

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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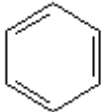

Background

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

KnowItAll Applications Used

- ChemWindow®

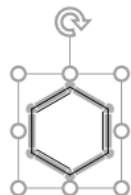
Begin a new structure drawing

	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>	



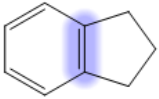



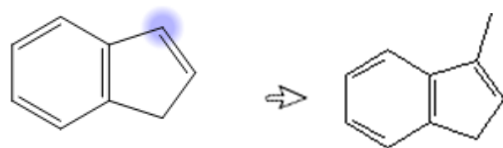
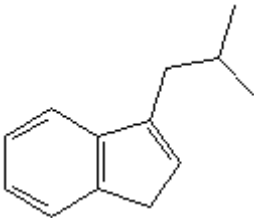
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Use the **Selection** tool  to select the structure and move it within the workspace.

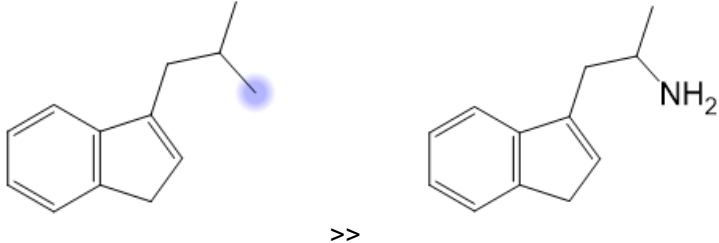
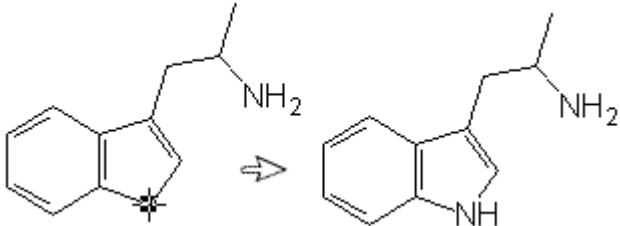
Graphic handles appear when the structure is selected.

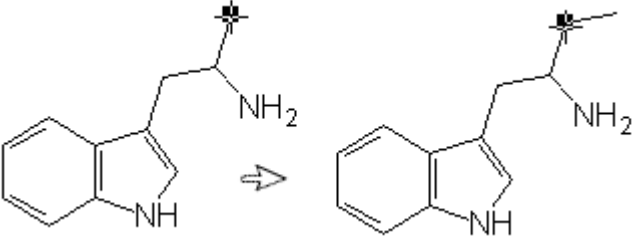
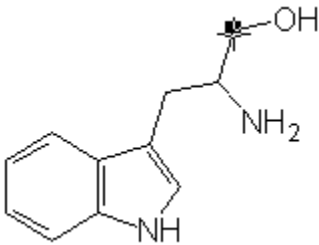
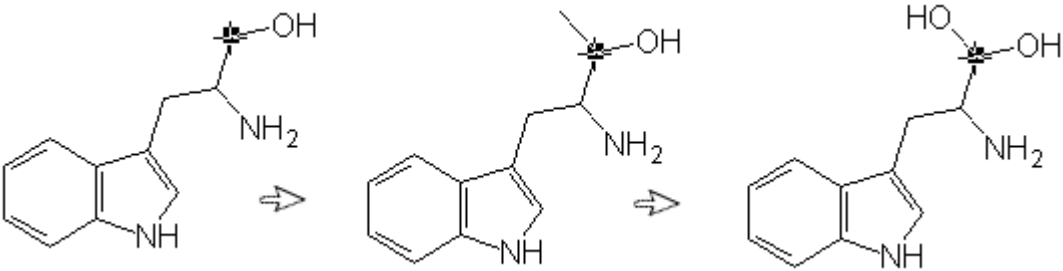


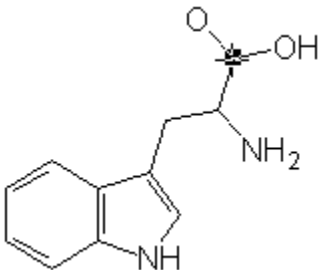
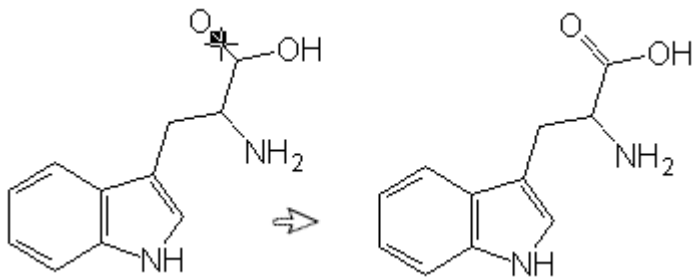
Add features to the structure

	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.	

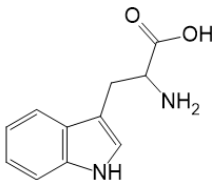
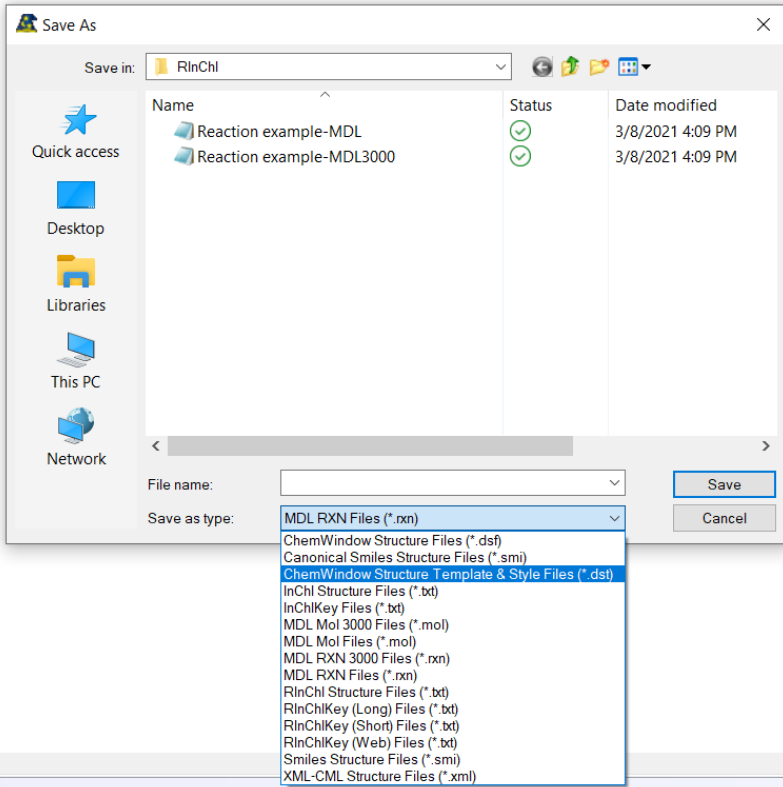
Use hot keys to add nitrogen and oxygen atoms

	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, a tryptophan molecule (indole ring with a 2-aminoethyl side chain) has a cursor (a small black square with a crosshair) 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 on the terminal carbon atom. An arrow points to the right, where the terminal carbon atom is now bonded to both a hydroxyl group (-OH) and the previously added single bond.</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 construction. The first stage is the tryptophan molecule with the cursor on the terminal carbon. An arrow points to the second stage, where a second single bond has been added to the terminal carbon. A second arrow points to the final stage, where the terminal carbon atom is bonded to two hydroxyl groups (-OH).</p>


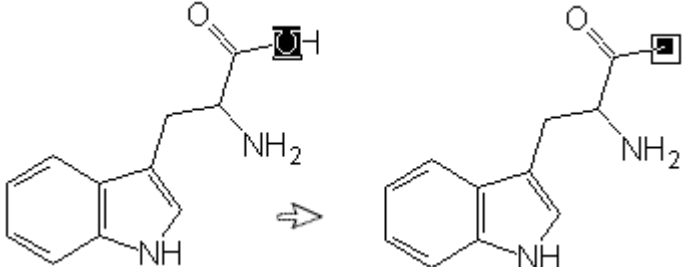
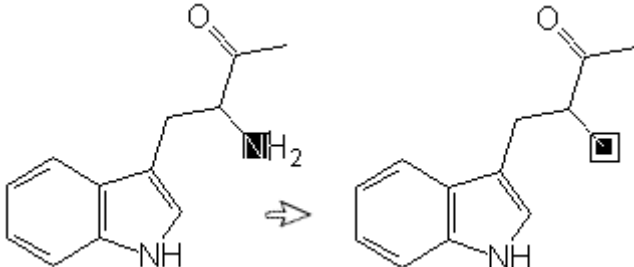

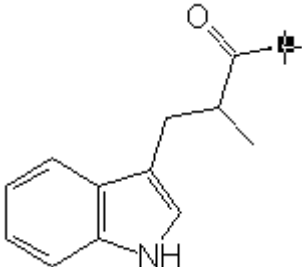
6	<p>Press o again to remove the hydrogen.</p> <p>Note: When using a hot key, you can change the number of hydrogens attached to the atom by pressing the hot key repeatedly.</p>	 <p>The diagram shows the chemical structure of tryptophan. A small square hit box is placed over the C-H bond of the hydroxyl group (-OH) on the side chain. The side chain is attached to the 3-position of the indole ring.</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 hydroxyl group (-OH) has a hit box on its C-H bond. An arrow points to the right, where the structure is shown with a double bond between the carbon and oxygen, and the hydrogen removed, forming a carboxylic acid group (-COOH).</p>

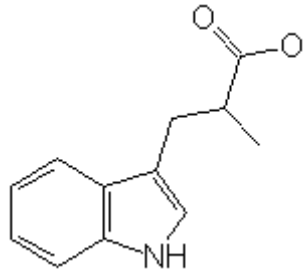

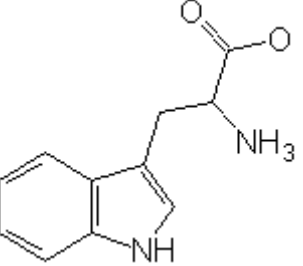

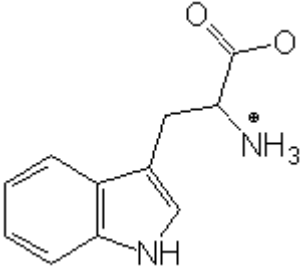
Save the structure


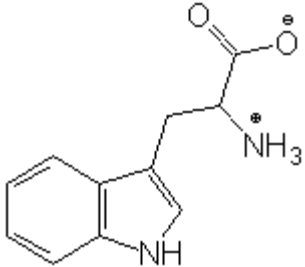
	Action	Result
1	<p>Choose File > Save.</p> <p>Note: You can also click the Save button on the toolbar or press Ctrl+S.</p>	<p>The Save As dialog box opens. The default file type (ChemWindow structure file, *.dsf) is already selected, and will be used for this structure. Other file types include ChemWindow Structure Template & Style (*.dst) and MDL Mol file (*.mol).</p>   <p>The screenshot shows the 'Save As' dialog box with the 'Save in' location set to 'RlnChl'. The 'Save as type' dropdown menu is open, displaying a list of file formats. The 'ChemWindow Structure Template & Style Files (*.dst)' option is highlighted in blue.</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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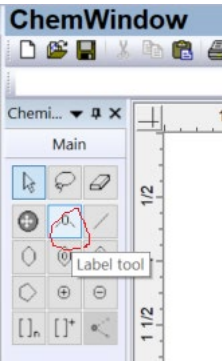
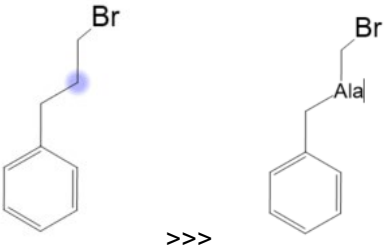
Edit the structure and use atom labels and atom tags

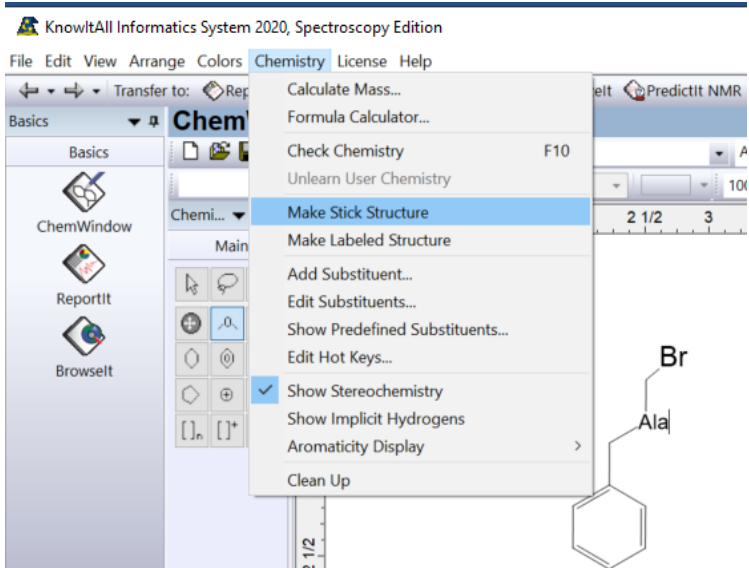
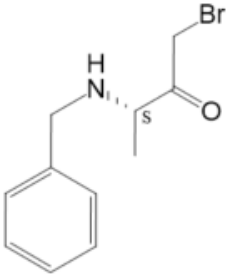
	Action	Result
1	Select the Eraser tool  , then click to remove the hydroxyl.	
2	Click to remove amino groups.	
3	Open the Main group on the Drawing Toolbar and select the Atom Label tool  . Then click where the hydroxyl group was located.	

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 anion (COO⁻), with the oxygen atoms explicitly labeled 'O'.</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 shows the tryptophan molecule with the carboxylate group removed and replaced by an ammonium group (NH₃⁺), where the '3' is a subscript.</p>
6	<p>Select the Positive Charge Atom Tag tool  to add a positive charge to the atom.</p>	 <p>The structure shows the tryptophan molecule with the ammonium group (NH₃⁺), where the positive charge is explicitly shown as a '+' sign next to the nitrogen atom.</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>

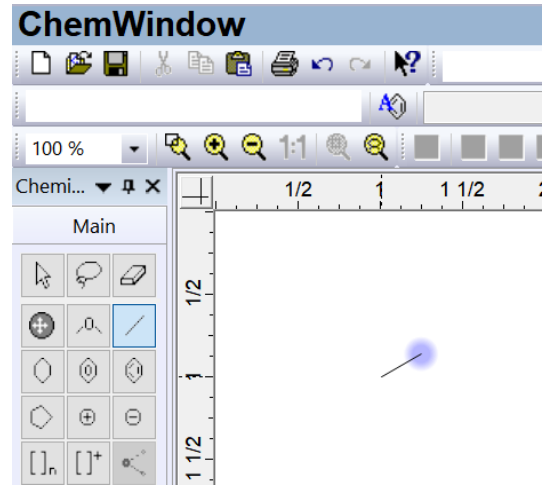
	Action	Result
7	Repeat with the Negative Charge Atom Tag tool  to add a negative charge to the oxygen atom.	 <p>The image shows the chemical structure of tryptophan. It consists of an indole ring system (a benzene ring fused to a pyrrole ring) attached to a side chain. The side chain is a 2-amino-3-(carboxymethyl)propyl group. The amino group is shown as NH₃⁺ with a positive charge symbol. The carboxylate group is shown as COO⁻ with a negative charge symbol on the oxygen atom.</p>
8	Choose File > Save As to save the structure with file name tryptophan2.dsf .	

Use pre-defined substituents

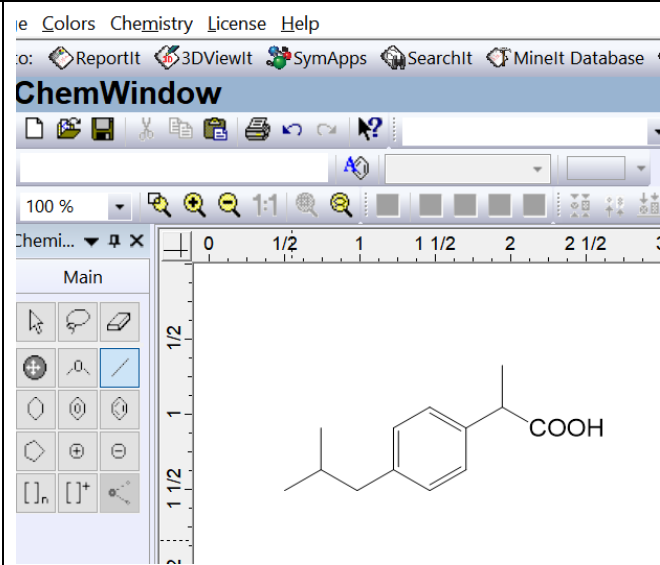
	Action	Result
1	Click on the Label tool.	 A screenshot of the ChemWindow software interface. The title bar reads 'ChemWindow'. Below it is a toolbar with various icons. A 'Main' toolbar is also visible, containing several icons. One icon, representing a label tool, is circled in red. A tooltip labeled 'Label tool' is positioned over this icon. The background shows a portion of a chemical structure with a vertical scale on the right side.
2	Select an atom and click to type Ala (a pre-defined substituent).	 A diagram illustrating the application of a pre-defined substituent. On the left, a benzene ring is shown with a blue highlight on one of its carbon atoms. A 'Br' atom is attached to this carbon via a single bond. An arrow with three right-pointing chevrons (>>>) points to the right. On the right, the same benzene ring is shown, but the 'Br' atom has been replaced by the text 'Ala', representing the pre-defined substituent.

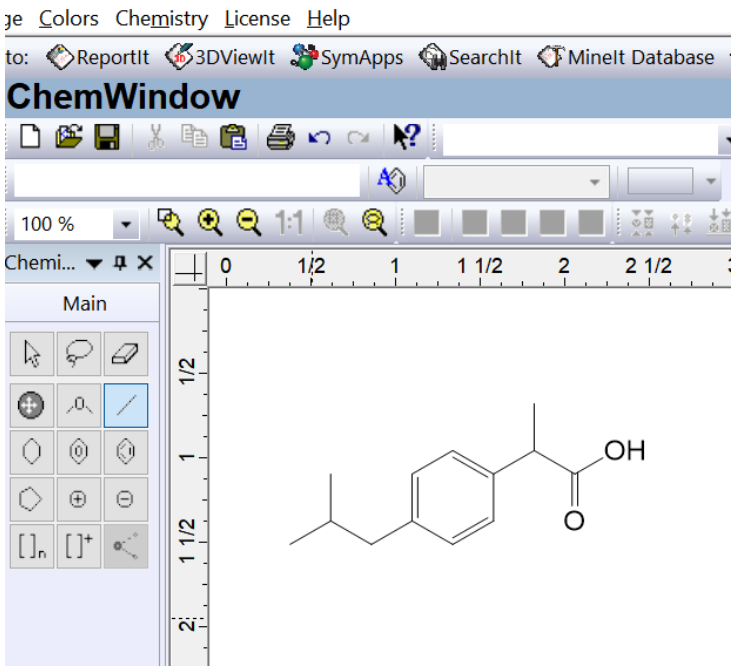
	Action	Result
3	Click Chemistry > Make Stick Structure .	 <p>The screenshot shows the 'Chemistry' menu open in the software. The 'Make Stick Structure' option is highlighted. The resulting chemical structure is a benzene ring with a -CH₂-CH₂-Br substituent.</p>
4		 <p>The above is the expanded structure.</p>

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. The title bar reads "ChemWindow". Below the title bar is a menu bar with icons for file operations (New, Open, Save, Print, Undo, Redo, Help) and a search icon. Below the menu bar is a toolbar with zooming icons (100%, 150%, 200%, 1:1, 50%) and a search icon. Below the toolbar is a ruler with markings at 1/2, 1, and 1 1/2. Below the ruler is a "Main" toolbox with various icons for drawing chemical structures. The "Standard bond" tool is highlighted in blue. To the right of the toolbox is a structure pane with a grid. A single bond is being drawn on the grid, and the end of the bond is highlighted with a blue glow.</p>

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

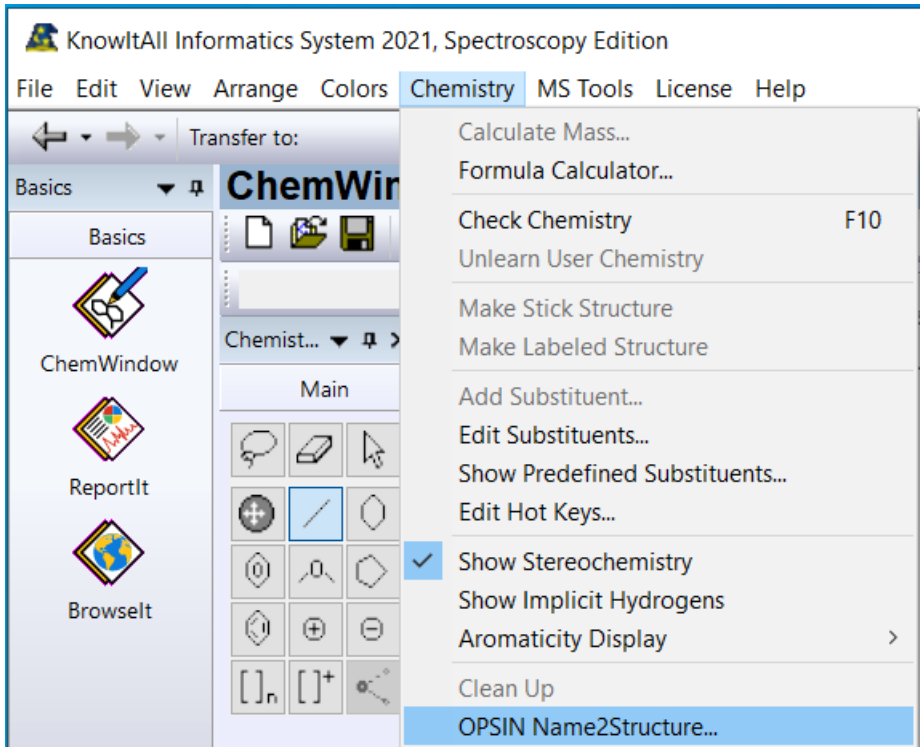


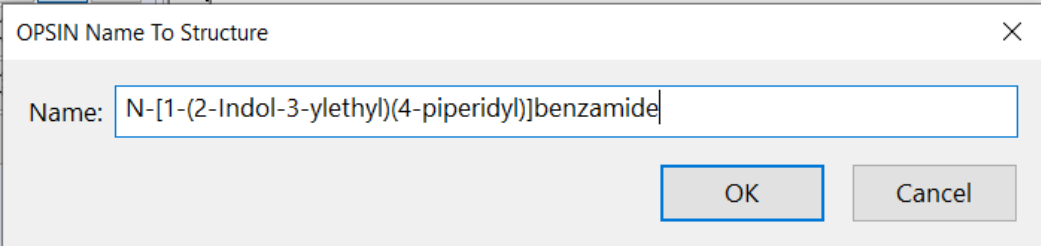
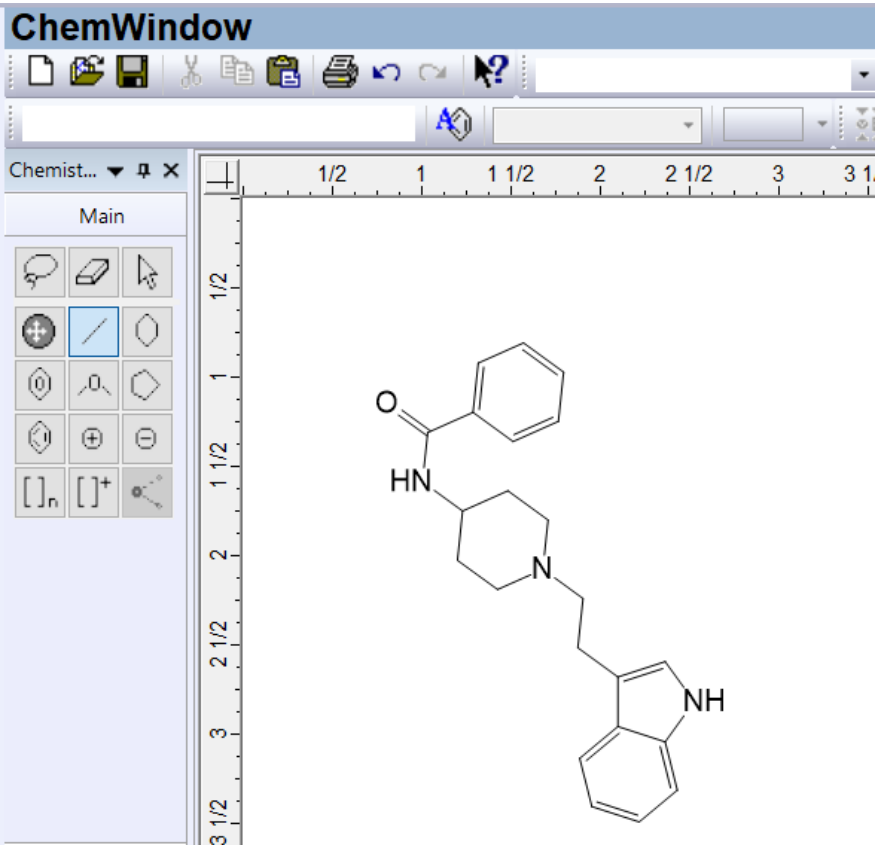
	Action	Result
3	Click Chemistry > Make Stick Structure .	 <p>The above is the expanded structure.</p>

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 'Chemistry' menu is open, and the 'OPSIN Name2Structure...' option is highlighted at the bottom. The interface includes a menu bar with 'File', 'Edit', 'View', 'Arrange', 'Colors', 'Chemistry', 'MS Tools', 'License', and 'Help'. A toolbar with various icons is visible below the menu bar. The left sidebar contains icons for 'ChemWindow', 'ReportIt', and 'BrowseIt'. The main window area shows a 'Basics' tab and a 'Main' tab with various drawing tools.</p>

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

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
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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.

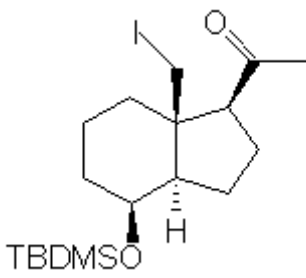
Training Files Used in This Lesson

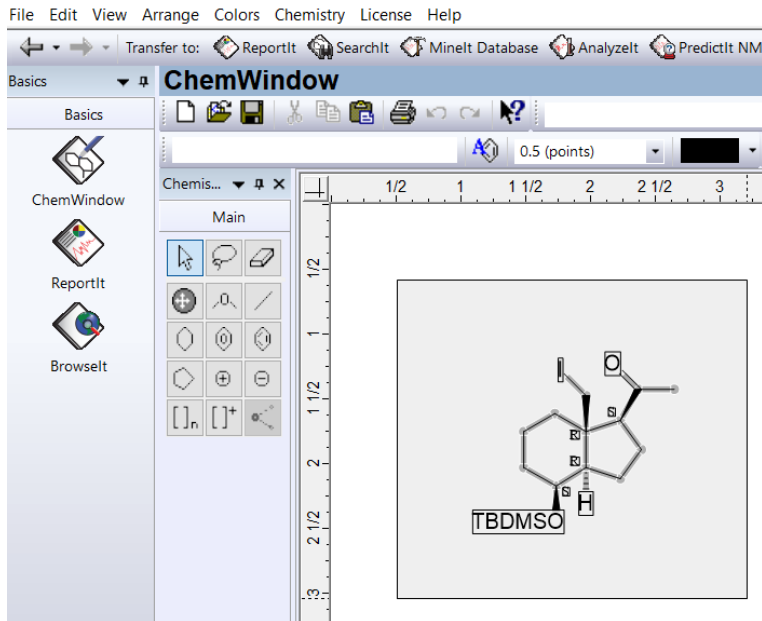
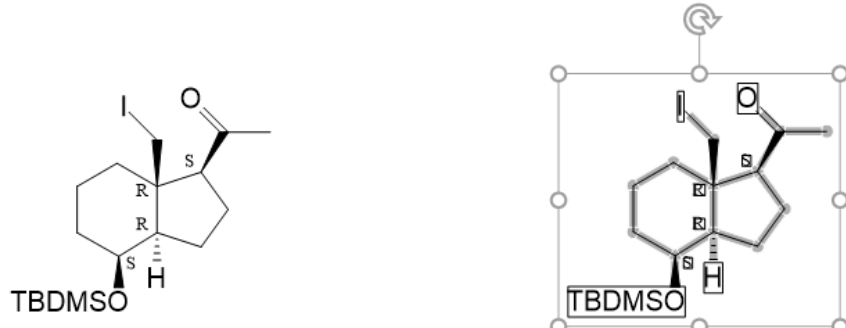
- Structure 1.dsf

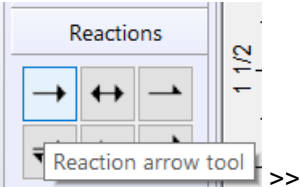

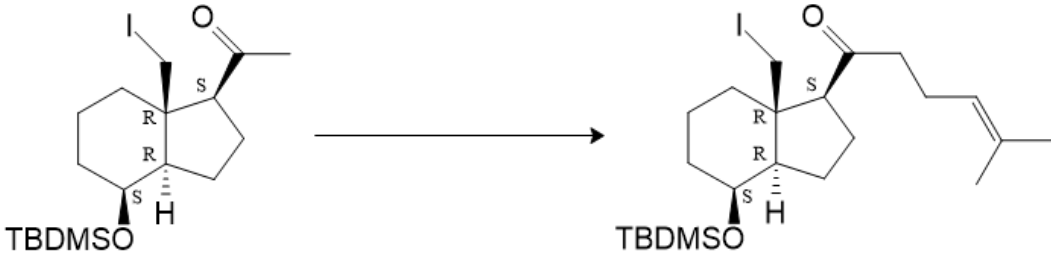
KnowItAll Applications Used

- ChemWindow®

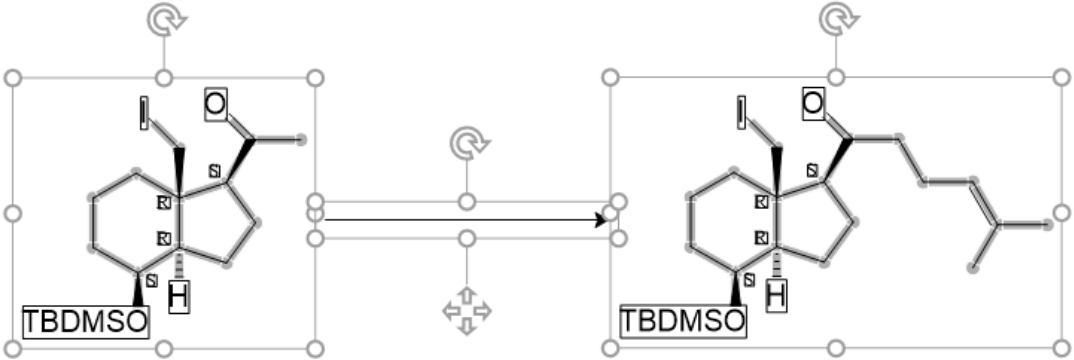
Draw Chemical Reactions

	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.  <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 a tert-butyldimethylsilyloxy (TBDMSO) group attached to one of its carbons. The five-membered ring has a hydrogen atom (H) attached to one of its carbons. There is also a carbonyl group (C=O) attached to the five-membered ring.</p>

<p>3 Select the structure.</p>	
<p>4 Navigate to Edit > Copy, then Edit > Paste.</p>	

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.	

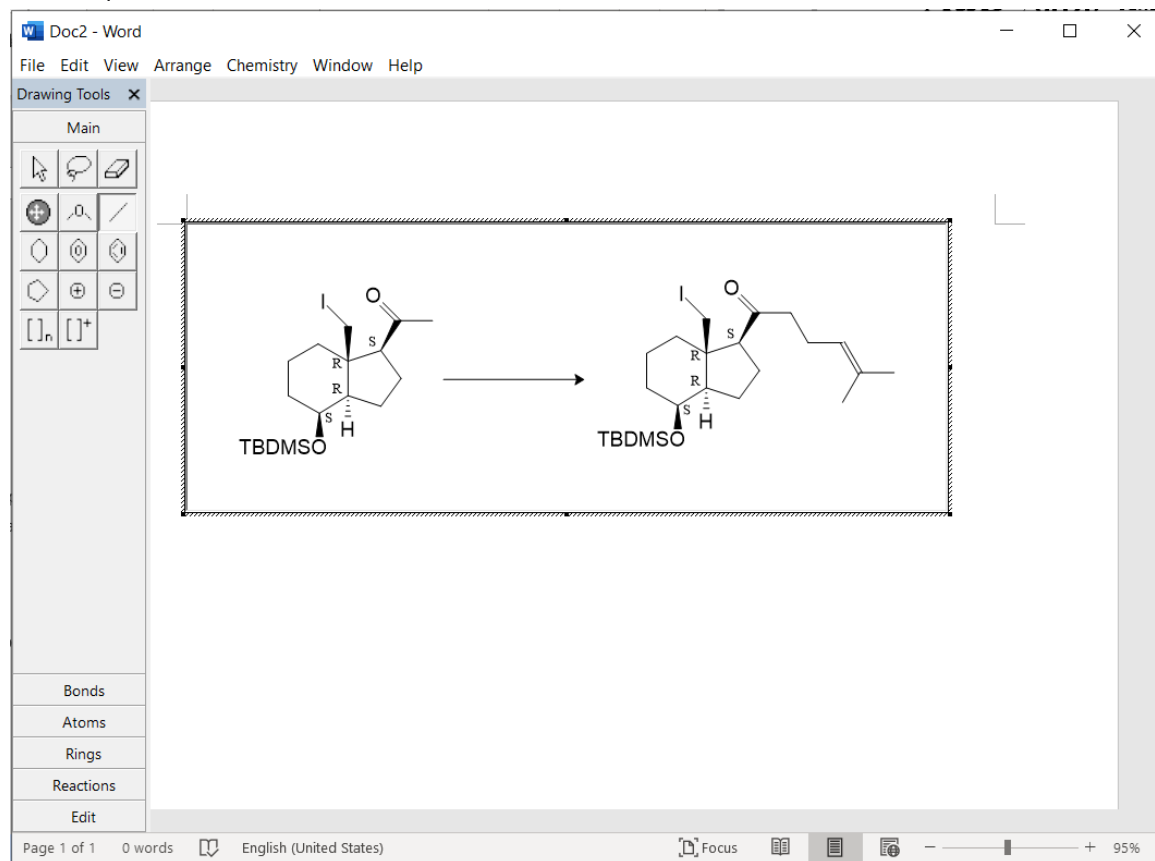
OLE connection with MS Office tools

	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.

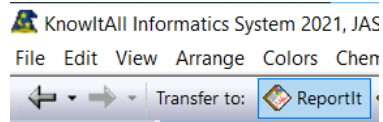
Double-click on the KnowItAll object saved.

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
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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.

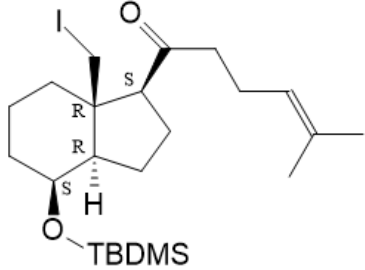
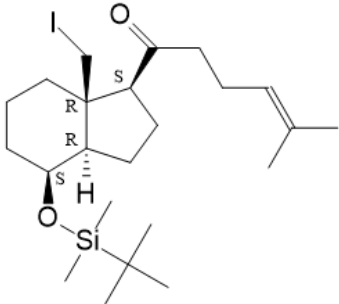
Training Files Used in This Lesson

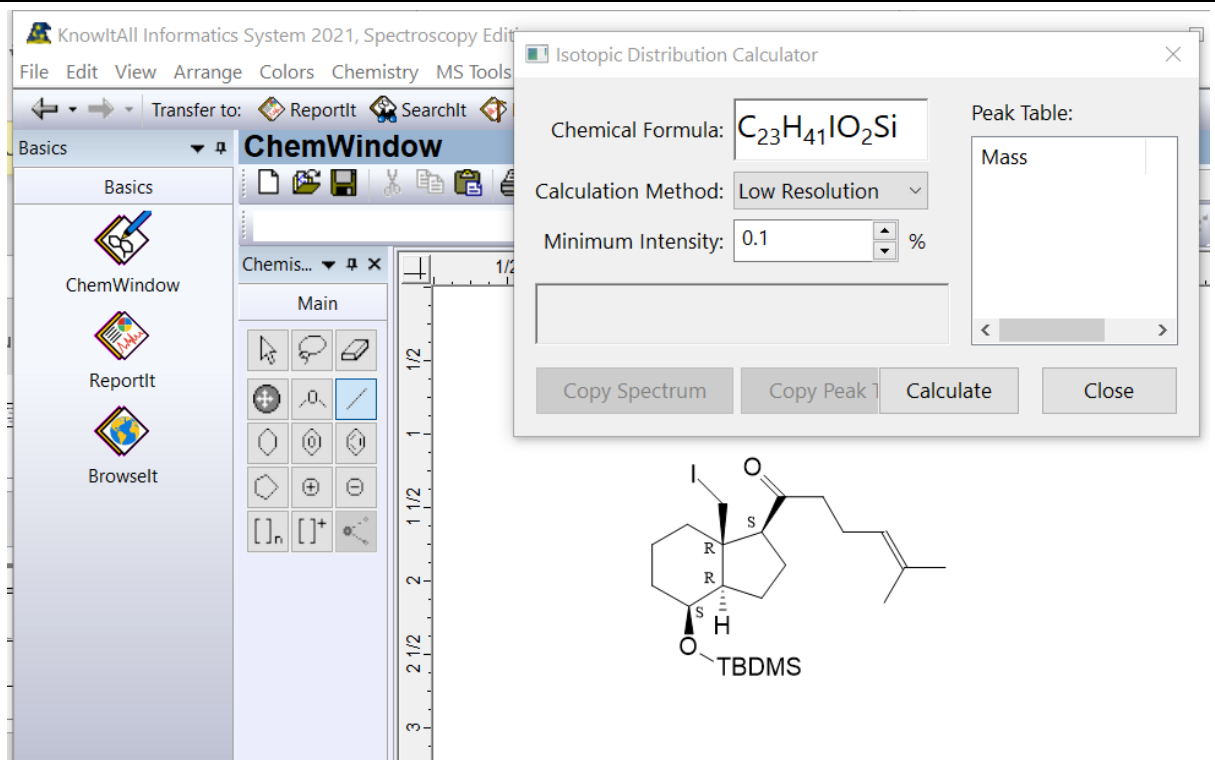
- Structure 2.dsf

KnowItAll Applications Used

- ChemWindow®

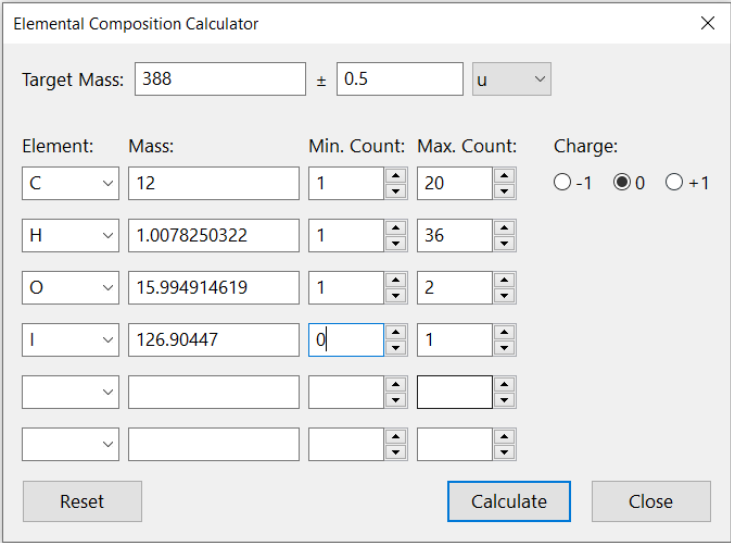
Isotopic Distribution

	Action	Result
1	<p>Navigate to File > Open, then navigate to KnowItAll Training Files > 8 - Drawing Structures and Reactions.</p> <p>Select Structure 2.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 hydrogen atom (H) attached with a dashed bond. The five-membered ring has a ketone group (C=O) attached with a wedge bond and a hydrogen atom (H) attached with a dashed bond. A tert-butyldimethylsilyloxy (TBDMS) group is attached to the oxygen of the alcohol group on the six-membered ring. A side chain is attached to the five-membered ring, consisting of a propyl chain ending in a terminal alkene with a methyl group.</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 3D representation of the same bicyclic compound shown in row 1. It uses wedge and dash notation to indicate stereochemistry. The iodine atom and the ketone group are on wedges, while the hydrogen atoms are on dashes. The TBDMS group is shown as a silicon atom bonded to an oxygen atom, which is bonded to the carbon of the alcohol group. The side chain is also shown in a stick representation.</p>

<p>3</p> <p>Navigate to MS Tools > Calculate Isotopic Distribution.</p> <p>In the pop-up window, click Calculate.</p>	 <p>KnowItAll Informatics System 2021, Spectroscopy Editor</p> <p>File Edit View Arrange Colors Chemistry MS Tools</p> <p>Transfer to: ReportIt SearchIt</p> <p>Basics ChemWindow</p> <p>Basics</p> <p>ChemWindow</p> <p>ReportIt</p> <p>Browselt</p> <p>Chemis... Main</p> <p>Isotopic Distribution Calculator</p> <p>Chemical Formula: $C_{23}H_{41}IO_2Si$</p> <p>Calculation Method: Low Resolution</p> <p>Minimum Intensity: 0.1 %</p> <p>Peak Table:</p> <p>Mass</p> <p>Copy Spectrum Copy Peak Calculate Close</p> <p>I</p> <p>O</p> <p>S</p> <p>R</p> <p>R</p> <p>R</p> <p>S</p> <p>H</p> <p>O</p> <p>TBDMS</p>
<p>4</p> <p>Open the MS Word document.</p> <p>Double-click on the KnowItAll object saved.</p>	

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></td></tr><tr><td>O</td><td>15.994914619</td><td>1</td><td>2</td><td></td></tr><tr><td>I</td><td>126.90447</td><td>0</td><td>1</td><td></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		O	15.994914619	1	2		I	126.90447	0	1											
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																																		
O	15.994914619	1	2																																		
I	126.90447	0	1																																		

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

Combinations of elements are displayed.

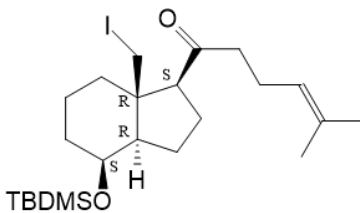
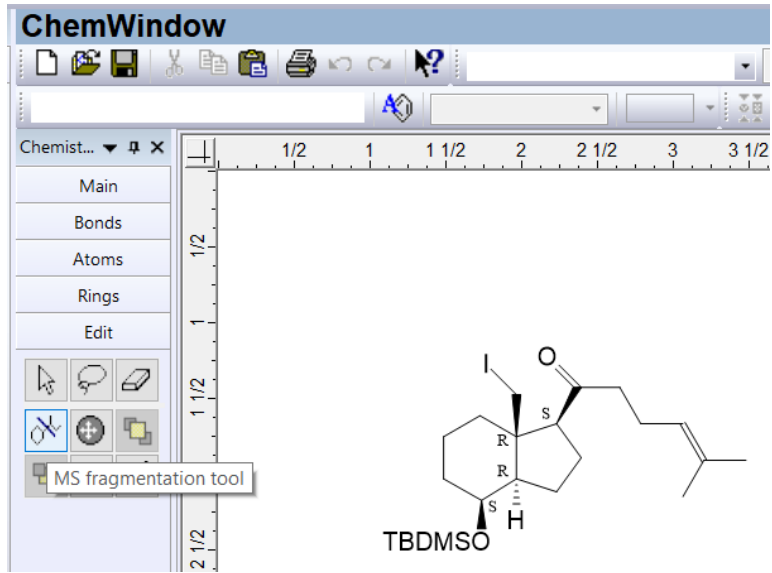
Elemental Composition Results

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

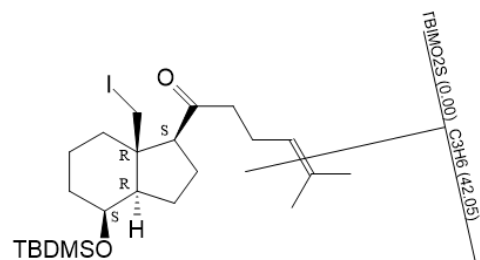
C	H	O	I	m	Δm [u]	Δm [ppm]
18	13	2	1	387.9960	-0.0040	-10.2457
19	17	1	1	388.0324	0.0324	83.5314
20	5	1	1	387.9385	-0.0615	-158.4799
17	25	2	1	388.0899	0.0899	231.7656
19	1	2	1	387.9021	-0.0979	-252.2570
18	29	1	1	388.1263	0.1263	325.5427

Copy To Clipboard Close

MS Fragmentation

	Action	Result
1	<p>Navigate to File > Open. Then navigate to KnowItAll Training Files > 8 - Drawing Structures and Reactions.</p> <p>Select Structure 2.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 application window. The title bar reads 'Chemist...'. The menu bar includes 'Main', 'Bonds', 'Atoms', 'Rings', and 'Edit'. The 'Edit' menu is open, showing various tools. The 'MS fragmentation tool' is highlighted with a tooltip. The main window displays the chemical structure from the previous step.</p>

3



You can clip the structure into two fragments.