skc** (Mac=**trichlor**) from the Files list box. (If the file name does not appear in the list box, change to the SAMPLE directory first.) The molecule appears in the drawing area.

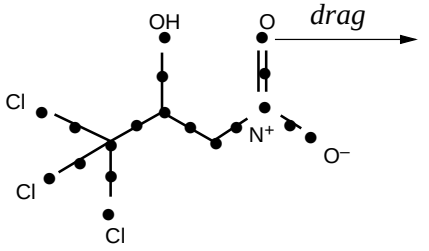
Exercise: Moving a molecule – use the select tool

1. Click the **Select** tool.
2. Double-click any atom to select all of the atoms and bonds in the molecule:



✎ To move a molecule with the Select tool, you must select *all* of the atoms and bonds. If some of the atoms or bonds are not selected, the molecule will distort when you move it.

3. Point to any atom in the molecule and drag it. The entire molecule moves to the new position:



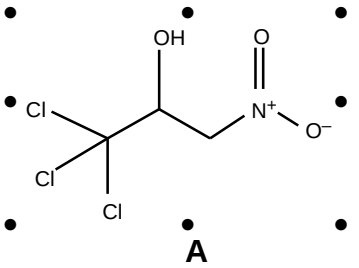
4. Release the mouse button to fix the molecule in place.

You can also use this method to join two molecules together. When the atom you use to drag the first structure touches an atom in the second structure, the two structures fuse. See “Join” in the *ISIS/Draw Reference* index.

Exercise: Moving a molecule – use the component tool

You use the Component tool to select *whole* molecules. Usually you select these molecules to define them as reaction components. But you can also use the Component tool to quickly select molecules that you want to move. When you select a molecule with the Component tool, you *cannot* move or edit the individual atoms and bonds, and you cannot fuse two molecules together.

1. Click the **Component** tool.
2. Click the center of the molecule. Eight selection handles appear around the molecule and the letter A appears underneath:



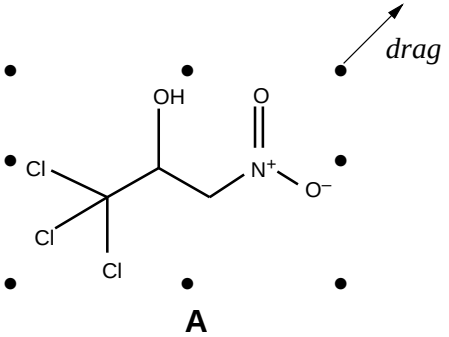
3. Point to the center of the molecule (not on a selection handle).
4. Drag the molecule to a new position. Release the mouse button to fix the molecule in place.

Exercise: Resizing a molecule – use the component tool

In this exercise, you will resize a molecule using the Component tool.

1. Verify that the **Component** tool is highlighted and that the molecule is selected.

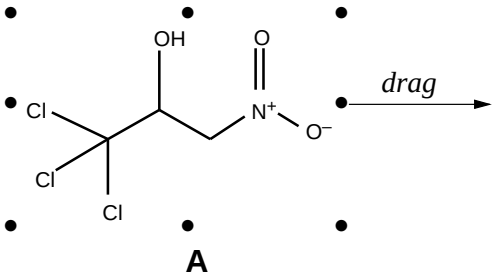
2. Point to a *corner* selection handle and drag the handle diagonally and outward. The molecule increases in size, keeping its original proportions:



A

3. Drag a corner selection handle diagonally and inward. The molecule decreases in size, keeping its original proportions.

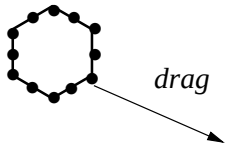
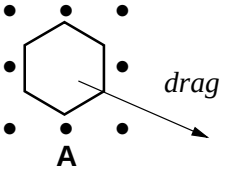
4. Now point to a selection handle on the right or left side (*not* a corner handle.) Drag the handle outward. The molecule stretches horizontally, losing its original proportions:



A

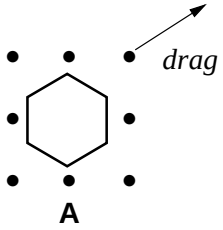
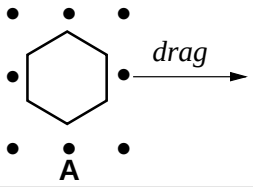
5. Drag a non-corner handle on the top or bottom of the molecule. The molecule stretches vertically, losing its original proportions.

Summary: Two ways to move a molecule

Choose one method	
Click the Select tool. Double-click any atom to select all atoms and bonds. Point to an atom or bond and drag the molecule to new position.	
Click the Component tool. Click the molecule. Point to center of molecule and drag to new position.	

Summary: Two ways to resize a molecule

Click the Component tool. Select the molecule. Then:

Choose one method	
Point to a corner handle and drag. The molecule keeps its original proportions.	
Point to a non-corner handle and drag. The molecule loses its original proportions.	

WHERE TO GO FROM HERE

You now have all the basic skills needed to draw molecules with ISIS/Draw. Depending on your job tasks, you may want to:

- *Practice drawing and learn additional techniques.* For some advanced drawing exercises, see the section "Drawing Examples" near the beginning of the chapter "Drawing a Molecule or Reaction" in the *ISIS/Draw Reference*.
- *Read about other drawing procedures.* For a comprehensive collection of drawing procedures, see the chapter "Drawing a Molecule or Reaction" in the *ISIS/Draw Reference*.
- *Learn how to draw reactions.* See the chapter "Drawing a Reaction" in this tutorial. These reactions are suitable for storing in a database or for use as reaction search queries.
- *Learn how to draw graphics for written reports or overhead transparencies.* See the chapter "Drawing a Presentation Graphic" in this tutorial.
- *Learn how to search databases.* See the *ISIS/Base Database Searching* book.

DEFAULTS AFFECTING MOLECULE DRAWING

Certain program defaults affect the way ISIS/Draw draws molecules. If you change these defaults from their factory settings, the drawing instructions in the tutorial and the *ISIS/Draw Reference* will not work as described. For a complete list of program defaults, see the chapter "ISIS/Draw Commands" in the *ISIS/Draw Reference*. To see which of the following defaults are set for your workstation, choose **Preferences...** from the **Options** menu.

Page 1

Standard bond length

Factory default: 0.25 inches.

Reset to Select tool after using a tool

Factory default: checkbox is unchecked. If checked, ISIS/Draw automatically activates the Select tool when you finish using another tool.

Highlight last drawn atoms and bonds

Factory default: checkbox is checked. If checked, ISIS/Draw automatically selects the last atom or bond that you drew. This allows you to immediately perform an operation on the atom or bond.

Delete atom when deleting all its bonds

Factory default: checkbox is checked. If checked, ISIS/Draw automatically deletes an atom if you delete all the bonds attached to that atom.

Abbreviate typed-in templates

Factory default: checkbox is unchecked. If checked, ISIS/Draw automatically abbreviates any template that you attach using a keyboard command to its name. You do not see the actual chemical structure.

Show “Valence exceeded” message

Factory default: checkbox is checked. If checked, ISIS/Draw warns you if you attach more bonds to an atom than the standard valence allows.

Use compass to draw bonds

Factory default: checkbox is checked, along with “Hard Compass.” ISIS/Draw restricts the length of bonds that you draw to standard bond length. It also restricts the angle for any bond you draw to a 15-degree increment.

Page 2

Atom number text size

Factory default: 6 points.

Adjust single and double bonds in aromatic rings

Factory default: checkbox is checked. If checked, ISIS/Draw automatically adjusts the bond order when you fuse aromatic rings.

Mark reacting centers automatically

Factory default: checkbox is unchecked. If checked, ISIS/Draw automatically marks reacting centers on any reaction you assemble, provided that the reaction components are atom-atom mapped.

Use open stereo wedge

Factory default: checkbox is unchecked. If checked, ISIS/Draw uses the open-wedge style for stereo up bonds.

Prompt Before Fusing Overlapped Atoms

Factory default: checkbox is unchecked. If checked, prevents new fusion when you attach a new template or bond to a structure and atoms overlap.

Select With Lasso/Select With Frame

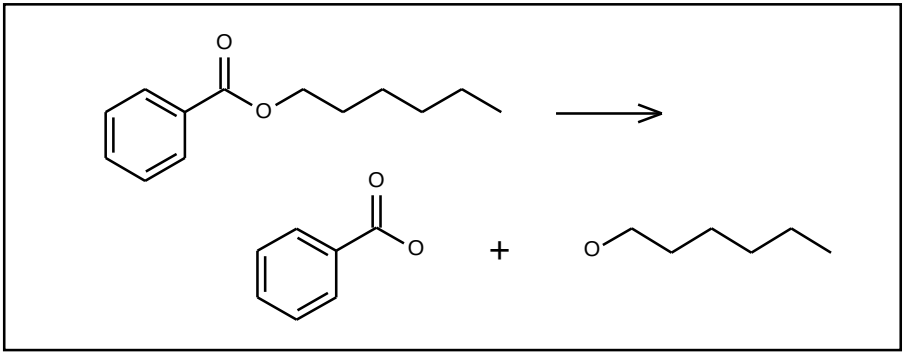
Factory default: Select with Frame checkbox is checked. Allows you to change between the lasso and frame to select objects when the **Select**, **Rotate**, or **Component** tool is active.

✎ Make sure that the **Select with Frame** radio button is selected for the rest of the tutorial.

2
Drawing A Reaction

You must complete Chapter 1, "Drawing a Molecule," before you begin this chapter. Chapter 1 teaches basic program operations and drawing techniques that you need to complete this chapter successfully.

This chapter teaches you how to draw *chemically significant* reactions. This means that you can store the reactions in an ISIS/Base or REACCS database and search for them based on the structures and chemical interactions of the component molecules. You will draw and edit the following reaction:



When you complete this chapter you will know how to:

- Assemble a reaction
- Move reaction components
- Move and resize a reaction
- Edit a reactant or product
- Dissolve a reaction

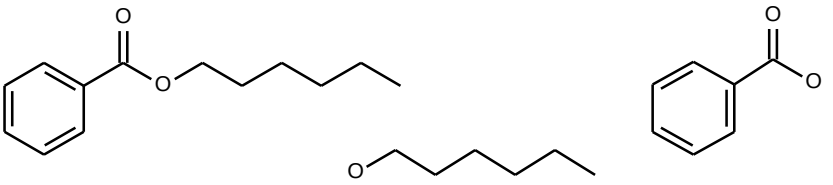
DRAWING REACTANTS AND PRODUCTS

To draw a reaction, you must first draw the molecules that compose the reaction. For the reaction to be chemically significant, you must draw the molecules using the molecule tools.

Before you begin, verify that Molecule is highlighted, and delete any objects in the window.

Exercise: Drawing the reaction components

In this exercise, you will draw the following reactants and products:



To save time, the first molecule is provided for you. You will retrieve the molecule from a sketch file.

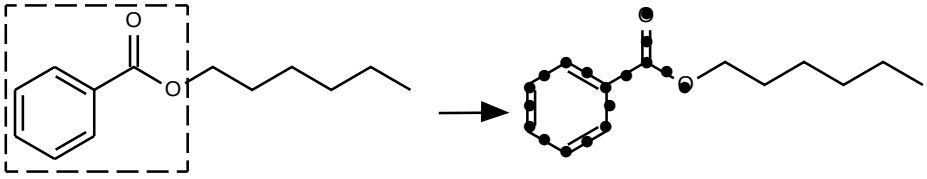
Retrieve the first molecule

1. Choose **Insert** from the **File** menu. A dialog box appears.
2. Click **reactant.skc** (Mac=**reactant**) from the list of file names. If the file name does not appear in the list box, change to the SAMPLE directory or folder. (If you did not follow the recommended installation, your work directory or folder may have a different name.)
3. Click **OK** (Mac=**Open**). The molecule stored in the sketch file REACTANT.SKC appears in the drawing area:

Draw the second molecule

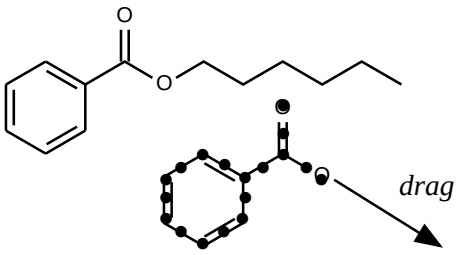
Often, the reactants and products in a reaction are structurally similar. If this is the case, you can draw one structure, *duplicate* it, and then modify the copy to create the next molecule. In this example, you will duplicate *part* of the first molecule to create the second molecule:

1. Click the **Select** tool if it is not already highlighted.
2. Drag the mouse to draw a frame around the ring portion of the molecule:



✎ It is important that you select all of the atoms and bonds that you want to duplicate. If some of the atoms or bonds are not selected, shift-click to select them. If some atoms or bonds that you do *not* want to duplicate are selected, shift-click to deselect them.

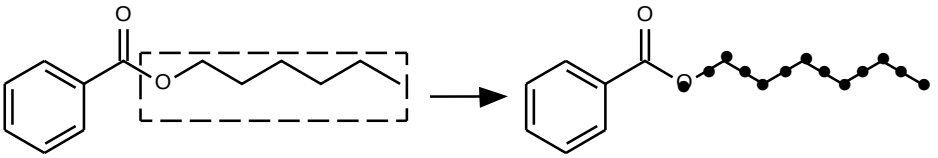
3. Choose **Duplicate** from the **Edit** menu. A duplicate of the selected atoms and bonds appears next to the original structure.
4. Point to any atom on the duplicate structure and drag it away from the original:



Draw the third molecule

You will duplicate a different part of the first molecule to create the third molecule.

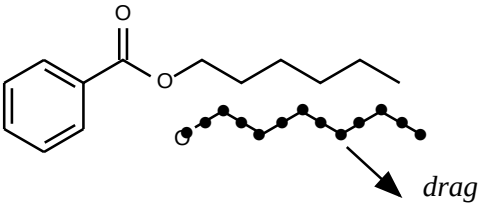
1. Select the chain portion of the first molecule:



✎ Make sure that all the atoms and bonds that you want to duplicate are selected before you go on to the next step.

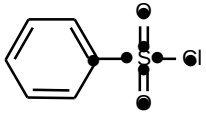
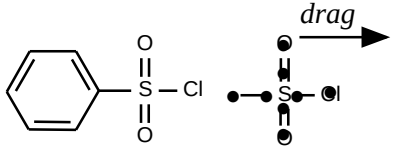
2. Choose **Duplicate** from the **Edit** menu.

3. Point to any atom on the duplicate structure and drag it away from the original:



You now have three molecules in the drawing area and are ready to assemble them into a reaction.

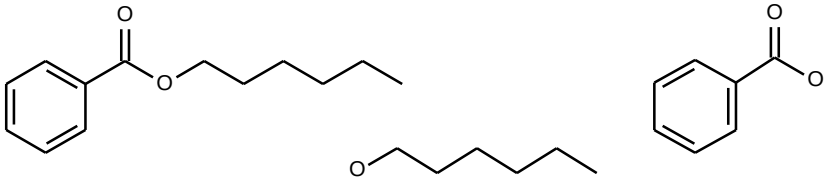
Summary: To duplicate a molecule

Follow these steps	
1. Select the atoms and bonds.	
2. Choose Duplicate from the Edit menu. Drag the duplicate structure away from the original.	

ASSEMBLING A REACTION

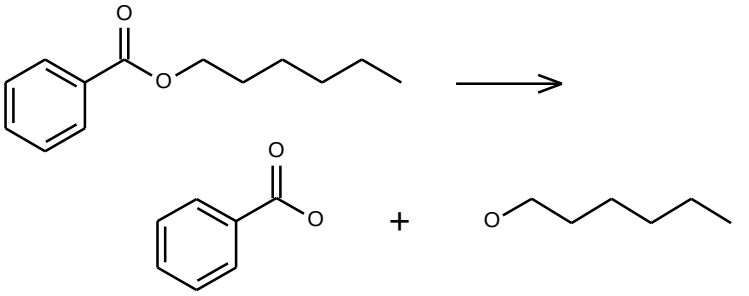
To assemble molecules into a reaction, you must use the *Component tool* to select the molecules that compose the reaction. The Component tool is only available when Molecule is highlighted.

Before you begin the exercise below, the following molecules must be displayed in the drawing area:

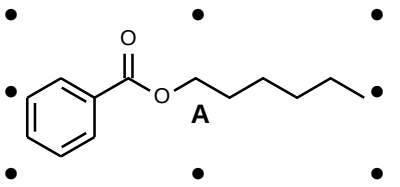


Exercise: Assemble the reaction

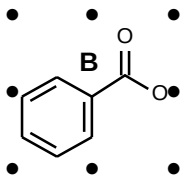
You will now assemble the following reaction:



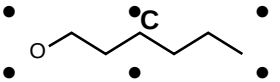
1. Click the **Component** tool .
2. Click the first molecule in the reaction. Eight selection handles appear around the molecule and the letter A appears in the center:



3. Shift-click the second molecule in the reaction. It displays the letter B:



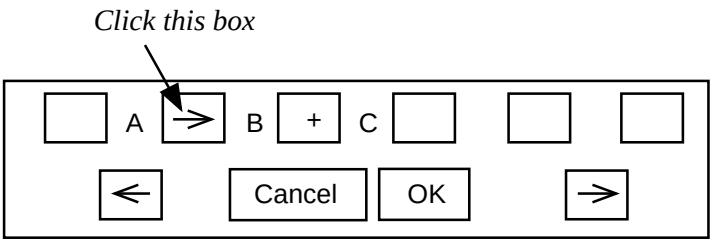
4. Shift-click the third molecule in the reaction. It displays the letter C:



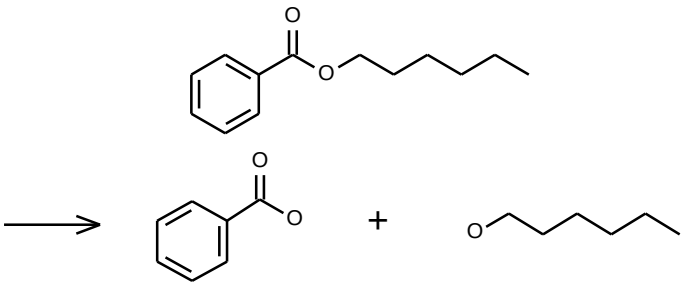
✎ You must select all three molecules in the proper sequence. If you made a mistake, click an empty space in the drawing area. All of the selection handles disappear. Now try to select the molecules again.

5. Choose **Reaction** from the **Chem** menu. The Reaction Assembly dialog box appears.

6. Click the box between A and B to place the reaction arrow:



7. Click **OK**. The reaction symbols (plus sign and arrow) appear in the drawing area:



The molecules in your reaction may be arranged differently. This is not important. In the next section, you will learn how to move the reaction components into the desired arrangement.

Exercise: Saving the reaction

You always save reactions in a *sketch file*. Sketch files save an image of the reaction, exactly as it is displayed on the screen, with all of the chemical information intact.

1. Choose **Save As** from the **File** menu. A dialog box appears.

2. Change to the SAMPLE directory or folder if it is not current. (If you did not follow the recommended installation, your work directory or folder may have a different name.)

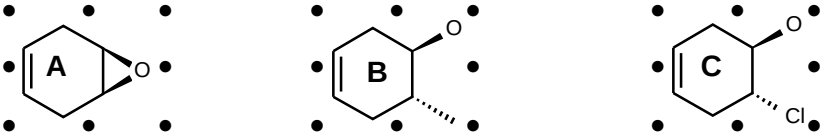
3. Type the file name **reaction.skc** in the Save As File Name text box. (Macintosh users type **reaction** in the Save the work in progress? text box.)

4. Click **OK** (Mac=**Save**). The sketch file is saved on disk, and you see the name of the sketch in the title bar of the window.

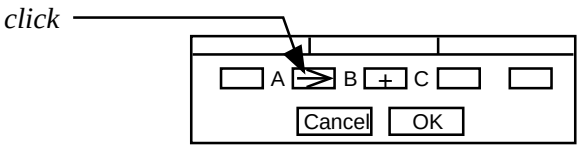
Summary: To assemble a reaction

Follow these steps

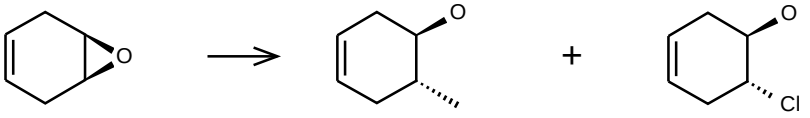
1. Click the Component tool. Select the reactants and products in sequence.



2. Choose Reaction from the Chem menu. Click a box to place the reaction arrow.



3. Click OK.



MOVING REACTION COMPONENTS

You can move the components of a reaction (molecules, plus signs, arrow) without affecting the reaction sequence.

If the reaction you drew in the last exercise is currently displayed, go directly to the Exercise below. If the reaction is *not* displayed, retrieve it from the sketch file REACTION.SKC:

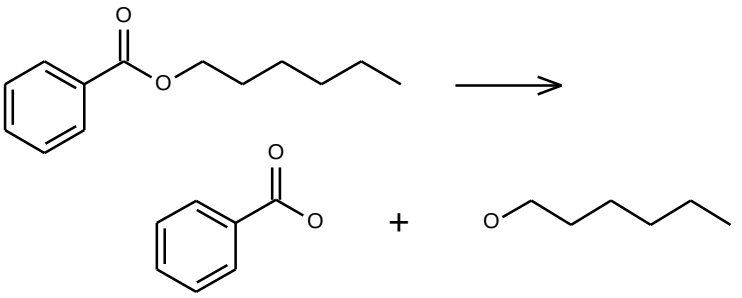
1. Choose **Insert** from the **File** menu.

2. Double-click the name **reaction.skc** (Mac=**reaction**) from the list box. (If the file name does not appear in the list box, change to the SAMPLE directory or folder.) The reaction appears in the drawing area.

Exercise: Moving reaction components

1. Click the **Component** tool if it is not already highlighted.

2. Select any molecule or symbol and drag it to a new position. Rearrange the reaction to look like this:



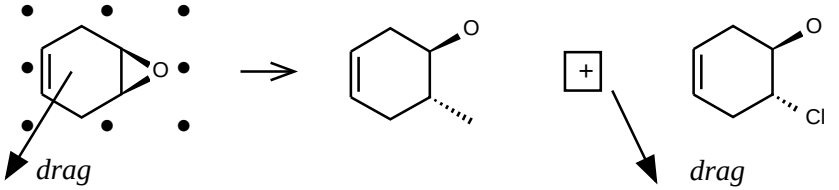
3. When you are satisfied with the reaction arrangement, choose **Save** on the **File** menu. The reaction is automatically saved to the current sketch file, REACTION.SKC.

   Use Save As when you want to name a *new* file. Use Save when you want to update an *existing* file. In this case, the new version of REACTION.SKC replaces the old version of the file on the disk.

Summary: To move reaction components

Follow these steps

1. Click the Component tool.
2. Select and then drag any molecule or reaction symbol to a new position.



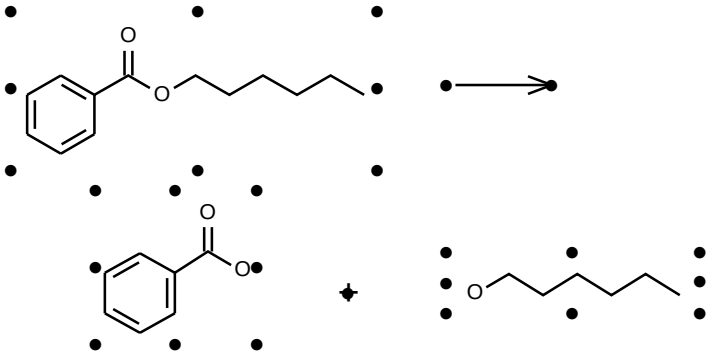
MOVING AND RESIZING A REACTION

If the reaction you drew in the last exercise is not displayed in the drawing area, retrieve it from the REACTION.SKC file.

Exercise: Moving a reaction

1. Click the **Component** tool if it is not already highlighted.

2. Double-click any of the molecules in the reaction, the plus sign, or the arrow. Selection handles appear around each of the reaction components:

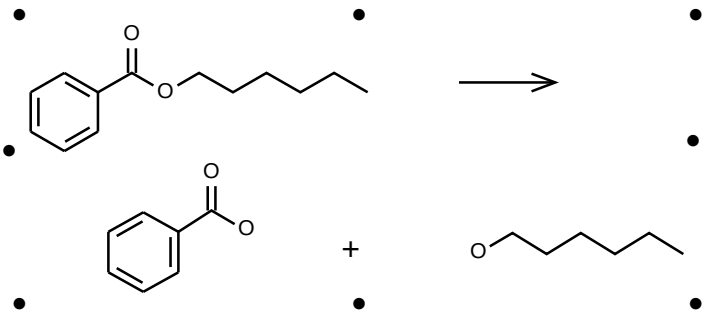


3. Point to the center of any molecule (not on a selection handle) and drag it. The entire reaction moves to the new position. Release the mouse button.

Exercise: Alternate method for moving a reaction

In this exercise, you will use the *sketch tools* to move a reaction. In general, use this method when you are drawing a sketch, such as an overhead transparency. *When you use the sketch tools, you cannot move or edit the individual reaction components.*

1. Click **Sketch** on the top menu bar. The sketch tools appear on the side menu. The **Select** tool is automatically highlighted.
2. Click any molecule in the reaction. Eight selection handles appear around the *entire* reaction:



3. Point to the center of the reaction (not on a selection handle) and drag it. The reaction moves to the new position. Release the mouse button.

Exercise: Resizing a reaction

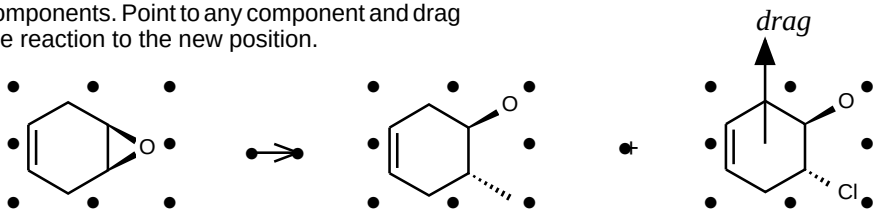
In this exercise, you will resize a reaction using the sketch tools.

1. Verify that **Sketch** is highlighted on the top menu bar.
2. Select the reaction.
3. Point to a *corner* selection handle and drag it diagonally. All the reaction components resize, keeping their original proportions.
4. Point to a *non-corner* selection handle and drag it. All of the reaction components resize, but they lose their original proportions.

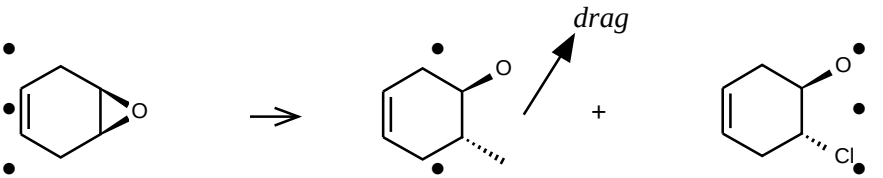
Summary: Two ways to move a reaction

Choose one method

Click the Component tool. Double-click any molecule or symbol to select all of the reaction components. Point to any component and drag the reaction to the new position.

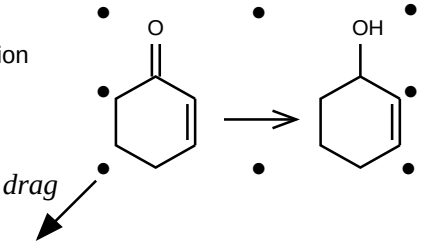
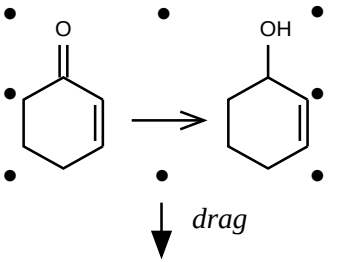


Click Sketch. Select the entire reaction. Point to the center of the reaction and drag it to the new position.



Summary: Two ways to resize a reaction

Click Sketch. Select the reaction. Then:

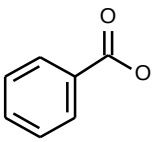
Choose one method	
Point to a corner handle and drag. The reaction keeps its original proportions.	
Point to a non-corner handle and drag. The reaction loses its original proportions.	

EDITING A REACTANT OR PRODUCT

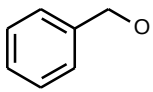
If the last reaction you drew is not currently displayed, retrieve it from the REACTION.SKC sketch file.

Exercise: Editing a molecule in a reaction

In this example, one of the product structures is incorrect. You must use the molecule tools to edit the structure:

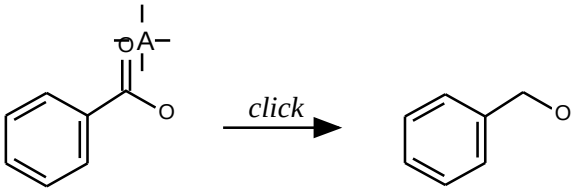


incorrect product

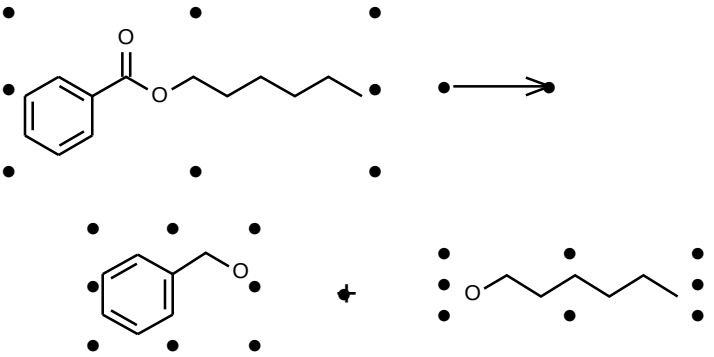


correct product

1. Click **Molecule** if it is not already highlighted.
2. Click the **Eraser** tool.
3. Click the oxygen atom to delete it:



4. To verify that the reaction is still assembled, click the **Component** tool. Double-click the molecule you edited. All three molecules and the reaction symbols are selected:



edited molecule

You can edit a reaction by editing any molecule in the reaction, but if you *delete* a molecule, the reaction dissolves.

5. Click an empty space in the drawing area to deselect the reaction components.

Summary: To edit a reactant or product

Follow these steps
1. Use the molecule tools to edit the reactant or product.
2. To verify that the reaction is assembled, click the Component tool. Double-click any molecule. All the molecules and reaction symbols should highlight.

DISSOLVING A REACTION

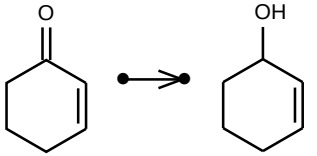
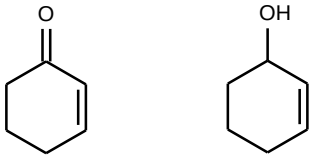
You can dissolve a reaction into its component molecules by deleting the plus sign, arrow, or any of the molecules.

Before you begin, a reaction must be displayed in the drawing area.

Exercise: Dissolving a reaction

1. Verify that the **Component** tool is highlighted.
2. Select any reaction symbol (either the plus sign or the arrow).
3. Choose **Cut** from the **Edit** menu. All the reaction symbols disappear.
4. To verify that the reaction has dissolved, double-click one of the molecules. If no other molecules highlight, the reaction is dissolved.

Summary: To dissolve a reaction

Follow these steps	
1. Click the Component tool. Select any reaction symbol.	
2. Choose Cut from the Edit menu.	

WHERE TO GO FROM HERE

You now have the basic skills needed to draw reactions with ISIS/Draw. Depending on your job tasks, you may want to:

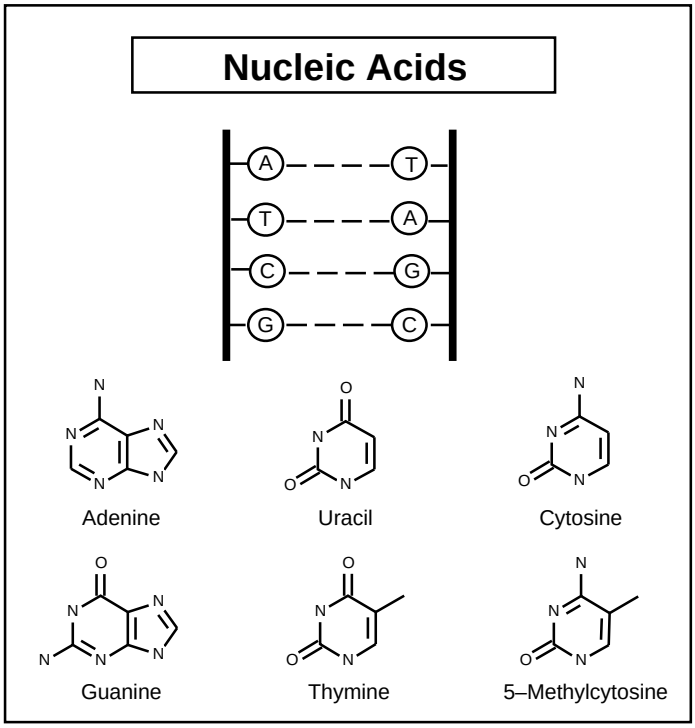
- *Read about other drawing procedures.* See the chapter "Drawing a Molecule or Reaction," in the *Reference* for a comprehensive collection of drawing procedures.
- *Learn how to search databases.* See the ISIS/Base *Database Searching* book.
- *Learn how to draw graphics for written reports or overhead transparencies.* See the chapter "Drawing a Presentation Graphic" in this tutorial.

3

Drawing a Presentation Graphic

In this chapter you create a complete presentation graphic. If you only want to add text or draw lines and boxes to embellish a molecule drawing, you can simply look up the relevant procedures in the *Reference* instead of completing this chapter.

You will create the following full–page graphic:



The graphic you create is an ISIS/Draw *sketch*. A sketch can contain objects that you draw with the ISIS/Draw molecule and sketch tools, or images that you import from other programs, such as analytical spectra or graphs. You can print sketches on paper, insert them in a document, or make them into overhead transparencies.

When you complete this chapter, you will know how to:

- Create a title
- Insert objects (such as molecules) from an existing sketch file
- Type and align text
- Draw a figure using the sketch tools
- Adjust the page layout

CREATING THE TITLE

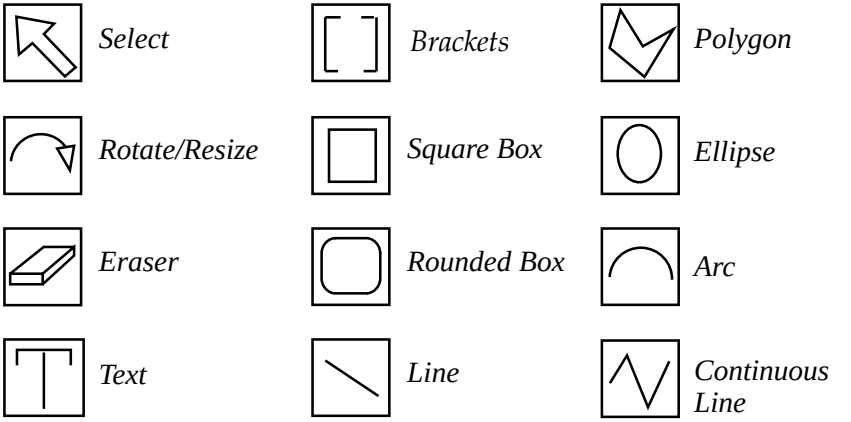
First, you will create the title. The title consists of text with a box around it:

Nucleic Acids

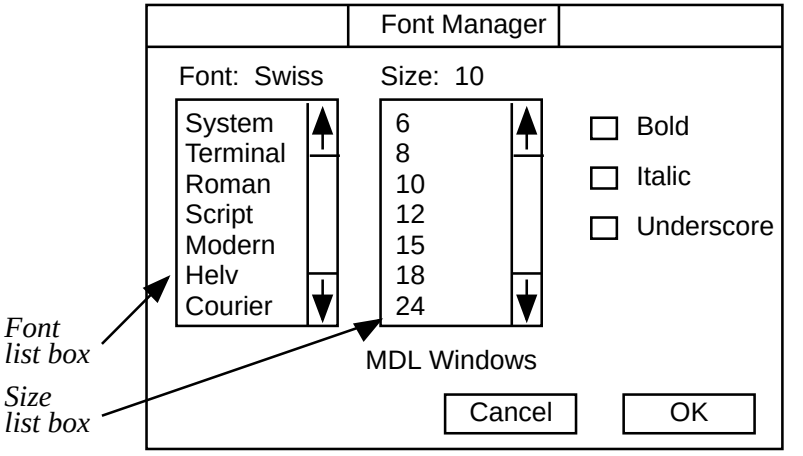
Typing the title

The text in the title is Helvetica font, size 28, with bold text style. Before you begin typing the title, choose the font, size, and text style:

1. You must first retrieve the sketch tools. Click **Sketch** to retrieve them. The sketch tools appear on the side menu:



2. Point to **Style** on the menu bar and press *and hold* the mouse button. The Style menu appears. Move the pointer down the menu commands until **Font** highlights. A cascading menu appears. Move the pointer onto the cascading menu and highlight **Font Manager**. Release the mouse button. The Font Manager dialog box appears:

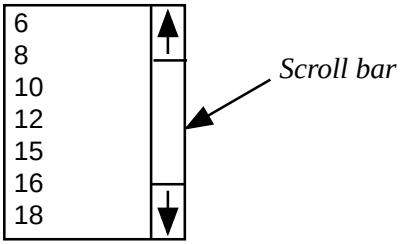


✎ We usually abbreviate these instructions to “Highlight Font on the Style menu, and then choose Font Manager .”

3. Click **Helv** (or **Helvetica**) in the Font *list box*. The available sizes for that font appear in the Size list box.

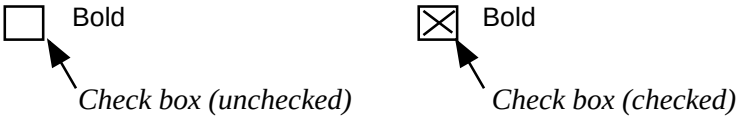
✎ The fonts and sizes that appear in the list boxes depend on the fonts and sizes available on your particular computer. If Helvetica 28 is not available, use any large-size font that you have.

4. If necessary, click the down-arrow on the Size *scroll bar* until **28** appears:



5. Click **28** to choose the font size. The text "MDL Windows" appears in the current font, size, and text style.

6. Click the *check box* for Bold to check it. This switches on the bold text style:



7. Click **OK**.

8. Click the **Text** tool T.

9. Click any position in the drawing area near the upper left corner. A blinking cursor appears. The blinking cursor is the *insertion point* for your text.

10. Type **Nucleic Acids**.

ISIS/Draw types text in the current font, size, and style. This means that all new text will be boldface Helvetica 28 until you change it. If you make a typing mistake, use these editing keys:

To do this:	IBM	Mac
Move cursor left	←	←
Move cursor right	→	→
Delete left character	Backspace	Delete

The blinking cursor disappears when you choose a new tool.

Drawing a box

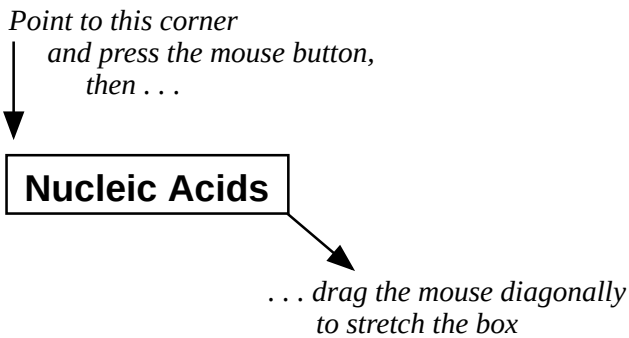
Now you want to draw a box around your title.

To draw a box

1. Click the **Square Box** tool □.

2. Move the pointer above the upper left corner of your title. This is where you will begin drawing the box.

3. Press *and hold down* the mouse button as you move the mouse to the lower right corner of your title. The box stretches from the origin to your pointer:



You can continue to stretch the box as long as you hold the mouse button.

✎ We usually use the word *drag* to mean "press and hold down the mouse button while you move the mouse."

4. When you are satisfied with the size of the box, release the mouse button. The box is fixed in place.

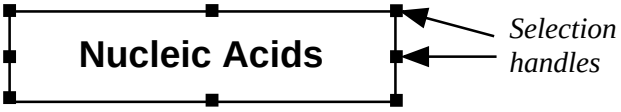
Resizing an object

If you are not satisfied with the size or shape of the box you drew, you can resize it.

To resize an object

1. Click the **Select** tool.

   You use this tool to *select* objects so that you can then *edit* them. For example, you must select a box before you can resize it. In this case, the selection handles around the box show that it is already selected:



2. Point to any selection handle (the pointer changes to an S) and drag it to stretch the box to the desired size and shape.

3. Release the mouse button.

Correcting mistakes

If you drew the title and box correctly, go directly to the next step, "Saving your sketch." If you made a drawing mistake and want to erase part or all of your sketch, see one of the procedures below:

To undo a command (optional)

If you made a mistake and want to immediately *undo* the last command, follow this step:

1. Choose **Undo** from the **Edit** menu.

Not all commands can be reversed with Undo. If this is the case, the Undo command is dimmed on the menu, and you cannot choose it.

To delete objects (optional)

If you drew an object by mistake and now want to delete it, follow these steps:

1. Click the **Select** tool.
2. Click the object that you want to delete. Selection handles appear around the object.
3. Choose **Cut** from the **Edit** menu. The object disappears.

To delete all objects in the window (optional)

If you made a mistake and you want to start drawing again from the beginning, follow these steps:

1. Choose **Select All** from the **Edit** menu.
2. Choose **Cut** from the **Edit** menu.

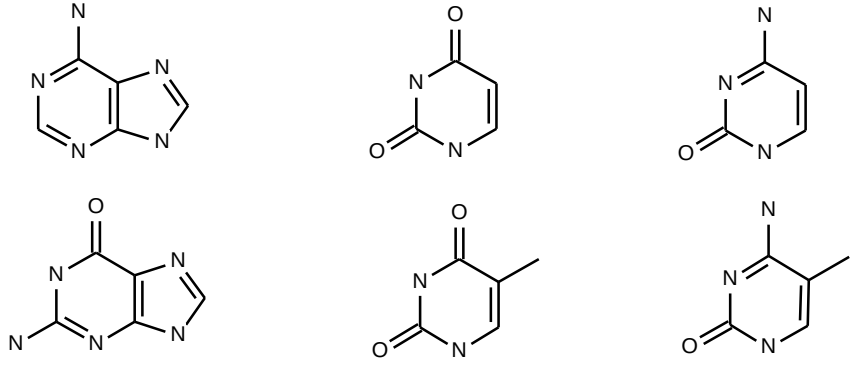
Saving your sketch

It is a good idea to save your work periodically. You will now save your sketch to a file on disk:

1. Choose **Save As** from the **File** menu. A dialog box appears.
2. Change to the SAMPLE directory or folder if it is not already current. (If you did not follow the recommended installation procedure, your work directory or folder may have a different name.)
3. Type the file name **dna.skc** in the Save As File Name text box. (Macintosh users type **dna** in the Save the work in progress? text box.) On IBM computers, the file-name extension .SKC identifies the file as a sketch file.
4. Click **OK** (Mac=**Save**). The sketch file is saved on disk, and you see the name of the sketch in the title bar of the window.

INSERTING A SKETCH

You will now insert six molecules at the bottom of the page:



Instead of drawing the structures, you will retrieve them from a sketch file.

Changing object scale

In order to position the molecules at the bottom of the page, you need to see the full page on the screen. To fit a full page in the window, reduce the object scale to 25% of actual size:

1. Highlight **Zoom** on the **Options** menu, and then choose **25% Size**. A boxed area appears in the window.

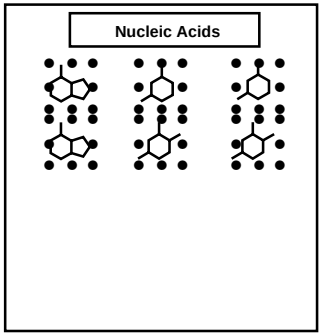
   The boxed area represents the size of a full page. The sketch objects are shown in a reduced scale to fit the page representation.

Inserting a sketch

The six molecules are stored in a sketch file named SIXMOLS. You will now insert the contents of SIXMOLS into your current sketch:

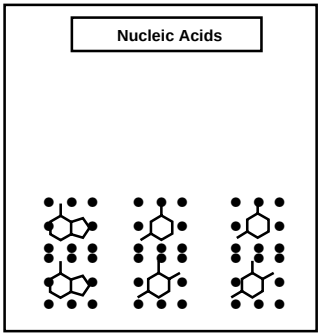
1. Choose **Insert** from the **File** menu. A dialog box appears.
2. Click **sixmols.skc** (Mac=**sixmols**). If this name does not appear in the list box, change to the SAMPLE directory or folder first. (If you did not follow the recommended installation procedure, your work directory or folder may have a different name.)

3. Click **OK** (Mac=**Open**). The six molecules appear in the boxed area. All of the molecules are automatically selected:



4. Click the **Select** tool if it is not already highlighted.

5. Point to the center of one of the molecules, and drag it to a position near the bottom of the page. Because all of the molecules are selected, all six molecules move together:

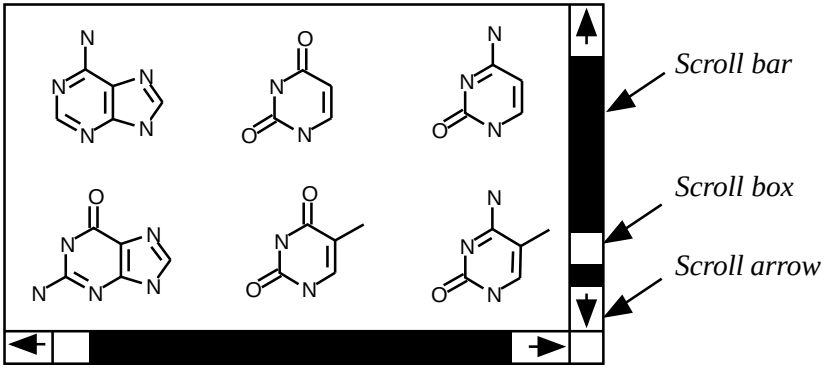


6. Release the mouse button to fix the molecules in place.

7. Click an empty space in the drawing area to deselect the molecules.

8. Highlight **Zoom** on the **Options** menu, and then choose **Actual Size**.

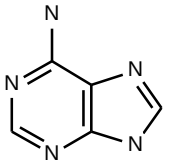
9. Scroll the window to the bottom of the page so that you can see the molecules. To do so, click near the bottom of the vertical scroll bar. Each time you click the scroll bar, ISIS/Draw scrolls the page by one window length:



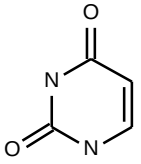
The scroll box indicates your position on the page. To slowly scroll the window up or down, click the up- or down-arrow on the vertical scroll bar. To scroll the window left or right, use the horizontal scroll bar. If the display does not move, you are at the limit of the drawing area in that direction. Try to scroll the window in a different direction.

TYPING AND ALIGNING TEXT

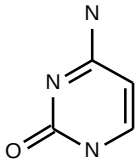
Now you want to type the name of each molecule below the structure:



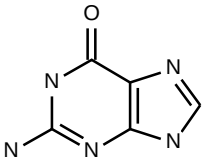
Adenine



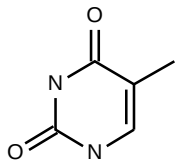
Uracil



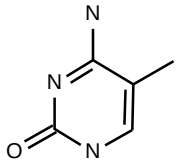
Cytosine



Guanine



Thymine



5–Methylcytosine

Typing text

Type the text using the Times Roman font, size 12, with plain text style (if these choices are not available on your particular computer, choose any mid-sized font):

1. Click the **Text** tool.
2. Highlight **Font** on the **Style** menu, and then choose **Font Manager**.
3. Click **Tms Rmn** (or **Times**) from the font list box.
4. Click **12** from the size list box.
5. Click the check box for **Bold** to uncheck it.
6. Click **OK**.
7. Click a position below the adenine structure. A blinking cursor appears.
8. Type **Adenine**.

Repeat Steps 7 and 8 to type the name of each molecule below the structure. The molecule names are Adenine, Uracil, Cytosine, Guanine, Thymine, and 5-Methylcytosine. The exact placement is not important now.

Moving text

Center the names under each structure:

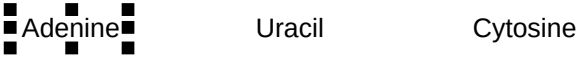
1. Click the **Select** tool.
2. Click the middle of the molecule name to select the text:

3. Move the pointer over the text. Do *not* point to a selection handle; you know you are pointing to a selection handle if you see the arrow change to S.
4. Drag the text to center it under the molecule structure.
5. Release the mouse button to fix the text in place.

Aligning text horizontally

Now that the names are centered under each structure, you will horizontally align the names into precise rows:

1. The Select tool is still highlighted. Click the name Adenine to select it:

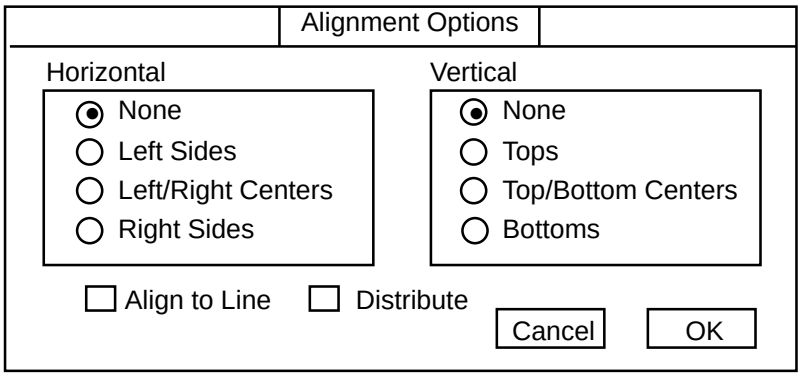


2. To select the next name in the row, press and hold the **Shift** key. Then click Uracil:

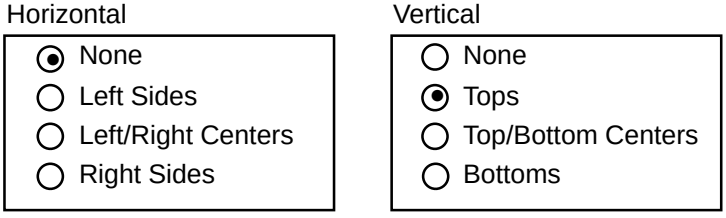
✎ We use the word *shift-click* to mean “press and hold the Shift key as you click an object.” You must shift-click to select more than one object at a time. If you click a second object *without* pressing the Shift key, the second object is selected but the first object is then *deselected.*

3. Shift-click Cytosine:

4. Choose **Align** from the **Object** menu. The Alignment Options dialog box appears:



5. To align the tops of the names, make sure that the radio button for **None** is highlighted in the **Horizontal** box. Then click the radio button for **Tops** in the **Vertical** box:



6. Click **OK**. The tops of the selected names are aligned.

7. To select the second row of names, click Guanine, and then shift–click Thymine and 5–Methylcytosine:

8. Choose **Align** from the **Object** menu.

9. Click the radio button for **Bottoms** in the **Vertical** box.

10. Click **OK**. The bottoms of the selected names are aligned.

11. Click an empty space in the drawing area to deselect the names.

Updating the sketch file

To protect your work, save the sketch:

1. Choose **Save** from the **File** menu. The sketch is automatically saved to the current file.

   ✎ Use Save As when you want to name a *new* file. Use Save when you want to update an *existing* file. In this case, the new version of DNA replaces the old version of the file on the disk.

STOP You are now at an optional stopping point. If you want to continue, go to "Drawing a Figure" below. If you wish to stop, you may exit the program now. When you are ready to begin again:

1. Start ISIS/Draw.

2. Choose **Open** from the **File** menu.

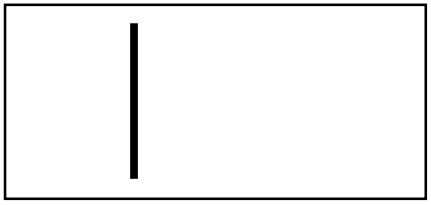
3. Click **dna.skc** (Mac=**dna**). (If this name does not appear in the list box, change to the SAMPLE directory or folder first.)

4. Click **OK** (Mac= **Open**).

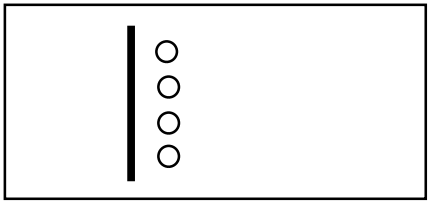
5. Click **Sketch** to retrieve the sketch tools.

DRAWING A FIGURE

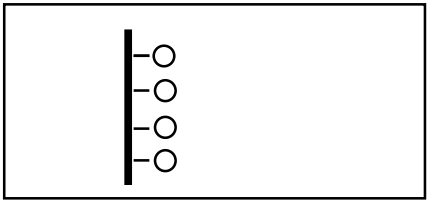
You will now draw the DNA figure in the center of the page. The figure is composed of simple geometric shapes and some text. The diagrams below summarize the drawing steps. Detailed instructions will follow:



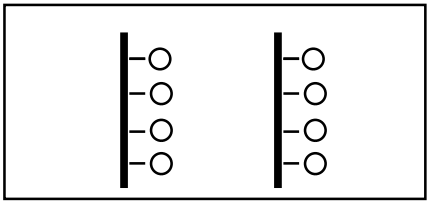
1. Draw a vertical line using a thick pen width.



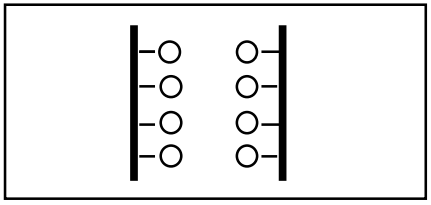
2. Draw a circle and duplicate it three times.



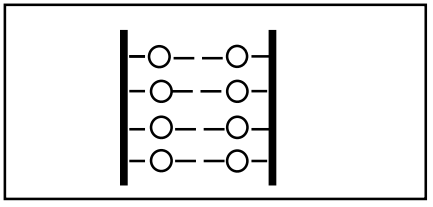
3. Draw four horizontal lines.



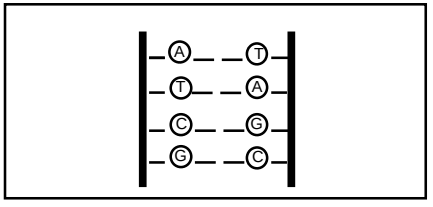
4. Duplicate the image.



5. Flip the right image.



6. Draw the dashed lines between the circles.

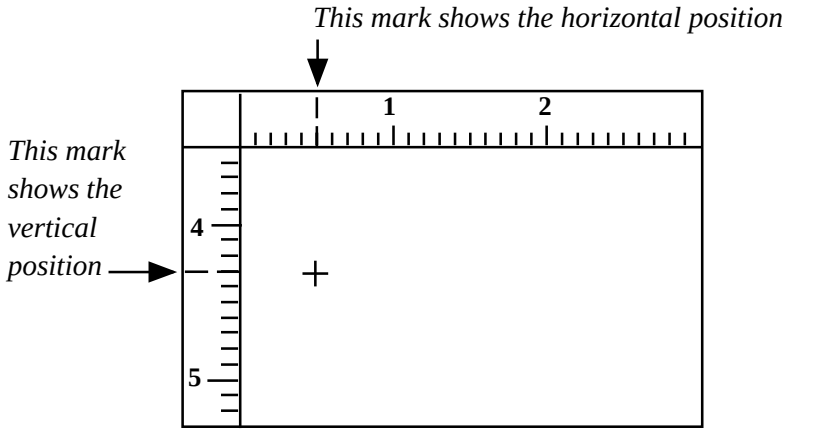


7. Type the base letters

Drawing a vertical line

You will now draw a vertical line using a thick *pen width* and the *ruler*:

1. Scroll the window to the blank area in the middle of the page.
2. Choose **Show Ruler** from the **Options** menu. Rulers appear at the top and side of the drawing area.
3. Choose **Snap To Ruler** from the **Options** menu. The pointer snaps to each division on the ruler as you draw. This helps you to measure the line precisely.
4. Click the **Line** tool .
5. Highlight **Pen Width** on the **Style** menu, and then choose the third pen width.
6. Position the pointer near the upper left corner of the window. A mark on each ruler shows the current pointer position. For example:



7. Press the **Shift** key. This activates the compass to help you draw a perfectly straight vertical line.

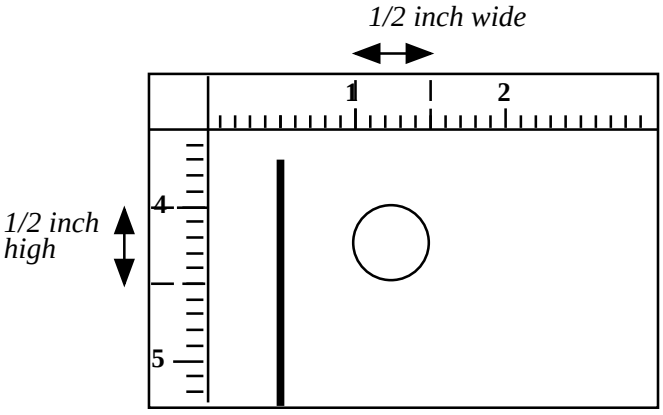
   The *compass* is a device that allows you to draw lines at angles constrained to 15-degree increments. As you draw a line, it snaps to the nearest 15-degree increment, ensuring a precise angle. In this case, you use the compass to draw a line at a 90 degree vertical.

8. Drag the mouse downward to draw the line. Watch the vertical ruler as you draw.
9. When the distance between the marks on the ruler measures approximately 3 inches (7 cm.), release the mouse button to end the line.
10. Release the **Shift** key.

Drawing a circle

A circle is a type of ellipse. To draw a circle, draw an ellipse and use the ruler to ensure a uniform diameter:

1. Click the **Ellipse** tool ⬭.
2. Highlight **Pen Width** from the **Style** menu, and then choose the first pen width.
3. Position the pointer approximately 1/2 inch (1 cm.) away from the vertical line, near the top of the line.
4. Drag the mouse until the ellipse is 1/2 inch (1 cm.) wide and 1/2 inch (1 cm.) high. Watch the marks on the ruler as you draw. The uniform diameter ensures a perfect circle:



5. Release the mouse button.

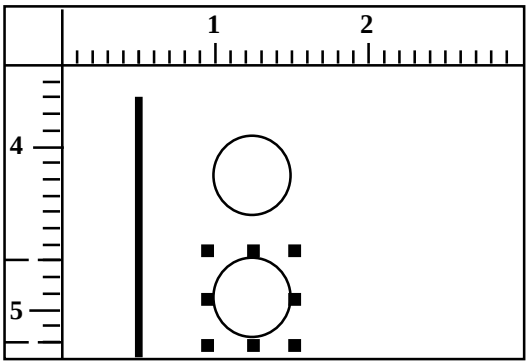
An alternative way to draw circles is to use the compass: Click the Ellipse tool, and then press Shift (Mac=Command) to activate the compass. Drag the mouse at a 45–degree angle. ISIS draws a perfect circle.

Duplicating an object

You will now duplicate the circle three times:

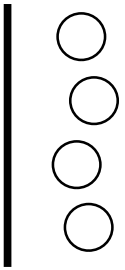
1. Verify that the circle is selected.
2. Choose **Duplicate** from the **Edit** menu. A copy of the circle appears, overlapping the original.

   You can also use the *keyboard accelerator* to quickly duplicate the selected object. The keyboard accelerator for a command is shown on the menu next to the command name.
3. Click the **Select** tool.
4. Point to the center of the duplicate circle and drag it to a position 1/4 inch (0.5 cm.) below the first circle:



The alignment of the circles is not important now. Later, you will use a command to automatically align the circles into a precise column.

Repeat the above procedure two times to draw two more circles. When you finish, the figure will look like this:



If necessary, move the line up or down to match the position of the circles:

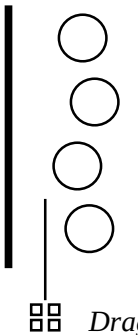
1. Click the middle of the line to select it.
2. Drag the line up or down to position it.

Aligning the circles to a line

You will now align the four circles exactly 1/2 inch (1 cm.) away from the vertical line:

1. The Select tool is still highlighted. Click the first circle to select it, and then shift-click to select the other three circles.
2. Choose the **Align** command on the **Object** menu.
3. Click the radio button for **Left Sides** in the **Horizontal** box.
4. Click the radio button for **None** in the **Vertical** box.
5. Click the check box for **Align to Line** to check it.
6. Click **OK**. The dialog box disappears and the pointer changes to a square shape.
7. Point to any position 1/2 inch (1 cm.) away from the vertical line.
8. Press **Shift** to activate the compass. This helps you to draw a perfectly vertical line.

9. Drag the mouse downward to indicate a straight, vertical line:



Drag the cursor to draw a vertical line

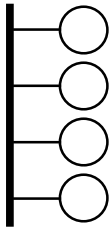
You do not need to draw a long line. A short line is sufficient to show the alignment position.

10. Release the mouse button. Release the **Shift** key. The circles align vertically, exactly 1/2 inch from the vertical line.

11. Choose **Show Ruler** from the **Options** menu to switch off the ruler.

Drawing horizontal lines

You will now draw the four horizontal lines that connect the vertical line to the circles:



1. Click the **Line** tool.

2. Point to the left side of the first circle. The pointer changes to an S .

3. Press the **Shift** key. This activates the compass.

4. Drag the mouse to the left until it touches the vertical line.

5. Release the mouse button.

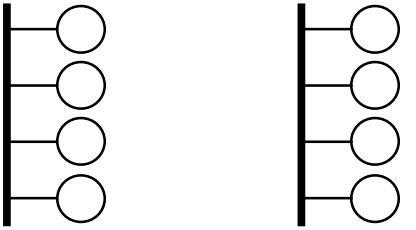
6. Release the **Shift** key.

Repeat the above procedure three times to draw horizontal lines from each circle to the vertical line.

Choose **Save** from the **File** menu. This updates the existing DNA.SKC file.

Duplicating a figure

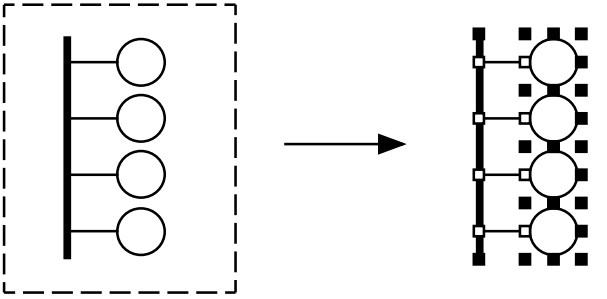
You have completed half of the DNA figure. Because the figure is symmetrical, you can duplicate the left half to create the right half:



To duplicate the left half, you must select all of the components:

1. Click the **Select** tool. To quickly select all of the figure components, you will draw a *frame* around the figure.

2. Point to the upper left corner of the figure. Then drag the mouse diagonally; the frame stretches from the origin to your pointer. When the frame encloses the figure, release the mouse button. All of the objects in the frame are selected:



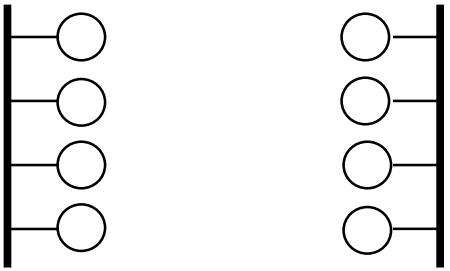
✎ It is important that all of the objects that you want to duplicate are selected. If some objects are not selected, shift-click to select them. Or, click an empty space to deselect all objects and then try to draw the selection frame again.

3. Choose **Duplicate** from the **Edit** menu. A copy of the figure appears.

4. Point to the center of any selected circle and drag the entire copy to the right side of the window.

Flipping a figure

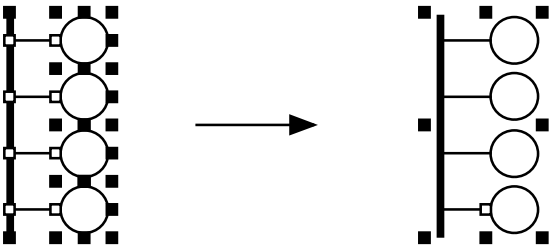
Now you want to *flip* the right half of the figure so that the circles are in the center:



Before you can flip the right half of the figure, you must group the components so that they act as a single object:

1. Verify that the objects composing the right half of the figure are selected.

2. Choose **Group** from the **Object** menu. The selection handles change to indicate that the components are now part of a *single* object:



Now flip the group:

1. Verify that the group is selected.
2. Highlight **Flip** on the **Object** menu, and then choose **Horizontal**. The group rotates 180 degrees in the horizontal plane.

Aligning two figures

Now you want to align the two halves. But before you can align them, you must group the components in *each half* so that you have *two objects*. The components in the right half are already grouped. To group the components in the left half of the figure:

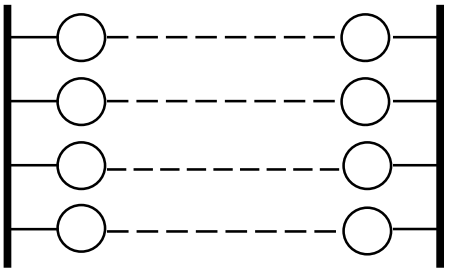
1. Verify that the **Select** tool is highlighted.
2. Draw a frame around the components in the left half of the figure. All of the components are selected.
3. Choose **Group** from the **Object** menu.

Now that the two halves compose two objects, align the bottoms:

1. The left group is already selected. Shift-click the right group to select it.
2. Choose **Align** from the **Object** menu.
3. Click the radio button for **None** in the **Horizontal** box.
4. Click the radio button for **Bottoms** in the **Vertical** box.
5. Click the check box for **Align to Line** to uncheck it.
6. Click **OK**. The two halves of the figure align.

Drawing dashed lines

You will now draw the dashed lines that connect the circles:



When each half of the figure is grouped into a single object, you cannot attach lines to the individual circles. You must *ungroup* the components before you draw the dashed lines:

1. Verify that the two halves are selected.
2. Choose **Ungroup** from the **Object** menu. The two groups dissolve and the individual components highlight.
3. Click an empty space in the drawing area to deselect all of the objects.

Now draw the four dashed lines:

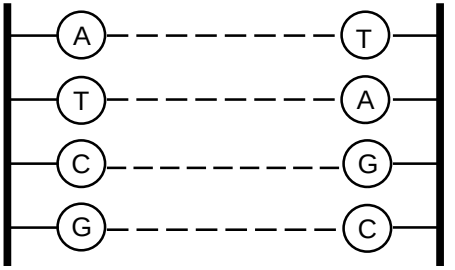
1. Click the **Line** tool.
2. Highlight **Line** on the **Style** menu, and then choose the third line style.
3. Point to the side of the first circle on the left. The pointer changes to an S.
4. Press the **Shift** key. This activates the compass.
5. Drag the mouse until the pointer touches the circle on the right.
6. Release the mouse button.
7. Release the **Shift** key.

Repeat the above procedure three times to draw the other three lines.

Choose **Save** from the **File** menu to save the sketch.

Typing single letters

Use the Helvetica font, point size 18, to type the base letters:



1. Click the **Text** tool.
2. Highlight **Font** on the **Style** menu, and then choose **Font Manager**.
3. Click **Helv** (or **Helvetica**) in the font list box.
4. Click **18** in the size list box.
5. Click **OK**.
6. Click the center of the first circle.
7. Type **A**.
8. Repeat Steps 6 and 7, typing the appropriate letter in each circle.

Moving single letters

Now move the base letters to the center of each circle. Each letter is a separate object:

1. Select the letter that you want to move.
2. Drag the letter to the center of the circle.
3. Release the mouse button.

Repeat the above procedure to center the letters in each circle. Choose **Save** from the **File** menu to save the sketch.

ADJUSTING THE SKETCH LAYOUT

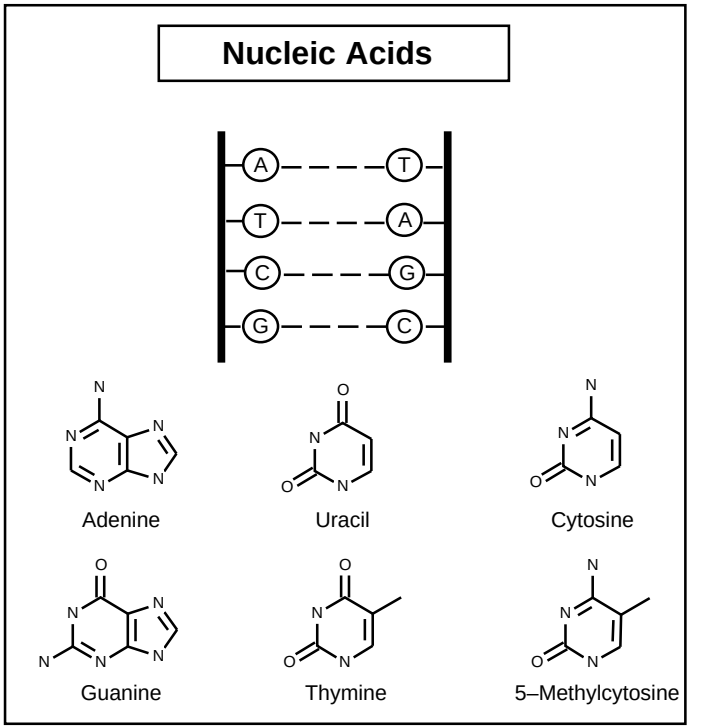
You have finished drawing all of the sketch components. Now you can adjust the page layout.

First, reduce the object scale so that you can see the position of each object on the page. To do this, highlight **Zoom** on the **Options** menu, and then choose **25% Size**.

Now you want to move the major figures in the sketch (the title, the DNA figure, the two rows of structures) to their proper positions on the page, but you do not want to move the individual objects (such as a circle or a row of text) out of alignment. Before you move the major figures, *group* the individual objects so that they move as a single unit:

1. To quickly select all of the objects in a figure, click the **Select** tool, and then draw a frame around the figure.
2. Choose **Group** from the **Object** menu. Eight selection handles appear around the entire group.
3. Point to the center of the group, and drag the figure to its new position.

Use this strategy to move the title, the DNA figure, and the two rows of structures to their proper positions on the page:



When you are satisfied with the sketch layout, highlight **Zoom** on the **Options** menu, and then choose **Actual Size**.

Finally, choose **Save** from the **File** menu to save the sketch.

WHERE TO GO FROM HERE

You now have the basic skills needed to draw sketches with ISIS/Draw. Depending on your job tasks, you may want to:

- *Insert the sketch into a document.* See the chapter "Exporting Files from ISIS" in the *Reference*.
- *Print the sketch.* See your system chapter in the *Reference*.
- *Practice drawing and learn additional techniques.* See "Creating Other Images" on page 77 for examples of other images that you can draw or import.

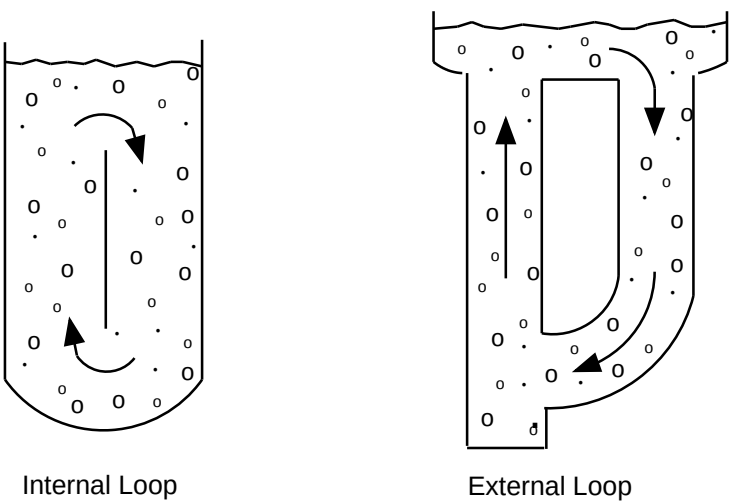
- *Read about other drawing procedures.* See the *Reference* for a comprehensive collection of drawing procedures.
- *Learn how to draw molecules and reactions.* See the chapters “Drawing a Molecule” and “Drawing a Reaction” in this tutorial.

CREATING OTHER IMAGES

This section contains examples of various kinds of images that you can create with ISIS/Draw. You can insert these images into a document, print them, or use them in an overhead transparency. To insert images into documents or export them to other programs, see the chapter “Exporting Files from ISIS” in the *Reference*. To print images, see your system chapter in the *Reference*.

Geometric objects and text

Geometric objects include boxes, ellipses, arcs, lines, polygons, and arrow heads. You can draw text in a wide variety of fonts and sizes, and you can add text styles such as boldface and italics. To draw geometric objects and text, you use the ISIS/Draw *sketch tools*. The following example is composed entirely of geometric objects and text:



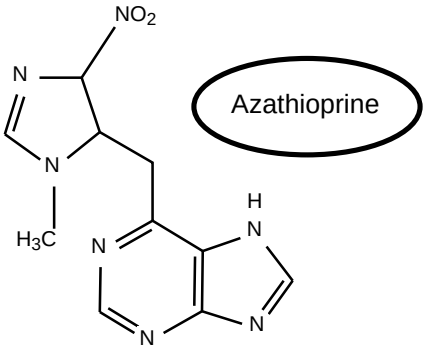
To create this image, draw *lines* and *arcs* (for the curved lines) to draw the bioreactor walls. Draw *circles* and *periods* to draw the bubbles. Use the Continuous Line tool to draw short, choppy, lines for the water surface. Add *arrow heads* to lines and arcs to draw the arrows. Use *Helvetica text* for the labels, with *underscore text style* for the title. For more information, see the following chapters in the *Reference*:

- Drawing Geometric Objects
- Typing Text
- Manipulating Objects

Structures, geometric objects, and text

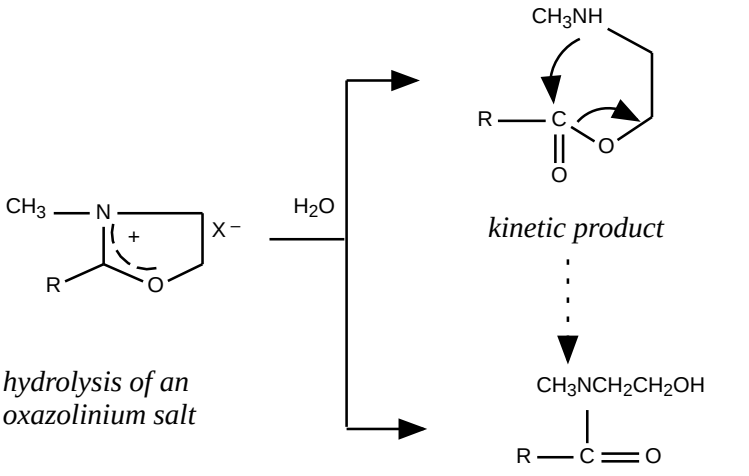
The following images combine chemically significant molecules and reactions with explanatory text and geometric objects.

This sketch contains a molecule, text, and an ellipse:



The molecule is chemically significant (if you draw it with the molecule tools), but the ellipse and text are not. You can store the entire sketch, including the geometric objects, in a *local* ISIS database, but only the molecule is searchable. Remote databases, such as MACCS–II and REACCS, strip the geometric objects from the sketch before registering the molecule into the database.

This sketch describes a chemical reaction, but it does *not* contain a chemically significant reaction:



The arrows showing the change from reactant to kinetic and thermodynamic products are geometric objects. Because the reaction was not created with the molecule tools, it is *not* chemically significant. You cannot store this reaction in a database.

The oxazolinium salt structure also contains geometric objects: a dashed arc and a plus sign. This molecule is *not* chemically significant.

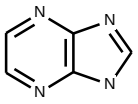
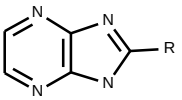
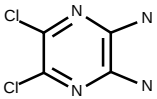
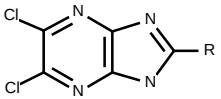
For more information, see the following chapters in the *Reference*:

- Drawing a Molecule or Reaction
- Drawing Geometric Objects
- Typing Text
- Manipulating Objects

Sketch tables

A *sketch table* consists of text, molecules, and/or geometric objects arranged into columns and rows:

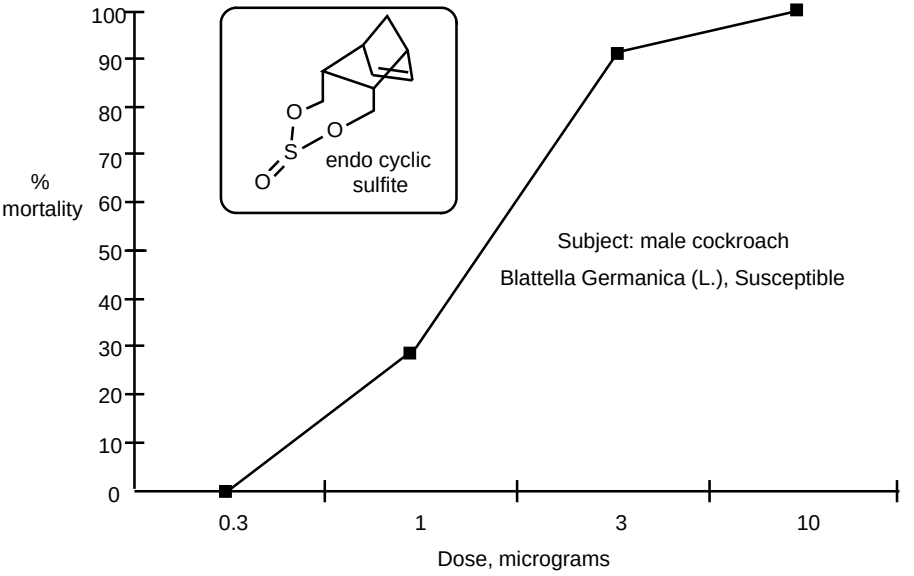
Preliminary Results of Alpha Compounds

Compound	Formula	Target Heterocycle	Amt.	Activity % T/C	Batch Number
	$C_5H_4N_4$		5.5032	100	1214–75
	$C_4H_4N_4Cl_2$		5.36	95	1470–67

To create this sketch, draw the molecules and text and then *align* them into columns and rows. Draw vertical and horizontal lines to separate the data. You can use a variety of fonts and font sizes for the table data and title. See the chapter “Drawing Sketch Tables” in the *Reference* for more information.

Imported images

Sketches can contain images that you import from other programs. This sketch contains an imported graph, a chemically significant molecule, a rounded box (geometric object), and text:



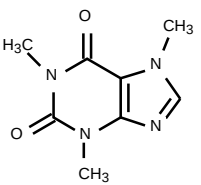
This sketch consists of a form with data imported from ISIS/Base:

NATURAL ALKALOID DATABASE

NAME: Caffeine (1,3,7–trimethylxanthine)

Tested by, Lab number: N. Lawler, B147

Date Tested: 6/7/88



	CNS Stimulation	Respiratory Stimulation	
Caffeine	1	1	
Theophylline	2	2	
Theobromine	3	3	(1 = most potent)

For more information, see the following chapters in the *Reference*:

- Importing Files into ISIS
- Drawing a Molecule or Reaction
- Drawing Geometric Objects
- Typing Text
- Manipulating Objects