

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
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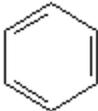
Background

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	<p>If desired, use tools on the zoom toolbar to change the magnification.</p> <p>Note: Choose View > Zoom Toolbar to toggle the toolbar display.</p>  <p>The ctrl + scroll function can also be used to zoom in and out quickly.</p>	

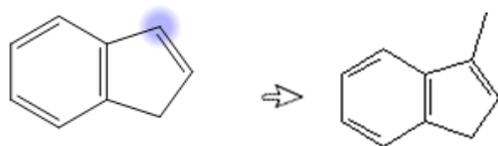
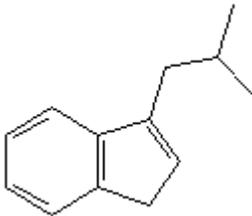
5

Use the **Selection** tool  to select the structure and move it within the workspace.

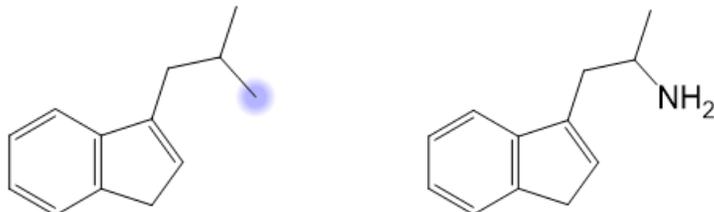
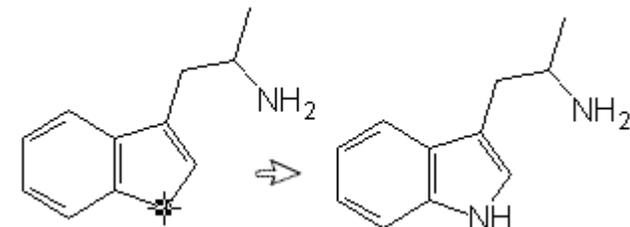
Graphic handles appear when the structure is selected.

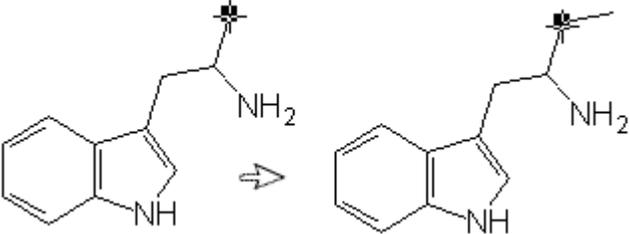
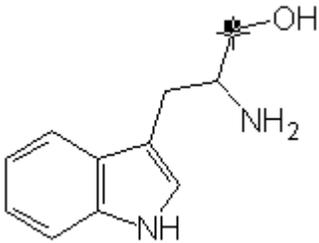
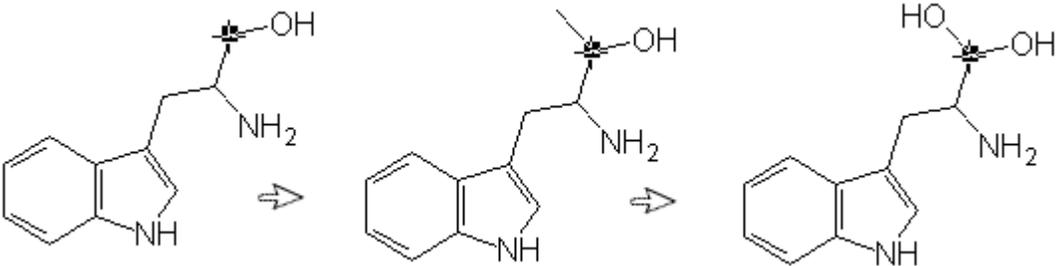


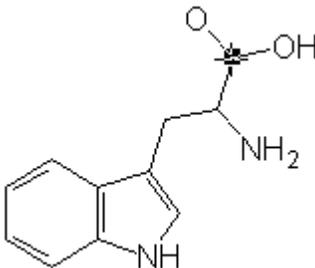
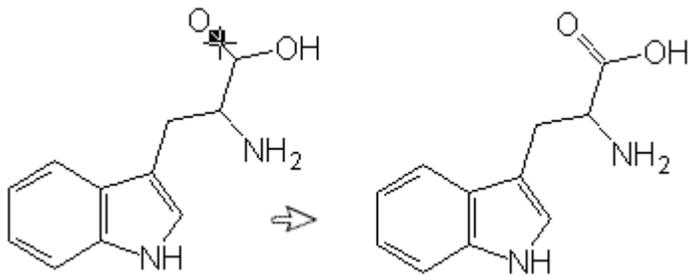
Add features to the structure

	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.	

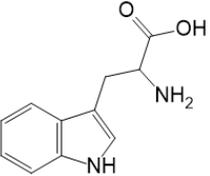
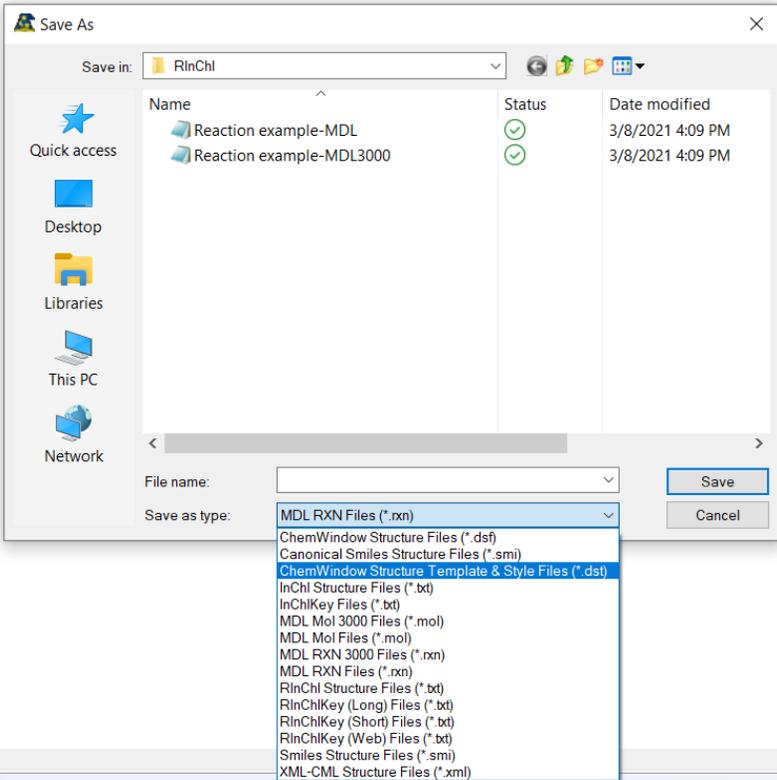
Use hot keys to add nitrogen and oxygen atoms

	Action	Result
1	Move the cursor over the terminal carbon. Then press n on your keyboard.	<p>NH₂ appears at the end of the bond.</p>  <p>Note: Numbers are automatically displayed as subscripts when using hot keys, which are shortcut keys you can use to quickly label atoms.</p> <p>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.</p>
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.	 <p>The diagram shows two stages of a chemical structure. On the left is a tryptophan molecule (indole ring with a 2-aminoethyl side chain). A cursor is positioned over the terminal carbon atom of the side chain. An arrow points to the right, where the same molecule is shown but with an additional single bond extending from the terminal carbon atom.</p>
4	Without moving the cursor, press o on your keyboard.	 <p>The diagram shows the tryptophan molecule from the previous step. The cursor remains over the terminal carbon atom. An arrow points to the right, where the terminal carbon atom is now bonded to a hydroxyl group (-OH) in addition to the existing bonds.</p>
5	Click to sprout another single bond. Then press o on the keyboard to add a hydroxyl group.	 <p>The diagram shows three stages of the molecule's modification. The first stage is the tryptophan molecule with one hydroxyl group. An arrow points to the second stage, where a cursor is over the terminal carbon atom and a new single bond is being added. A second arrow points to the final stage, where the terminal carbon atom is bonded to two hydroxyl groups (-OH).</p>

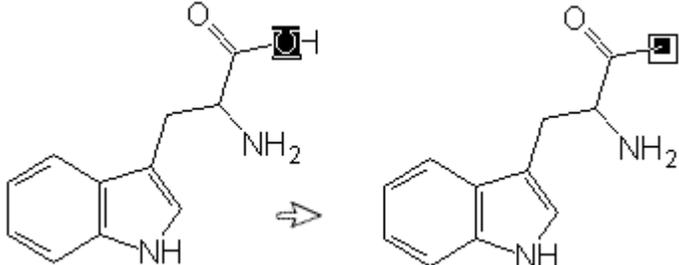
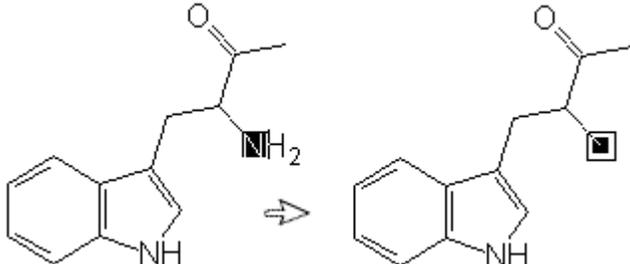
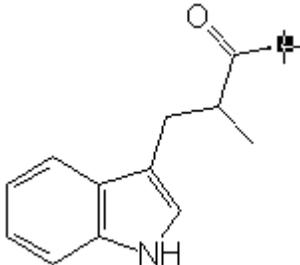
6	<p>Press o again to remove the hydrogen.</p> <p>Note: When using a hot key, you can change the number of hydrogens attached to the atom by pressing the hot key repeatedly.</p>	 <p>The diagram shows the chemical structure of tryptophan. A small black square with a white crosshair (a hit box) is placed over the C-H bond of the hydroxyl group (-OH) attached to the alpha carbon. The rest of the molecule, including the indole ring and the amino group (-NH₂), is shown in a standard skeletal representation.</p>
7	<p>Move the cursor to the hit box on the bond. Then click to create a double bond.</p>	 <p>The diagram illustrates the transformation of the tryptophan structure. On the left, the structure is identical to the one in step 6, with a hit box on the C-H bond of the hydroxyl group. An arrow points to the right, where the resulting structure is shown. In this structure, the C-H bond has been replaced by a C=O double bond, and the hydrogen atom has been removed, forming a carboxylic acid group (-COOH).</p>

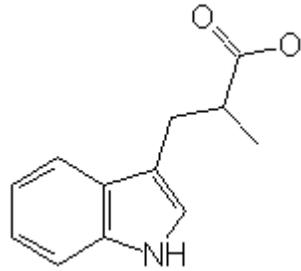
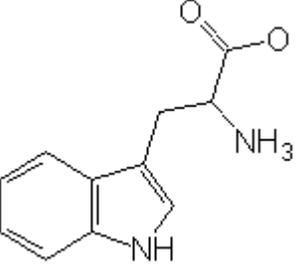
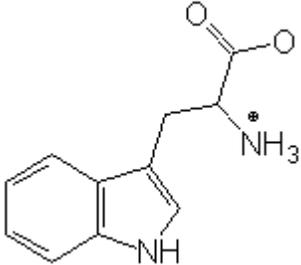
Save the structure

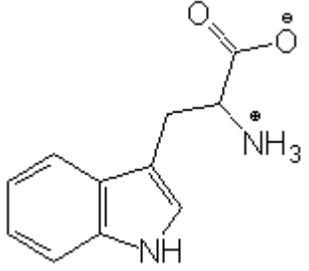
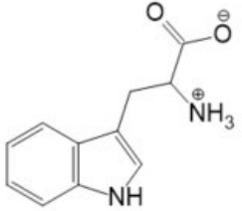
	Action	Result
1	<p>Choose File > Save.</p> <p>Note: You can also click the Save button on the toolbar or press Ctrl+S.</p>	<p>The Save As dialog box opens. The default file type (ChemWindow structure file, *.dsf) is already selected, and will be used for this structure. Other file types include ChemWindow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

3	Click Save .	The structure is saved, and the file name is displayed on the drawing tab.
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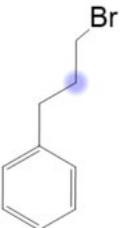
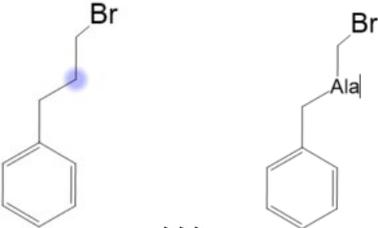
Edit the structure and use atom labels and atom tags

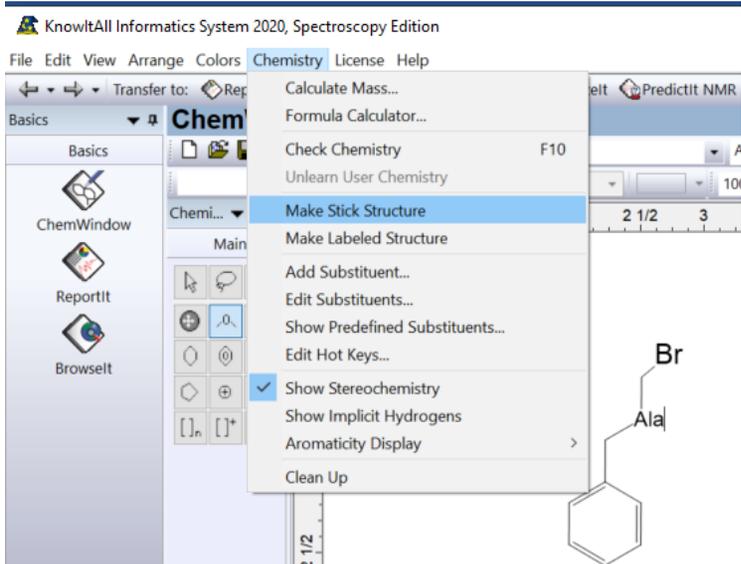
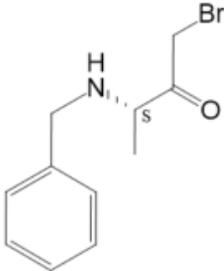
	Action	Result
1	Select the Eraser tool  , then click to remove the hydroxyl.	
2	Click to remove amino groups.	
3	Open the Main group on the Drawing Toolbar and select the Atom Label tool  . Then click where the hydroxyl group was located.	

4	<p>Type uppercase O.</p> <p>Note: Atom labels are case-sensitive.</p>	 <p>The structure shows a tryptophan molecule where the carboxyl group is drawn as a carboxylate ion (COO-). The nitrogen atom of the amino group is labeled 'NH'.</p>
5	<p>Move to the other atom and type uppercase NH3.</p> <p>Note: Numbers are automatically displayed as subscripts if the Text Style toolbar's Formula tool  is selected.</p>	 <p>The structure is identical to the previous one, but the amino group is now labeled 'NH3'.</p>
6	<p>Select the Positive Charge Atom Tag tool  to add a positive charge to the atom.</p>	 <p>The structure is identical to the previous one, but a positive charge symbol (⊕) is placed above the nitrogen atom, which is now labeled 'NH3'.</p>
	<p>TIP</p>	<p>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.</p>

	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 .	
9	Click the "x" at the bottom tab to close this drawing Click No at saving file prompt This would start a new blank ChemWindow screen.	 

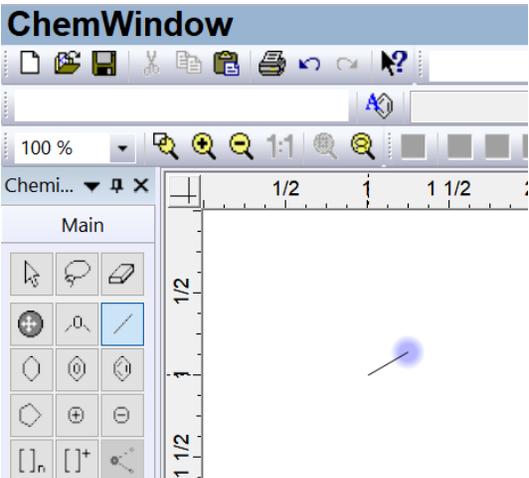
Use pre-defined substituents

	Action	Result
1	Draw the structure shown:	
2	<p>Label the atom highlighted with the text Ala using either:</p> <ul style="list-style-type: none">a) the Label tool  under the Main group orb) by clicking enter with the atom highlighted. <p>Note: Ala is a pre-defined substituent.</p>	

	Action	Result
3	Click Chemistry > Make Stick Structure .	 <p>KnowItAll Informatics System 2020, Spectroscopy Edition</p> <p>File Edit View Arrange Colors Chemistry License Help</p> <p>Transfer to: Reg</p> <p>Basics ChemWindow Reportit Browseit</p> <p>Chemistry menu options:</p> <ul style="list-style-type: none">Calculate Mass...Formula Calculator...Check Chemistry F10Unlearn User ChemistryMake Stick StructureMake Labeled StructureAdd Substituent...Edit Substituents...Show Predefined Substituents...Edit Hot Keys...<input checked="" type="checkbox"/> Show StereochemistryShow Implicit HydrogensAromaticity DisplayClean Up <p>Structure shown: <chem>BrCCc1ccccc1</chem></p>
4	Note: A table showing all predefined substituents can be viewed by selecting Chemistry > Show Predefined Substituents .	 <p>The above is the expanded structure.</p>

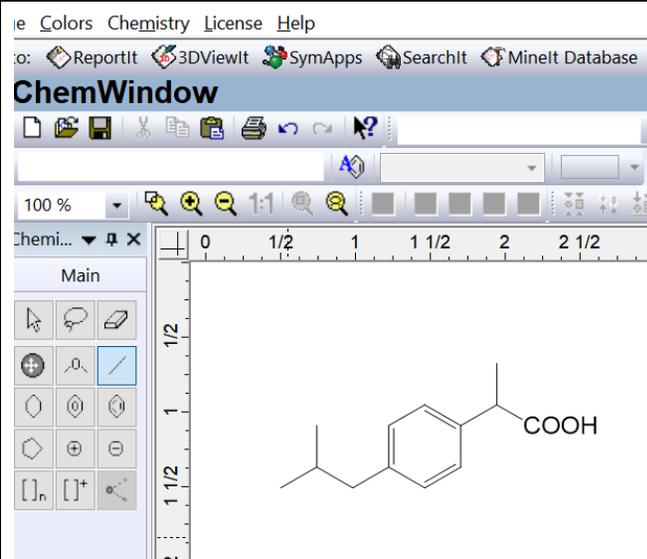
5	<p>Click the "x" at the bottom tab to close this drawing.</p> <p>Click No at saving file prompt.</p> <p>This would start a new blank ChemWindow screen.</p>	
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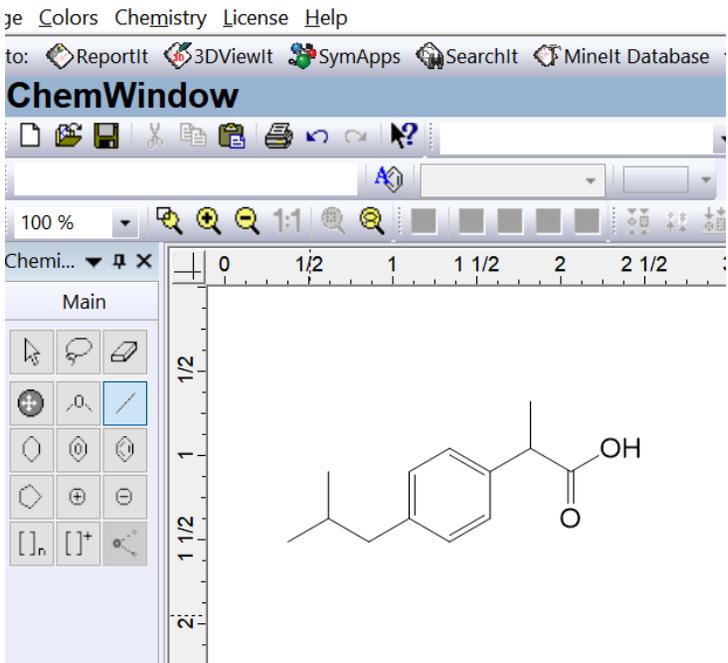
Use Hotkeys

	Action	Result
1	<p>In the Main toolbox, select the Standard bond tool.</p> <p>Click the structure pane to insert the single bond. The end of the bond will be highlighted automatically.</p>	 <p>The screenshot shows the ChemWindow interface. At the top is a menu bar with icons for file operations. Below it is a toolbar with various drawing tools. A 'Main' toolbox is visible on the left, containing icons for selection, erasing, and drawing bonds. The 'Standard bond' tool is highlighted. The main workspace shows a single bond being drawn, with a blue highlight at its end. A ruler is visible at the bottom of the workspace.</p>

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

(Note that hot keys involving capital letters use shift + letter, not caps lock + letter.)

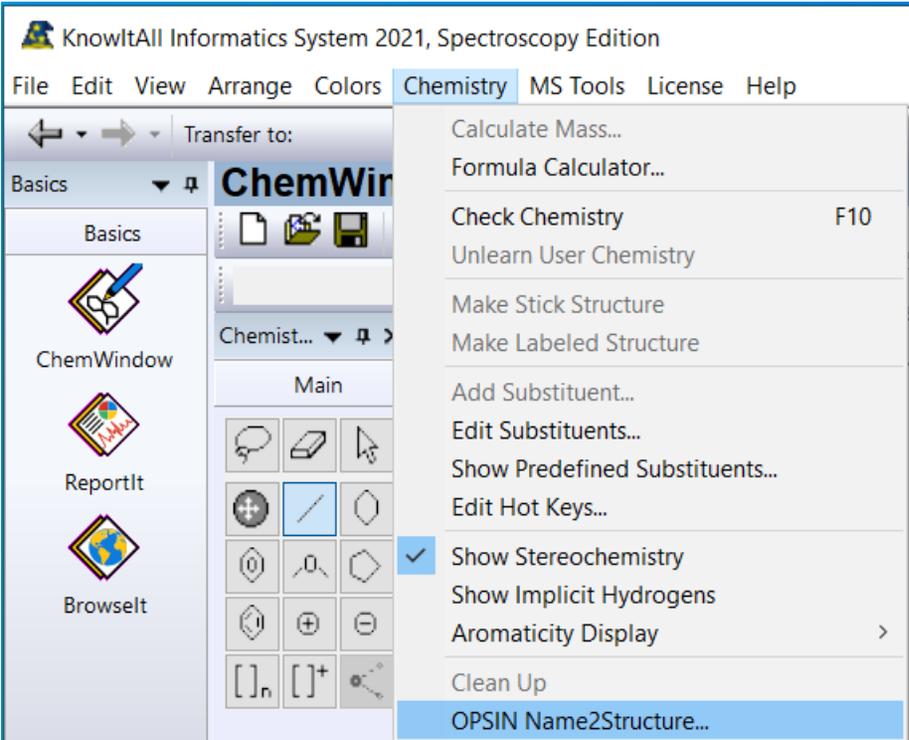


	Action	Result
3	Click Chemistry > Make Stick Structure .	 <p>The above is the expanded structure.</p>
4	Click the "x" at the bottom tab to close this drawing. Click No at saving file prompt. This would start a new blank ChemWindow screen.	

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 .	 <p>The screenshot shows the ChemWin software interface. The menu bar includes File, Edit, View, Arrange, Colors, Chemistry, MS Tools, License, and Help. The 'Chemistry' menu is open, displaying a list of options: Calculate Mass..., Formula Calculator..., Check Chemistry (F10), Unlearn User Chemistry, Make Stick Structure, Make Labeled Structure, Add Substituent..., Edit Substituents..., Show Predefined Substituents..., Edit Hot Keys..., Show Stereochemistry (checked), Show Implicit Hydrogens, Aromaticity Display (with a right arrow), Clean Up, and OPSIN Name2Structure... (highlighted in blue). The left sidebar shows icons for ChemWindow, ReportIt, and Browselt. The main workspace contains a grid of drawing tools.</p>

2	<p>Enter N-[1-(2-Indol-3-ylethyl)(4-piperidyl)]benzamide. Click OK.</p> <div data-bbox="697 272 1734 521"><p>OPSPIN Name To Structure X</p><p>Name: <input type="text" value="N-[1-(2-Indol-3-ylethyl)(4-piperidyl)]benzamide"/></p><p style="text-align: right;"><input type="button" value="OK"/> <input type="button" value="Cancel"/></p></div>
3	<p>The resulting structure is displayed.</p> <div data-bbox="697 573 1566 1409"><p>ChemWindow</p><p>Chemist... X</p><p>Main</p><p>The image shows the ChemWindow interface with the chemical structure of N-[1-(2-Indol-3-ylethyl)(4-piperidyl)]benzamide. The structure consists of a benzamide group (a benzene ring attached to a carbonyl group, which is attached to an NH group) connected to a piperidine ring. The piperidine ring is further connected via a two-carbon chain to the 1-position of an indole ring.</p></div>

4	Click the "x" at the bottom tab to close this drawing Click No at saving file prompt This would start a new blank ChemWindow screen.	
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Example 2 – common name

Repeat steps 1 – 4, now entering a common name such as 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
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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

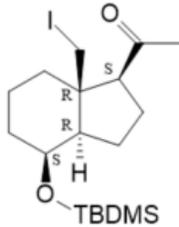
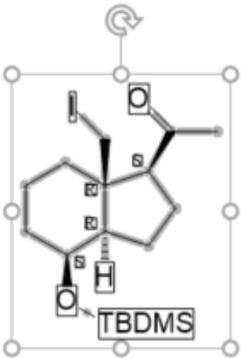
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions

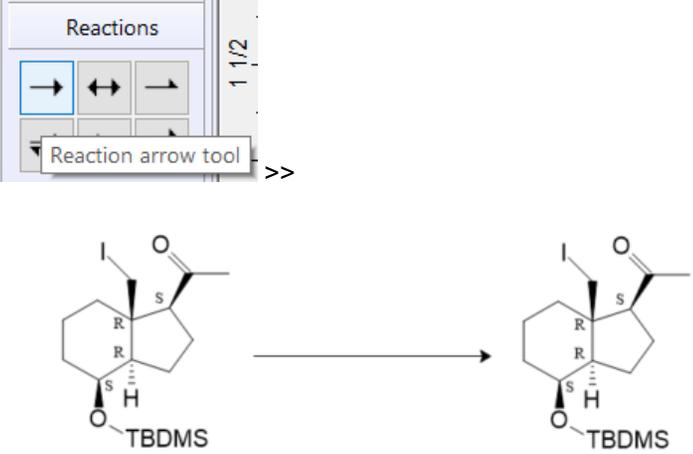
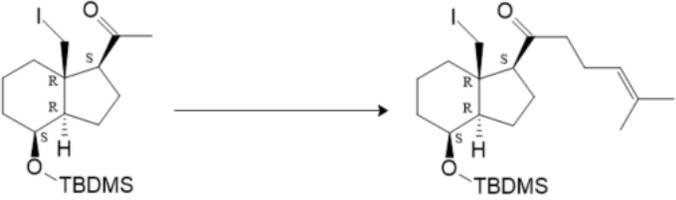
- Reactant.dsf

KnowItAll Applications Used

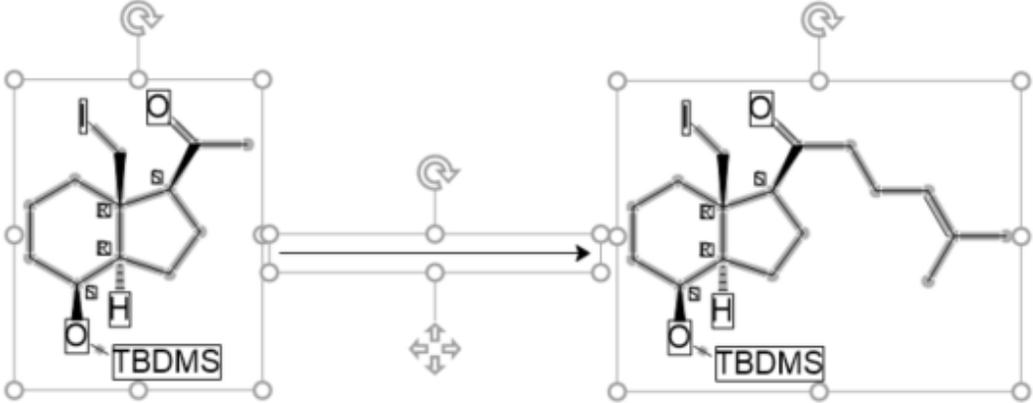
- ChemWindow®

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 C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions . Select Reactant.dsf . Click Open .	The file opens in the workspace. 
3	Select the structure.	

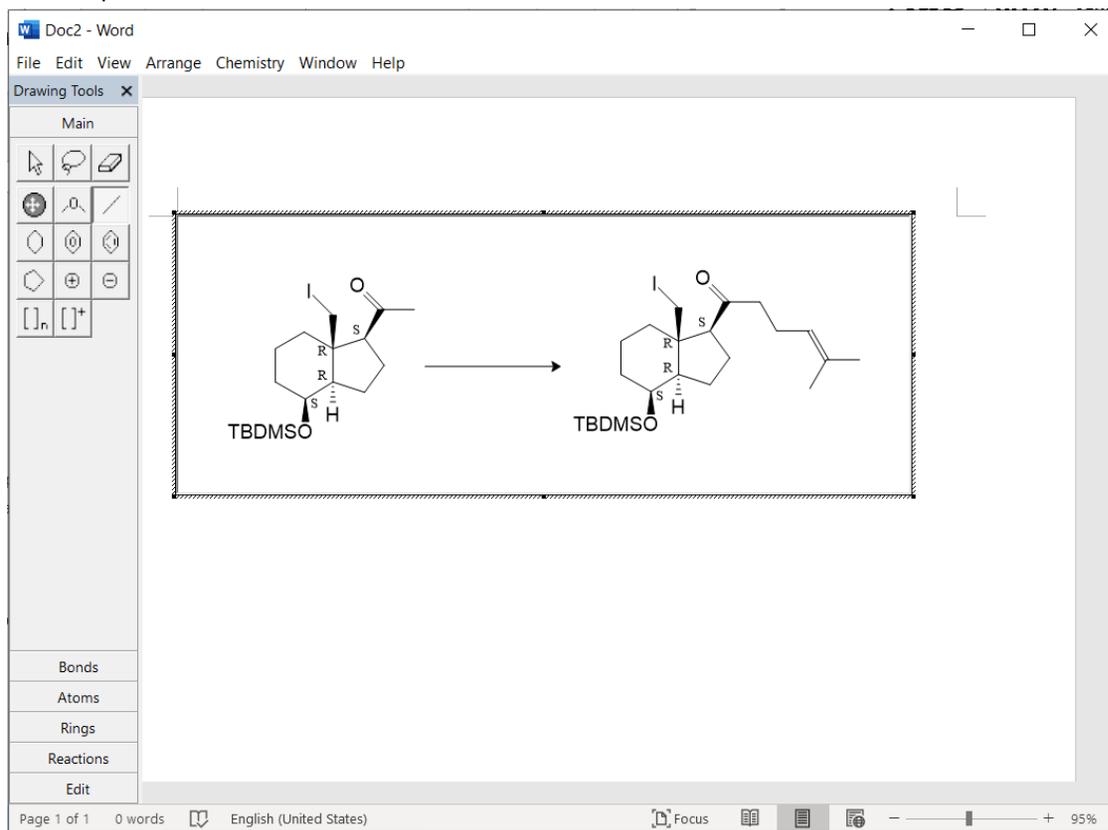
4	Navigate to Edit > Copy , then Edit > Paste .	
5	In the Reactions toolbox, select Reaction arrow tool and draw between the two structures.	
6	Modify the structure on right to be the product.	

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.	

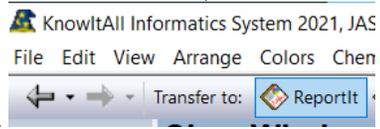
3 In the MS Word document, double-click on the KnowItAll object saved.

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.

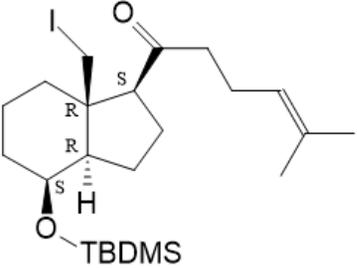
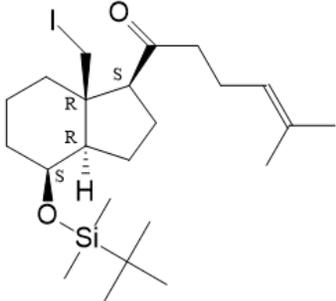
Training Files Used in This Lesson

- Structure 2.dsf

KnowItAll Applications Used

- ChemWindow®

Isotopic Distribution

	Action	Result
1	<p>Navigate to File > Open, then navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions folder.</p> <p>Select Product.dsf.</p> <p>Click Open.</p>	 <p>The chemical structure shows a bicyclic system consisting of a six-membered ring fused to a five-membered ring. The six-membered ring has an iodine atom (I) attached with a wedge bond and a carbonyl group (C=O) attached with a wedge bond. The five-membered ring has a hydrogen atom (H) attached with a dashed bond and a TBDMS group (tert-butyldimethylsilyloxy) attached with a wedge bond. A side chain is attached to the carbonyl group, consisting of a propyl chain ending in a terminal alkene with a methyl substituent.</p> <p>You can calculate Isotopic Distributions for a database record structure.</p>
2	<p>Navigate to Chemistry > Make Stick Structure.</p>	 <p>The stick structure is a simplified representation of the same bicyclic compound shown in the previous row, using lines to represent bonds and atoms. It includes the iodine atom, carbonyl group, TBDMS group, and the side chain.</p>

3 Navigate to **MS Tools > Calculate Isotopic Distribution**.

In the pop-up window, click **Calculate**.

KnowItAll Informatics System 2021, Spectroscopy Editor

ChemWindow

Isotopic Distribution Calculator

Chemical Formula: $C_{23}H_{41}IO_2Si$

Calculation Method: Low Resolution

Minimum Intensity: 0.1 %

Peak Table:

Mass	Intensity
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Copy Spectrum Copy Peak Table Calculate Close

TBDMS

4

Isotopic Distribution Calculator

Chemical Formula: $C_{23}H_{41}IO_2Si$

Calculation Method: Low Resolution

Minimum Intensity: 0.1 %

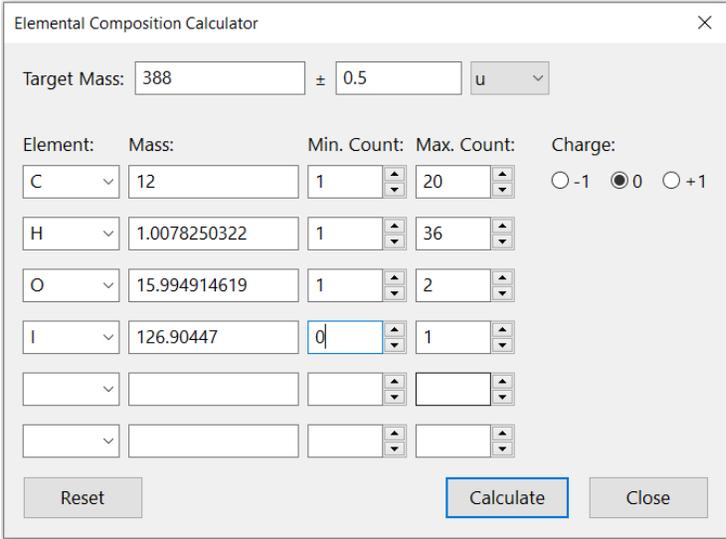
Peak Table:

Mass	Intensity
504	100.0000
505	29.9539
506	7.9809
507	1.3092

Copy Spectrum Copy Peak Table Calculate Close

Isotopic Elemental Composition

This tool is not associated with a database record structure.

	Action	Results																																			
1	Navigate to MS Tools > Calculate Elemental Composition .	<p>This dialog shows up.</p>  <p>Elemental Composition Calculator</p> <p>Target Mass: 388 ± 0.5 u</p> <table border="1"><thead><tr><th>Element</th><th>Mass</th><th>Min. Count</th><th>Max. Count</th><th>Charge</th></tr></thead><tbody><tr><td>C</td><td>12</td><td>1</td><td>20</td><td><input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1</td></tr><tr><td>H</td><td>1.0078250322</td><td>1</td><td>36</td><td><input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1</td></tr><tr><td>O</td><td>15.994914619</td><td>1</td><td>2</td><td><input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1</td></tr><tr><td>I</td><td>126.90447</td><td>0</td><td>1</td><td><input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1</td></tr><tr><td></td><td></td><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td><td></td><td></td></tr></tbody></table> <p>Reset Calculate Close</p>	Element	Mass	Min. Count	Max. Count	Charge	C	12	1	20	<input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1	H	1.0078250322	1	36	<input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1	O	15.994914619	1	2	<input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1	I	126.90447	0	1	<input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1										
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H	1.0078250322	1	36	<input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1																																	
O	15.994914619	1	2	<input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1																																	
I	126.90447	0	1	<input type="radio"/> -1 <input checked="" type="radio"/> 0 <input type="radio"/> +1																																	

2 Fill in elements and occurrences and click **Calculate**.

Combinations of elements are displayed.

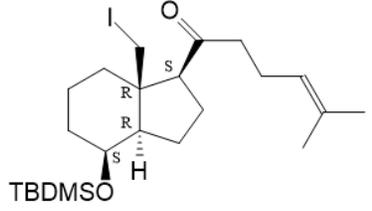
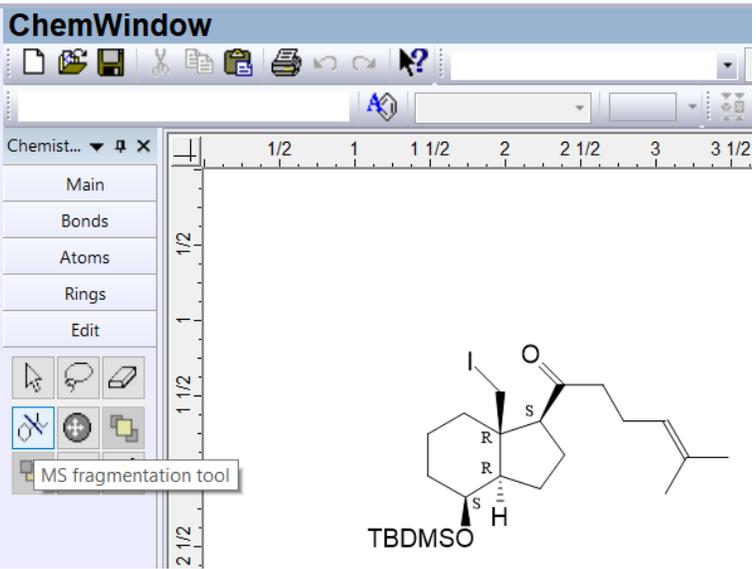
Elemental Composition Results

Target Mass: 388 ± 0.5 u
Charge: 0 Result Count: 6

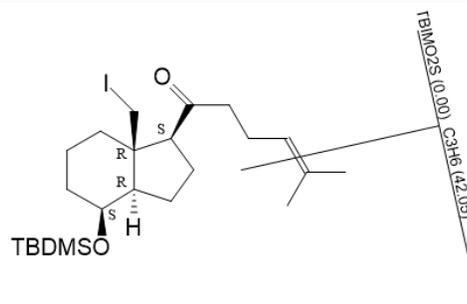
C	H	O	I	m	Δm [u]	Δm [ppm]
18	13	2	1	387.9960	-0.0040	-10.2457
19	17	1	1	388.0324	0.0324	83.5314
20	5	1	1	387.9385	-0.0615	-158.4799
17	25	2	1	388.0899	0.0899	231.7656
19	1	2	1	387.9021	-0.0979	-252.2570
18	29	1	1	388.1263	0.1263	325.5427

Copy To Clipboard Close

MS Fragmentation

	Action	Result
1	<p>Navigate to File > Open. Then navigate to C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions folder.</p> <p>Select Product.dsf.</p> <p>Click Open.</p>	 <p>You can calculate Isotopic Distributions for a database record structure.</p>
2	<p>In the Edit toolbox, select the MS fragmentation tool.</p>	 <p>The screenshot shows the ChemWindow interface with the 'MS fragmentation tool' highlighted in the 'Edit' toolbox. The main window displays the same chemical structure as in the previous step.</p>

3



You can clip the structure into two fragments.