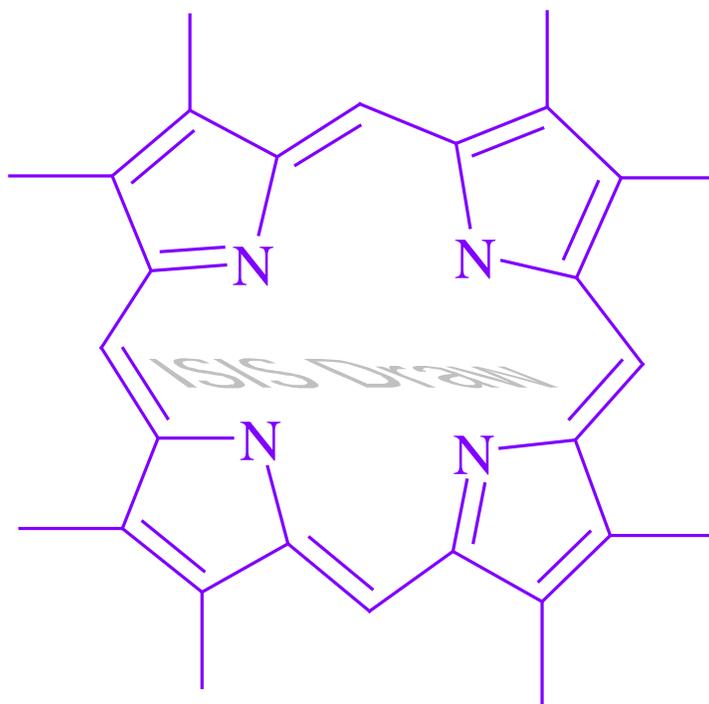


Introduction to ISIS Draw

A Chemical Drawing Tool Program



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Introduction

The program ISIS Draw is designed to draw chemical, amino acid or simplified protein structures and reaction schemes for presentation and/or journal publications. There are other useful features within the program such as ChemInspector to check the chemical structure for validity and molecular property calculation for molecular weight, molecular formula and molecular composition.

This manual is NOT intended to teach you the chemistry or physical meaning of chemical structures, instead, this manual provides you with instructions on how to use the drawing tool to present your research data and to create graphics for presentation and publication use.

It is assumed that the user of this manual is familiar with the Windows or Mac operating system and know how to move and scroll windows, select objects, and choose menu commands. It is also assumed that the user knows how to use Copy and Paste and how to edit text prior to using the ISIS program.

NOTE: This software should ONLY be loaded onto your desktop computer by your Computer Support Person (CSP). The NIEHS computers are being checked for Y2K compliance and individuals should not load or remove any software or hardware on their computers.

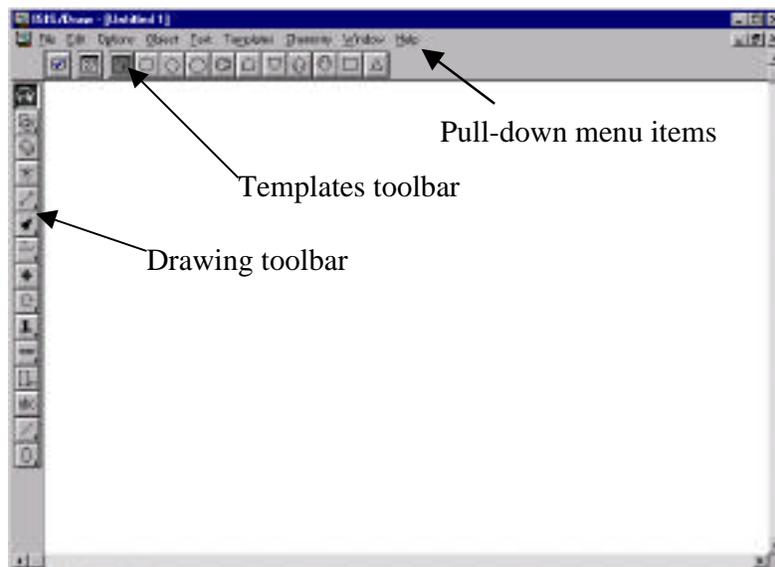
Launch the ISIS/Draw Program

From the **Start** bar, select **Program, ISIS Draw 2.2.1 Standalone, ISIS Draw 2.2.1**

Or you may double click on the ISIS/Draw program icon to launch the program if you have set up an alias for the program on your desktop.



When the program starts, you will see the following window.



On the screen you will see pull-down menu, horizontal templates and a vertical drawing tool bars (see the Appendix A for more details on each of drawing tools).

Chapter 1

Drawing Molecules

1.0 Introduction

A molecule (i.e. chemical structure) is made of atoms and chemical bonds. An atom is represented by a chemical symbol (i.e. element) such as **C** (carbon), **N** (nitrogen) or **O** (Oxygen). The chemical bond is a “linker” between atoms to make up a molecule.

1.1 Basic Strategy

To draw molecules, do the following:

1. Draw the basic framework with template tools, templates from a template page, and drawing tools.
2. Edit atoms, bonds, and molecules as necessary. All atoms are **carbons** unless otherwise specified.

1.2 Drawing Structures with Template Tools and Template Pages

Templates are pre-saved structural fragments or molecules that you can use as building blocks for your own structures. A **template tool** allows you to use one specific structure, whereas a **template page** contains many structures from which to choose.

1.2.1 To Use a Template Tool

1. Click one of the template-tool icons on the horizontal tool bar:



2. Do one of the following:
 - To **place** the template anywhere, click an empty area.
 - To **fuse** the template to an existing bond, click on the existing bond.
 - To **attach** the template by a single bond to an existing atom, click the atom

Exercise 1.1: Create Your First Molecule Using a Template Tool

1. Click on benzene icon on the horizontal tool bar as shown below.

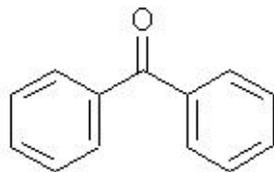


2. Click on any place on the program screen. Now you have created a benzene molecule.

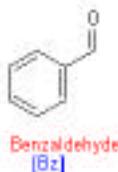
1.2.2 To Use a Template from a Template Page

1. Choose a template page (e.g. amino acid, aromatics, etc) from the **Templates** menu. You see the template page in a window.
2. Find the structural fragment or molecule that you want to add to your sketch.
3. Click an atom or bond in the structural fragment or molecule. The template page goes behind the sketch window.
4. Do one of the following:
 - To **place** the template anywhere, click an empty area.
 - To **fuse** the template to an existing bond, click on the bond.
 - To **attach** the template by a single bond to an existing atom, click on the atom.

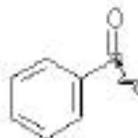
Exercise 1.2: Drawing a Chemical Structures Using the Template Page



1. From the menu items, choose **Template, Aromatics**.
2. From the Aromatics templates, select by clicking on the molecule.



3. Move your cursor in any work area and click once, you see the molecule shown on the screen.
4. Click  on the horizontal template tool bar and place your cursor on the carbon of carbonyl group as shown:



5. Click once. Congratulations, you have just created another chemical structure.

1.3 Drawing Bonds and Chains

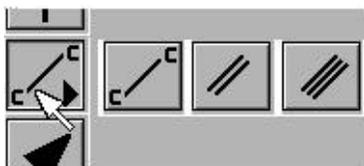
Drawing bonds: To draw bonds, click a bond tool on the vertical tool bar, such as bond tool  or other bond tool . Then, click the mouse to add a bond to the drawing area, or drag the mouse from an existing atom toward the direction where you will draw the next atom.

Default values: Any atoms, bonds, or other objects that you draw use pre-set default values. For information on changing these default values, see section **1.13 Changing ISIS/Draw Settings**.

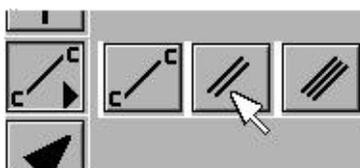
1. Some tool icons have a small triangle/arrow head in the bottom right corner. For example, the single-bond tool:



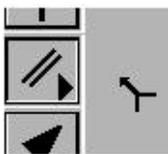
2. This indicates that there are **additional tools** available. For example, to change the tool to a double bond, first click and hold on the single-bond tool:



3. Keeping the mouse click down, drag the mouse onto the double-bond tool:

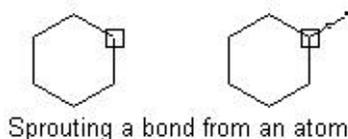


4. Finally, release the mouse. You see:



The double-bond tool is now the default tool. The cursor indicates that you can draw double bonds. (Click the mouse to draw a double bond.)

Sprouting: To sprout a bond from an atom, click  (or any other bond tool), and then click the atom:



Stereo Bond: (*Up/Down/Either*): To draw an Up, Down, or Either bond, click the appropriate tool icon. Then, click the mouse over the drawing area to draw the bond. The bond you chose displays on the tool bar, and is now the default bond.

Bond Type: To change the bond type of an existing bond, click a **different** bond tool and then click the bond. The bond changes to the default bond type shown on the tool bar.

Stereo Bond Direction: To reverse the direction of a stereo bond, click one of the stereo bond tools, then click the **middle** of the bond.

Bond Rotation: To rotate the position of a single bond, click the selection tool , select the free end of the bond, click, hold and drag to the desired position and length.

Standard Bond Length: To change the standard bond length, choose **Options, Settings**, and then click the **Chemical Drawing** tab. Click the **Standard bond/grid length** box, and enter or choose a bond length. Then, choose the unit of measure. For more information on changing default values, see *1.13 Changing ISIS/Draw Settings*.

Drawing Chains: To draw chains in one direction, click the chain tool  and then press and drag the mouse. To draw continuous bonds that follow the position of your mouse, click  and then click and drag the mouse in the desired direction. You can draw rings and other molecules of specific shapes with this tool.

Other Objects: You draw other objects, such as lines, boxes, arrows, and polygons as follows: Click the appropriate tool, and then click, hold and drag the mouse to draw the object.

Help on Tools: To see help information for **any** of the tools on the horizontal or vertical tool bars, move the cursor over the tool, and then click and hold the mouse.

To turn this help on or off, choose **Options, Settings**, click the **General** tab, and set **Show toolbar help messages**. You can also find more information in **Tools** on the **ISIS/Draw Table of Contents**.

Exercise 1.3: Create the following molecule.



1. Click the bond tool  and place your cursor on any area of the program. Click once, you now see a line (bond) on your work area.
2. Point your cursor on one end of the bond as shown  and click once.



3. Repeat the last step so you have the molecule on your work area.



4. Click  and hold on mouse key and drag your cursor to highlight the "Double bond" as shown:



5. Place the cursor at the middle of molecule as shown and click once.



6. You now have the structure, save your work as *test1*.

-
- (Optional) Use ChemInspector to ensure that the molecule's chemistry is correct. For more information, see Section 2.4 for details.
 - (Optional) To ensure that a molecule has uniform bond lengths and angles, select the molecule by clicking once on it, and then from the menu items, choose **Object, Clean Molecule**.
-

1.4 Drawing Atoms

Drawing atoms: To draw an atom, click the atom tool  and then click the mouse where you want the atom to appear. You see a text entry field where you can either enter an atom symbol or choose one from a list. Then, click elsewhere. As you type in the atom symbol, you can also type in charges, radicals, or isotopes.

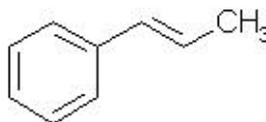
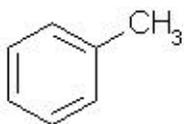
Note: If you enter a standard atom symbol, such as **br**, ISIS/Draw capitalizes it and treats it as the atom symbol **Br**. If you enter text that is **not** an atom symbol, such as **bu**, ISIS/Draw treats the text as an atom alias that is not chemically significant as a search query. For information on atom aliases and other **chemically insignificant text**, see **1.11 Drawing structures for presentation graphics**.

Repeating atom symbols: To repeat an atom symbol that you just entered, press **Ctrl** on a PC or **Command** on a Macintosh and click another atom to replace its current symbol. Or click in the drawing area to add a new atom of the same value.

Editing atoms: To edit an atom, first click either of the selection tools , and then double-click the atom. The **Edit Atom** dialog box will open so that you can edit the atom. For more information, see **Section 1.7 Editing Atoms, bonds, and structures**.

Exercise 1.4: Create the following molecule.

You may use the last molecule created as a template. This exercise uses tools from both Section 1.3 and 1.4.



You should still have the last created molecule on your work area, if not, open the file, *test1.skc*.

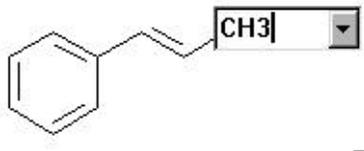
1. Click once on the **benzene ring** tool from the horizontal template tool.



2. Place your cursor on one end of the molecule as shown and click once.



- Click on atom tool  and place your cursor on the other end of the single bond.
- Click once and type in CH3 in the text box and press **Enter** key as shown:



- You got it! Now go to **File, Save** and type in *test2* and click **Save**.

1.4.1 Chemically-Significant Text

Chemically-significant text is any atom symbol (element) or set of atom symbols (elements) that you specify. You can include charges, radicals, and isotopes.

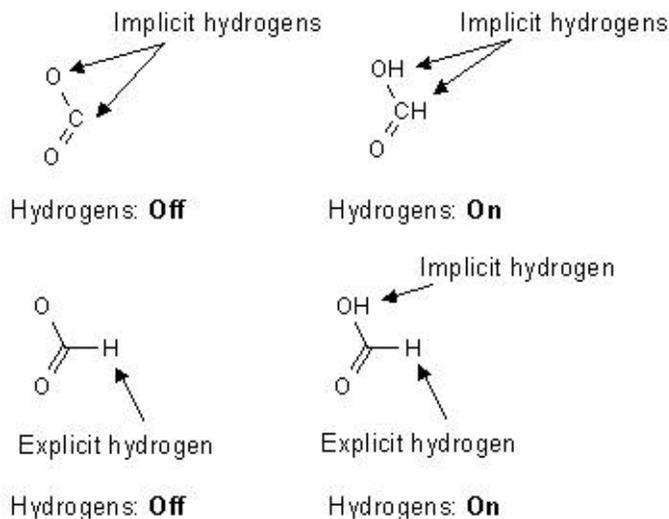
Specifying charges: To specify a charge, enter a plus (+) or a minus (-) **after** the appropriate character. For example, **N2+**.

Specifying radicals: To specify a radical, enter one of the following characters **after** the atom symbol:

: (singlet diradical)
· (doublet monoradical)
^^ (triplet diradical)

Specifying isotopes: To specify an isotope, enter the isotope number **before** the atom symbol. For example, **16O**.

Sprouting explicit hydrogens: An explicit hydrogen is a hydrogen with a bond attached to an atom. An implicit hydrogen is **either** a hydrogen that you know to be present at a specific position in a structure (implied), but it is not visible **or**, if the hydrogen is visible, it is drawn without the bond attached to the atom.

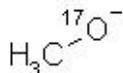


To sprout an explicit hydrogen, sprout a single bond, select the atom and then choose **Object, Edit Atom**. Click the **Symbol** box and choose **H**.

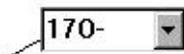
1.4.2 Chemically-Insignificant Text

Chemically-insignificant text is any text that you enter from the keyboard. For information on atom aliases and other chemically-insignificant text, see **1.11 Drawing structures for presentation graphics**.

Exercise 1.5: Create the following molecule.



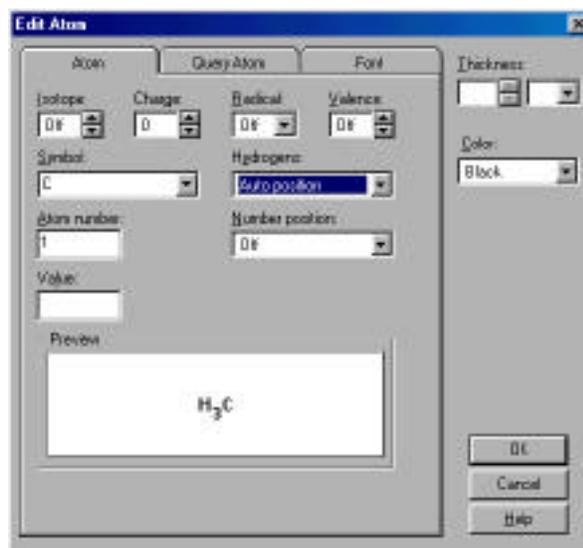
1. Clear the work area by selecting **File, New**.
2. Click the single bond tool  and place it on the empty work area.
3. Click the atom tool  and place it on the end of bond. Type in **17O-** in the text box (as shown below) and press **Enter** key:



4. Click the lasso selection tool  and select the other end of bond as shown:



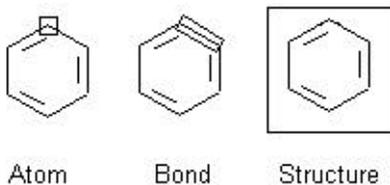
5. Edit the atom by choosing **Object, Edit Atom** or right click the mouse then select **Edit Atom**. The Edit Atom window appears as shown below. Click on the selection box for **Hydrogen** and choose “**Auto Position**” then click **OK**.



6. Now you have completed the structure.

1.5 Selecting and Deselecting Atoms, Bonds, and Structures

When you move the cursor over an item in the drawing area, ISIS/Draw indicates whether the item is an **atom**, a **bond**, or an **object**:



In the following instructions, if you **double-click** an atom, bond, structure, or **any** object instead of single-clicking, you see a dialog box where you can edit the object.

1.5.1 Selecting Atoms, Bonds, and Structures

There are three **Select tools** that you can use: , , and . Which one you use is an individual preference.

- Use lasso  or select  to select **individual atoms or bonds, whole structures, and non-chemical objects**.
- Use the lasso tool  if you prefer to select objects within a lasso, or use select tool  if you prefer a rectangular frame.
- Use the molecule selection tool  to select **whole molecules or non-chemical objects** only. You **cannot** select individual atoms or bonds using this tool.

To switch between the three Select tools: Click the **Select tool** that appears on the tool bar, then drag the mouse over to one of the other tools and release the mouse.

To select **one atom or bond**, first click  or , and then click the atom or bond.

To select **multiple atoms, bonds, or structures**, do one of the following:

- Click either  or , and then click one atom or bond. Press the **Shift** key and then click additional atoms or bonds.
- Click either  or  and drag the mouse around the atoms, bonds, or structures that you want to select.

To select one structure, do one of the following:

- Click the molecule select tool  and then click the structure.
- Click  or , then press **Ctrl** (PC) or **Command** (Mac) key and click the structure.

Other Objects: You select other objects, such as lines, boxes, arrows, and polygons as follows: Click any of the selection tools , , or , then click **one** object, **or** click and drag the mouse around multiple objects.

Windows users only: When you select **one or more objects** and press the **right mouse button**, you see a pop-up menu with commands that apply to the objects that you selected.

For example, if you select a structure and press the right mouse button, you see a pop-up menu that includes **Cut, Copy, Select All, Duplicate** and **Edit Molecules**. The commands that you see on the menu vary according to the objects that you select.

1.5.2 Deselecting Atoms, Bonds, and Structures

To deselect an item and leave other items selected, press the **Shift** key and click on an already selected item to deselect.

To deselect **all** the items that you selected, simply click an empty area of the window.

Other objects: You deselect other objects, such as lines, boxes, arrows, or polygons, as follows: Press the **Shift** key and click one already selected object to deselect, or click an empty area to deselect all.

1.6 Deleting Atoms, Bonds, and Structures

Select one or more atoms, bonds, or structures. Then, do one of the following:

- Press the **Delete** key.
- Choose **Edit, Cut**.

To delete atoms or bonds **one at a time**, click the erase tool , then click an atom or bond.

Note: When you delete an atom, any bonds attached to that atom are **also** deleted.

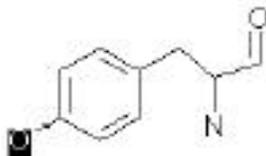
Other objects: You delete other types of objects, such as lines, arrows, boxes, Rgroup labels, and so on, as follows: Click  and then click an object; or select the objects and press the **Delete** key or choose **Edit, Cut**.

Deleting all objects in the drawing area: To delete **all** of the objects in the drawing area, first choose **Edit, Select All**, and then press the **Delete** key or choose **Edit, Cut**.

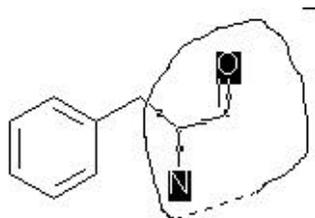
Exercise 1.6: Select, deselect and Delete atoms, bonds and structures.

From the menu bar, select **Template, Amino Acids**. Choose **Tyrosyl [Tyr]** and place it on your work area.

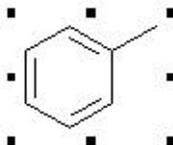
1. Click the lasso selection tool . Hold down the **Shift** key and highlight the **O** atom and the bond next to it as shown



2. Press the **Delete** key to remove highlighted fragment.
3. Highlight the portion of the molecule by using the lasso selection tool as shown.



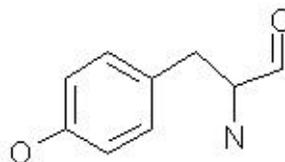
4. From the menu items, select **Edit, Cut**.
5. Switch to  and highlight the rest of molecule by dragging a rectangle frame to cover the structure. Deselect the structure by clicking any area outside the box. You now see:



6. Click  and drag the cursor to make a rectangle frame covering the structure and release the mouse to erase the whole structure.

1.7 Editing Atoms, Bonds, and Structures

You can edit an atom, bond, or structure. This can include such things as changing the atom symbols, adding a charge, or changing a bond from a double to a triple bond.



To edit atoms, bonds, or structures, do the following:

1. Click the selection tool  or . Select the molecule tool  if you want to edit an entire structure, not individual atoms or bonds.
2. Select the atoms, bonds, or structures to edit.
3. Do one of the following:
 - a. Double-click one of the selected atoms, bonds, or structures.
 - b. Choose **Object, Edit**.

You see the Edit dialog box:



4. Click the tab that identifies the type of change that you want to make. You see **only** tabs that apply to the atoms, bonds, or structures that you selected. To find information for an item on a tab, click **Help**.

Note: The wording of the **Object, Edit** menu command varies depending on what you select. For example:

- If you select a bond, the command reads **Edit Bond**.
- If you select at least one atom and one bond, the command reads **Edit Molecule**.
- If you select different types of objects, such as text, atoms, and a box, the command reads **Edit Objects**.

Other objects: You edit other types of objects, such as lines, arrows, boxes, Rgroup labels, and so on, as follows:

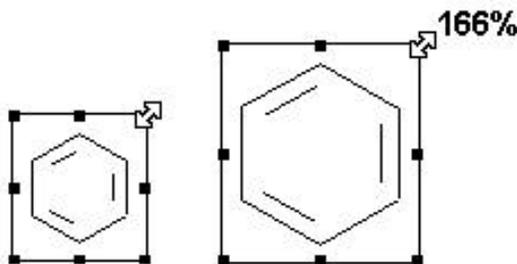
- Click on one of the selection tools, , or . Then, select the objects to edit, and then choose **Object, Edit Objects**.

Note: On the PC, if you select an OLE object, the **Edit <object>** command is not available.

1.8 Resizing or Scaling Structures

At times you may need to reduce the size of your structures or scale them to fit more on one screen. Doing this is very similar to other drawing software packages.

- To **resize** a structure, select it by clicking on it once, then drag one of the **corner** handles. ISIS/Draw displays the percentage by which you



are resizing the structure.

Note: If you drag a **non-corner** handle, the structure becomes distorted.

- To **scale** a structure, select it, and then choose **Object, Scale, Percent**. Enter a number - **without** a % sign - to scale the structure.

Note: If you resize or scale **all** of the molecules in the drawing area, you see a dialog box where you specify if you want your settings to reflect the resizing or scaling. Click **Yes** to have the settings modified so that any **new** molecules that you draw are drawn in the same scale. Click **No** to leave the settings as they are.

- **Other objects:** You resize or scale other types of objects, such as lines, polygons, boxes, and so on, as follows: Select the object, then drag a corner handle, or choose **Object, Scale, Percent**.

1.9 Moving Atoms, Bonds, and Structures

To **move** atoms, bonds, or structures, first select them. Then, press the mouse and drag the items to the new location (the cursor changes to a hand).

Other objects: You move other types of objects, such as lines, polygons, boxes, and so on, as follows: Select the object, press the mouse, then drag the object to the new location.

Note: When the cursor looks like a **hand**, you can move the atom, bond, or object. When the cursor looks like a **double-arrow**, move the cursor over the item so that it changes to a hand. Otherwise, you will re-scale or distort the object instead of moving it.

Exercise 1.7: Edit and move atoms, bonds and molecules and resize the structure.

From the template tool, select  and place it on the work area.

1. Use the select tool to highlight the bottom atom and use  to change it to **atom O** as shown below



2. Click the bond tool . Select one of the double bond and click once to change it to **Triple bond**.
3. Click once again will change it to “**single bond**” as shown:

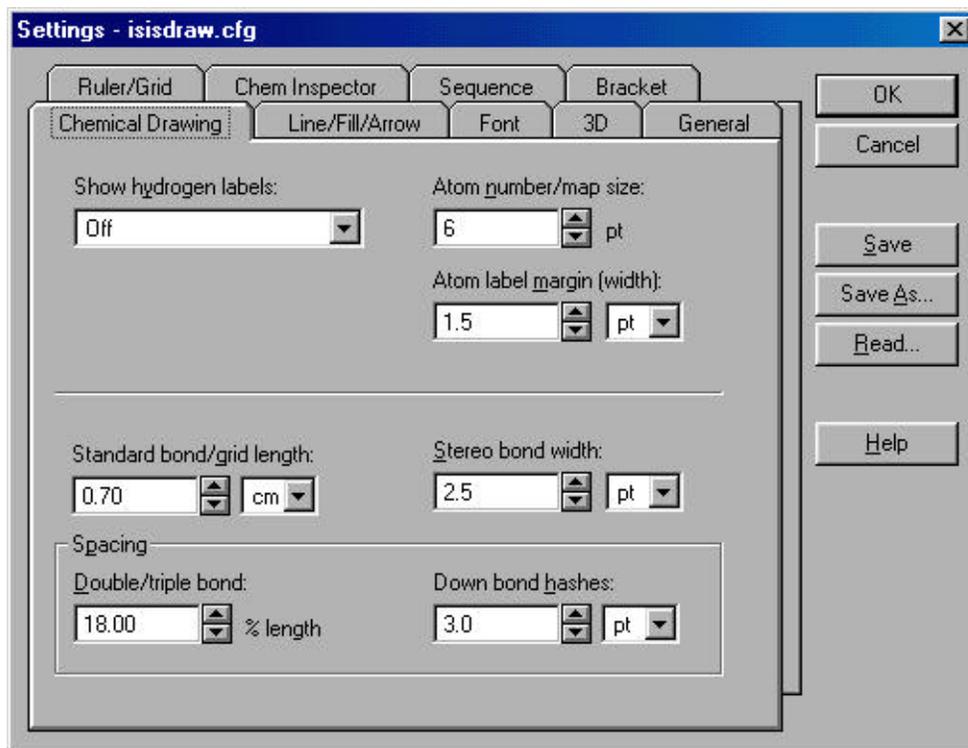


4. Use any of the three selection tools , , or  to select the whole molecule.
 5. Move your cursor into the highlighted box until you see the hand symbol. Click and hold the mouse to move the structure to other area. Release the mouse key to place it.
 6. Resize the structure by dragging one of corners and moving upward to enlarge it and downward to shrink it. When asked to **change settings to match the sketch**, click on the **No** button.
-

1.10 Changing ISIS/Draw Settings

You can modify the settings in ISIS/Draw' to suit your drawing needs. To modify any setting, choose **Options, Settings**, and then click the tabs to view the program defaults that you can modify.

Below is the screen shot showing what settings you can change within the program.



To save any modifications you made to the settings, click **Save**, otherwise any changes you make to settings apply only until you exit from ISIS/Draw.

To obtain information on the individual items on a tab, click **Help**.

For more information, see **Settings** in the *ISIS/Draw Contents* from the Help menu.

1.11 Aliases, Superscript, Subscript, Positioning, Deleting and Displaying Text and Numeric Information

You can draw structures that contain atom aliases. An **atom alias** is text that you attach to an atom that is not chemically significant but is used in presentations. The atom alias hides the existing atom but **does not** replace it. The chemical significance of the atom underneath does not change in any way. An atom alias can be any text or numerical value.

Creating atom aliases: To create an atom alias do one of the following:

1. To specify an atom alias **by itself**, click the atom tool  and then click where you want the alias to appear. Enter the atom alias text into the text entry field, then click elsewhere.
2. To add an atom alias to an existing structure, click  and then click the atom to which you want to attach the atom alias. Enter the atom alias text into the text entry field, then click elsewhere. Do not use all uppercase letters when you type in the atom symbol.

Note: If you use all uppercase letters when you type in the atom alias, ISIS/Draw **might** add an abbreviated structure to the sketch **instead** of the atom alias. In addition, when you create an atom alias, numerical values are **automatically** subscripted.

To enter letters or numerical values that are **superscript**, enter **\S** before and after the letter or number. You **must** use a capital letter **S**.

For example: To specify $^{32}\text{PO}_4$, enter **\S32\SPO4**.

To enter letters that are **subscript**, enter **\s** before and after the letter. You **must** use a lower case letter **s**.

To enter numerical values that are **not subscripts**, enter **\n** before and after the number. You **must** use a lower case letter **n**.

For example: To specify $^4\text{PO}_4^-$, enter **\n4PO\s4\S-**.

Positioning atom charges within an alias: To place a charge at the **left** of an atom, click the atom tool , click the atom, and then enter the charge and atom alias text. Click elsewhere on the screen.

For example, to specify ^+PO , enter **\S+\SPO**.

Editing or deleting atom aliases: To edit or delete an atom alias, click  and then click the atom containing the atom alias. Delete or edit the text in the text entry field, then click elsewhere.

Displaying hydrogen labels: To display hydrogen labels, choose **Options, Settings** and then click the **Chemical Drawing** tab. Click the **Show hydrogen labels** box and choose the types of atoms on which to display hydrogen labels: Off, On Hetero, On Hetero or Terminal, and On All.

Positioning hydrogen attachments: To specify the position of hydrogens on an atom, click  or  and double-click the atom. Click the **Atom** tab and then click the **Hydrogens** box and choose where you want the hydrogens to appear.

1.11.1 Sprout One Bond from a Typed-In Formula (Atom Alias)

Use this procedure to sprout one bond from a typed-in formula (atom alias). For example, to sprout an explicit hydrogen from a carbon atom that exists as an atom alias:



1. Click  and click in the drawing area.
2. Enter the formula. Include a caret (^) **before** the character you want the bond to be attached to. For example, enter **CH^CH2** to have the attachment point be at the second carbon.

Note: You can include **only one** caret for one attachment point.

3. Click one of the bond tools.
4. Draw a bond under the text string. The bond attaches itself to the correct site.
5. Click the atom tool .
6. Click the end of the bond and enter the atom label **H**.

Note: When you use this procedure, the numerical values that you enter are **automatically subscripted**, and the text string and bond are automatically grouped.

1.11.2 Sprout Two or More Bonds from a Typed-In Formula (Atom Alias)

Use this procedure to sprout **two or more** bonds from a typed-in formula (atom alias). For example, to sprout two or more explicit hydrogens from different carbon atoms that exist as atom aliases:



1. Click on the text tool .
2. Enter the formula, such as **CHCH2**.
3. (Optional) If the formula contains numerical values that should be subscripted, select the formula and choose **Text, Formula**.
4. Click the single bond tool .
5. Draw the bonds. The bonds are the standard bond length.
6. (Optional) Click the atom tool  and enter any atom labels, such as an explicit H, that you want to be attached to the bonds.
7. To keep the objects together, select all of the objects and choose **Object, Group**.

1.11.3 To Draw a Ring that Contains an Aromatic Designation

Use this procedure to draw a **chemically-insignificant** ring with an aromatic designation, such as Benzene:

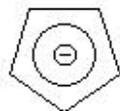


Note: This ring **cannot** be used as a query to search databases in ISIS/Base.

1. Use a template tool to draw the ring of your choice.
2. Click Ellipse tool . (Click and hold the rectangle tool to choose this.)
3. Press the **Shift** key as you draw a circle that is smaller than the ring.
4. Select the circle and move it inside the ring.
5. To keep the objects together, select all of the objects and choose **Object, Group**.

1.11.4 Drawing Charged Aromatic Rings

Use this procedure to draw **chemically-insignificant charged aromatic rings**, such as the following:



1. Use a template tool to draw the ring of your choice.
2. Click 
3. Press the **Shift** key as you draw a circle that is smaller than the ring.
4. Select the circle and move it inside the ring.
5. Press the **Shift** key as you draw a smaller circle.
6. Select the smaller circle and move it inside the larger circle.
7. Click the text tool  and type a - (minus).
8. Highlight the minus and move it inside the smaller circle.
9. To keep the objects together, select all of the objects and choose **Object, Group**.

1.12 Recovering from Problems

Occasionally there will be times when you ask the program to do something you didn't really mean to do or times where you want to change what you've already done. Below are some suggestions for correcting these problems.

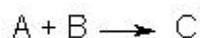
1. To reverse your last action, choose **Edit, Undo** from the menu items.
2. To leave a dialog box without changing anything, click **Cancel**.
3. To avoid many problems, **save your work often**. Save different versions (each with their own unique names i.e. version1, version 2) if you aren't quite sure which one you like the best.
4. If you prefer, you can always close the sketch without saving changes. If you saved your work recently, you will not lose many changes.

Chapter 2

Drawing Reactions

2.0 Introduction

A chemical reaction is two or more chemical components react to produce new product(s). A simple representation of chemical reaction is:



2.1 Basic Strategy

1. Draw the molecule components of the reaction with template tools, template pages, and/or drawing tools. (See **Chapter 1 Drawing Molecules** for more information.)
2. Use the  tool to add arrows. Use the  tool to add a plus, or click  and type a plus at the cursor position of your choice.
3. (Optional) To add reaction conditions to the reaction, click , enter the conditions, and place them at the position of your choice.

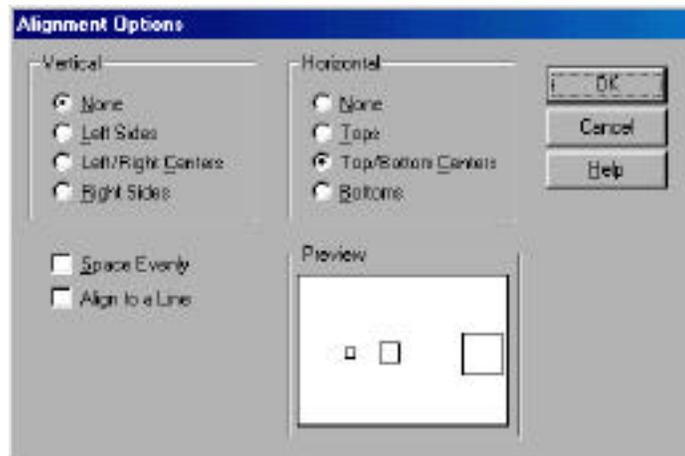
For example, to add 60°C above an arrow, click  and enter the degree symbol as a lower case, superscripted "o" symbol.

2.2 Editing a Reaction

1. Add, edit, delete, or move reaction elements as necessary.
2. To align an **entire reaction**, including arrow and plus signs, select the reaction and choose **Object, Align**. Use the **Alignment Options** dialog to specify how to align the reaction.
 - To align a reaction by **molecular components** only, first select one atom from each component. Then, choose **Object, Align** and specify how to align the reaction.
 - If you do not like the way the reaction is aligned, choose **Edit, Undo**.

For example, A + B → C

1. Select all components by choosing **Edit, Select All** from the menu items, or clicking on selected items while holding down the shift key.
2. Click **Object, Align**.
3. In the **Align Option** window, select Top/Bottom center for the Horizontal as shown below and click **OK**.



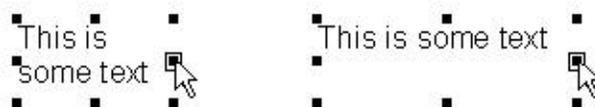
4. Now all components are aligned as shown. A + B → C

2.3 Working with Text

To **enter text**, click , and then click where you want the text to appear. Now, enter the text. Alternatively, you can enter text by pasting it in from the Clipboard.

To **edit text**, click , click the text, and then edit it as you would with a word processor.

To **reformat text**, click , click the text, and then drag a non-corner handle:



To **change text properties**, such as making text bold, select the text and do one of the following:

- Choose **Object, Edit Text**.
- Double-click the text.
- Choose one of the commands on the Text menu.

To set text **defaults**, choose **Options, Settings**, and then click the **Font** tab. To **save** any modifications you made to the settings, click **Save**, otherwise any changes you make to settings apply **only** until you exit from ISIS/Draw.

- If this is a **new** sketch, the new font settings are applied to any **new** text you enter.
- If this sketch contains **existing** text, a dialog asks if you want to apply the new font settings to the existing text.

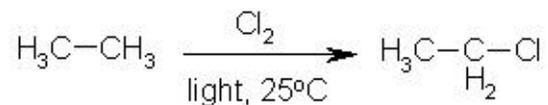
To enter **reaction conditions** (text that is above or below reactants, products, or the reaction arrow): Click , then click where you want the reaction condition to appear, and then enter the text.

2.4 Chem Inspector and Calculate Mol_Values

You may use ChemInspector to verify the chemistry of sketches.

1. Click the Run Chem Inspector tool  or choose **Chemistry, Run Chem Inspector** from the menu items.
2. Do one of the following:
 - To verify the entire sketch, click Check entire sketch.
 - To verify part of the sketch, first select the objects that you want to verify, and then click Check selected objects.
 - Or you may use Calculate MolValues to calculate molecular properties of sketches such as molecular weight, mass, formula and compositions.
3. Choose **Chemistry, Calculate MolValues, Calculate**.

Exercise 2.1: Create the following reaction scheme.



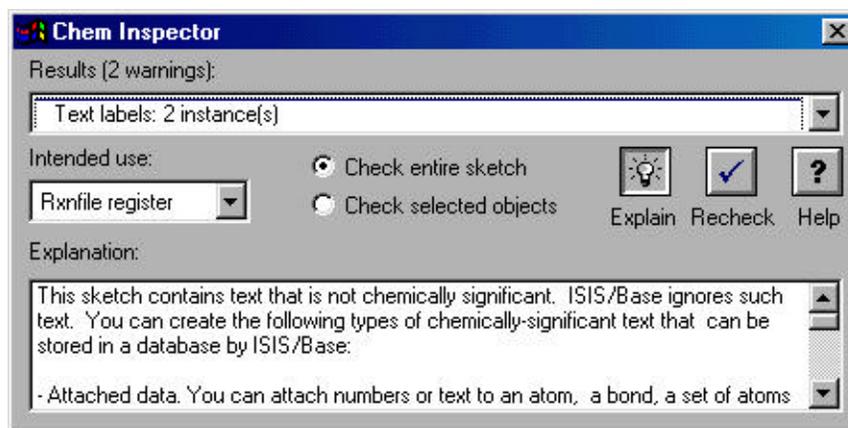
1. Clear the work area by selecting **File, New**.
2. Click  and place the cursor in the work area and click once.
3. Type in **CH3** in the text box and press enter. Click on **CH3** and hold the mouse key to drag toward your right. Release the mouse key when you see a line drawn. Press **Enter** key when you see.



4. Select  and click on the right side of the molecule, CH₃-CH₃, to draw a arrow. You may want to lengthen the arrow to allow enough space for some texts later.
5. Click  and place the text cursor at the top of the arrow and type in **Cl2**. You can change this into Cl₂ by highlighting the number **2** and select **Text, Subscript** or highlight Cl2 and select **Text, Formula**.
6. Place the text cursor below the arrow and click to type in **light, 25oC**. Change **o** to superscript by highlighting it and select **Text, Superscript**.
7. Select  again and click the area next to the arrow head. Create **CH3-CH2-Cl** by following the same procedures described in step 3.
8. You may now try to align the texts and make it look nicer.
9. Save your work as *test3*.

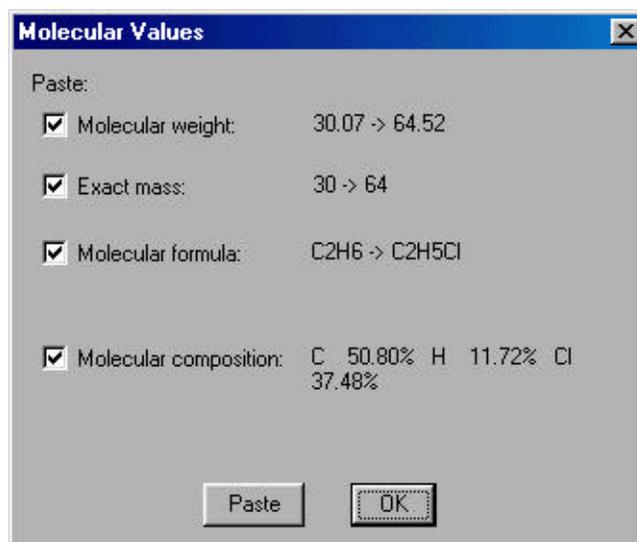
Exercise 2.2: (Optional)

1. Use the above reaction scheme (test3.skc)
2. Click  or choose **Chemistry, Run ChemInspector**.
3. You should see the following window appears.



You may scroll down the Explanation window for more information. Click **OK** when done reading.

4. Choose **Chemistry, Calculate MolValues, Calculate**. You now see the following with molecular properties displayed.



5. Click **OK** to close the window.
-

Chapter 3

Biopolymers

3.0 Introduction

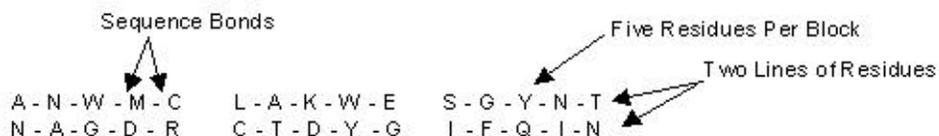
A biopolymer sequence is a linear chain of connected repeating structures that are called residues. In the following example, you see the residue codes for one of the protein Bovine Insulin, which contains 21 amino acid residues:

H2N-G I V E Q C C A S V C S L Y Q L E N Y C N-COOH

In ISIS, the list of residue codes that you can use are defined in a Residue Map file that uses the structures from a Residue Template file. In this example, the Residue Map file contains the list of 1-letter residue codes for the amino acid residues. MDL provides you with Residue Map files for 1- and 3-letter residue codes for amino acids and for the nucleic acids DNA and RNA. The sequence bond between each residue is formed by the connection of atoms that are specified within the Residue Template file.

If the list of residue codes or their underlying structures are not sufficient for your specific needs, you can edit an existing **Residue Map file** or **Residue Template file** or create your own.

To improve the readability of a sequence, you can group residues into suitably sized blocks, limit the number of residues per line, or change the spacing between blocks or residues:



3.1 Customize the Display Settings

You can change the following default settings for drawing sequences:

1. Spacing Between Residues
2. Spacing Between Blocks
3. Spacing Between Lines
4. Number of Blocks in a Line
5. Number of Residues in a Block
6. Show/Hide Sequence Bonds
7. Show/Hide Crosslink Bonds
8. Show/Hide Residue Brackets
9. Show/Hide Leaving Groups
10. Define the Delimiter

To change these defaults, choose **Options, Settings** and click the **Sequence** Tab. Change the defaults of your choice, and then click **OK**.

3.1.1 To Specify the List of Residue Code

Use the following procedure to specify the list of residue codes that you want to use to build a biopolymer sequence. Every list of residue codes that are available for use **must** be listed on the Sequence menu.

1. Choose **Chemistry, Sequence**, and then choose the list of residue codes that you want. The program provides you with the following lists of residue codes on the Sequence menu: **Amino Acids - 1 letter** (for 1-letter amino acid structures); **Amino Acids- 3 letter** (for 3-letter amino acid structures); **DNA - 1 letter** (for deoxyribonucleic acid structures); or **RNA - 1 letter** (for ribonucleic acid structures).

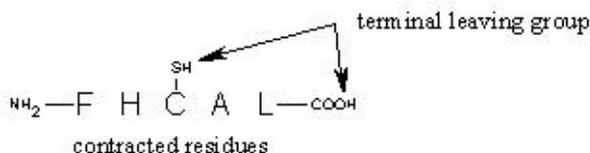
Note: To use a list of residue codes that is not on the Sequence menu or to customize a list, click **Customizing a List of Residue Codes**.

2. To view the current list of residue codes that you chose in Step 1, choose **Chemistry, Sequence**. You should check the box next to **Show Residue List**.
3. If you do not see the current list, click the sequence tool .

3.2 Create a Sequence from the Keyboard or the Residue List

You can type a sequence of residues directly from the keyboard:

1. Click the sequence tool .
2. Type in the residue codes of your choice. You see the contracted residues and terminal leaving groups. For example:



3. To specify the end of a block of residues as you enter residues into the ISIS/Draw window, press the **Space** key.

Caution: If you do not specify the number of residues per line, all the residue codes that you type will remain on a single line that might extend past the drawing window. However, you can insert a line break anywhere if you press the **Return** key.

4. You can also create the sequence by double-clicking from the list of residues, choose **Chemistry, Sequence**. You should check the box next to **Show Residue List**.



3.3 *Editing Sequences*

There are a variety of things that you can do to edit sequences that you create in ISIS/Draw.

3.3.1 Delete Contracted Residues

1. Click the sequence tool .
2. Click the residue that you want to delete. You see the cursor at the left of the residue code.
3. Do one of the following:
 - To delete the residue at the left of the cursor, press the **Back Space** key on the PC or on the Macintosh use either the Back Space or Delete key.
 - For the PC only: To delete the residue at the right of the cursor, press the **Delete** key.

3.3.2 Insert a Contracted Residue into a Sequence at any Location

1. Click the sequence tool  (if it is not highlighted).
2. Click the exact middle of the residue that is at the right of your insertion point. You see a box around the residue.
3. Type in the residue codes of your choice. (Alternatively, double-click the residue from the list of residues.) The insertion of a new residue moves the succeeding residues one position to the right.

Caution: If you previously specified a default setting for the number of residues per line and the insertion of your residue exceeds that default setting, a new line is not created.

4. Insertions can create gaps (additional spacing) between succeeding residues. To eliminate a gap, click . Choose **Edit, Objects**, and then click the **Sequence** tab. Edit the sequence.

3.3.3 Renaming the Residue Code of a Contracted Residue

- Click .
- Select the residue code that you want to rename.
- Choose **Chemistry, Residue, Rename**.
- Enter a unique name for the residue code.
- Click **OK**.

3.3.4 Specifying Blocks of Residues in a Sequence to Improve the Readability of Contracted Residues

Do one of the following:

- To specify the end of a block of residues as you type in residues via the keyboard into the ISIS/Draw window, press the **Space** key. (You cannot use the **Space** key if you click residues from a list of residue codes.)
- To specify the default number of residues per block, choose **Options, Settings**. You see the **Settings** dialog box. Click the **Sequence** tab, and then click the number of residues that you want per block in the **Blocksize** list box. You can enter a value between 0 and 999. A

default setting of 0 (zero) specifies that there are no blocks of residues (zero residues per block.)

To save the specifications that you entered and to apply them to your current work, click **Save**, click **OK**, and then click **Yes**. (Or, click **No** to apply these settings solely to future work.)

Note: To change the block size for a sequence that you already entered, select the sequence, choose **Edit, Objects**, and then click the **Sequence Tab**. Click the number of residues that you want per block in the **Blocksize** list box.

3.3.5 Specifying Lines of Contracted Residues in a Sequence

You must specify a new line for the residues in a sequence that would otherwise extend past the drawing window.

Do one of the following:

- To specify the end of a line of residues as you enter residues into the ISIS/Draw window, press the **Return** key.
- To specify the default number of residues per line, choose **Options, Settings**. You see the **Settings** dialog box. Click the **Sequence Tab**, and then click the number of residues that you want per line in the **Wrap after** list box. You can enter a value between 0 and 999. A default setting of 0 (zero) specifies that there is solely a single line of residues.

To save the specifications that you entered and to apply them to your current work, click **Save**, click **OK**, and then click **Yes**. (Or, click **No** to apply these settings solely to future work.)

Note: To change the number of residues per line for a sequence that you already entered, select the sequence, choose **Edit, Objects**, and then click the **Sequence Tab**. Click the number of residues that you want per line in the **Wrap after** list box.

Use this procedure to cleave a sequence that is in the ISIS/Draw window **into smaller sequences**

1. Click erase tool .
2. Click the sequence bond where you want to cleave or cut apart the sequence. You see the leaving groups on the cleaved residues.

3.3.6 Joining Two Sequences

1. Click the selection tool .
2. Press and hold the mouse button on a terminal leaving group of one of the sequences.
3. Drag the mouse to a terminal leaving group on the other sequence, and then release it. The sequences join together.
4. To undo Steps 2 and 3, choose **Edit, Undo**. The sequences move back to their original location.

3.3.7 Shaping Sequences

1. Click the sequence shape tool  (you may have to change the tool from the default).
2. Press and hold the mouse button on a residue. This residue is now the anchor.
3. Drag the mouse to the shape of your choice, and then release it. The residues that succeed the anchor move to the new shape.

3.3.8 Snap a Sequence to a Pre-Existing Object (Shape Template)

This procedure assumes that you have a pre-existing shape template in ISIS/Draw. A shape template can be any circle or line object that is created in ISIS/Draw with the Sketch tools.

1. Choose **Options, Snap To Object**.
2. Click the sequence shape tool .
3. Do one of the following:

- If you have a sequence in the ISIS/Draw window, press and hold the mouse button on a residue. This residue is now the **anchor**. Drag the mouse to the shape of the object, and then release it. The residues that succeed the anchor move to the new shape.
- If you do not have a sequence in the ISIS/Draw window, position the cursor on the shape template where you want to see the first residue. Type the letter codes for the residues of your choice. Each residue snaps to the object along the sequence path that the object creates via its shape.

3.3.9 Expanding Contracted Residues

Caution: This procedure might produce overlapping structures or structures that are difficult to edit. Thus, we recommend that you expand a single residue code in the Edit window.

1. Click the selection tool .
2. Select the set of residues that you want to expand.
3. Choose **Chemistry, Residue, Expand**. You see the chemical structures.
4. You can edit the underlying chemical structures.
5. To change the display of the residues, click any of the following:

Residue Brackets:	Display/Hide
Leaving Groups:	Delete, Display/Hide,
Sequence Bonds:	Display/Hide
Crosslink Bonds:	Add, Delete, Display/Hide
6. To contract a set of expanded structures in the ISIS/Draw window, select them, and then choose **Chemistry, Residue, Contract**.

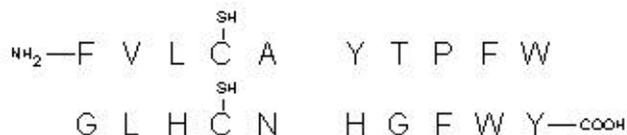
3.3.10 Configure Chemical Groups on Specific Residues in the Up- or Down-Configuration

This procedure assumes that you have a set of expanded residues in the ISIS/Draw window.

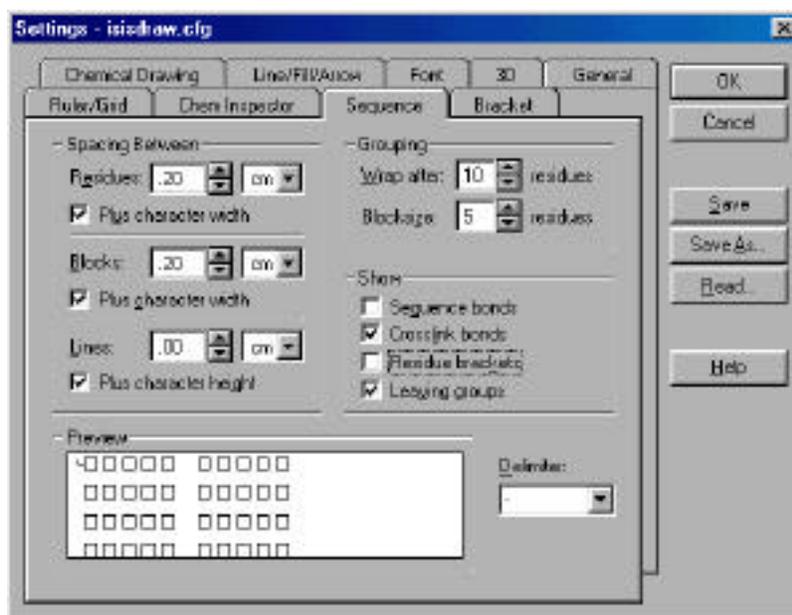
1. Select a residue whose chemical group you want to configure in the opposite orientation. (You can select more than one residue by using the selection tool if the residues are in succession.)

2. Choose **Options, Flip, Chem Group**.

Exercise 3.1: Create the following sequence.



1. Clear the work area by choosing **File, New**.
2. Make sure **Chemistry, Sequence, Amino Acids – 1 letter** was checked.
3. Change the sequence setting by selecting **Options, Settings** and click on the **Sequence** tab. Make changes in **Grouping – Wrap after 10** residues and **Blocksize 5** residues as shown. Notice the preview window changes as you type in those numbers. Click **OK** when done.



4. Select the sequence tool  and click on the empty work area.
5. Type in **FVLCA YTPFW GLHCN HGFWY** on the screen. You have now created the sequence as shown above.
6. Save your work as **test4**.

Chapter 4

Create Presentation/Publication Graphics

4.0 Introduction

This chapter is intended to show you other useful features and techniques within the ISIS Draw program to make nice graphics for presentation and publication.

4.1 Drawing for journal publication

ISIS Draw includes journal settings for the following publications:

- Journal of American Chemical Society
- Journal of Chemical Information & Computer Sciences
- Journal of Medicinal Chemistry
- Journal of Organic Chemistry
- Perkin I/Perkin II
- Synthesis/Synthesis Letters
- Tetrahedron/Tetrahedron Letters

4.1.1 Apply Journal Settings to a New Sketch

Use this procedure to apply journal settings to a new sketch.

- From the menu items, choose **File, New**.
- Choose **Options, Read Journal or Custom Settings**.
- Select the journal settings file whose settings you want to apply to the sketch.
- Click on **OK**
- Choose **Options, Apply Settings**. The journal settings are applied to any new objects that you draw.

Note: The same procedure can be used to apply the journal settings to the existing sketch by opening the file and following the above steps 2-5.

4.1.2 Modify the Journal Settings

Use this procedure to modify a journal setting file. You might do this if publication style requirements change. Journal settings files are read-only, so save your modified settings under another name.

- From the menu items, choose **Options, Settings**.
- Click on **Read**.
- Select the journal settings file whose settings you want to modify.
- Click on **OK**.
- Click a tab and select any option to modify.
- Click on **Save As**.
- Enter a name for the new settings file.
- Click **OK**.

Note: The similar procedures can be used to create any new journal settings.

4.2 Create Presentation Graphics

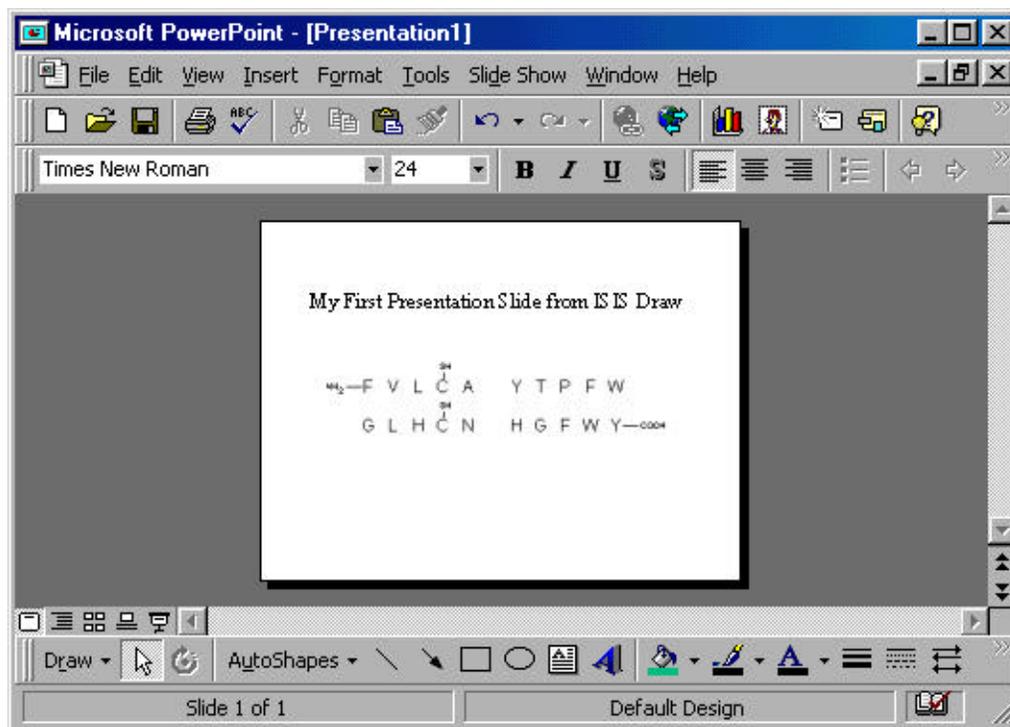
Since the ISIS Draw program does not have good import/export functions for most of other applications, such as Word or PowerPoint, the only alternative to create a presentation graphic from the program is to do **Cut-and-Paste**.

1. First create your sketch with colors and fonts you would like to present.
2. With any presentation/graphical program open, you can cut and paste your sketch.

Exercise 4.1: Create your presentation slide with ISIS Draw sketch

- Open your last saved sequence file, **test4.skc**.
- From the menu items, choose **Edit, Select All**.
- From the menu items, select **Edit, Copy**.
- Open Microsoft PowerPoint, then

3. Choose **Blank Presentation**
 4. Then select the **blank slide** from the slide template choices.
- Choose **Edit, Paste**. You should see the sketch appear on the PowerPoint slide. You now can move or resize to fit your need. Type in a title.
 - If you need to modify the sketch, simply highlight the sketch and double click on it. It will automatically open up the sketch in the ISIS Draw program. When done editing, select **File, Exit and Return to Microsoft PowerPoint**.



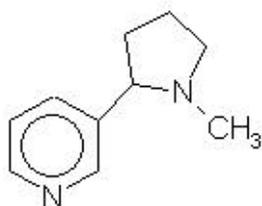
- You may perform any operations as you used to do with PowerPoint program.

Appendix A

A. Optional Exercises

The following optional exercises are designed for the advanced users or for those who are interested in learning more techniques in using ISIS draw program.

Exercise A.1. Create the following sketch. This exercise combines all tools and techniques mentioned in Chapter 1.

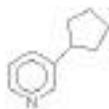


Nicotine

A tobacco alkaloid

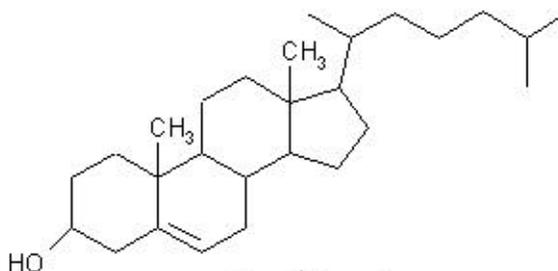
1. Clear the work area by choosing **File, New**.
2. Click  and place it on the work area.
3. Choose  and click on the bottom of the hexagon. Type in **N** in the text box and press **Enter**.
4. Click on the shape tool and select Ellipse . Press and drag the mouse key to draw a circle within the hexagon.
5. Use the select tool to highlight it and move it to the center as shown:

6. Choose the bond tool  and click on the right hand corner of the sketch.
7. Choose the five-member ring  and click on the end of the single bond as shown.



8. Choose the atom tool  and click on the corner of the pentagon next to the single and type in **N** in the text box.
9. Press on **N** (pentagon) and drag to make a bond. Type in **CH3** and press enter.
10. Click the text tool  and place it below the sketch.
11. Type in “**Nicotine**” and Make it bold by choosing **Text, Bold** from the menu items.
12. Type in “***A tobacco alkaloid***” and Make it italic by choosing **Text, Italic**.
13. Change the font color by highlighting the text and double-clicking on it. When the window opens, change the color to red.
14. You got it! Save your work as **exerciseA1.sk**.

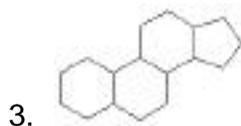
Exercise A.2. Create the following sketch. This exercise combines all tools and techniques mentioned in Chapter 1 and 2.



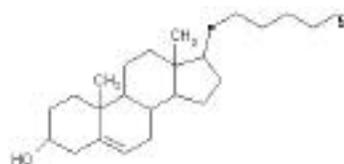
Cholesterol

A steroid occurs in all animal tissues

1. Create a new work area by choosing **File, New** from the menu items.
2. Click the hexagon tool     and click once to place in the work area. Place the cursor on one side of hexagon and click once. You shall see the second hexagon join to it. Repeat the same step with one more hexagon and one pentagon as shown:

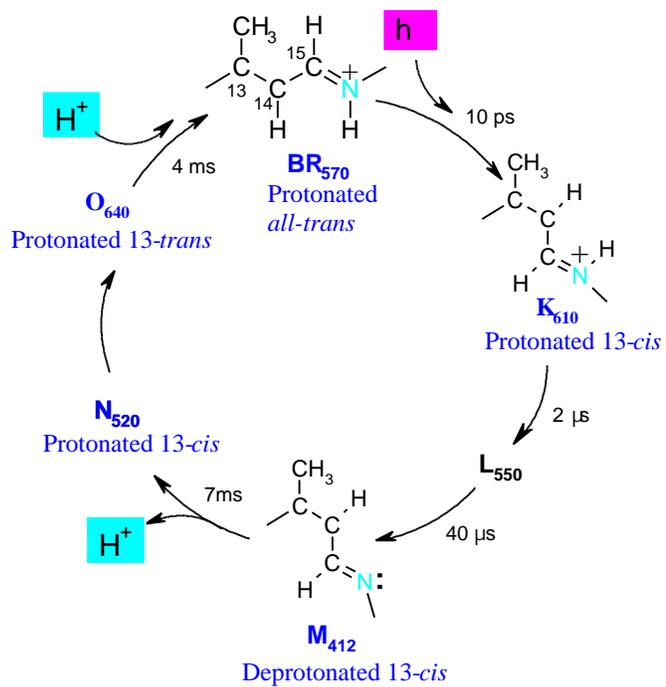


4. Click  and add a double bond to the second hexagon in the position as shown in the final sketch.
5. Click  and add three chemical groups, **OH** and 2 **CH₃** as shown above. Change the font size to **10** by highlighting individuals and double click on it to **Edit Text**.
6. Click  and add a single bond to one end of pentagon as shown in the final sketch.
7. Click on chain tool,  and press on the end of single bond and drag until you see **5** shown at the end of chain as shown. Release the mouse key.



8. Click  and add two more bonds to the sketch. Add final texts and save your work as **exerciseA2.sk**.

Exercise A.3. The Photocycle of Bacteriorhodopin. See if you can create the following graph for your presentation.



Appendix B

Descriptions of Tool Bar

I. Select Tools:



Lasso Tool	
Press-drag:	Select the objects inside a lasso
Click on an object:	Select the object
with Ctrl key:	Select entire molecule
Press-drag on an object:	Move an object
Press-drag on a selection handle:	Resize an object
Double-click an object:	Edit the object properties



Molecule Select Tool	
Press-drag:	Select the molecules/objects inside a frame
Click on a molecule/object:	Select the molecule/object
Press-drag on a molecule/object:	Move a molecule/object
Press-drag on a selection handle:	Resize a molecule/object
Double-click a molecule/object:	Edit the molecule/object properties

II. Rotate Tools:



2D Rotate Tool	
Press-drag the pivot:	Move the center of rotation
Press-drag around objects:	Select the objects inside a lasso
Press-drag selected objects:	Rotate the objects around the pivot
Ctrl-click a molecule:	Select a molecule



3D Rotate Tool

Press-drag around molecules:	Select the molecules inside a frame
Press-drag selected molecules:	Rotate the molecules in 3 dimensions
with Shift key:	Constrain rotation to X or Y axis
with Ctrl key:	Constrain rotation to Z axis

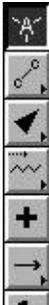
III. Erase Tool:



Eraser Tool

Click on an object:	Delete the object
with Ctrl key:	Delete the structure
Press-drag:	Delete the objects inside a frame

IV. Atom Tool:



Atom Tool

Use the **keyboard** to enter symbols, charges, isotopes, radicals, hydrogens, and query properties.

Click an atom and type:	Edit the atom
Click and type:	Create an atom
Press-drag an atom:	Create an atom at the end of a bond
Ctrl-click an atom:	Repeat previous atom symbol

V. Bond Tools:




Single Bond Tool

Click:	Sprout a single bond
Press-drag:	Draw a single bond
Click a bond:	Change to a single bond
Repeat click:	Switch between single, double, and triple bond



Double Bond Tool

Click:	Sprout a double bond
Press-drag:	Draw a double bond
Click a bond:	Change to a double bond
Repeat click:	Change position of the double-bond side



Triple Bond Tool

Click:	Sprout a triple bond
Press-drag:	Draw a triple bond
Click a bond:	Change to a triple bond

VI. Other Bond Tools:




Up Wedge Tool

Click:	Sprout an up wedge bond
Press-drag:	Draw an up wedge bond
Click a bond:	Change to an up wedge bond
Repeat click:	Reverse the direction of the bond



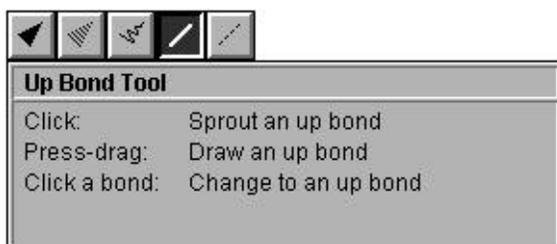
Down Wedge Tool

Click:	Sprout a down wedge bond
Press-drag:	Draw a down wedge bond
Click a bond:	Change to a down wedge bond
Repeat click:	Reverse the direction of the bond

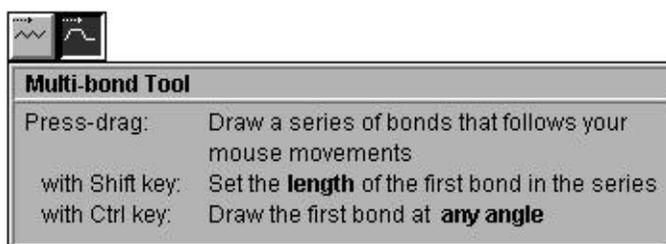
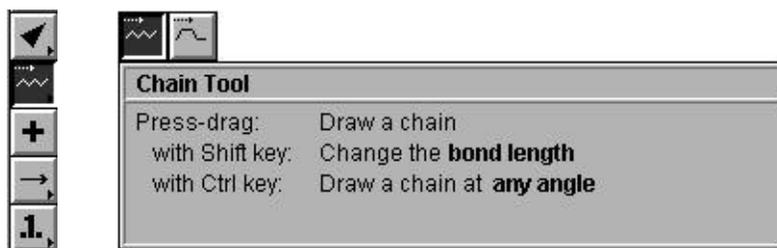


Either Bond Tool

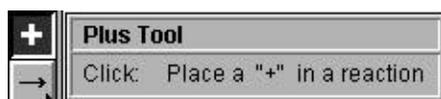
Click:	Sprout an either bond
Press-drag:	Draw an either bond
Click a bond:	Change to an either bond
Repeat click:	Reverse the direction of the bond



VII. Chain Tool:



VIII. Plus Tool:



IX. Arrow Tool:

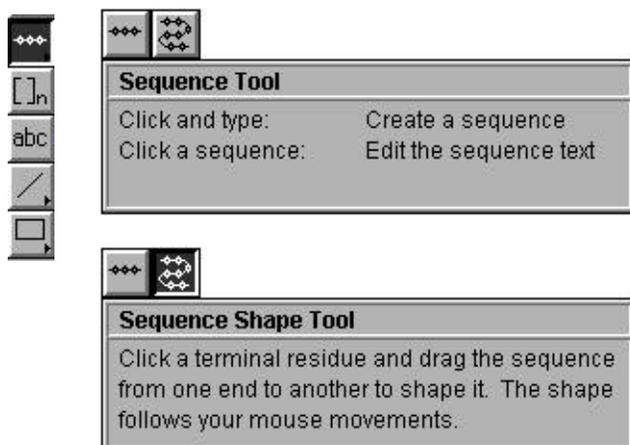
Arrow Tool (valid for ISIS/Base reactions)	
	Click: Place an arrow
	Press-drag: Draw an arrow
	with Shift key: Draw an arrow at any angle
	Repeat click: Alternate between left, right, and double arrowhead

X. Mapping Tool:

Atom-Atom Map Tool (use only with a reaction)	
	Click two atoms: Map a pair of atoms
	Click an atom and drag to another atom: Map a pair of atoms
	Click a bond: Alternate between reacting center types

Delete Atom-Atom Map Tool (use only with a reaction containing atom maps)	
	Click an atom: Delete an atom-atom map
	Click a bond: Delete a reacting center
	Press-drag: Delete multiple atom-atom maps inside a frame

XI. Sequence Tool:

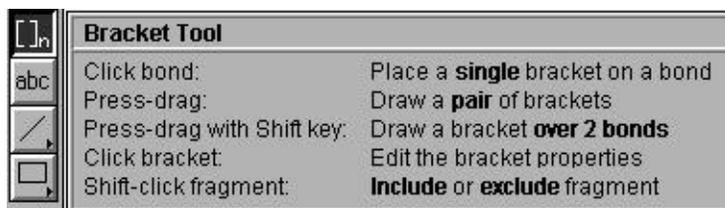


The image shows two tool panels for the Sequence Tool and Sequence Shape Tool. On the left, there is a vertical toolbar with icons for sequence creation, editing, and shaping. The Sequence Tool panel has two icons: a horizontal sequence and a curved sequence. The Sequence Shape Tool panel has two icons: a horizontal sequence and a curved sequence.

Sequence Tool	
Click and type:	Create a sequence
Click a sequence:	Edit the sequence text

Sequence Shape Tool	
Click a terminal residue and drag the sequence from one end to another to shape it. The shape follows your mouse movements.	

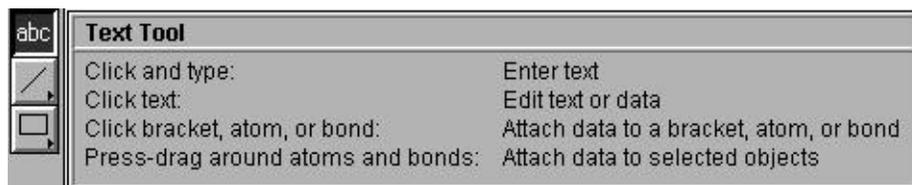
XII. Bracket Tool:



The image shows the Bracket Tool panel with a vertical toolbar on the left containing icons for bracket creation and editing. The main panel contains a table of actions and their descriptions.

Bracket Tool	
Click bond:	Place a single bracket on a bond
Press-drag:	Draw a pair of brackets
Press-drag with Shift key:	Draw a bracket over 2 bonds
Click bracket:	Edit the bracket properties
Shift-click fragment:	Include or exclude fragment

XIII. Text Tool:



The image shows the Text Tool panel with a vertical toolbar on the left containing icons for text entry and attachment. The main panel contains a table of actions and their descriptions.

Text Tool	
Click and type:	Enter text
Click text:	Edit text or data
Click bracket, atom, or bond:	Attach data to a bracket, atom, or bond
Press-drag around atoms and bonds:	Attach data to selected objects

XVI. Line Tool:



Straight Line Tool

Press-drag:	Draw a line at any angle
with Shift key:	Draw a line constrained to 15 degree increments



Continuous Line Tool

Click and move mouse:	Define the segments
Double-click:	Finish the last segment



Circular Arc Tool

Press-drag:	Draw an arc
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XV. Shape Tool:

Rounded Rectangle Tool

Press-drag:	Draw a rounded rectangle
with Shift key:	Draw a rounded square



Polygon Tool

Click and move mouse: Define the segments
Double-click: Finish the last segment and close the polygon



Ellipse Tool

Press-drag: Draw an ellipse
with Shift key: Draw a **circle**



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