KnowItAll Software Training

Drawing Structures and Reactions

Drawing Structures and Reactions

How to Use ChemWindow to Create and Edit Structures

Purpose

The ChemWindow application is a full-featured 2-dimensional structure drawing program. You can use the ChemWindow application to create chemical structures that can be used throughout the KnowItAll Informatics System for searching, prediction and reporting chemical composition.

Objectives

This exercise will teach you:

- How to use basic ChemWindow tools to create and edit a structure drawing
- How to save a structure for further use
- How to send structure from ChemWindow to MS office documents

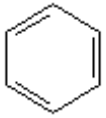
Background

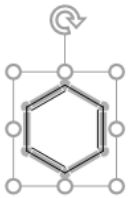
Chemical structures can be used throughout the KnowItAll Informatics System for searching, prediction and reporting chemical composition.

KnowItAll Applications Used

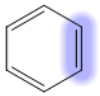
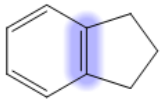
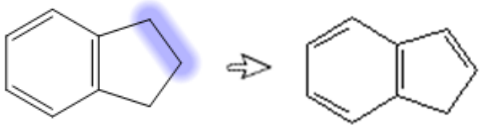
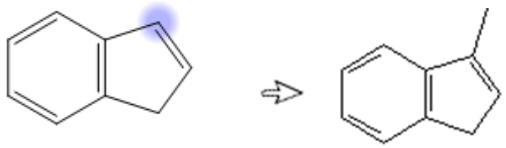
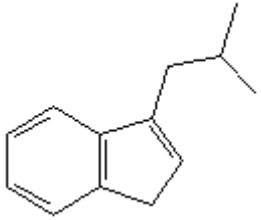
- ChemWindow®

Begin a new structure drawing

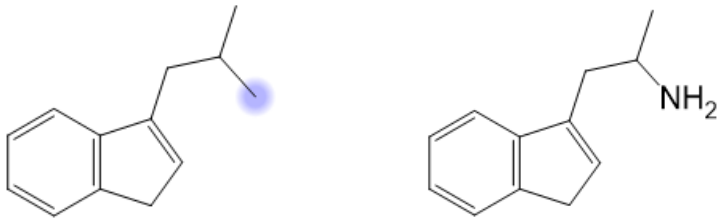
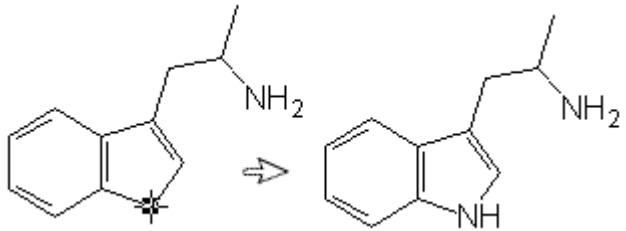
	Action	Result
1	Click the **ChemWindow** icon in the **Basics** toolbox.	The **ChemWindow** application opens to a blank drawing pane.
2	Select the **Benzene Ring** tool  in the **Main** section of the **Chemistry Toolbar**.	
3	Move the cursor into the drawing area, then click to draw a benzene ring.	The benzene ring structure is placed in the drawing area. 
4	If desired, use tools on the zoom toolbar to change the magnification. **Note**: Choose **View > Zoom Toolbar** to toggle the toolbar display.  The **ctrl** + **scroll** function can also be used to zoom in and out quickly.	

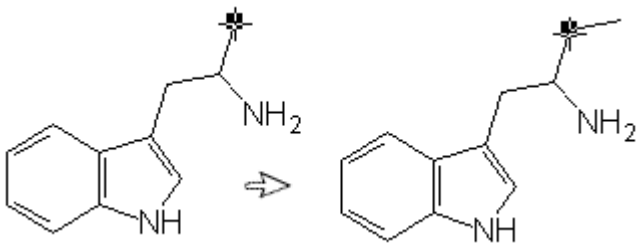
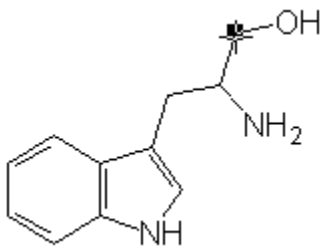
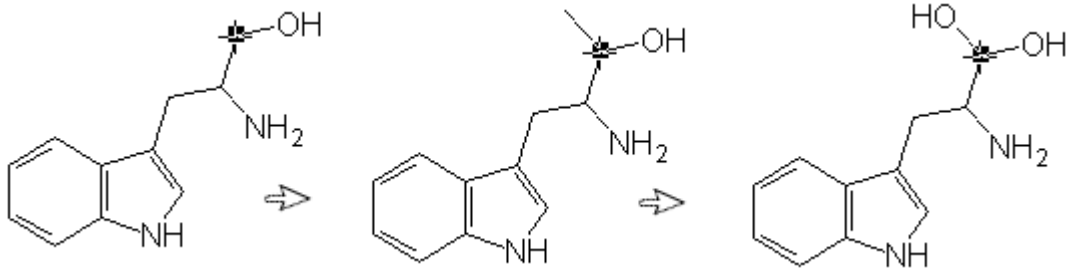
5	Use the **Selection** tool  to select the structure and move it within the workspace.	Graphic handles appear when the structure is selected. 

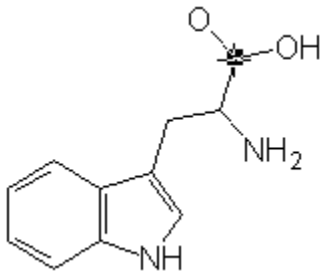
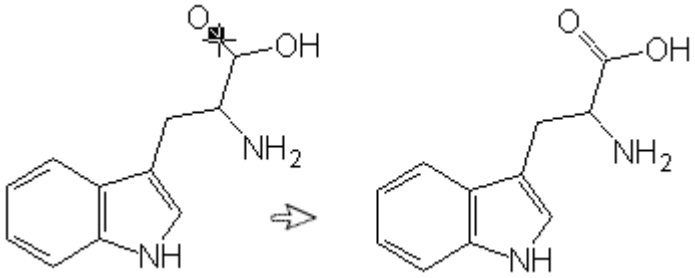
Add features to the structure

	Action	Result
1	Select the **Cyclopentane** tool, then move the cursor to the highlighted bond on the benzene ring.	
2	Click to join a cyclopentane ring to the benzene ring.	
3	Open the **Bonds** group in the **Drawing Toolbar** and select the **Inside Double Bond** tool. Then use it to add a double bond to the structure.	
4	Select the **Single Bond** tool. Then move the cursor over the atom's hit box as shown. Click to create a single bond.	 **Note**: If you don't release the cursor, you can control the bond direction by dragging.
5	Continue adding single bonds by clicking on hit boxes on atoms.	

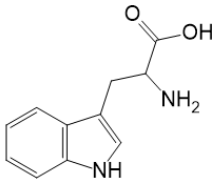
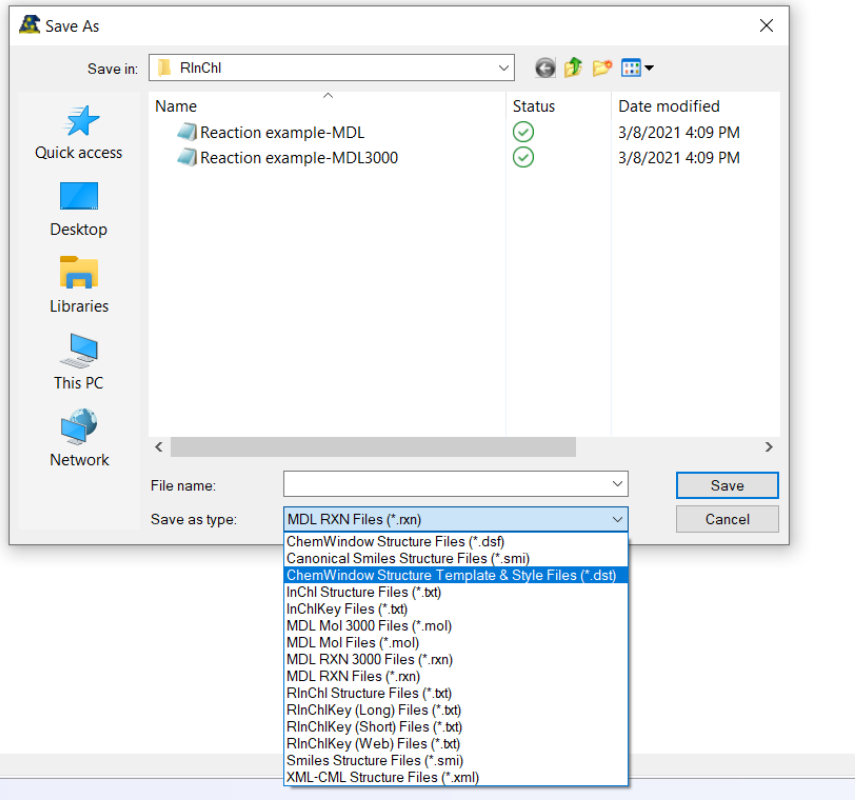
Use hot keys to add nitrogen and oxygen atoms

	Action	Result
1	Move the cursor over the terminal carbon. Then press **n** on your keyboard.	**NH_2** appears at the end of the bond.  >> **Note**: Numbers are automatically displayed as subscripts when using hot keys, which are shortcut keys you can use to quickly label atoms. You can also use the atom label tool to add atoms to a drawing. However, unlike atoms added while using a bond tool, atoms in atom labels are not actually part of the structure and will not be included when calculating the mass or chemical formula.
2	Repeat to replace a carbon atom with **NH**.	

3	With the single bond tool still selected, place your cursor over the terminal carbon atom and click to add another single bond.	
4	Without moving the cursor, press **o** on your keyboard.	
5	Click to sprout another single bond. Then press **o** on the keyboard to add a hydroxyl group.	

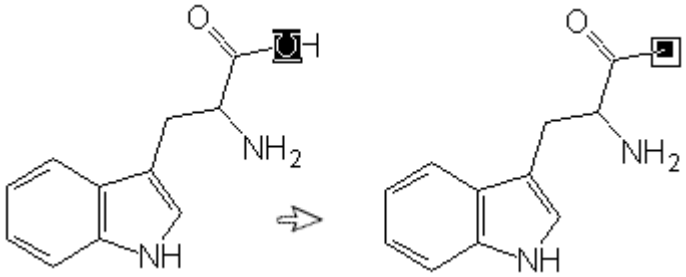
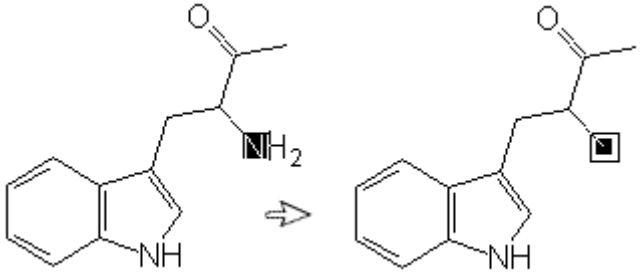
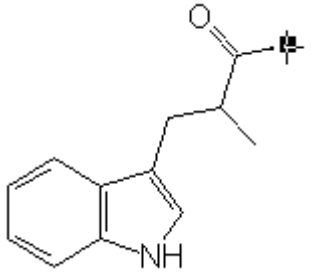
6	Press **o** again to remove the hydrogen. **Note**: When using a hot key, you can change the number of hydrogens attached to the atom by pressing the hot key repeatedly.	
7	Move the cursor to the hit box on the bond. Then click to create a double bond.	

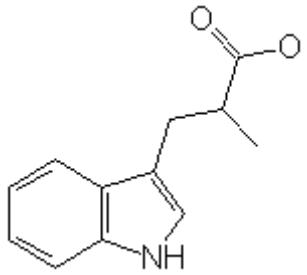
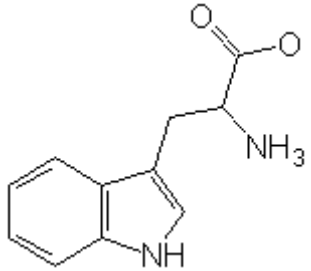
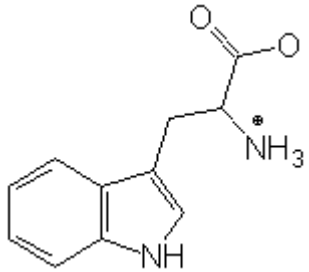
Save the structure

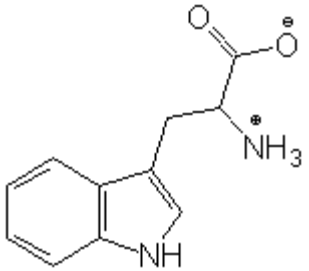
	Action	Result
1	Choose **File > Save**. **Note**: You can also click the **Save** button on the toolbar or press Ctrl+S.	The **Save As** dialog box opens. The default file type (**ChemWindow** structure file, *.dsf) is already selected, and will be used for this structure. Other file types include **ChemWindow** Structure Template & Style (*.dst) and MDL Mol file (*.mol).  
2	Navigate to the folder where you wish to save the structure file, then type in the file name “tryptophan.”	

3	Click **Save**.	The structure is saved, and the file name is displayed on the drawing tab.

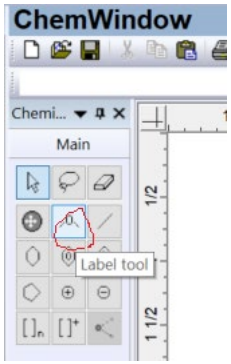
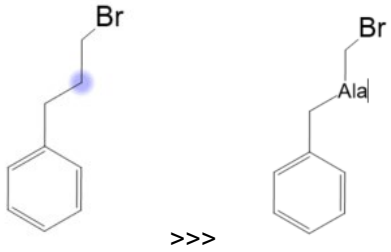
Edit the structure and use atom labels and atom tags

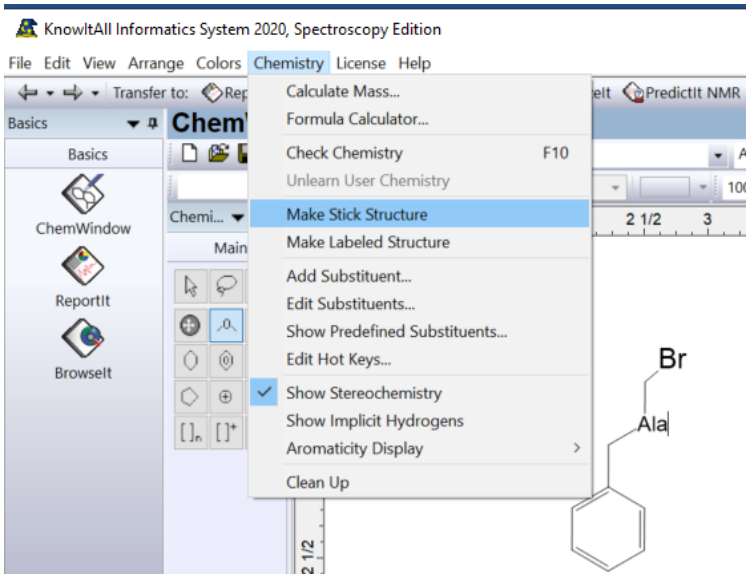
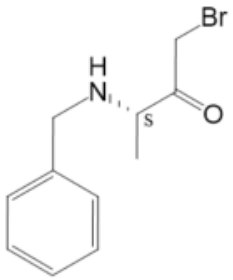
	Action	Result
1	Select the **Eraser** tool  , then click to remove the hydroxyl.	
2	Click to remove amino groups.	
3	Open the **Main** group on the **Drawing Toolbar** and select the **Atom Label** tool  . Then click where the hydroxyl group was located.	

4	Type uppercase **O**. **Note**: Atom labels are case-sensitive.	
5	Move to the other atom and type uppercase NH3. **Note**: Numbers are automatically displayed as subscripts if the **Text Style** toolbar's **Formula** tool CH2 is selected.	
6	Select the **Positive Charge Atom Tag** tool ⊕ to add a positive charge to the atom.	
	TIP	Clicking and dragging a charge allows you more control over the placement of the charge. You can also use the **Lasso** tool to move the charge.

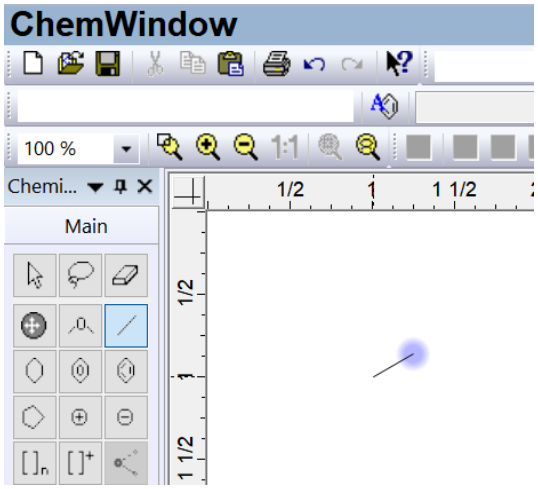
	Action	Result
7	Repeat with the **Negative Charge Atom Tag** tool ⊖ to add a negative charge to the oxygen atom.	
8	Choose **File > Save As** to save the structure with file name **tryptophan2.dsf**.	

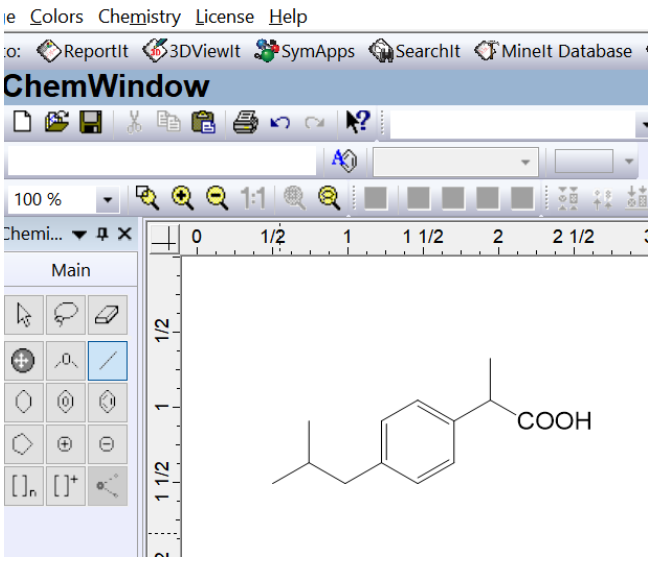
Use pre-defined substituents

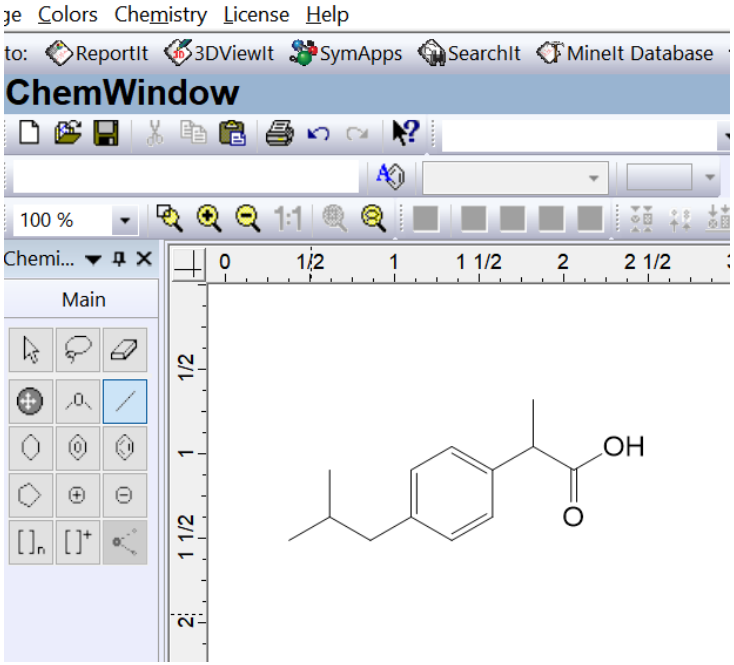
	Action	Result
1	Click on the **Label** tool.	
2	Select an atom and click to type **Ala** (a pre-defined substituent).	

	Action	Result
3	Click **Chemistry** > **Make Stick Structure**.	
4		 The above is the expanded structure.

Use Hotkeys

	Action	Result
1	In the Main toolbox, select the **Standard bond** tool. Click the structure pane to insert the single bond. The end of the bond will be highlighted automatically.	

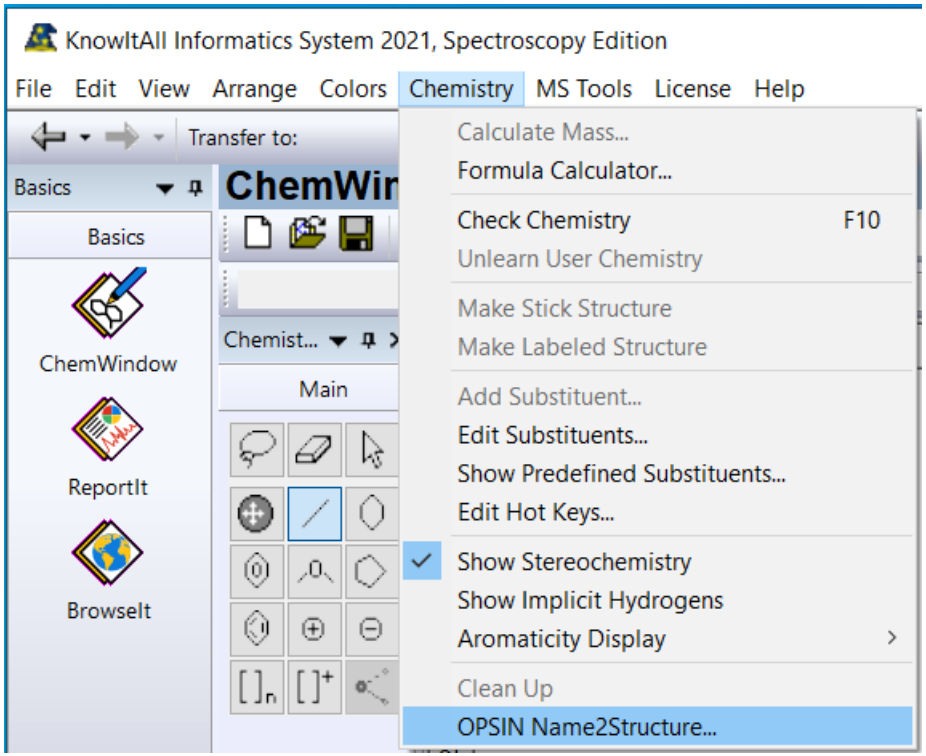
2	Type the following characters on your keyboard: 9, 1, 3, 9, O (Capital letter O).	

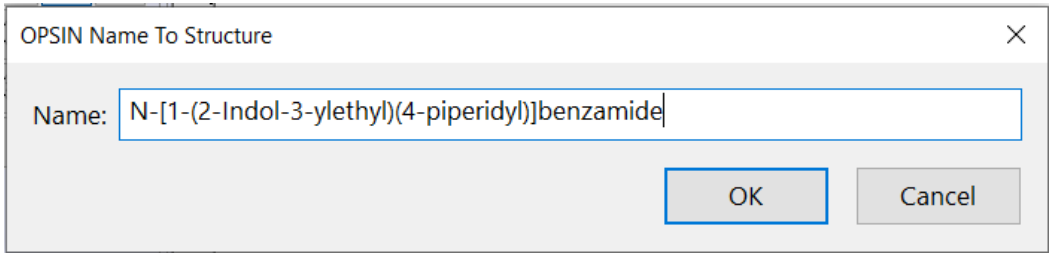
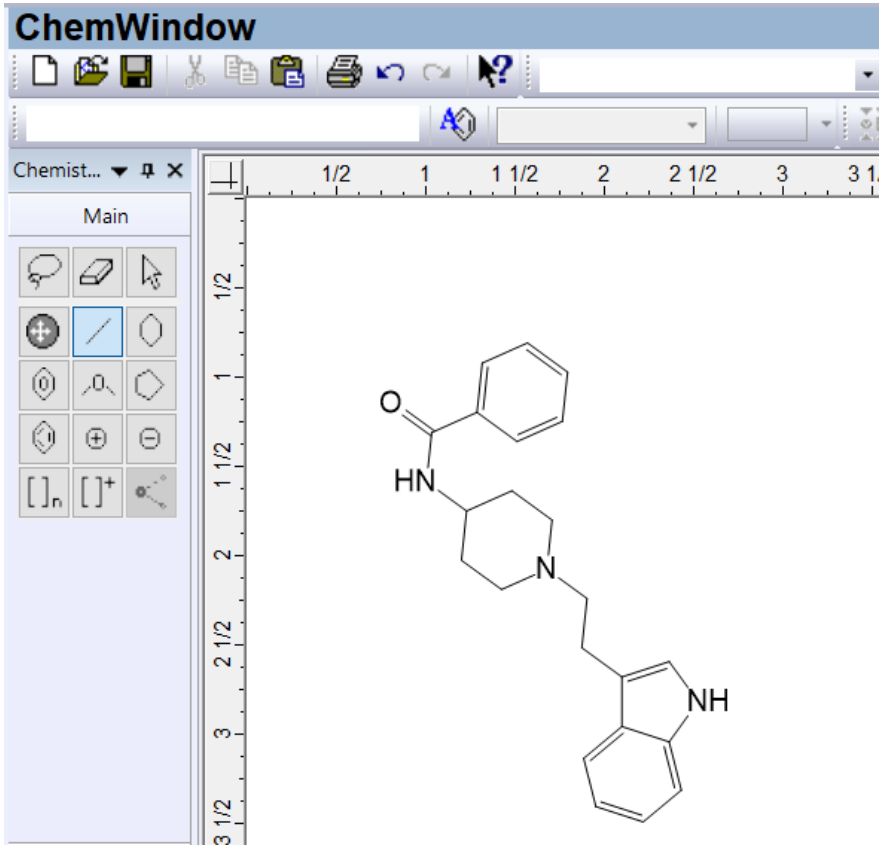
	Action	Result
3	Click **Chemistry** > **Make Stick Structure**.	 The above is the expanded structure.

NOTE: You can copy structures and paste to MS office tools. This capability is discussed further in the next session.

Use OPSIN Name2Structure

Example 1 – chemical name

	Action	Result
1	Navigate to Chemistry > OPSIN Name2Structure.	

2	Enter **N-[1-(2-Indol-3-ylethyl)(4-piperidyl)]benzamide**. Click **OK**.	
3		The resulting structure is displayed. 

Example 2 – common name

You can enter common name in step 2 (above). For example, cholesterol. **ChemWindow** displays it as a structure.

Drawing Reactions

How to Use ChemWindow to Draw Reactions

Purpose

ChemWindow to create reactions and transfer them to MS tools as well as ReportIt application.

Objectives

This exercise will teach you:

- How to draw chemical reactions
- How to work with MS office tools

Background

Scientists can use the KnowItAll's ChemWindow application to create reaction schemes to reports. This capability is useful to anyone communicating the results of laboratory procedures.

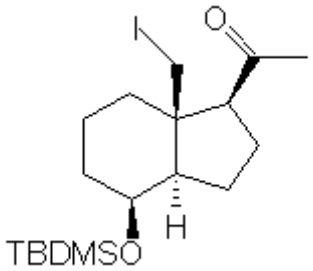
Training Files Used in This Lesson

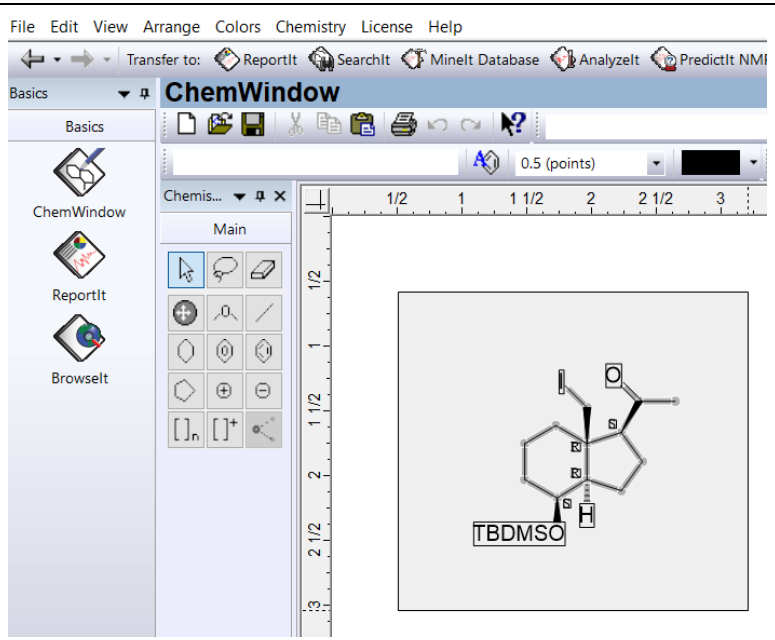
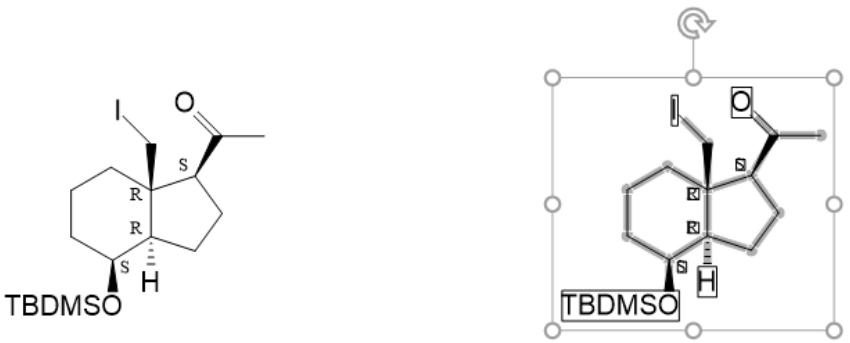
- Structure 1.dsf

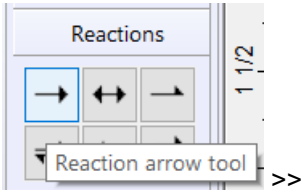
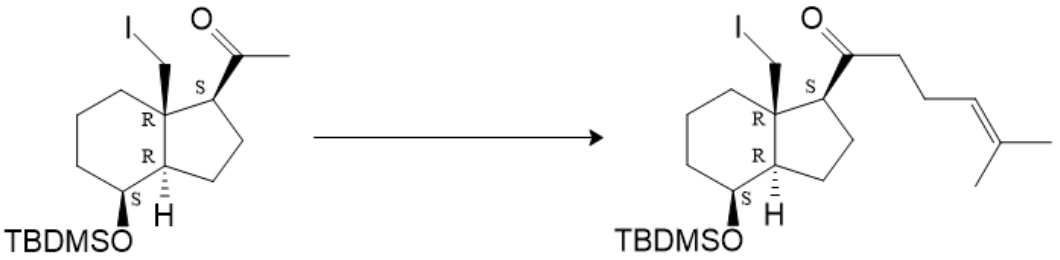
KnowItAll Applications Used

- ChemWindow®

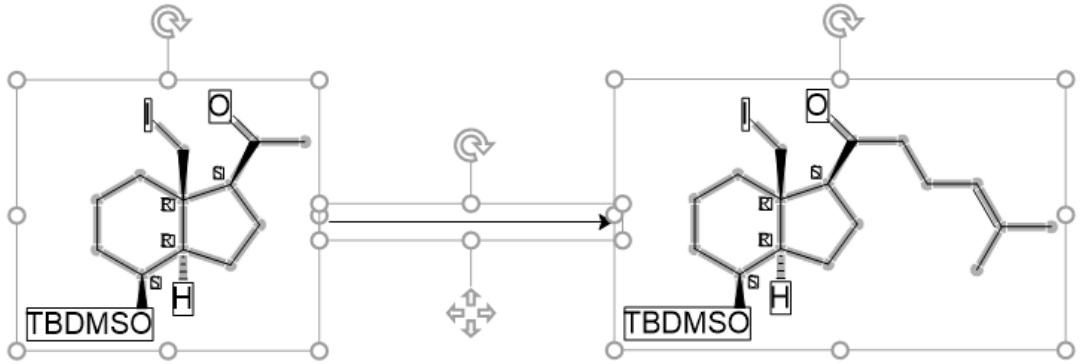
Draw Chemical Reactions

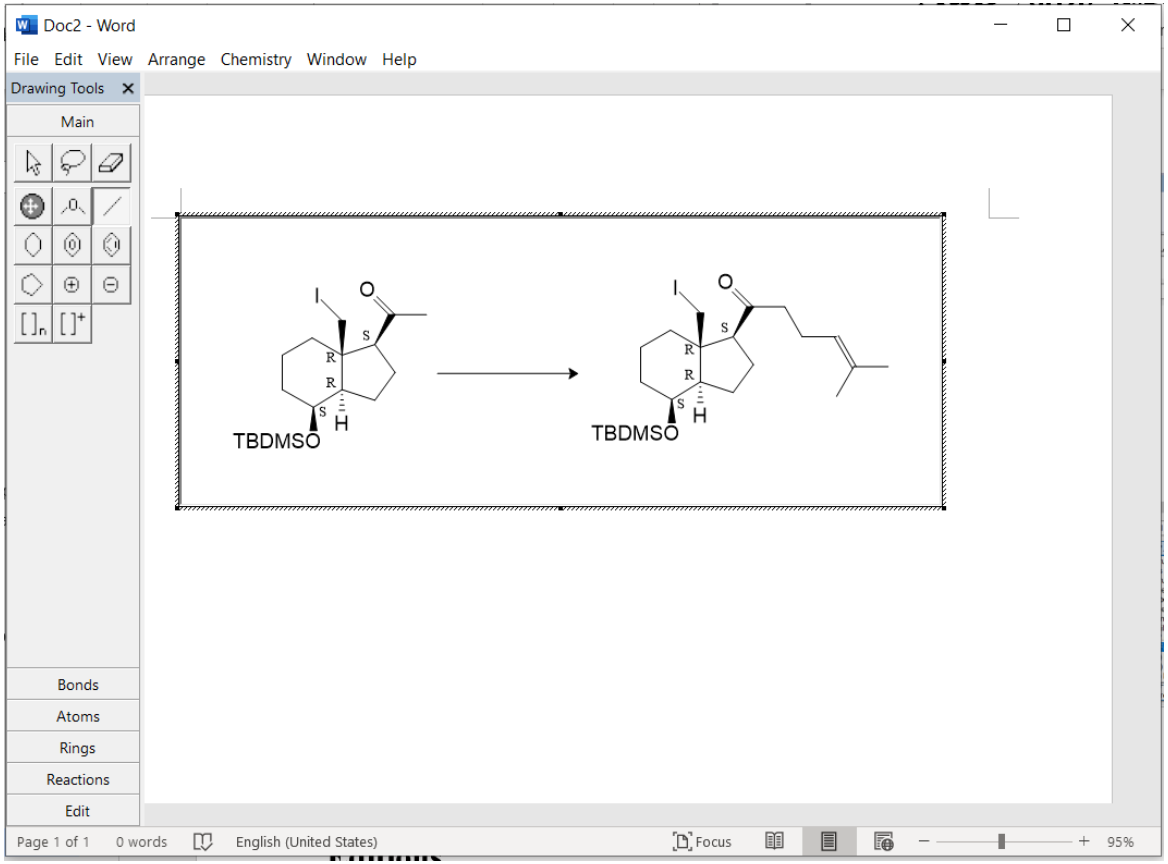
	Action	Result
1	Click the **ChemWindow** icon in the **Basics** toolbox.	The ChemWindow application opens to a blank drawing.
2	Navigate to **File > Open,** then navigate to **KnowItAll Training Files > 8 - Drawing Structures and Reactions**. Select **Structure 1.dsf**. Click **Open**.	The file opens in the workspace. 

3	Select the structure.	
4	Navigate to **Edit > Copy**, then **Edit > Paste**.	

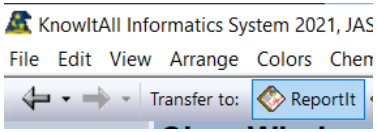
5	In the **Reactions** toolbox, select **Reaction arrow** tool and draw between the two structures.	 >> 
6	Modify the structure on right to be the product.	

OLE connection with MS Office tools

	Action	Result
1	Select the structure object and copy it.	
2	Paste in MS Word. Save the Word document. Close KnowItAll.	

3	Open the MS Word document. Double-click on the KnowItAll object saved.	You can perform ChemWindow actions from here.  **TIP**: You can work with other MS office tools in the same way.

NOTE: For complex text editing with structure and reactions, we recommend you transfer what is in **ChemWindow** to the **ReportIt** application. You can do this by using the **Transfer to: ReportIt** function.



Mass Spectrometry Tools

How to Use the Mass Spectrometry Tools in ChemWindow

Purpose

This exercise demonstrates how to use tools specially made for Mass Spectrometry.

Objectives

This exercise will teach you:

- How to calculate Isotopic Distribution for a structure
- How to calculate elemental composition
- How to use the MS fragmentation tool

Background

Scientists can use the KnowItAll's ChemWindow application to add reaction schemes to reports. This capability is useful to anyone communicating the results of laboratory procedures.

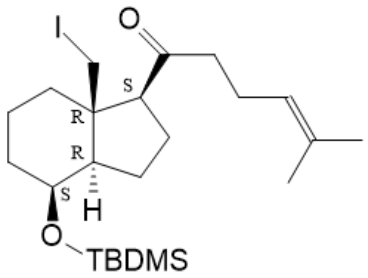
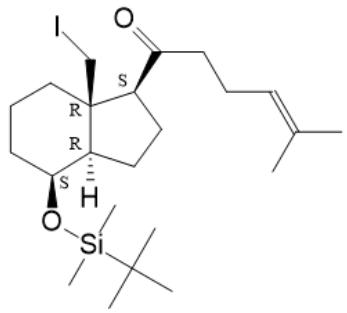
Training Files Used in This Lesson

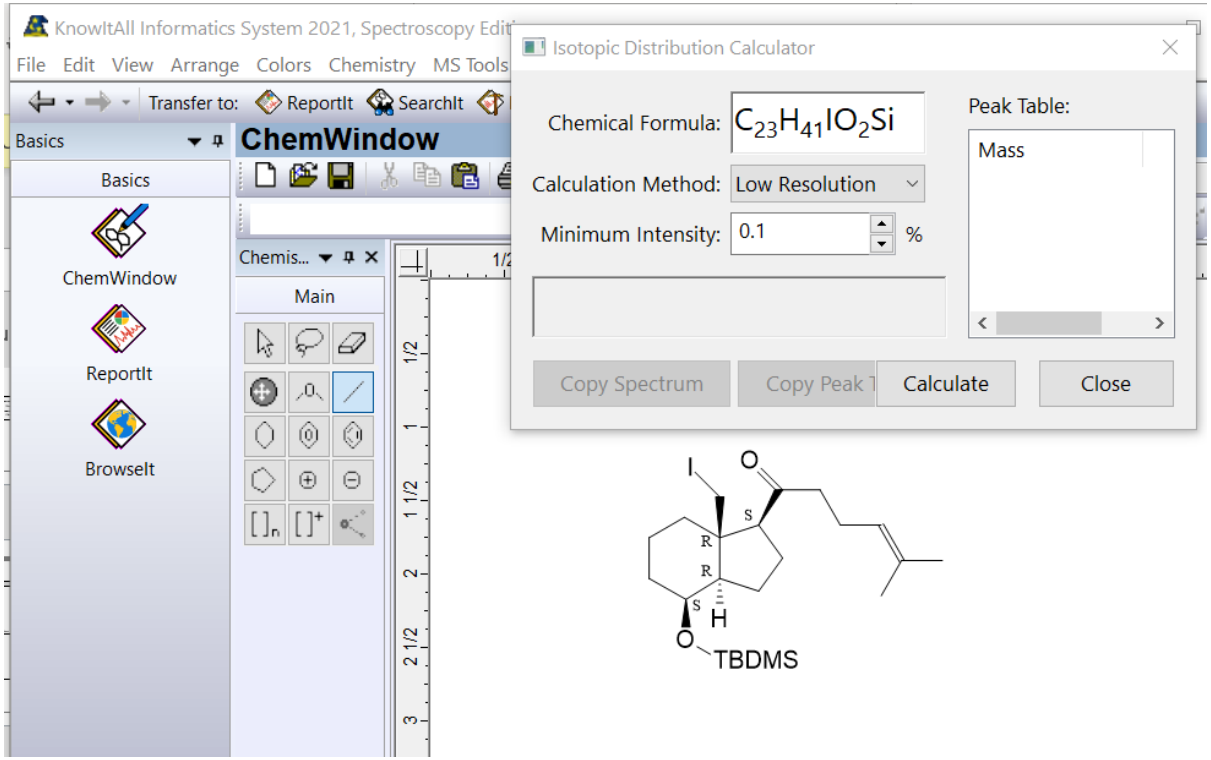
- Structure 2.dsf

KnowItAll Applications Used

- ChemWindow®

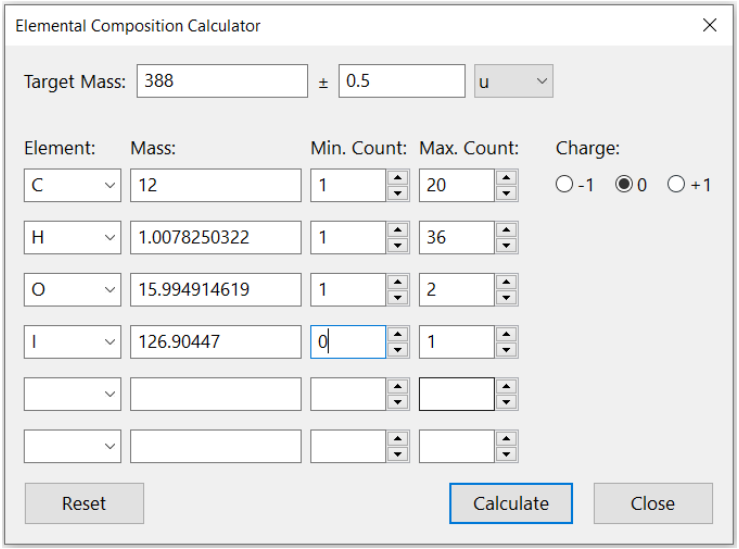
Isotopic Distribution

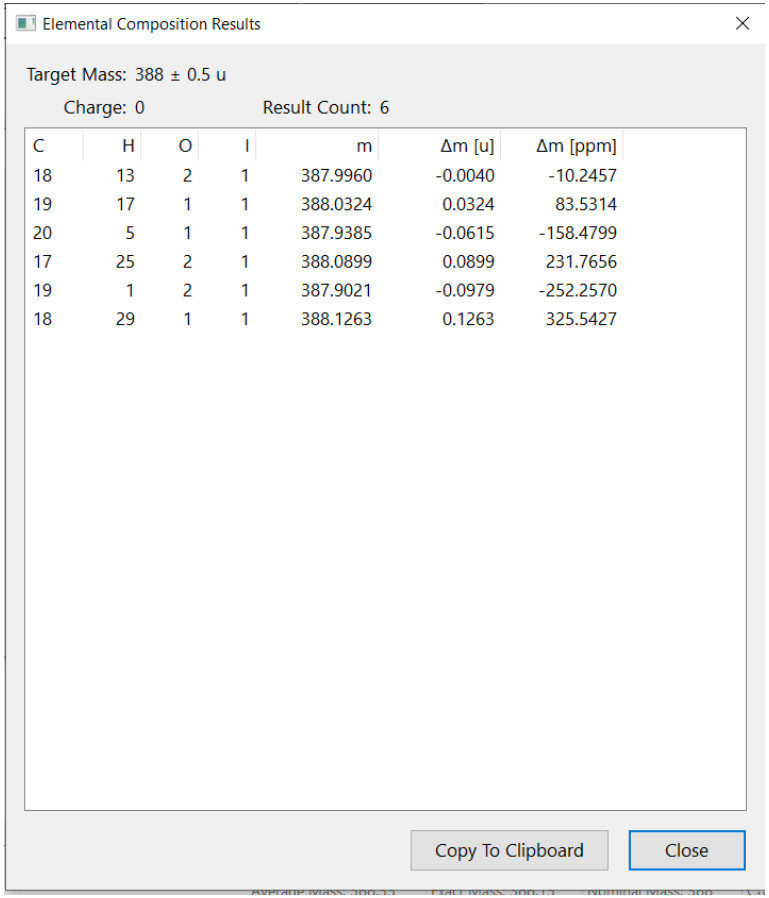
	Action	Result
1	Navigate to **File > Open,** then navigate to **KnowItAll Training Files > 8 - Drawing Structures and Reactions**. Select **Structure 2.dsf**. Click **Open**.	 You can calculate Isotopic Distributions for a database record structure.
2	Navigate to **Chemistry > Make Stick Structure**.	

3	Navigate to **MS Tools > Calculate Isotopic Distribution**. In the pop-up window, click **Calculate**.	
4	Open the MS Word document. Double-click on the KnowItAll object saved.	

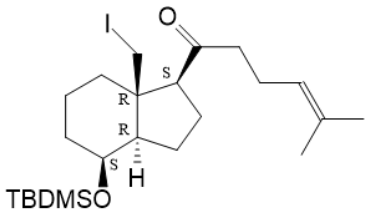
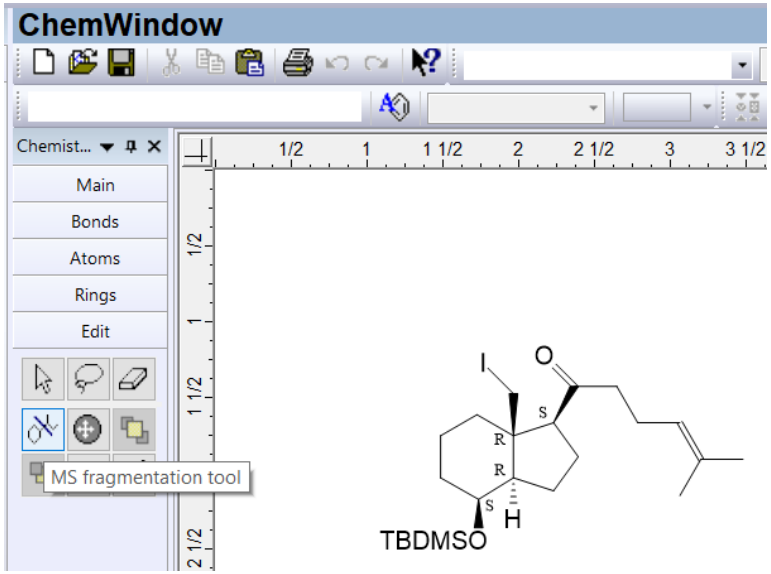
Isotopic Elemental Composition

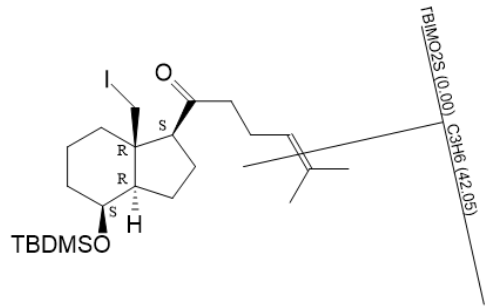
This tool is not associated with a database record structure.

	Action	Results
1	Navigate to **MS Tools > Calculate Elemental Composition**.	This dialog shows up. 

2	Fill in elements and occurrences and click **Calculate**.	Combinations of elements are displayed. 

MS Fragmentation

	Action	Result
1	Navigate to **File > Open.** Then navigate to **KnowItAll Training Files > 8 - Drawing Structures and Reactions**. Select **Structure 2.dsf**. Click **Open**.	 You can calculate Isotopic Distributions for a database record structure.
2	In the **Edit** toolbox**,** select the **MS fragmentation tool**.	

3		 You can clip the structure into two fragments.